



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:32 AM GMT

PDB ID : 3LW5  
Title : Improved model of plant photosystem I  
Authors : Nelson, N.; Toporik, H.  
Deposited on : 2010-02-23  
Resolution : 3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

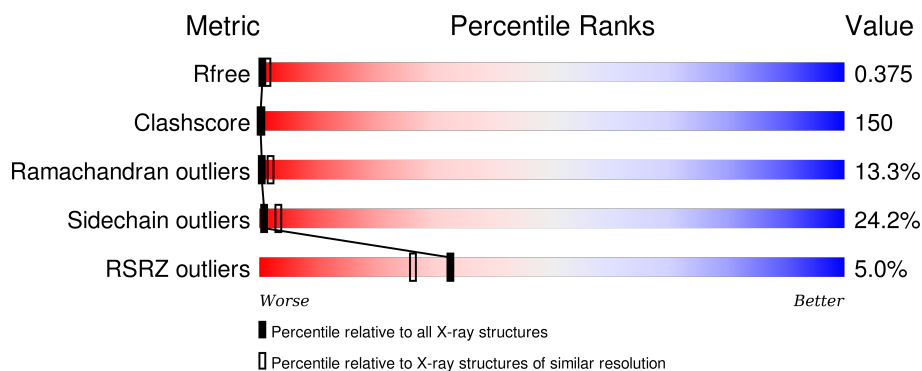
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	738	
2	B	733	
3	C	81	
4	D	138	
5	E	64	

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Mol	Chain	Length	Quality of chain
6	F	154	
7	G	95	
8	H	69	
9	I	30	
10	J	42	
11	K	84	
12	L	161	
13	N	85	
14	R	53	
15	1	170	
16	2	176	
17	3	172	
18	4	166	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	1	1001	X	-	-	-
19	CLA	1	1002	X	-	-	-
19	CLA	1	1003	X	-	-	-
19	CLA	1	1005	X	-	-	-
19	CLA	1	1006	X	-	-	X
19	CLA	1	1007	X	-	-	-
19	CLA	1	1008	X	-	-	-
19	CLA	1	1010	X	-	-	-
19	CLA	1	1011	X	-	-	-
19	CLA	1	1012	X	-	-	-
19	CLA	1	1013	X	-	-	-
19	CLA	1	1014	X	-	-	-
19	CLA	1	1015	X	-	-	-
19	CLA	1	1303	X	-	-	-
19	CLA	1	1310	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	2	1307	X	-	-	-
19	CLA	2	2001	X	-	-	-
19	CLA	2	2002	X	-	-	-
19	CLA	2	2003	X	-	-	-
19	CLA	2	2004	X	-	-	-
19	CLA	2	2005	X	-	-	-
19	CLA	2	2006	X	-	-	-
19	CLA	2	2007	X	-	-	-
19	CLA	2	2008	X	-	-	-
19	CLA	2	2010	X	-	-	-
19	CLA	2	2011	X	-	-	-
19	CLA	2	2012	X	-	-	-
19	CLA	2	2013	X	-	-	-
19	CLA	2	2014	X	-	X	-
19	CLA	2	4009	X	-	-	-
19	CLA	3	1118	X	-	-	-
19	CLA	3	1147	X	-	-	-
19	CLA	3	2009	X	-	X	-
19	CLA	3	3001	X	-	-	-
19	CLA	3	3002	X	-	-	-
19	CLA	3	3003	X	-	-	-
19	CLA	3	3004	X	-	-	-
19	CLA	3	3005	X	-	-	-
19	CLA	3	3006	X	-	-	-
19	CLA	3	3007	X	-	-	-
19	CLA	3	3008	X	-	-	-
19	CLA	3	3010	X	-	-	-
19	CLA	3	3011	X	-	-	-
19	CLA	3	3012	X	-	-	-
19	CLA	3	3013	X	-	-	-
19	CLA	3	3014	X	-	-	-
19	CLA	3	3015	X	-	-	-
19	CLA	3	3016	X	-	-	-
19	CLA	3	3017	X	-	-	-
19	CLA	4	1004	X	-	X	-
19	CLA	4	1009	X	-	-	-
19	CLA	4	1304	X	-	X	-
19	CLA	4	1306	X	-	-	-
19	CLA	4	4001	X	-	-	X
19	CLA	4	4002	X	-	X	-
19	CLA	4	4003	X	-	-	-
19	CLA	4	4004	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	4	4005	X	-	-	-
19	CLA	4	4006	X	-	-	-
19	CLA	4	4007	X	-	-	-
19	CLA	4	4010	X	-	-	-
19	CLA	4	4011	X	-	-	-
19	CLA	4	4012	X	-	-	-
19	CLA	4	4013	X	-	-	-
19	CLA	4	4014	X	-	-	-
19	CLA	4	4015	X	-	-	-
19	CLA	A	1101	X	-	-	-
19	CLA	A	1102	X	-	-	-
19	CLA	A	1103	X	-	-	-
19	CLA	A	1104	X	-	-	-
19	CLA	A	1105	X	-	X	-
19	CLA	A	1106	X	-	X	-
19	CLA	A	1107	X	-	X	-
19	CLA	A	1108	X	-	-	-
19	CLA	A	1109	X	-	-	-
19	CLA	A	1110	X	-	-	-
19	CLA	A	1111	X	-	X	-
19	CLA	A	1112	X	-	X	X
19	CLA	A	1113	X	-	-	-
19	CLA	A	1115	X	-	X	-
19	CLA	A	1116	X	-	-	-
19	CLA	A	1117	X	-	X	-
19	CLA	A	1119	X	-	X	X
19	CLA	A	1120	X	-	-	-
19	CLA	A	1121	X	-	-	-
19	CLA	A	1122	X	-	X	-
19	CLA	A	1123	X	-	X	-
19	CLA	A	1124	X	-	X	-
19	CLA	A	1125	X	-	X	-
19	CLA	A	1126	X	-	X	-
19	CLA	A	1127	X	-	-	-
19	CLA	A	1128	X	-	X	-
19	CLA	A	1129	X	-	-	-
19	CLA	A	1131	X	-	X	-
19	CLA	A	1132	X	-	-	-
19	CLA	A	1133	X	-	X	-
19	CLA	A	1134	X	-	-	-
19	CLA	A	1135	X	-	X	-
19	CLA	A	1136	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A	1137	X	-	-	-
19	CLA	A	1138	X	-	X	-
19	CLA	A	1139	X	-	X	-
19	CLA	A	1140	X	-	X	-
19	CLA	A	1141	X	-	X	-
19	CLA	A	1149	X	-	-	-
19	CLA	A	1151	X	-	-	-
19	CLA	A	1237	X	-	X	-
19	CLA	A	1309	X	-	-	-
19	CLA	A	9011	X	-	-	-
19	CLA	A	9012	X	-	X	-
19	CLA	A	9013	X	-	X	-
19	CLA	A	9022	X	-	X	-
19	CLA	A	9023	X	-	X	-
19	CLA	B	1201	X	-	-	X
19	CLA	B	1202	X	-	X	-
19	CLA	B	1203	X	-	-	-
19	CLA	B	1205	X	-	X	-
19	CLA	B	1206	X	-	-	-
19	CLA	B	1208	X	-	-	-
19	CLA	B	1209	X	-	-	-
19	CLA	B	1210	X	-	X	-
19	CLA	B	1211	X	-	-	-
19	CLA	B	1212	X	-	-	-
19	CLA	B	1213	X	-	-	X
19	CLA	B	1214	X	-	X	-
19	CLA	B	1215	X	-	-	-
19	CLA	B	1216	X	-	-	-
19	CLA	B	1217	X	-	-	-
19	CLA	B	1218	X	-	-	-
19	CLA	B	1219	X	-	-	-
19	CLA	B	1220	X	-	X	-
19	CLA	B	1221	X	-	X	-
19	CLA	B	1222	X	-	X	-
19	CLA	B	1223	X	-	X	-
19	CLA	B	1224	X	-	-	-
19	CLA	B	1225	X	-	X	-
19	CLA	B	1226	X	-	X	-
19	CLA	B	1227	X	-	-	-
19	CLA	B	1228	X	-	-	-
19	CLA	B	1229	X	-	-	-
19	CLA	B	1230	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B	1231	X	-	-	-
19	CLA	B	1232	X	-	-	X
19	CLA	B	1233	X	-	-	-
19	CLA	B	1234	X	-	-	-
19	CLA	B	1235	X	-	X	-
19	CLA	B	1236	X	-	X	-
19	CLA	B	1238	X	-	X	-
19	CLA	B	1239	X	-	X	-
19	CLA	B	1301	X	-	-	-
19	CLA	B	9010	X	-	-	-
19	CLA	F	1240	X	-	-	-
19	CLA	F	1302	X	-	-	-
19	CLA	F	1305	X	-	-	-
19	CLA	G	1242	X	-	-	-
19	CLA	H	1145	X	-	X	-
19	CLA	H	1207	X	-	X	-
19	CLA	H	1241	X	-	-	-
19	CLA	H	1505	X	-	-	-
19	CLA	I	1204	X	-	-	-
19	CLA	J	1308	X	-	X	-
19	CLA	J	1311	X	-	-	-
19	CLA	K	1142	X	-	-	-
19	CLA	K	1143	X	-	X	-
19	CLA	K	1146	X	-	-	-
19	CLA	K	3009	X	-	-	-
19	CLA	L	1130	X	-	X	-
19	CLA	L	1148	X	-	X	-
19	CLA	L	1501	X	-	-	-
19	CLA	L	1502	X	-	X	-
19	CLA	L	1503	X	-	-	-
19	CLA	L	1504	X	-	X	X
19	CLA	R	1144	X	-	-	-
19	CLA	R	1150	X	-	-	-
20	PQN	A	5001	X	-	-	-
20	PQN	B	5002	X	-	X	-
21	BCR	A	6002	-	-	X	X
21	BCR	A	6007	-	-	X	X
21	BCR	A	6008	-	-	X	X
21	BCR	A	6011	-	-	X	-
21	BCR	B	6010	-	-	X	-
21	BCR	B	6017	-	-	X	X
21	BCR	B	6020	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	BCR	F	6014	-	-	X	-
21	BCR	F	6016	-	-	X	-
21	BCR	I	6021	-	-	X	-
21	BCR	J	6012	-	-	X	-
21	BCR	L	6019	-	-	X	-
22	LMU	3	7005	-	-	X	-
22	LMU	4	7034	-	-	X	-
22	LMU	4	7052	-	-	X	-
22	LMU	D	7050	-	-	X	-
24	SF4	A	8001	-	-	X	-
24	SF4	C	8002	-	-	X	-
24	SF4	C	8003	-	-	X	-



## 2 Entry composition [i](#)

There are 24 unique types of molecules in this entry. The entry contains 36370 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	730	Total	C	N	O	S	0	0	0
			5739	3762	974	985	18			

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	733	Total	C	N	O	S	0	0	0
			5844	3841	997	993	13			

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	81	Total	C	N	O	S	0	0	0
			619	384	108	115	12			

- Molecule 4 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	138	Total	C	N	O	S	0	0	0
			1097	704	191	199	3			

- Molecule 5 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	64	Total	C	N	O	0	0	0
			513	327	90	96			

- Molecule 6 is a protein called Photosystem I reaction center subunit III, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	154	Total	C	N	O	S	0	0	0
			1221	794	207	217	3			

- Molecule 7 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	95	Total	C	N	O	0	0	0
			738	481	120	137			

- Molecule 8 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	H	69	Total	C	N	O	0	0	0
			517	334	80	103			

- Molecule 9 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	30	Total	C	N	O	S	0	0	0
			229	158	34	35	2			

- Molecule 10 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	42	Total	C	N	O	S	0	0	0
			334	228	51	54	1			

- Molecule 11 is a protein called Photosystem I reaction center subunit X psaK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	84	Total	C	N	O	S	0	0	0
			592	377	102	110	3			

- Molecule 12 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	161	Total	C	N	O	S	0	0	0
			1209	797	192	219	1			

- Molecule 13 is a protein called Photosystem I-N subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	85	Total	C	N	O	S	0	0	0
			685	436	113	132	4			

- Molecule 14 is a protein called CHAIN R.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	R	53	Total	C	N	O	0	0	0
			265	159	53	53			

- Molecule 15 is a protein called AT3g54890.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	1	165	Total	C	N	O	S	0	0	0
			1257	816	208	229	4			

- Molecule 16 is a protein called Type II chlorophyll a/b binding protein from photosystem I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	2	176	Total	C	N	O	S	0	0	0
			1367	895	223	245	4			

- Molecule 17 is a protein called Chlorophyll a-b binding protein 3, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	3	156	Total	C	N	O	S	0	0	0
			1197	784	199	209	5			

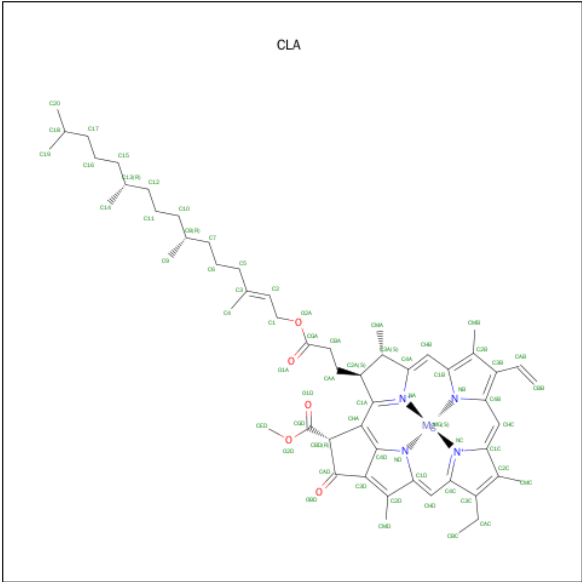
- Molecule 18 is a protein called Chlorophyll a-b binding protein P4, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	4	166	Total	C	N	O	S	0	0	0
			1309	856	216	234	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	?	-	ALA	SEE REMARK 999	UNP Q9SQL2

- Molecule 19 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	1	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	1	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	1	1	Total 25	C 20	Mg 1	N 4		0	0
19	A	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
19	A	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
19	A	1	Total 57	C 47	Mg 1	N 4	O 5	0	0
19	A	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
19	A	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
19	A	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
19	A	1	Total 54	C 44	Mg 1	N 4	O 5	0	0
19	A	1	Total 54	C 44	Mg 1	N 4	O 5	0	0
19	A	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
19	A	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
19	A	1	Total 52	C 42	Mg 1	N 4	O 5	0	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
19	3	1	Total 36	C 30	Mg 1	N 4	O 1	0	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
19	A	1	Total 51	C 41	Mg 1	N 4	O 5	0	0
19	A	1	Total 42	C 34	Mg 1	N 4	O 3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	K	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	K	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	R	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
19	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	K	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	R	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	I	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	F	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	G	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	F	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
19	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	F	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	J	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	J	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	L	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	3	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	3	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		

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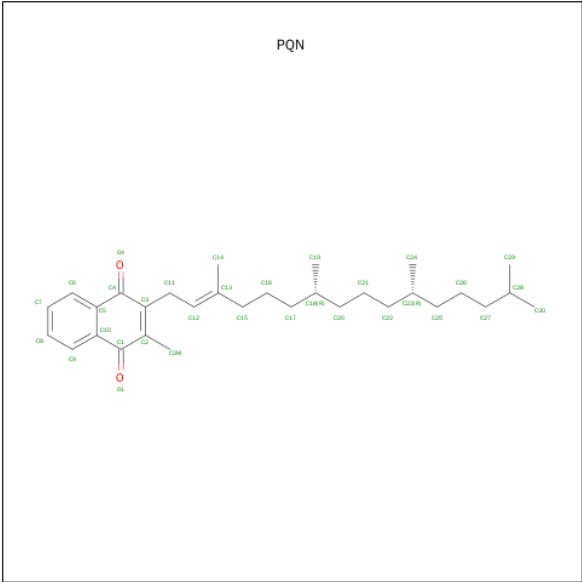
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
19	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
19	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
19	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	3	1	Total	C	Mg	N		0
			25	20	1	4		
19	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	3	1	Total	C	Mg	N		0
			25	20	1	4		
19	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	3	1	Total	C	Mg	N		0
			25	20	1	4		
19	3	1	Total	C	Mg	N		0
			25	20	1	4		
19	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	4	1	Total	C	Mg	N		0
			25	20	1	4		
19	4	1	Total	C	Mg	N		0
			25	20	1	4		
19	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

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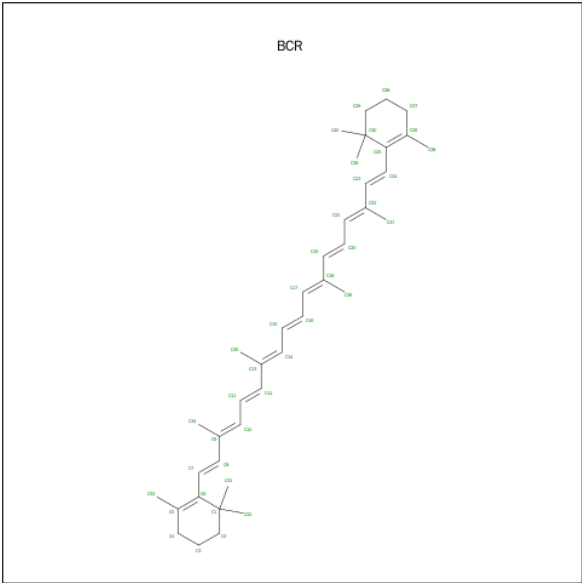
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	4	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	4	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 20 is PHYLLOQUINONE (three-letter code: PQN) (formula: C<sub>31</sub>H<sub>46</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	1	Total	C	O	0
			33	31	2	
20	B	1	Total	C	O	0
			33	31	2	

- Molecule 21 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



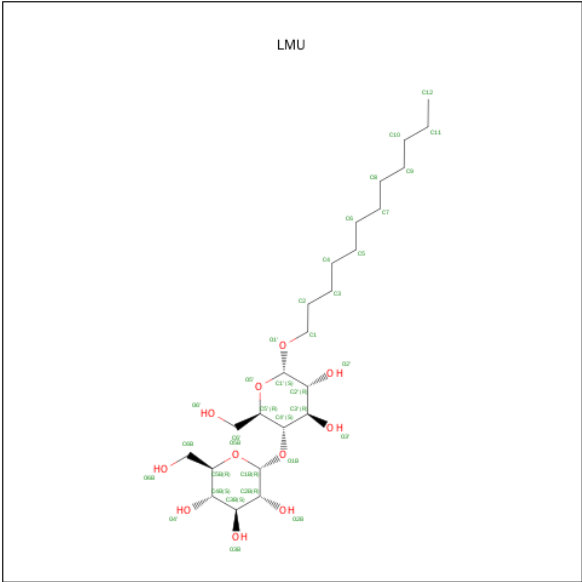
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	1	Total	C		0
			40	40		
21	A	1	Total	C		0
			40	40		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0
21	J	1	Total C 40 40	0	0
21	F	1	Total C 40 40	0	0
21	F	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	I	1	Total C 40 40	0	0
21	L	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	I	1	Total C 40 40	0	0
21	3	1	Total C 40 40	0	0
21	1	1	Total C 40 40	0	0

- Molecule 22 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula:  $C_{24}H_{46}O_{11}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	K	1	Total	C	O	0	0
			35	24	11		
22	H	1	Total	C	O	0	0
			35	24	11		
22	3	1	Total	C	O	0	0
			35	24	11		
22	1	1	Total	C	O	0	0
			35	24	11		
22	3	1	Total	C	O	0	0
			35	24	11		
22	2	1	Total	C	O	0	0
			35	24	11		
22	R	1	Total	C	O	0	0
			35	24	11		
22	4	1	Total	C	O	0	0
			35	24	11		
22	4	1	Total	C	O	0	0
			34	23	11		
22	A	1	Total	C	O	0	0
			35	24	11		
22	H	1	Total	C	O	0	0
			35	24	11		
22	B	1	Total	C	O	0	0
			25	14	11		
22	1	1	Total	C	O	0	0
			35	24	11		
22	R	1	Total	C	O	0	0
			35	24	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	C	1	Total	C	O	0	0
			35	24	11		
22	A	1	Total	C	O	0	0
			35	24	11		
22	H	1	Total	C	O	0	0
			35	24	11		
22	4	1	Total	C	O	0	0
			35	24	11		
22	4	1	Total	C	O	0	0
			35	24	11		
22	R	1	Total	C	O	0	0
			35	24	11		
22	R	1	Total	C	O	0	0
			35	24	11		
22	R	1	Total	C	O	0	0
			35	24	11		
22	A	1	Total	C	O	0	0
			35	24	11		
22	R	1	Total	C	O	0	0
			35	24	11		
22	R	1	Total	C	O	0	0
			35	24	11		
22	G	1	Total	C	O	0	0
			35	24	11		
22	2	1	Total	C	O	0	0
			35	24	11		
22	H	1	Total	C	O	0	0
			35	24	11		
22	L	1	Total	C	O	0	0
			35	24	11		
22	H	1	Total	C	O	0	0
			35	24	11		
22	2	1	Total	C	O	0	0
			35	24	11		
22	H	1	Total	C	O	0	0
			35	24	11		
22	4	1	Total	C	O	0	0
			35	24	11		
22	4	1	Total	C	O	0	0
			35	24	11		
22	A	1	Total	C	O	0	0
			35	24	11		

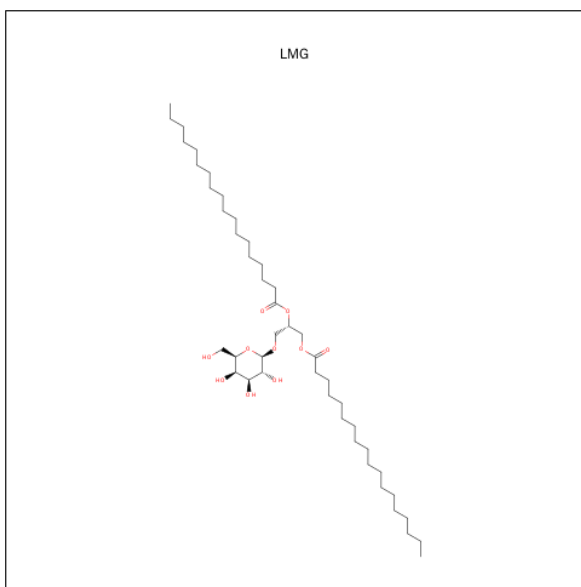
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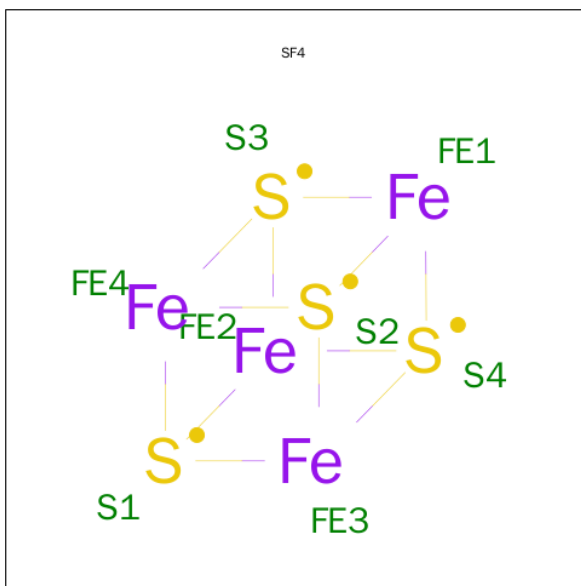
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	F	1	Total	C	O	0	0
			34	23	11		
22	E	1	Total	C	O	0	0
			35	24	11		
22	B	1	Total	C	O	0	0
			35	24	11		
22	G	1	Total	C	O	0	0
			35	24	11		
22	B	1	Total	C	O	0	0
			35	24	11		
22	K	1	Total	C	O	0	0
			35	24	11		
22	K	1	Total	C	O	0	0
			35	24	11		
22	H	1	Total	C	O	0	0
			35	24	11		
22	A	1	Total	C	O	0	0
			35	24	11		
22	A	1	Total	C	O	0	0
			35	24	11		
22	2	1	Total	C	O	0	0
			35	24	11		
22	K	1	Total	C	O	0	0
			35	24	11		
22	E	1	Total	C	O	0	0
			35	24	11		
22	N	1	Total	C	O	0	0
			35	24	11		
22	D	1	Total	C	O	0	0
			35	24	11		
22	G	1	Total	C	O	0	0
			35	24	11		
22	4	1	Total	C	O	0	0
			35	24	11		
22	4	1	Total	C	O	0	0
			34	23	11		

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	B	1	Total	C	O	0	0
			49	39	10		

- Molecule 24 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).

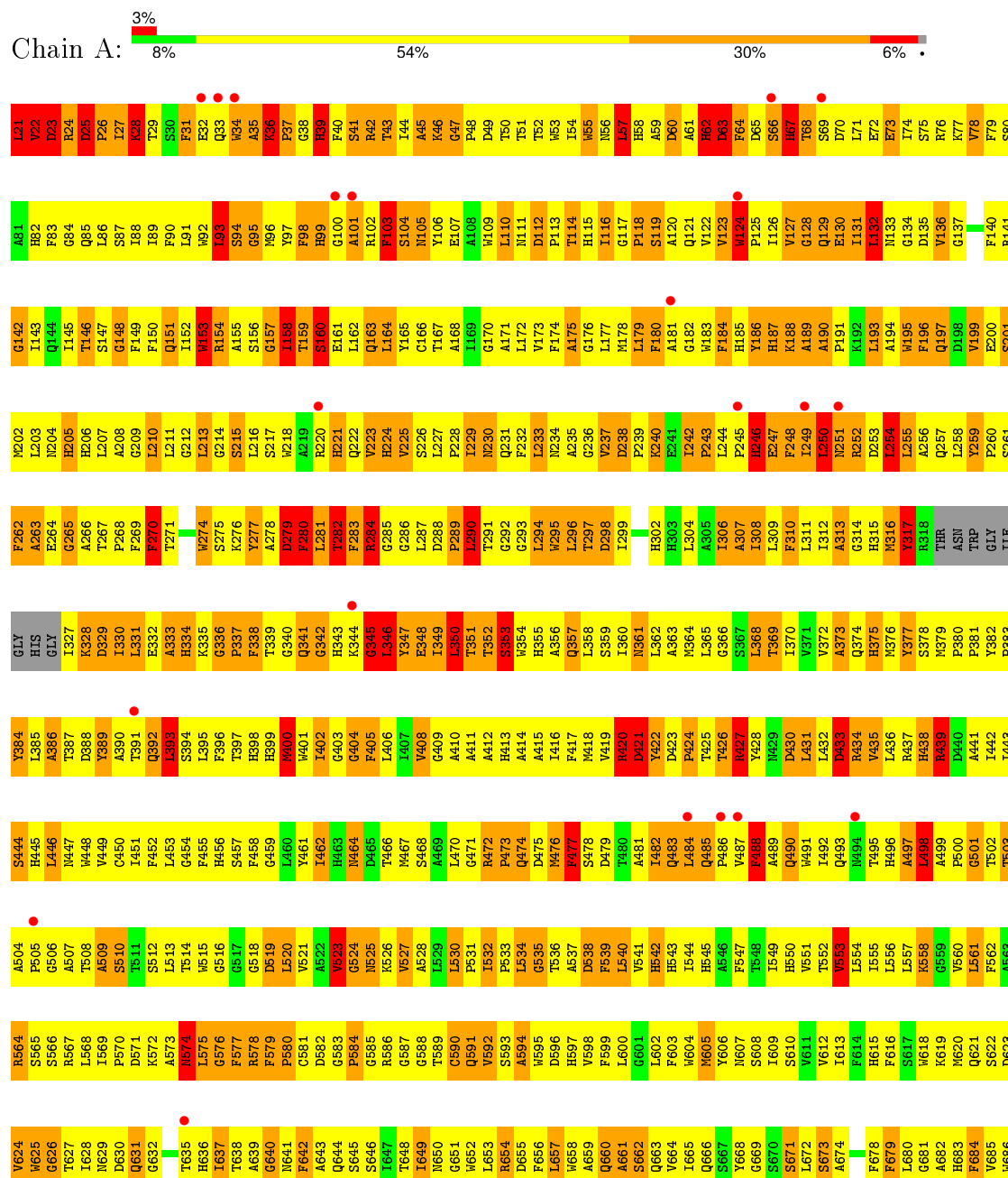


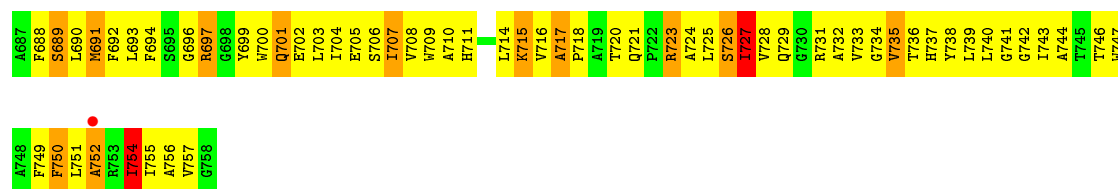
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	A	1	Total	Fe	S	0	0
			8	4	4		
24	C	1	Total	Fe	S	0	0
			8	4	4		
24	C	1	Total	Fe	S	0	0
			8	4	4		

### 3 Residue-property plots

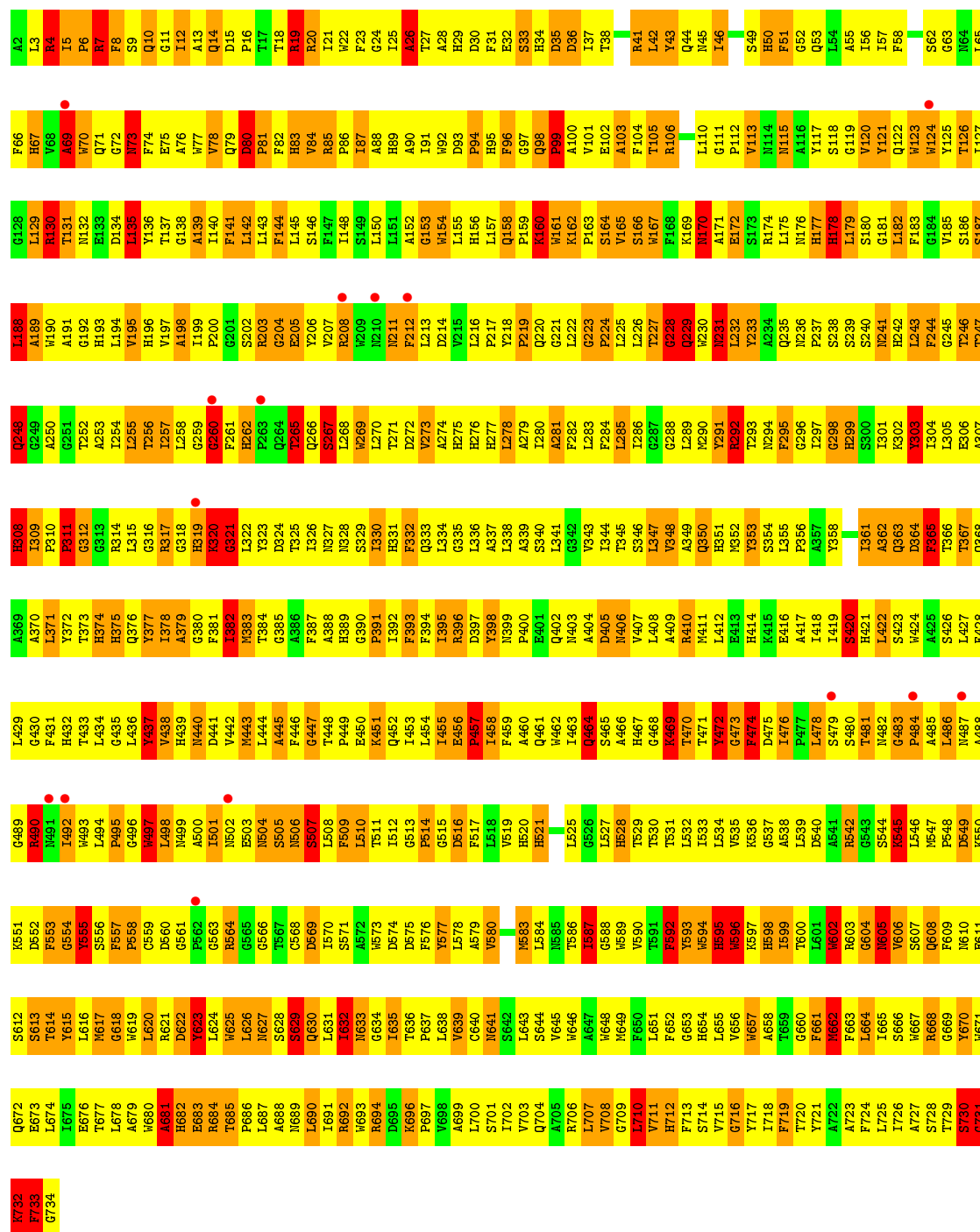
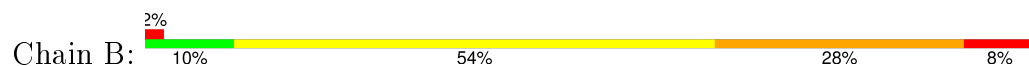
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

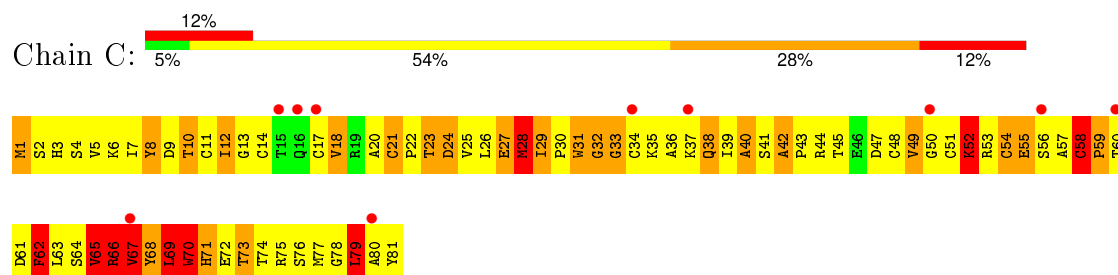




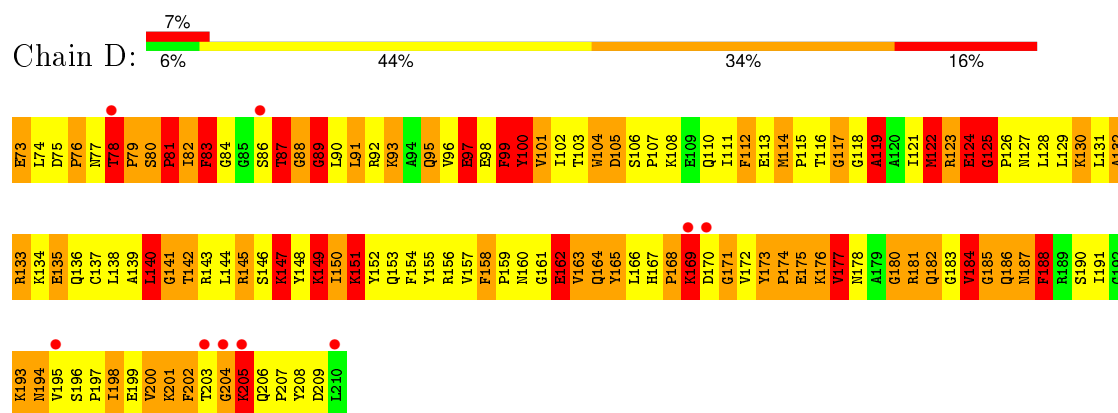
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



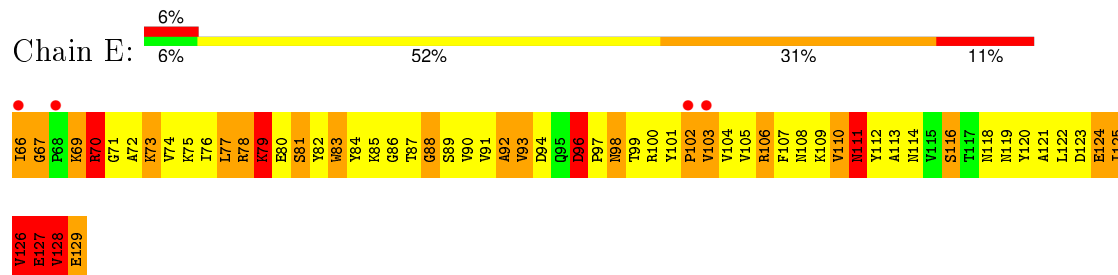
- Molecule 3: Photosystem I iron-sulfur center



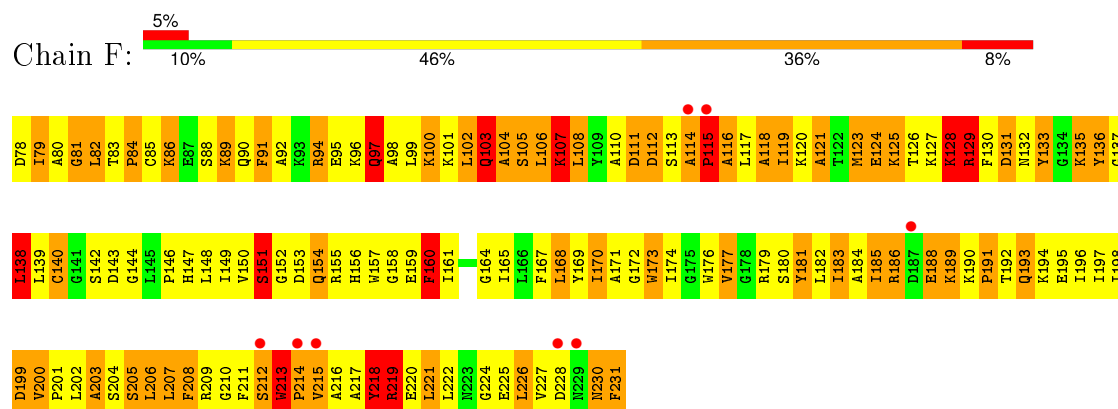
- Molecule 4: Putative uncharacterized protein



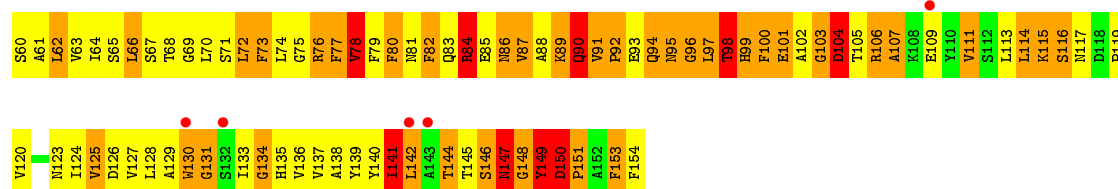
- Molecule 5: Putative uncharacterized protein



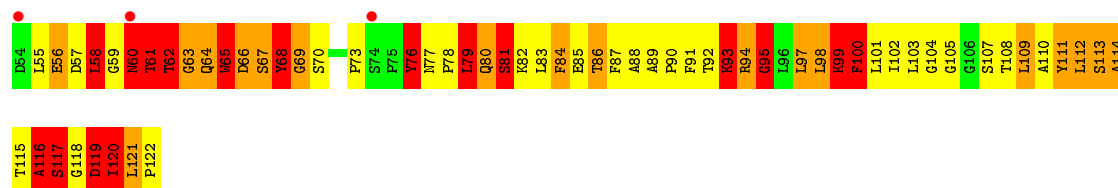
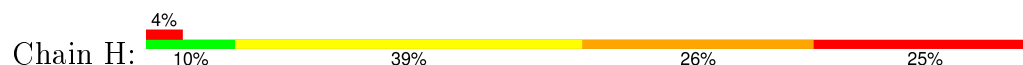
- Molecule 6: Photosystem I reaction center subunit III, chloroplastic



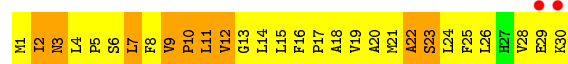
- Molecule 7: Putative uncharacterized protein



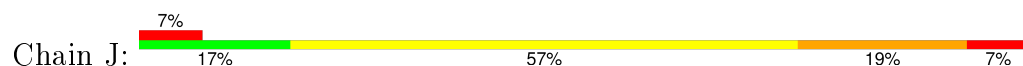
• Molecule 8: Putative uncharacterized protein



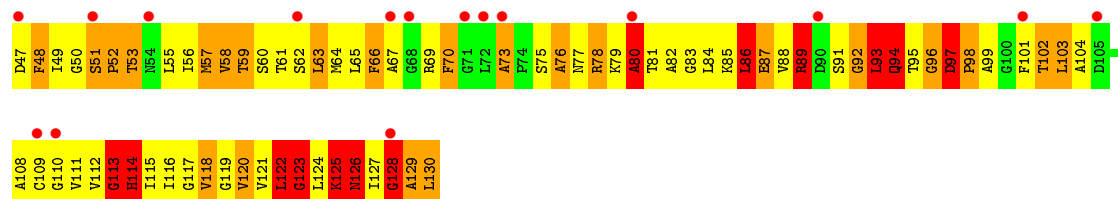
• Molecule 9: Photosystem I reaction center subunit VIII



• Molecule 10: Photosystem I reaction center subunit IX

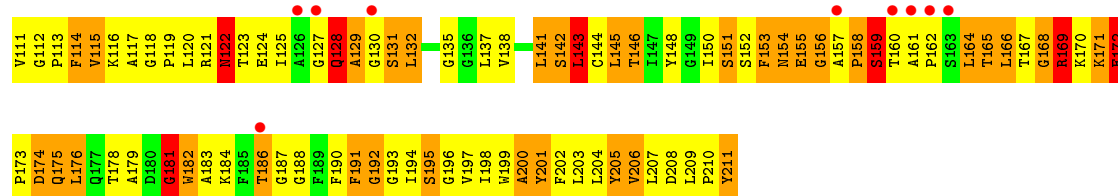


• Molecule 11: Photosystem I reaction center subunit X psaK

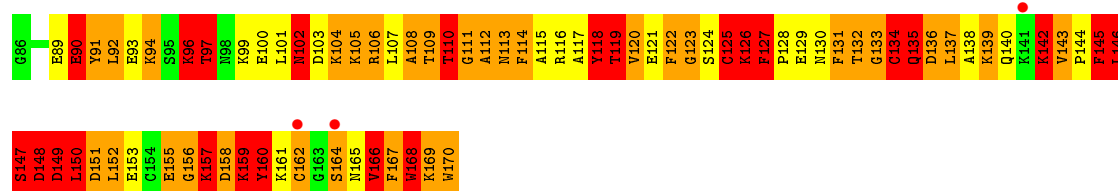


• Molecule 12: Putative uncharacterized protein

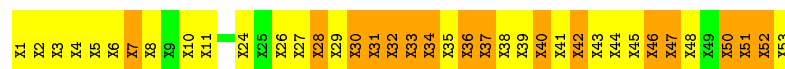




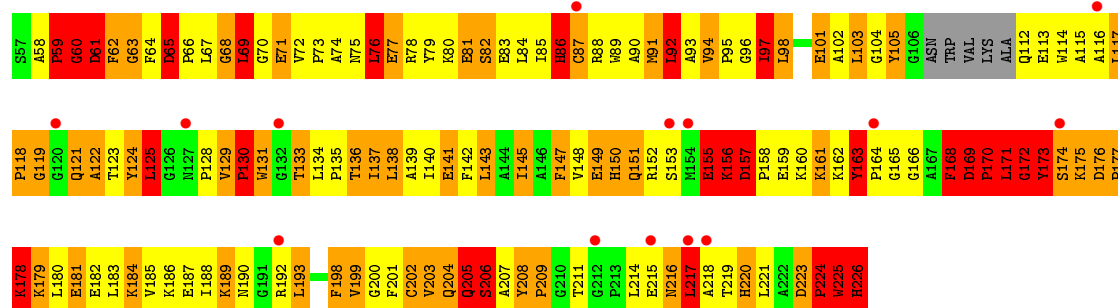
• Molecule 13: Photosystem I-N subunit



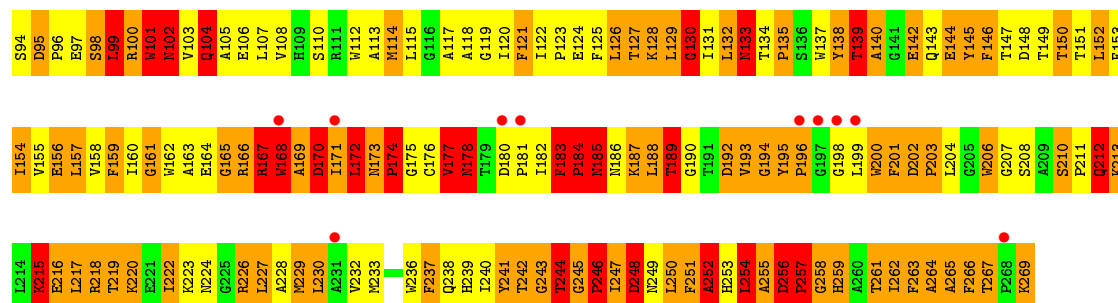
• Molecule 14: CHAIN R



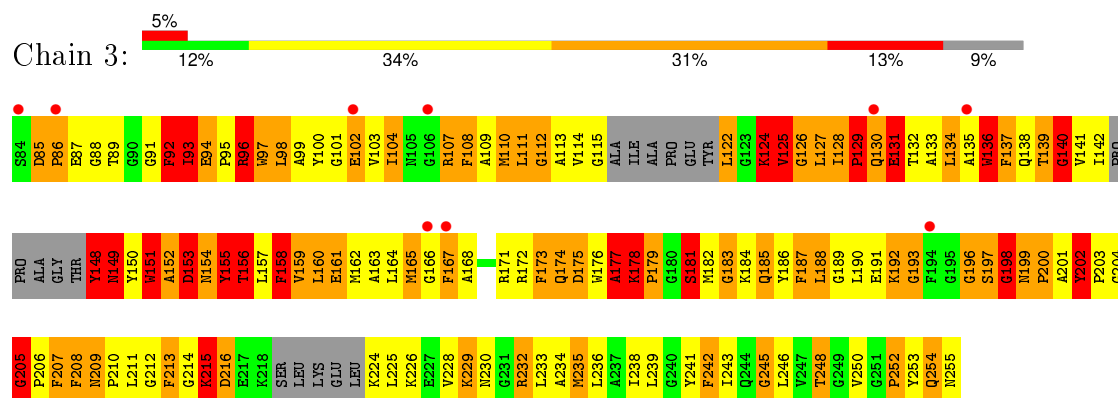
• Molecule 15: AT3g54890



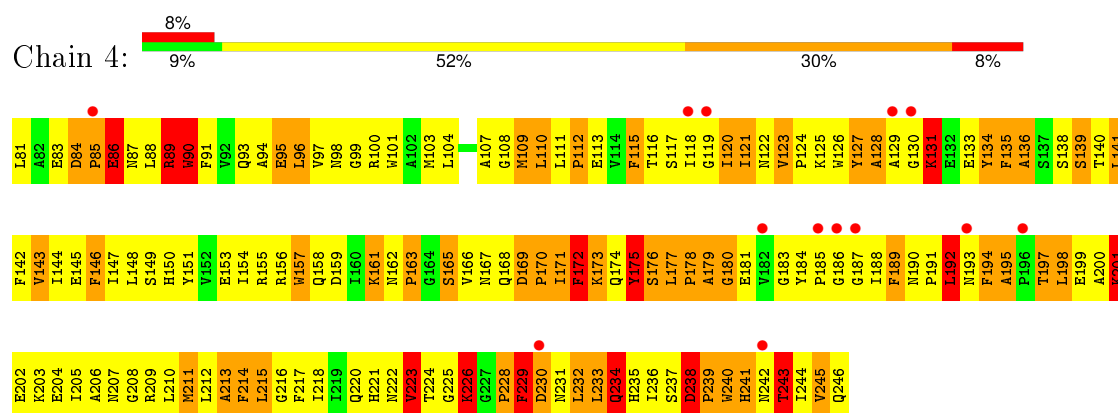
• Molecule 16: Type II chlorophyll a/b binding protein from photosystem I



• Molecule 17: Chlorophyll a-b binding protein 3, chloroplastic



• Molecule 18: Chlorophyll a-b binding protein P4, chloroplastic





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.66Å 189.09Å 129.39Å 90.00° 91.24° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30 49.14 – 3.21	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-3.30) 99.0 (49.14-3.21)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.56 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.349 , 0.383 0.352 , 0.375	Depositor DCC
$R_{free}$ test set	4349 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	77.2	Xtriage
Anisotropy	0.691	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.16 , 93.8	EDS
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 93858 reflections	Xtriage
$F_o, F_c$ correlation	0.79	EDS
Total number of atoms	36370	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, CLA, PQN, LMU, BCR, LMG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.88	5/5932 (0.1%)	1.20	49/8096 (0.6%)
2	B	0.96	8/6054 (0.1%)	1.16	35/8273 (0.4%)
3	C	1.10	1/632 (0.2%)	1.35	5/856 (0.6%)
4	D	1.13	2/1124 (0.2%)	1.49	15/1516 (1.0%)
5	E	1.26	2/523 (0.4%)	1.38	7/710 (1.0%)
6	F	0.98	0/1250	1.29	10/1687 (0.6%)
7	G	1.00	3/757 (0.4%)	1.41	5/1031 (0.5%)
8	H	1.12	3/530 (0.6%)	1.58	11/722 (1.5%)
9	I	0.82	0/235	0.88	0/320
10	J	0.83	0/344	0.99	0/469
11	K	1.14	4/599 (0.7%)	1.50	8/811 (1.0%)
12	L	1.07	3/1244 (0.2%)	1.32	10/1703 (0.6%)
13	N	1.11	3/699 (0.4%)	1.51	10/936 (1.1%)
15	1	1.50	20/1295 (1.5%)	1.51	21/1763 (1.2%)
16	2	1.16	9/1413 (0.6%)	1.51	30/1934 (1.6%)
17	3	1.09	9/1231 (0.7%)	1.37	18/1658 (1.1%)
18	4	1.13	6/1349 (0.4%)	1.56	13/1839 (0.7%)
All	All	1.04	78/25211 (0.3%)	1.32	247/34324 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	81
2	B	0	83
3	C	0	14
4	D	0	37
5	E	0	10
6	F	0	27

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	G	1	24
8	H	2	22
11	K	0	21
12	L	0	23
13	N	0	40
14	R	0	17
15	1	0	37
16	2	0	45
17	3	0	35
18	4	0	28
All	All	3	544

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	1	119	GLY	N-CA	13.83	1.66	1.46
15	1	172	GLY	C-O	12.76	1.44	1.23
15	1	63	GLY	C-O	11.60	1.42	1.23
15	1	225	TRP	C-N	10.48	1.58	1.34
2	B	94	PRO	N-CD	-10.34	1.33	1.47
15	1	60	GLY	CA-C	-9.76	1.36	1.51
16	2	194	GLY	N-CA	8.95	1.59	1.46
1	A	337	PRO	N-CD	-8.94	1.35	1.47
15	1	225	TRP	C-O	8.79	1.40	1.23
15	1	171	LEU	C-O	8.58	1.39	1.23
15	1	63	GLY	CA-C	8.39	1.65	1.51
15	1	166	GLY	N-CA	8.32	1.58	1.46
16	2	133	ASN	C-O	8.31	1.39	1.23
2	B	99	PRO	N-CD	-8.30	1.36	1.47
12	L	64	PRO	N-CD	-8.29	1.36	1.47
15	1	60	GLY	N-CA	7.95	1.57	1.46
2	B	219	PRO	N-CD	-7.88	1.36	1.47
11	K	123	GLY	C-N	7.83	1.52	1.34
17	3	198	GLY	N-CA	7.75	1.57	1.46
18	4	239	PRO	N-CD	-7.30	1.37	1.47
15	1	172	GLY	CA-C	7.23	1.63	1.51
15	1	225	TRP	CB-CG	7.21	1.63	1.50
17	3	158	PHE	C-O	7.20	1.37	1.23
2	B	457	PRO	N-CD	-7.19	1.37	1.47
13	N	157	LYS	C-N	6.90	1.50	1.34
16	2	167	ARG	CZ-NH1	6.75	1.41	1.33
16	2	184	PRO	C-N	6.71	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	1	172	GLY	N-CA	6.67	1.56	1.46
15	1	173	TYR	CD2-CE2	-6.47	1.29	1.39
17	3	129	PRO	N-CD	-6.38	1.39	1.47
16	2	165	GLY	C-O	6.38	1.33	1.23
13	N	157	LYS	C-O	6.33	1.35	1.23
4	D	188	PHE	CB-CG	-6.25	1.40	1.51
1	A	21	LEU	C-O	6.15	1.35	1.23
18	4	129	ALA	N-CA	6.14	1.58	1.46
2	B	229	GLN	C-O	6.03	1.34	1.23
17	3	196	GLY	C-O	6.02	1.33	1.23
16	2	130	GLY	C-O	-6.00	1.14	1.23
1	A	153	TRP	CB-CG	-5.96	1.39	1.50
13	N	146	LEU	N-CA	5.96	1.58	1.46
5	E	127	GLU	CG-CD	-5.96	1.43	1.51
16	2	177	VAL	CB-CG1	5.96	1.65	1.52
15	1	61	ASP	N-CA	-5.94	1.34	1.46
7	G	149	TYR	C-N	5.89	1.47	1.34
18	4	176	SER	CB-OG	5.80	1.49	1.42
8	H	95	GLY	N-CA	5.79	1.54	1.46
7	G	107	ALA	N-CA	5.73	1.57	1.46
1	A	137	GLY	N-CA	5.71	1.54	1.46
2	B	167	TRP	CB-CG	-5.71	1.40	1.50
18	4	234	GLN	N-CA	5.70	1.57	1.46
15	1	215	GLU	CB-CG	5.65	1.62	1.52
17	3	158	PHE	C-N	5.65	1.47	1.34
16	2	175	GLY	N-CA	5.62	1.54	1.46
7	G	151	PRO	N-CD	-5.60	1.40	1.47
16	2	178	ASN	CG-OD1	5.56	1.36	1.24
11	K	92	GLY	N-CA	5.55	1.54	1.46
3	C	31	TRP	CB-CG	5.53	1.60	1.50
2	B	497	TRP	CB-CG	-5.47	1.40	1.50
11	K	96	GLY	CA-C	5.46	1.60	1.51
12	L	62	GLY	N-CA	5.43	1.54	1.46
15	1	226	HIS	N-CA	5.42	1.57	1.46
8	H	65	TRP	C-N	5.38	1.46	1.34
4	D	185	GLY	N-CA	5.36	1.54	1.46
15	1	226	HIS	CA-C	5.32	1.66	1.52
17	3	102	GLU	CB-CG	5.29	1.62	1.52
2	B	205	GLU	CB-CG	5.28	1.62	1.52
5	E	81	SER	CB-OG	5.22	1.49	1.42
17	3	124	LYS	CD-CE	5.22	1.64	1.51
1	A	55	TRP	CB-CG	-5.21	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	148	TYR	CG-CD2	5.20	1.46	1.39
17	3	126	GLY	N-CA	5.15	1.53	1.46
18	4	229	PHE	C-O	5.08	1.33	1.23
12	L	172	GLU	CG-CD	-5.05	1.44	1.51
15	1	173	TYR	C-O	-5.04	1.13	1.23
18	4	90	TRP	CB-CG	-5.04	1.41	1.50
11	K	128	GLY	C-O	5.03	1.31	1.23
15	1	209	PRO	N-CD	5.02	1.54	1.47
8	H	116	ALA	C-N	5.01	1.45	1.34

All (247) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	84	ASP	C-N-CD	-31.95	50.30	120.60
16	2	184	PRO	O-C-N	11.36	140.88	122.70
16	2	258	GLY	N-CA-C	10.50	139.35	113.10
4	D	123	ARG	NE-CZ-NH2	-10.44	115.08	120.30
18	4	186	GLY	N-CA-C	10.00	138.11	113.10
12	L	84	SER	N-CA-C	9.30	136.11	111.00
11	K	113	GLY	N-CA-C	-9.14	90.24	113.10
11	K	114	HIS	N-CA-C	-9.09	86.47	111.00
16	2	184	PRO	CA-C-O	-8.94	98.75	120.20
1	A	524	GLY	N-CA-C	8.71	134.87	113.10
1	A	47	GLY	N-CA-C	-8.64	91.49	113.10
16	2	132	LEU	CA-CB-CG	8.59	135.06	115.30
1	A	284	ARG	N-CA-C	8.51	133.98	111.00
18	4	169	ASP	N-CA-C	8.15	133.01	111.00
15	1	225	TRP	C-N-CA	-7.99	101.72	121.70
6	F	103	GLN	O-C-N	-7.92	110.03	122.70
4	D	141	GLY	N-CA-C	-7.83	93.53	113.10
2	B	602	TRP	N-CA-C	7.78	132.00	111.00
4	D	169	LYS	N-CA-C	7.72	131.84	111.00
11	K	97	ASP	N-CA-C	7.65	131.64	111.00
13	N	134	CYS	N-CA-C	-7.63	90.40	111.00
13	N	159	LYS	N-CA-C	7.60	131.53	111.00
1	A	238	ASP	N-CA-C	-7.51	90.73	111.00
4	D	125	GLY	N-CA-C	7.46	131.76	113.10
17	3	131	GLU	N-CA-C	-7.46	90.86	111.00
17	3	158	PHE	N-CA-C	-7.45	90.89	111.00
16	2	126	LEU	N-CA-C	-7.41	90.99	111.00
5	E	128	VAL	N-CA-C	-7.30	91.29	111.00
18	4	234	GLN	N-CA-C	7.27	130.62	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	242	ILE	N-CA-C	7.18	130.39	111.00
17	3	154	ASN	N-CA-C	7.12	130.22	111.00
12	L	132	LEU	CA-CB-CG	7.05	131.53	115.30
1	A	346	LEU	CA-CB-CG	-7.05	99.09	115.30
4	D	122	MET	N-CA-C	7.04	130.01	111.00
2	B	72	GLY	N-CA-C	-7.03	95.53	113.10
15	1	202	CYS	CA-CB-SG	-6.98	101.43	114.00
1	A	350	LEU	CA-CB-CG	-6.98	99.24	115.30
16	2	252	ALA	N-CA-C	-6.97	92.18	111.00
15	1	65	ASP	C-N-CD	-6.95	105.31	120.60
1	A	336	GLY	C-N-CD	-6.94	105.33	120.60
16	2	102	ASN	N-CA-C	-6.93	92.28	111.00
1	A	534	LEU	N-CA-C	6.83	129.44	111.00
8	H	60	ASN	N-CA-C	6.80	129.37	111.00
7	G	72	LEU	CA-CB-CG	6.79	130.91	115.30
13	N	149	ASP	N-CA-C	-6.77	92.73	111.00
2	B	632	ILE	C-N-CA	-6.76	104.81	121.70
16	2	185	ASN	N-CA-C	6.75	129.21	111.00
5	E	98	ASN	N-CA-C	6.73	129.17	111.00
4	D	99	PHE	N-CA-C	6.72	129.15	111.00
15	1	143	LEU	CA-CB-CG	-6.72	99.85	115.30
5	E	127	GLU	N-CA-CB	-6.67	98.59	110.60
5	E	127	GLU	N-CA-C	6.66	128.99	111.00
18	4	175	TYR	N-CA-C	-6.65	93.06	111.00
1	A	348	GLU	N-CA-C	-6.59	93.20	111.00
4	D	100	TYR	N-CA-C	6.59	128.79	111.00
4	D	205	LYS	N-CA-C	6.56	128.72	111.00
1	A	295	TRP	O-C-N	6.55	133.18	122.70
1	A	28	LYS	N-CA-C	6.55	128.68	111.00
2	B	99	PRO	CA-N-CD	-6.51	102.38	111.50
1	A	345	GLY	N-CA-C	-6.47	96.92	113.10
16	2	127	THR	CB-CA-C	-6.47	94.12	111.60
18	4	194	PHE	N-CA-C	6.46	128.45	111.00
16	2	253	HIS	CB-CA-C	6.46	123.32	110.40
17	3	183	GLY	N-CA-C	-6.44	97.01	113.10
2	B	625	TRP	N-CA-C	6.42	128.33	111.00
3	C	67	VAL	CB-CA-C	-6.41	99.23	111.40
18	4	215	LEU	C-N-CA	-6.36	108.95	122.30
1	A	116	ILE	N-CA-C	6.35	128.15	111.00
5	E	70	ARG	N-CA-C	6.34	128.12	111.00
15	1	168	PHE	N-CA-C	6.34	128.11	111.00
3	C	79	LEU	CA-CB-CG	6.33	129.87	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	353	SER	N-CA-C	6.31	128.03	111.00
4	D	180	GLY	N-CA-C	6.29	128.82	113.10
4	D	177	VAL	CB-CA-C	-6.28	99.48	111.40
16	2	130	GLY	CA-C-N	-6.27	103.40	117.20
13	N	145	PHE	C-N-CA	-6.27	106.02	121.70
13	N	126	LYS	N-CA-C	6.25	127.86	111.00
13	N	166	VAL	N-CA-C	-6.24	94.16	111.00
15	1	69	LEU	O-C-N	-6.23	112.61	123.20
1	A	246	HIS	N-CA-C	6.22	127.81	111.00
15	1	165	GLY	C-N-CA	-6.20	109.28	122.30
18	4	180	GLY	N-CA-C	-6.20	97.61	113.10
1	A	290	LEU	CA-CB-CG	6.19	129.54	115.30
2	B	243	LEU	CA-CB-CG	6.17	129.49	115.30
16	2	183	PHE	N-CA-C	6.16	127.64	111.00
2	B	710	LEU	N-CA-C	-6.13	94.44	111.00
5	E	126	VAL	CB-CA-C	-6.11	99.78	111.40
15	1	63	GLY	CA-C-O	6.11	131.59	120.60
12	L	64	PRO	CA-N-CD	-6.09	102.97	111.50
11	K	94	GLN	N-CA-C	6.09	127.45	111.00
1	A	295	TRP	CA-C-N	-6.08	103.83	117.20
1	A	503	THR	N-CA-C	-6.08	94.59	111.00
17	3	104	ILE	CB-CA-C	-6.08	99.44	111.60
2	B	321	GLY	N-CA-C	6.07	128.28	113.10
2	B	19	ARG	N-CA-C	-6.07	94.62	111.00
1	A	158	ILE	N-CA-C	-6.06	94.64	111.00
16	2	129	LEU	N-CA-C	-6.04	94.69	111.00
1	A	265	GLY	N-CA-C	6.03	128.17	113.10
17	3	155	TYR	N-CA-C	6.03	127.27	111.00
17	3	125	VAL	C-N-CA	-6.01	109.68	122.30
18	4	215	LEU	N-CA-C	-6.01	94.78	111.00
1	A	530	LEU	CA-CB-CG	6.01	129.12	115.30
15	1	163	TYR	N-CA-C	-6.00	94.80	111.00
2	B	553	PHE	N-CA-C	-5.98	94.84	111.00
8	H	61	THR	CA-C-N	-5.96	104.10	117.20
1	A	337	PRO	CA-N-CD	-5.94	103.19	111.50
2	B	483	GLY	N-CA-C	-5.93	98.26	113.10
2	B	14	GLN	N-CA-C	5.91	126.95	111.00
15	1	92	LEU	CA-CB-CG	5.90	128.86	115.30
8	H	58	LEU	CA-CB-CG	5.89	128.86	115.30
8	H	68	TYR	N-CA-C	5.89	126.92	111.00
2	B	228	GLY	N-CA-C	-5.89	98.37	113.10
6	F	226	LEU	N-CA-C	-5.89	95.09	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	159	VAL	CB-CA-C	-5.89	100.21	111.40
16	2	161	GLY	N-CA-C	-5.88	98.39	113.10
2	B	469	LYS	C-N-CA	-5.86	107.05	121.70
1	A	62	HIS	N-CA-C	-5.85	95.21	111.00
2	B	303	TYR	CB-CA-C	-5.84	98.71	110.40
17	3	196	GLY	N-CA-C	5.84	127.71	113.10
16	2	130	GLY	N-CA-C	-5.82	98.56	113.10
2	B	626	LEU	CA-CB-CG	5.79	128.62	115.30
17	3	166	GLY	N-CA-C	-5.77	98.67	113.10
16	2	171	ILE	CB-CA-C	-5.77	100.06	111.60
6	F	219	ARG	N-CA-C	5.76	126.56	111.00
18	4	230	ASP	N-CA-C	5.76	126.55	111.00
17	3	205	GLY	N-CA-C	-5.72	98.79	113.10
6	F	114	ALA	N-CA-C	5.71	126.41	111.00
15	1	171	LEU	O-C-N	5.70	132.89	123.20
1	A	101	ALA	C-N-CA	-5.70	107.46	121.70
15	1	172	GLY	CA-C-N	-5.70	104.67	117.20
15	1	82	SER	N-CA-C	-5.69	95.63	111.00
13	N	157	LYS	C-N-CA	-5.69	107.47	121.70
6	F	206	LEU	CA-CB-CG	-5.69	102.22	115.30
6	F	82	LEU	CA-CB-CG	-5.68	102.23	115.30
17	3	151	TRP	N-CA-C	-5.68	95.67	111.00
16	2	216	GLU	N-CA-C	-5.67	95.69	111.00
7	G	150	ASP	N-CA-C	5.63	126.21	111.00
16	2	194	GLY	N-CA-C	5.62	127.14	113.10
2	B	456	GLU	N-CA-C	-5.61	95.84	111.00
11	K	52	PRO	N-CA-C	-5.61	97.51	112.10
1	A	43	THR	N-CA-C	-5.61	95.86	111.00
2	B	219	PRO	CA-N-CD	-5.60	103.67	111.50
7	G	96	GLY	N-CA-C	-5.60	99.11	113.10
16	2	99	LEU	CA-CB-CG	-5.57	102.48	115.30
4	D	87	THR	N-CA-C	5.57	126.03	111.00
6	F	103	GLN	CA-C-N	5.56	129.44	117.20
4	D	140	LEU	CB-CG-CD2	-5.56	101.55	111.00
17	3	128	ILE	N-CA-C	5.56	126.00	111.00
2	B	255	LEU	CA-CB-CG	5.56	128.08	115.30
16	2	169	ALA	N-CA-C	-5.55	96.01	111.00
1	A	254	LEU	CA-CB-CG	-5.54	102.56	115.30
1	A	353	SER	CB-CA-C	-5.53	99.59	110.10
1	A	501	GLY	N-CA-C	-5.52	99.30	113.10
13	N	101	LEU	N-CA-C	-5.51	96.11	111.00
1	A	157	GLY	N-CA-C	-5.50	99.34	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	123	GLY	C-N-CA	-5.50	107.95	121.70
2	B	94	PRO	CA-N-CD	-5.50	103.80	111.50
2	B	623	TYR	N-CA-C	-5.50	96.16	111.00
15	1	86	HIS	N-CA-CB	-5.50	100.71	110.60
16	2	227	LEU	CA-CB-CG	5.49	127.93	115.30
4	D	188	PHE	CB-CG-CD1	-5.49	116.96	120.80
16	2	171	ILE	N-CA-C	-5.49	96.18	111.00
15	1	157	ASP	N-CA-C	5.46	125.74	111.00
16	2	254	LEU	CB-CG-CD1	5.45	120.27	111.00
4	D	142	THR	N-CA-C	-5.44	96.31	111.00
17	3	177	ALA	N-CA-C	-5.43	96.34	111.00
8	H	99	LYS	CA-C-O	-5.43	108.70	120.10
2	B	553	PHE	C-N-CA	-5.41	110.94	122.30
2	B	120	VAL	CB-CA-C	-5.41	101.13	111.40
15	1	172	GLY	CA-C-O	5.41	130.34	120.60
12	L	164	LEU	N-CA-C	5.40	125.58	111.00
12	L	93	VAL	N-CA-C	-5.39	96.43	111.00
1	A	22	VAL	N-CA-C	5.39	125.55	111.00
18	4	238	ASP	C-N-CD	-5.38	108.75	120.60
8	H	117	SER	N-CA-C	5.38	125.53	111.00
16	2	130	GLY	O-C-N	5.37	131.29	122.70
1	A	528	ALA	N-CA-C	5.36	125.48	111.00
8	H	84	PHE	N-CA-C	5.36	125.47	111.00
1	A	131	ILE	N-CA-C	-5.35	96.55	111.00
18	4	211	MET	CB-CA-C	5.35	121.10	110.40
2	B	312	GLY	N-CA-C	5.34	126.46	113.10
17	3	129	PRO	CA-N-CD	-5.33	104.04	111.50
2	B	731	GLY	N-CA-C	-5.33	99.79	113.10
12	L	159	SER	N-CA-C	5.32	125.35	111.00
2	B	605	ASN	N-CA-C	-5.31	96.66	111.00
11	K	57	MET	N-CA-C	-5.31	96.66	111.00
2	B	260	GLY	N-CA-C	5.30	126.36	113.10
16	2	127	THR	N-CA-CB	5.30	120.37	110.30
1	A	353	SER	N-CA-CB	-5.29	102.56	110.50
3	C	69	LEU	N-CA-C	5.29	125.29	111.00
12	L	146	THR	N-CA-CB	5.29	120.35	110.30
1	A	330	ILE	CB-CA-C	-5.29	101.03	111.60
12	L	89	TYR	N-CA-C	5.28	125.25	111.00
5	E	96	ASP	CB-CG-OD1	-5.26	113.56	118.30
13	N	102	ASN	N-CA-C	5.26	125.20	111.00
1	A	118	PRO	N-CA-C	5.25	125.76	112.10
2	B	683	GLU	N-CA-C	-5.25	96.84	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	SER	C-N-CA	-5.24	111.29	122.30
1	A	23	ASP	N-CA-C	-5.24	96.87	111.00
7	G	77	PHE	N-CA-C	5.24	125.14	111.00
1	A	281	LEU	CB-CG-CD2	-5.23	102.11	111.00
16	2	257	PRO	CA-C-N	5.23	126.66	116.20
17	3	149	ASN	CA-C-N	-5.23	105.70	117.20
3	C	70	TRP	N-CA-C	-5.22	96.91	111.00
15	1	69	LEU	CA-CB-CG	-5.21	103.31	115.30
16	2	172	LEU	N-CA-C	5.21	125.08	111.00
12	L	181	GLY	N-CA-C	-5.21	100.08	113.10
6	F	115	PRO	N-CA-C	5.21	125.64	112.10
2	B	69	ALA	N-CA-C	5.21	125.05	111.00
4	D	185	GLY	N-CA-C	-5.20	100.10	113.10
16	2	256	ASP	C-N-CD	-5.19	109.19	120.60
17	3	216	ASP	N-CA-C	-5.19	96.99	111.00
6	F	81	GLY	N-CA-C	-5.18	100.15	113.10
2	B	507	SER	N-CA-C	5.18	124.98	111.00
2	B	227	THR	N-CA-C	-5.16	97.06	111.00
7	G	131	GLY	N-CA-C	5.16	125.99	113.10
1	A	280	PHE	N-CA-C	5.14	124.88	111.00
1	A	282	THR	N-CA-C	-5.13	97.14	111.00
2	B	498	LEU	N-CA-C	-5.13	97.14	111.00
1	A	342	GLY	N-CA-C	-5.12	100.30	113.10
2	B	681	ALA	N-CA-C	-5.12	97.19	111.00
3	C	62	PHE	N-CA-C	-5.12	97.18	111.00
12	L	74	THR	CB-CA-C	-5.12	97.79	111.60
1	A	540	LEU	CA-CB-CG	5.11	127.05	115.30
1	A	63	ASP	N-CA-C	5.11	124.79	111.00
2	B	486	LEU	CA-CB-CG	5.09	127.02	115.30
2	B	684	ARG	N-CA-C	5.09	124.73	111.00
6	F	97	GLN	N-CA-C	-5.07	97.31	111.00
8	H	76	TYR	N-CA-C	5.07	124.68	111.00
15	1	76	LEU	N-CA-C	-5.07	97.32	111.00
15	1	129	VAL	N-CA-C	5.07	124.68	111.00
17	3	86	PRO	N-CA-C	5.07	125.28	112.10
8	H	121	LEU	CA-CB-CG	5.06	126.94	115.30
16	2	170	ASP	N-CA-C	5.06	124.66	111.00
8	H	81	SER	N-CA-C	-5.05	97.37	111.00
1	A	42	ARG	N-CA-C	5.04	124.61	111.00
16	2	246	PRO	N-CD-CG	-5.04	95.64	103.20
1	A	94	SER	N-CA-C	-5.04	97.40	111.00
11	K	98	PRO	CA-N-CD	-5.04	104.45	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	121	ILE	N-CA-C	-5.03	97.41	111.00
15	1	69	LEU	CA-C-N	5.02	126.25	116.20
8	H	99	LYS	CA-C-N	5.02	128.25	117.20
1	A	95	GLY	C-N-CA	-5.02	109.15	121.70
1	A	154	ARG	NE-CZ-NH2	-5.02	117.79	120.30
15	1	156	LYS	CA-C-N	5.02	128.24	117.20
13	N	143	VAL	C-N-CD	-5.02	109.56	120.60
1	A	193	LEU	CA-CB-CG	5.01	126.81	115.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	G	77	PHE	CA
8	H	60	ASN	CA
8	H	68	TYR	CA

All (544) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	1	105	TYR	Peptide
15	1	118	PRO	Peptide
15	1	121	GLN	Peptide
15	1	122	ALA	Peptide
15	1	125	LEU	Peptide
15	1	130	PRO	Peptide
15	1	155	GLU	Peptide
15	1	156	LYS	Peptide
15	1	157	ASP	Peptide
15	1	170	PRO	Peptide
15	1	171	LEU	Peptide
15	1	172	GLY	Peptide
15	1	174	SER	Peptide
15	1	176	ASP	Peptide
15	1	178	LYS	Peptide
15	1	179	LYS	Peptide
15	1	184	LYS	Peptide
15	1	185	VAL	Peptide
15	1	204	GLN	Peptide
15	1	205	GLN	Peptide
15	1	206	SER	Peptide
15	1	208	TYR	Peptide
15	1	216	ASN	Peptide

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
15	1	217	LEU	Peptide
15	1	224	PRO	Mainchain,Peptide
15	1	225	TRP	Peptide
15	1	59	PRO	Peptide
15	1	60	GLY	Peptide
15	1	61	ASP	Peptide
15	1	62	PHE	Peptide
15	1	63	GLY	Mainchain,Peptide
15	1	65	ASP	Peptide
15	1	68	GLY	Mainchain
15	1	69	LEU	Mainchain
15	1	97	ILE	Peptide
16	2	100	ARG	Peptide
16	2	101	TRP	Peptide
16	2	102	ASN	Peptide
16	2	130	GLY	Peptide
16	2	133	ASN	Peptide
16	2	138	TYR	Peptide
16	2	139	THR	Peptide
16	2	140	ALA	Peptide
16	2	142	GLU	Peptide
16	2	166	ARG	Peptide
16	2	170	ASP	Peptide
16	2	172	LEU	Peptide
16	2	174	PRO	Peptide
16	2	177	VAL	Peptide
16	2	178	ASN	Peptide
16	2	181	PRO	Peptide
16	2	184	PRO	Peptide
16	2	189	THR	Peptide
16	2	193	VAL	Peptide
16	2	199	LEU	Peptide
16	2	210	SER	Peptide
16	2	212	GLN	Peptide
16	2	213	LYS	Peptide
16	2	215	LYS	Peptide
16	2	216	GLU	Peptide
16	2	218	ARG	Peptide
16	2	243	GLY	Peptide
16	2	244	THR	Peptide
16	2	245	GLY	Peptide
16	2	246	PRO	Peptide

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Mol	Chain	Res	Type	Group
16	2	247	ILE	Peptide
16	2	248	ASP	Peptide
16	2	250	LEU	Peptide
16	2	252	ALA	Peptide
16	2	255	ALA	Peptide
16	2	256	ASP	Peptide
16	2	257	PRO	Peptide
16	2	261	THR	Peptide
16	2	262	ILE	Peptide
16	2	263	PHE	Peptide
16	2	264	ALA	Peptide
16	2	266	PHE	Peptide
16	2	267	THR	Peptide
16	2	98	SER	Peptide
16	2	99	LEU	Peptide
17	3	110	MET	Peptide
17	3	122	LEU	Peptide
17	3	125	VAL	Peptide
17	3	127	LEU	Peptide
17	3	128	ILE	Peptide
17	3	129	PRO	Peptide
17	3	130	GLN	Peptide
17	3	131	GLU	Peptide
17	3	136	TRP	Peptide
17	3	139	THR	Peptide
17	3	140	GLY	Peptide
17	3	148	TYR	Peptide
17	3	149	ASN	Peptide
17	3	153	ASP	Peptide
17	3	158	PHE	Peptide
17	3	177	ALA	Peptide
17	3	178	LYS	Peptide
17	3	179	PRO	Peptide
17	3	181	SER	Peptide
17	3	188	LEU	Peptide
17	3	189	GLY	Peptide
17	3	193	GLY	Peptide
17	3	196	GLY	Peptide
17	3	197	SER	Peptide
17	3	198	GLY	Peptide
17	3	199	ASN	Peptide
17	3	200	PRO	Peptide

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Mol	Chain	Res	Type	Group
17	3	205	GLY	Peptide
17	3	212	GLY	Peptide
17	3	213	PHE	Peptide
17	3	215	LYS	Peptide
17	3	85	ASP	Peptide
17	3	93	ILE	Peptide
17	3	96	ARG	Peptide
17	3	98	LEU	Peptide
18	4	110	LEU	Peptide
18	4	112	PRO	Peptide
18	4	119	GLY	Peptide
18	4	123	VAL	Peptide
18	4	127	TYR	Peptide
18	4	128	ALA	Peptide
18	4	130	GLY	Peptide
18	4	131	LYS	Peptide
18	4	135	PHE	Peptide
18	4	136	ALA	Peptide
18	4	170	PRO	Peptide
18	4	171	ILE	Peptide
18	4	172	PHE	Peptide
18	4	175	TYR	Mainchain,Peptide
18	4	178	PRO	Peptide
18	4	189	PHE	Peptide
18	4	197	THR	Peptide
18	4	198	LEU	Peptide
18	4	213	ALA	Peptide
18	4	223	VAL	Peptide
18	4	226	LYS	Peptide
18	4	229	PHE	Peptide
18	4	232	LEU	Peptide
18	4	233	LEU	Peptide
18	4	243	THR	Peptide
18	4	86	GLU	Peptide
18	4	89	ARG	Peptide
1	A	103	PHE	Peptide
1	A	114	THR	Peptide
1	A	117	GLY	Peptide
1	A	119	SER	Peptide
1	A	123	VAL	Peptide
1	A	128	GLY	Peptide
1	A	132	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	A	134	GLY	Peptide
1	A	136	VAL	Peptide
1	A	142	GLY	Peptide
1	A	146	THR	Peptide
1	A	148	GLY	Peptide
1	A	189	ALA	Peptide
1	A	197	GLN	Peptide
1	A	199	VAL	Peptide
1	A	201	SER	Peptide
1	A	21	LEU	Peptide
1	A	22	VAL	Peptide
1	A	23	ASP	Peptide
1	A	240	LYS	Peptide
1	A	246	HIS	Peptide
1	A	25	ASP	Peptide
1	A	250	LEU	Peptide
1	A	251	ASN	Peptide
1	A	257	GLN	Peptide
1	A	26	PRO	Peptide
1	A	262	PHE	Peptide
1	A	263	ALA	Peptide
1	A	27	ILE	Peptide
1	A	270	PHE	Peptide
1	A	274	TRP	Peptide
1	A	275	SER	Peptide
1	A	276	LYS	Peptide
1	A	279	ASP	Peptide
1	A	28	LYS	Peptide
1	A	280	PHE	Peptide
1	A	282	THR	Peptide
1	A	290	LEU	Peptide
1	A	316	MET	Peptide
1	A	345	GLY	Peptide
1	A	346	LEU	Peptide
1	A	349	ILE	Peptide
1	A	352	THR	Peptide
1	A	36	LYS	Peptide
1	A	37	PRO	Peptide
1	A	38	GLY	Peptide
1	A	39	HIS	Peptide
1	A	393	LEU	Peptide
1	A	420	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	A	427	ARG	Peptide
1	A	430	ASP	Peptide
1	A	45	ALA	Peptide
1	A	46	LYS	Peptide
1	A	47	GLY	Peptide
1	A	482	ILE	Peptide
1	A	483	GLN	Peptide
1	A	486	PRO	Peptide
1	A	488	PHE	Peptide
1	A	497	ALA	Peptide
1	A	501	GLY	Peptide
1	A	505	PRO	Peptide
1	A	506	GLY	Peptide
1	A	510	SER	Peptide
1	A	518	GLY	Peptide
1	A	519	ASP	Peptide
1	A	520	LEU	Peptide
1	A	525	ASN	Peptide
1	A	527	VAL	Peptide
1	A	535	GLY	Peptide
1	A	574	ASN	Peptide
1	A	575	LEU	Peptide
1	A	576	GLY	Peptide
1	A	62	HIS	Peptide
1	A	625	TRP	Peptide
1	A	626	GLY	Peptide
1	A	631	GLN	Peptide
1	A	64	PHE	Peptide
1	A	66	SER	Peptide
1	A	67	HIS	Peptide
1	A	73	GLU	Peptide
1	A	93	LEU	Peptide
2	B	103	ALA	Peptide
2	B	126	THR	Peptide
2	B	130	ARG	Peptide
2	B	135	LEU	Peptide
2	B	139	ALA	Peptide
2	B	162	LYS	Peptide
2	B	166	SER	Peptide
2	B	170	ASN	Peptide
2	B	203	ARG	Peptide
2	B	204	GLY	Peptide

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Mol	Chain	Res	Type	Group
2	B	211	ASN	Peptide
2	B	223	GLY	Peptide
2	B	224	PRO	Peptide
2	B	228	GLY	Peptide
2	B	229	GLN	Peptide
2	B	231	ASN	Peptide
2	B	232	LEU	Peptide
2	B	238	SER	Peptide
2	B	246	THR	Peptide
2	B	248	GLN	Peptide
2	B	256	THR	Peptide
2	B	257	ILE	Peptide
2	B	259	GLY	Peptide
2	B	26	ALA	Peptide
2	B	260	GLY	Peptide
2	B	265	THR	Peptide
2	B	267	SER	Peptide
2	B	292	ARG	Peptide
2	B	298	GLY	Peptide
2	B	303	TYR	Peptide
2	B	308	HIS	Peptide
2	B	311	PRO	Peptide
2	B	320	LYS	Peptide
2	B	33	SER	Peptide
2	B	36	ASP	Peptide
2	B	363	GLN	Peptide
2	B	364	ASP	Peptide
2	B	365	PHE	Peptide
2	B	377	TYR	Peptide
2	B	4	ARG	Peptide
2	B	405	ASP	Peptide
2	B	406	ASN	Peptide
2	B	445	ALA	Peptide
2	B	447	GLY	Peptide
2	B	458	ILE	Peptide
2	B	464	GLN	Peptide
2	B	468	GLY	Peptide
2	B	469	LYS	Peptide
2	B	472	TYR	Peptide
2	B	473	GLY	Peptide
2	B	474	PHE	Peptide
2	B	478	LEU	Peptide

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Mol	Chain	Res	Type	Group
2	B	481	THR	Peptide
2	B	483	GLY	Peptide
2	B	484	PRO	Peptide
2	B	5	ILE	Peptide
2	B	504	ASN	Peptide
2	B	507	SER	Peptide
2	B	510	LEU	Peptide
2	B	540	ASP	Peptide
2	B	549	ASP	Peptide
2	B	563	GLY	Peptide
2	B	595	HIS	Peptide
2	B	602	TRP	Peptide
2	B	603	ARG	Peptide
2	B	604	GLY	Peptide
2	B	605	ASN	Peptide
2	B	606	VAL	Peptide
2	B	618	GLY	Peptide
2	B	627	ASN	Peptide
2	B	632	ILE	Peptide
2	B	633	ASN	Peptide
2	B	635	ILE	Peptide
2	B	641	ASN	Peptide
2	B	69	ALA	Peptide
2	B	690	LEU	Peptide
2	B	7	ARG	Peptide
2	B	73	ASN	Peptide
2	B	730	SER	Peptide
2	B	732	LYS	Peptide
2	B	80	ASP	Peptide
2	B	84	VAL	Peptide
2	B	9	SER	Peptide
3	C	1	MET	Peptide
3	C	27	GLU	Peptide
3	C	28	MET	Peptide
3	C	29	ILE	Peptide
3	C	33	GLY	Peptide
3	C	42	ALA	Peptide
3	C	54	CYS	Peptide
3	C	65	VAL	Peptide
3	C	67	VAL	Peptide
3	C	68	TYR	Peptide
3	C	69	LEU	Peptide

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Mol	Chain	Res	Type	Group
3	C	70	TRP	Peptide
3	C	73	THR	Peptide
3	C	79	LEU	Peptide
4	D	108	LYS	Peptide
4	D	114	MET	Peptide
4	D	117	GLY	Peptide
4	D	118	GLY	Peptide
4	D	119	ALA	Peptide
4	D	124	GLU	Peptide
4	D	125	GLY	Peptide
4	D	145	ARG	Peptide
4	D	147	LYS	Peptide
4	D	150	ILE	Peptide
4	D	151	LYS	Peptide
4	D	158	PHE	Peptide
4	D	161	GLY	Peptide
4	D	162	GLU	Peptide
4	D	163	VAL	Peptide
4	D	168	PRO	Peptide
4	D	171	GLY	Peptide
4	D	174	PRO	Peptide
4	D	177	VAL	Peptide
4	D	181	ARG	Peptide
4	D	182	GLN	Peptide
4	D	184	VAL	Peptide
4	D	190	SER	Peptide
4	D	193	LYS	Peptide
4	D	194	ASN	Peptide
4	D	204	GLY	Peptide
4	D	209	ASP	Peptide
4	D	73	GLU	Peptide
4	D	78	THR	Peptide
4	D	79	PRO	Peptide
4	D	81	PRO	Peptide
4	D	83	PHE	Peptide
4	D	87	THR	Peptide
4	D	89	GLY	Peptide
4	D	91	LEU	Peptide
4	D	93	LYS	Peptide
4	D	97	GLU	Peptide
5	E	116	SER	Peptide
5	E	124	GLU	Peptide

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
5	E	125	ILE	Peptide
5	E	126	VAL	Mainchain
5	E	127	GLU	Peptide
5	E	67	GLY	Peptide
5	E	79	LYS	Peptide
5	E	88	GLY	Peptide
5	E	96	ASP	Peptide
5	E	97	PRO	Peptide
6	F	103	GLN	Mainchain
6	F	104	ALA	Peptide
6	F	105	SER	Peptide
6	F	107	LYS	Peptide
6	F	108	LEU	Peptide
6	F	111	ASP	Peptide
6	F	112	ASP	Peptide
6	F	115	PRO	Peptide
6	F	116	ALA	Peptide
6	F	118	ALA	Peptide
6	F	129	ARG	Peptide
6	F	133	TYR	Peptide
6	F	135	LYS	Peptide
6	F	137	GLY	Peptide
6	F	138	LEU	Peptide
6	F	151	SER	Peptide
6	F	185	ILE	Peptide
6	F	189	LYS	Peptide
6	F	196	ILE	Peptide
6	F	199	ASP	Peptide
6	F	203	ALA	Peptide
6	F	212	SER	Peptide
6	F	213	TRP	Peptide
6	F	218	TYR	Peptide
6	F	230	ASN	Peptide
6	F	79	ILE	Peptide
6	F	97	GLN	Mainchain
7	G	100	PHE	Peptide
7	G	103	GLY	Peptide
7	G	104	ASP	Peptide
7	G	106	ARG	Peptide
7	G	111	VAL	Peptide
7	G	114	LEU	Peptide
7	G	115	LYS	Peptide

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Mol	Chain	Res	Type	Group
7	G	134	GLY	Peptide
7	G	141	ILE	Peptide
7	G	146	SER	Peptide
7	G	147	ASN	Peptide
7	G	148	GLY	Peptide
7	G	149	TYR	Peptide
7	G	153	PHE	Peptide
7	G	71	SER	Peptide
7	G	78	VAL	Peptide
7	G	82	PHE	Peptide
7	G	84	ARG	Peptide
7	G	86	ASN	Peptide
7	G	90	GLN	Peptide
7	G	91	VAL	Peptide
7	G	95	ASN	Peptide
7	G	98	THR	Peptide
7	G	99	HIS	Peptide
8	H	114	ALA	Peptide
8	H	116	ALA	Peptide
8	H	118	GLY	Peptide
8	H	119	ASP	Peptide
8	H	120	ILE	Peptide
8	H	56	GLU	Peptide
8	H	58	LEU	Peptide
8	H	60	ASN	Peptide
8	H	61	THR	Peptide
8	H	62	THR	Peptide
8	H	63	GLY	Peptide
8	H	65	TRP	Peptide
8	H	67	SER	Peptide
8	H	68	TYR	Peptide
8	H	69	GLY	Peptide
8	H	79	LEU	Peptide
8	H	81	SER	Peptide
8	H	84	PHE	Peptide
8	H	86	THR	Peptide
8	H	93	LYS	Peptide
8	H	95	GLY	Peptide
8	H	97	LEU	Peptide
11	K	113	GLY	Peptide
11	K	118	VAL	Peptide
11	K	119	GLY	Peptide

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Mol	Chain	Res	Type	Group
11	K	120	VAL	Peptide
11	K	122	LEU	Peptide
11	K	123	GLY	Peptide
11	K	125	LYS	Peptide
11	K	126	ASN	Peptide
11	K	128	GLY	Peptide
11	K	129	ALA	Peptide
11	K	73	ALA	Peptide
11	K	76	ALA	Peptide
11	K	80	ALA	Peptide
11	K	86	LEU	Peptide
11	K	88	VAL	Peptide
11	K	89	ARG	Peptide
11	K	91	SER	Peptide
11	K	93	LEU	Peptide
11	K	94	GLN	Peptide
11	K	96	GLY	Peptide
11	K	97	ASP	Peptide
12	L	128	GLN	Peptide
12	L	129	ALA	Peptide
12	L	143	LEU	Peptide
12	L	152	SER	Peptide
12	L	154	ASN	Peptide
12	L	156	GLY	Peptide
12	L	157	ALA	Peptide
12	L	160	THR	Peptide
12	L	165	THR	Peptide
12	L	166	LEU	Peptide
12	L	168	GLY	Peptide
12	L	169	ARG	Peptide
12	L	174	ASP	Peptide
12	L	176	LEU	Peptide
12	L	206	VAL	Peptide
12	L	52	PRO	Peptide
12	L	61	ASN	Peptide
12	L	67	GLY	Peptide
12	L	68	SER	Peptide
12	L	73	VAL	Peptide
12	L	79	ILE	Peptide
12	L	88	ALA	Peptide
12	L	95	PRO	Peptide
13	N	100	GLU	Peptide

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Mol	Chain	Res	Type	Group
13	N	102	ASN	Peptide
13	N	108	ALA	Peptide
13	N	111	GLY	Peptide
13	N	112	ALA	Peptide
13	N	113	ASN	Peptide
13	N	118	TYR	Peptide
13	N	119	THR	Peptide
13	N	120	VAL	Peptide
13	N	123	GLY	Peptide
13	N	125	CYS	Peptide
13	N	126	LYS	Peptide
13	N	127	PHE	Peptide
13	N	129	GLU	Peptide
13	N	131	PHE	Peptide
13	N	133	GLY	Peptide
13	N	135	GLN	Peptide
13	N	136	ASP	Peptide
13	N	137	LEU	Peptide
13	N	142	LYS	Peptide
13	N	145	PHE	Peptide
13	N	147	SER	Peptide
13	N	148	ASP	Peptide
13	N	150	LEU	Peptide
13	N	151	ASP	Peptide
13	N	152	LEU	Peptide
13	N	155	GLU	Peptide
13	N	156	GLY	Peptide
13	N	157	LYS	Peptide
13	N	158	ASP	Peptide
13	N	160	TYR	Peptide
13	N	162	CYS	Peptide
13	N	164	SER	Peptide
13	N	166	VAL	Peptide
13	N	168	TRP	Peptide
13	N	169	LYS	Peptide
13	N	90	GLU	Peptide
13	N	92	LEU	Peptide
13	N	96	LYS	Peptide
13	N	97	THR	Peptide
14	R	28	UNK	Peptide
14	R	30	UNK	Peptide
14	R	31	UNK	Peptide

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Mol	Chain	Res	Type	Group
14	R	32	UNK	Peptide
14	R	33	UNK	Peptide
14	R	34	UNK	Peptide
14	R	36	UNK	Peptide
14	R	37	UNK	Peptide
14	R	40	UNK	Peptide
14	R	42	UNK	Peptide
14	R	46	UNK	Peptide
14	R	47	UNK	Peptide
14	R	48	UNK	Peptide
14	R	50	UNK	Peptide
14	R	51	UNK	Peptide
14	R	52	UNK	Peptide
14	R	7	UNK	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5739	0	5574	1922	6
2	B	5844	0	5648	1926	14
3	C	619	0	605	325	0
4	D	1097	0	1101	436	4
5	E	513	0	514	252	0
6	F	1221	0	1247	373	28
7	G	738	0	709	337	6
8	H	517	0	503	208	2
9	I	229	0	252	53	1
10	J	334	0	344	84	0
11	K	592	0	618	270	5
12	L	1209	0	1220	435	64
13	N	685	0	667	344	0
14	R	265	0	67	79	0
15	1	1257	0	1220	592	37
16	2	1367	0	1312	644	35
17	3	1197	0	1137	516	2
18	4	1309	0	1264	532	45
19	1	665	0	453	123	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	2	663	0	494	142	0
19	3	736	0	453	158	0
19	4	729	0	496	154	0
19	A	2676	0	2544	1037	0
19	B	2177	0	2072	680	0
19	F	130	0	85	21	0
19	G	51	0	40	9	0
19	H	240	0	237	61	0
19	I	60	0	58	7	0
19	J	116	0	107	51	0
19	K	210	0	179	40	8
19	L	322	0	275	118	0
19	R	122	0	123	13	0
20	A	33	0	45	9	0
20	B	33	0	46	22	0
21	1	40	0	54	6	0
21	3	40	0	54	6	0
21	A	200	0	271	162	0
21	B	240	0	323	116	0
21	F	80	0	107	61	0
21	I	80	0	111	46	0
21	J	40	0	52	32	0
21	L	40	0	53	34	0
22	1	70	0	92	10	0
22	2	140	0	184	14	0
22	3	70	0	90	38	0
22	4	278	0	357	69	0
22	A	210	0	275	27	0
22	B	95	0	115	11	0
22	C	35	0	46	0	0
22	D	35	0	45	21	0
22	E	70	0	92	24	0
22	F	34	0	41	12	0
22	G	105	0	138	14	0
22	H	245	0	322	40	0
22	K	140	0	184	37	2
22	L	35	0	46	11	0
22	N	35	0	46	9	0
22	R	245	0	322	34	0
23	B	49	0	71	19	0
24	A	8	0	0	2	0
24	C	16	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	36370	0	35200	10756	130

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 150.

All (10756) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:4:7034:LMU:C9	22:4:7052:LMU:H1'	1.24	1.64
2:B:459:PHE:CE2	19:B:1235:CLA:C2D	1.76	1.63
19:A:1125:CLA:HBB2	19:A:1133:CLA:CMA	1.18	1.60
1:A:244:LEU:CB	1:A:247:GLU:HG3	1.25	1.60
16:2:130:GLY:CA	16:2:131:ILE:HG13	1.29	1.60
2:B:459:PHE:CD2	19:B:1235:CLA:C3D	1.79	1.59
1:A:21:LEU:CA	1:A:22:VAL:HG12	1.16	1.59
15:1:177:PRO:HD2	15:1:180:LEU:CG	1.13	1.58
1:A:281:LEU:HD13	19:A:1115:CLA:CED	1.24	1.57
19:2:2007:CLA:CBC	19:3:2009:CLA:HED2	1.11	1.57
22:4:7034:LMU:C8	22:4:7052:LMU:H2'	1.09	1.56
16:2:130:GLY:HA2	16:2:131:ILE:CG1	1.29	1.56
5:E:89:SER:HB2	5:E:106:ARG:CZ	1.28	1.56
18:4:158:GLN:HB3	19:4:1004:CLA:CMA	1.12	1.56
22:4:7034:LMU:H81	22:4:7052:LMU:C2'	1.23	1.56
2:B:459:PHE:HD2	19:B:1235:CLA:C3D	0.91	1.56
15:1:177:PRO:CD	15:1:180:LEU:HG	1.08	1.55
8:H:61:THR:CA	8:H:62:THR:HG23	1.36	1.55
13:N:130:ASN:CB	13:N:139:LYS:HG2	1.36	1.55
18:4:120:ILE:CD1	18:4:226:LYS:HG3	1.12	1.54
15:1:93:ALA:HB1	19:1:1006:CLA:CHC	1.34	1.54
18:4:120:ILE:HD11	18:4:226:LYS:CG	1.24	1.54
3:C:44:ARG:NH2	4:D:181:ARG:CD	1.68	1.54
13:N:103:ASP:HB2	13:N:107:LEU:CD1	1.35	1.52
18:4:103:MET:CE	18:4:208:GLY:N	1.71	1.52
18:4:103:MET:HE2	18:4:208:GLY:CA	1.38	1.52
19:A:1125:CLA:CBB	19:A:1133:CLA:HMA2	1.04	1.52
17:3:103:VAL:HG13	17:3:107:ARG:CD	1.36	1.51
2:B:459:PHE:CD2	19:B:1235:CLA:C2D	1.82	1.51
8:H:58:LEU:CD1	8:H:62:THR:HG21	1.38	1.51
15:1:97:ILE:HD13	15:1:98:LEU:CA	1.10	1.51
18:4:103:MET:CE	18:4:208:GLY:CA	1.88	1.51
17:3:113:ALA:CB	17:3:239:LEU:HD11	1.34	1.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:R:32:UNK:CB	14:R:33:UNK:CB	1.85	1.51
2:B:314:ARG:NH1	15:1:67:LEU:HD21	1.22	1.50
18:4:172:PHE:CB	18:4:194:PHE:HE2	0.89	1.50
18:4:158:GLN:CB	19:4:1004:CLA:HMA3	1.37	1.50
8:H:61:THR:HA	8:H:62:THR:CG2	1.37	1.50
1:A:244:LEU:HB2	1:A:247:GLU:CG	1.40	1.49
18:4:172:PHE:HB2	18:4:194:PHE:CE2	1.00	1.49
6:F:190:LYS:NZ	6:F:192:THR:HG21	1.18	1.49
15:1:97:ILE:CD1	15:1:98:LEU:N	1.69	1.49
1:A:250:LEU:HB2	17:3:136:TRP:CH2	1.47	1.49
15:1:97:ILE:CD1	15:1:98:LEU:CA	1.85	1.49
19:1:1013:CLA:C6	19:1:1014:CLA:HED3	1.41	1.48
1:A:281:LEU:CD1	19:A:1115:CLA:HED1	1.41	1.47
3:C:62:PHE:CZ	5:E:80:GLU:CD	1.88	1.47
13:N:103:ASP:CB	13:N:107:LEU:HD12	1.43	1.47
19:L:1148:CLA:HED1	19:L:1148:CLA:C2	1.38	1.47
1:A:443:ILE:HD11	1:A:557:LEU:CD2	1.41	1.46
13:N:155:GLU:HB3	13:N:157:LYS:N	1.21	1.46
17:3:135:ALA:HB1	17:3:139:THR:CB	1.44	1.46
17:3:127:LEU:CB	19:3:1147:CLA:HED3	1.45	1.45
4:D:156:ARG:NH1	4:D:158:PHE:HE1	0.97	1.45
22:4:7034:LMU:H92	22:4:7052:LMU:C1'	1.42	1.45
1:A:249:ILE:CG2	17:3:136:TRP:HZ3	1.25	1.45
2:B:596:TRP:CH2	2:B:612:SER:O	1.68	1.44
2:B:123:TRP:HA	2:B:126:THR:CG2	1.44	1.44
2:B:294:ASN:ND2	7:G:94:GLN:HG3	1.25	1.44
2:B:89:HIS:C	2:B:113:VAL:HG11	1.10	1.44
8:H:58:LEU:CD1	8:H:62:THR:CG2	1.91	1.44
17:3:122:LEU:CD2	19:3:3006:CLA:CHA	1.94	1.44
19:4:4006:CLA:C10	22:4:7034:LMU:H121	1.47	1.44
18:4:87:ASN:HB2	18:4:90:TRP:CE3	1.51	1.44
15:1:176:ASP:HB3	15:1:180:LEU:CD1	1.46	1.43
1:A:308:ILE:CD1	19:A:1115:CLA:HHC	1.47	1.43
16:2:160:ILE:CG2	19:2:2012:CLA:CBB	1.95	1.43
2:B:633:ASN:CB	2:B:636:THR:HB	1.48	1.43
21:B:6020:BCR:C33	19:L:1502:CLA:C4B	1.95	1.43
16:2:133:ASN:ND2	16:2:134:THR:HB	1.28	1.43
13:N:146:LEU:CD1	17:3:142:ILE:O	1.66	1.43
18:4:175:TYR:O	18:4:194:PHE:CE1	1.69	1.42
17:3:103:VAL:CG1	17:3:107:ARG:HD3	1.47	1.42
22:3:7003:LMU:H3B	22:3:7005:LMU:C5B	1.46	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:14:CYS:HA	3:C:17:CYS:SG	1.58	1.41
4:D:167:HIS:NE2	4:D:172:VAL:HG11	1.12	1.41
16:2:133:ASN:HD22	16:2:134:THR:CB	1.33	1.41
6:F:190:LYS:NZ	6:F:192:THR:CG2	1.82	1.41
19:2:2007:CLA:CBC	19:3:2009:CLA:CED	1.95	1.40
4:D:167:HIS:NE2	4:D:172:VAL:CG1	1.84	1.40
16:2:168:TRP:HD1	16:2:171:ILE:CG2	1.35	1.40
1:A:154:ARG:NE	1:A:384:TYR:HE1	1.19	1.40
19:A:1115:CLA:CED	19:A:1115:CLA:H2A	1.49	1.39
13:N:139:LYS:CB	13:N:142:LYS:HD3	1.50	1.39
11:K:92:GLY:O	11:K:93:LEU:HG	1.22	1.39
17:3:150:TYR:CG	17:3:151:TRP:CD1	2.10	1.39
1:A:338:PHE:CE1	19:A:1151:CLA:CBB	2.06	1.39
16:2:122:ILE:HD11	19:2:2002:CLA:CAB	1.51	1.39
16:2:166:ARG:N	16:2:167:ARG:HB2	1.21	1.39
1:A:478:SER:CB	1:A:644:GLN:HE22	1.35	1.39
2:B:257:ILE:O	2:B:497:TRP:CE3	1.75	1.39
1:A:342:GLY:CA	1:A:430:ASP:HB2	1.48	1.39
13:N:155:GLU:C	13:N:157:LYS:CE	1.90	1.39
2:B:247:THR:HA	2:B:250:ALA:CB	1.52	1.39
22:4:7034:LMU:H111	22:4:7052:LMU:C4'	1.38	1.38
1:A:21:LEU:N	1:A:22:VAL:CG1	1.83	1.38
16:2:160:ILE:HG22	19:2:2012:CLA:CBB	1.52	1.38
17:3:127:LEU:CB	19:3:1147:CLA:CED	2.01	1.38
1:A:534:LEU:HD12	1:A:535:GLY:N	1.31	1.38
13:N:155:GLU:CB	13:N:157:LYS:H	1.37	1.38
1:A:21:LEU:CA	1:A:22:VAL:CG1	1.98	1.37
15:1:176:ASP:CB	15:1:180:LEU:HD12	1.54	1.37
18:4:158:GLN:NE2	19:4:1004:CLA:C1A	1.87	1.37
1:A:21:LEU:HA	1:A:22:VAL:CG1	1.54	1.37
13:N:130:ASN:HB2	13:N:139:LYS:CG	1.51	1.37
1:A:249:ILE:HG23	17:3:136:TRP:CZ3	1.60	1.37
16:2:168:TRP:CD1	16:2:171:ILE:HG21	1.59	1.37
16:2:118:ALA:HA	16:2:121:PHE:CE2	1.60	1.36
2:B:732:LYS:HG2	2:B:734:GLY:N	1.34	1.36
1:A:279:ASP:O	1:A:281:LEU:HG	1.24	1.36
2:B:459:PHE:HE2	19:B:1235:CLA:C1D	1.39	1.36
19:3:1147:CLA:HMC1	19:3:1147:CLA:CBC	1.46	1.36
13:N:132:THR:CG2	13:N:139:LYS:HD3	1.55	1.36
12:L:205:TYR:CD1	12:L:207:LEU:HD12	1.61	1.36
22:3:7003:LMU:H3B	22:3:7005:LMU:C4B	1.52	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:VAL:HA	2:B:123:TRP:CD1	1.61	1.35
17:3:150:TYR:N	17:3:152:ALA:HB2	1.40	1.35
19:3:2009:CLA:CGA	19:3:2009:CLA:HBD	1.56	1.35
7:G:98:THR:CB	7:G:101:GLU:CD	1.95	1.34
19:3:2009:CLA:C5	19:3:2009:CLA:H92	1.45	1.34
3:C:44:ARG:NH2	4:D:181:ARG:HD3	1.04	1.34
15:1:67:LEU:HD12	15:1:68:GLY:N	1.41	1.34
1:A:308:ILE:HD11	19:A:1115:CLA:CAB	1.56	1.34
4:D:114:MET:CG	4:D:115:PRO:O	1.76	1.34
18:4:103:MET:CE	18:4:208:GLY:HA2	1.49	1.34
7:G:89:LYS:CE	7:G:89:LYS:HA	1.55	1.33
20:B:5002:PQN:H162	21:B:6017:BCR:C33	1.54	1.33
13:N:114:PHE:CD1	13:N:117:ALA:HB2	1.62	1.33
16:2:134:THR:OG1	16:2:135:PRO:HD2	1.22	1.33
16:2:118:ALA:CA	16:2:121:PHE:HE2	1.40	1.33
18:4:145:GLU:HG3	18:4:146:PHE:CD1	1.62	1.32
1:A:744:ALA:CB	21:A:6011:BCR:H391	1.59	1.32
3:C:64:SER:O	3:C:65:VAL:HG12	1.16	1.32
19:A:1119:CLA:H92	21:A:6007:BCR:C37	1.57	1.32
5:E:89:SER:OG	5:E:106:ARG:CD	1.78	1.32
4:D:140:LEU:CD1	4:D:141:GLY:N	1.92	1.32
19:L:1148:CLA:CED	19:L:1148:CLA:H2	1.57	1.32
2:B:304:ILE:CD1	19:B:1216:CLA:HED2	1.59	1.31
17:3:150:TYR:CD2	17:3:151:TRP:CD1	2.18	1.31
5:E:89:SER:OG	5:E:106:ARG:HD3	1.28	1.31
15:1:91:MET:O	15:1:95:PRO:HD3	1.20	1.31
7:G:98:THR:HG21	7:G:101:GLU:OE2	1.18	1.31
19:L:1148:CLA:HAA1	19:L:1148:CLA:CGD	1.60	1.31
16:2:186:ASN:OD1	16:2:188:LEU:HD11	1.27	1.31
2:B:36:ASP:O	2:B:41:ARG:NH1	1.63	1.31
16:2:117:ALA:CB	16:2:230:LEU:HG	1.58	1.31
3:C:62:PHE:CE2	5:E:80:GLU:HG3	1.65	1.31
1:A:120:ALA:H	1:A:145:ILE:CD1	1.41	1.30
2:B:257:ILE:O	2:B:497:TRP:CZ3	1.84	1.30
19:A:1115:CLA:C2A	19:A:1115:CLA:HED3	1.61	1.30
8:H:78:PRO:HD3	19:L:1501:CLA:CMD	1.61	1.30
17:3:113:ALA:HB2	17:3:239:LEU:CD1	1.62	1.30
16:2:165:GLY:C	16:2:167:ARG:HB2	1.50	1.30
15:1:189:LYS:CG	19:1:1007:CLA:HMC2	1.62	1.30
17:3:111:LEU:O	17:3:114:VAL:N	1.65	1.30
1:A:338:PHE:CE1	19:A:1151:CLA:HBB1	1.65	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:155:GLU:C	13:N:157:LYS:HE2	1.49	1.29
15:1:88:ARG:O	15:1:92:LEU:HB2	1.28	1.29
21:B:6020:BCR:H333	19:L:1502:CLA:C4B	1.56	1.29
2:B:732:LYS:HG2	2:B:733:PHE:C	1.52	1.29
1:A:281:LEU:CD2	19:A:1115:CLA:CMA	2.07	1.29
17:3:150:TYR:CD2	17:3:151:TRP:NE1	2.01	1.29
19:K:1143:CLA:CAC	22:K:7001:LMU:O3B	1.79	1.29
16:2:96:PRO:HD2	17:3:85:ASP:OD2	1.30	1.29
1:A:21:LEU:N	1:A:22:VAL:HG12	0.99	1.28
7:G:98:THR:CG2	7:G:101:GLU:OE2	1.77	1.28
13:N:132:THR:HG21	13:N:139:LYS:CD	1.62	1.28
12:L:154:ASN:O	12:L:178:THR:HG23	1.18	1.28
8:H:119:ASP:O	8:H:120:ILE:HG22	1.24	1.28
1:A:246:HIS:HA	1:A:248:PHE:CE2	1.67	1.28
19:3:2009:CLA:H52	19:3:2009:CLA:C9	1.54	1.28
1:A:157:GLY:HA3	1:A:229:ILE:CG2	1.60	1.28
2:B:122:GLN:O	2:B:126:THR:CB	1.80	1.28
1:A:668:TYR:CD1	2:B:445:ALA:HB2	1.68	1.28
16:2:134:THR:OG1	16:2:135:PRO:CD	1.80	1.28
19:2:2007:CLA:HAC2	19:3:2009:CLA:CED	1.62	1.28
18:4:167:ASN:OD1	19:4:4014:CLA:C2	1.80	1.27
4:D:140:LEU:HD12	4:D:141:GLY:N	0.95	1.27
2:B:229:GLN:C	7:G:63:VAL:HG21	1.55	1.27
22:4:7034:LMU:C11	22:4:7052:LMU:C4'	2.12	1.27
11:K:49:ILE:O	11:K:52:PRO:CG	1.80	1.27
11:K:49:ILE:O	11:K:52:PRO:HG2	1.14	1.27
1:A:368:LEU:HD21	19:A:1117:CLA:C9	1.63	1.27
15:1:95:PRO:O	15:1:98:LEU:HB3	1.30	1.27
1:A:157:GLY:O	1:A:158:ILE:CG2	1.79	1.27
19:2:2007:CLA:CAC	19:3:2009:CLA:CED	2.11	1.27
5:E:89:SER:CB	5:E:106:ARG:CZ	2.11	1.27
4:D:156:ARG:NH1	4:D:158:PHE:CE1	1.74	1.27
4:D:123:ARG:NH2	22:D:7050:LMU:C4B	1.98	1.27
1:A:162:LEU:O	1:A:165:TYR:HB3	1.34	1.27
15:1:97:ILE:HD13	15:1:98:LEU:N	0.94	1.27
2:B:317:ARG:NH1	2:B:405:ASP:O	1.68	1.27
7:G:72:LEU:HD23	7:G:124:ILE:CD1	1.65	1.27
15:1:77:GLU:HA	15:1:80:LYS:CG	1.65	1.27
12:L:129:ALA:O	12:L:201:TYR:HB3	1.35	1.27
1:A:744:ALA:HB2	21:A:6011:BCR:C39	1.64	1.26
5:E:107:PHE:CE2	5:E:109:LYS:HG3	1.69	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3:109:ALA:C	17:3:111:LEU:HB3	1.55	1.26
12:L:209:LEU:CD1	12:L:210:PRO:HD2	1.64	1.26
12:L:60:ILE:CG2	12:L:61:ASN:H	1.43	1.26
15:1:95:PRO:O	15:1:98:LEU:CB	1.83	1.26
1:A:242:ILE:HG13	1:A:243:PRO:CD	1.65	1.26
16:2:130:GLY:CA	16:2:131:ILE:CG1	1.97	1.26
4:D:123:ARG:NH2	22:D:7050:LMU:O4'	1.67	1.26
6:F:200:VAL:CG1	10:J:7:TYR:HB2	1.65	1.26
7:G:98:THR:HB	7:G:101:GLU:CD	1.54	1.26
4:D:167:HIS:CD2	4:D:172:VAL:HG21	1.68	1.26
2:B:232:LEU:CD1	2:B:235:GLN:HG3	1.66	1.26
2:B:317:ARG:NH2	2:B:410:ARG:HG2	1.49	1.26
2:B:459:PHE:CE2	19:B:1235:CLA:CMD	2.18	1.26
13:N:155:GLU:O	13:N:157:LYS:HE3	1.22	1.26
4:D:200:VAL:HG21	4:D:206:GLN:NE2	1.48	1.26
1:A:242:ILE:CG1	1:A:243:PRO:HD3	1.64	1.25
16:2:226:ARG:HD2	16:2:230:LEU:CD2	1.67	1.25
17:3:103:VAL:HG13	17:3:107:ARG:NE	1.49	1.25
2:B:160:LYS:HD3	2:B:161:TRP:CE2	1.70	1.25
2:B:403:ASN:O	2:B:406:ASN:HB3	1.34	1.25
3:C:5:VAL:CG2	3:C:65:VAL:HG23	1.66	1.25
11:K:127:ILE:C	11:K:129:ALA:HA	1.56	1.25
19:B:1209:CLA:HAC2	19:B:1210:CLA:CBB	1.65	1.25
19:B:1209:CLA:CAC	19:B:1210:CLA:HBB2	1.65	1.25
8:H:76:TYR:OH	12:L:90:ARG:NE	1.68	1.25
13:N:139:LYS:CG	13:N:142:LYS:HD3	1.66	1.24
1:A:281:LEU:CD1	19:A:1115:CLA:CED	2.00	1.24
4:D:156:ARG:CZ	4:D:158:PHE:HE1	1.48	1.24
2:B:5:ILE:HG22	2:B:6:PRO:CD	1.67	1.24
16:2:254:LEU:HD22	16:2:255:ALA:N	1.49	1.24
11:K:49:ILE:C	11:K:52:PRO:CG	2.05	1.24
18:4:146:PHE:HZ	19:4:4013:CLA:C4C	1.50	1.24
19:A:9012:CLA:H11	2:B:616:LEU:CD1	1.66	1.24
7:G:98:THR:HB	7:G:101:GLU:OE1	1.15	1.23
1:A:284:ARG:HA	1:A:284:ARG:NH1	1.50	1.23
2:B:36:ASP:O	2:B:41:ARG:CZ	1.86	1.23
7:G:72:LEU:CD2	7:G:124:ILE:CD1	2.15	1.23
2:B:225:LEU:HD13	2:B:233:TYR:OH	1.33	1.23
8:H:76:TYR:OH	12:L:90:ARG:CD	1.84	1.23
22:4:7034:LMU:C11	22:4:7052:LMU:H4'	1.67	1.23
19:A:1119:CLA:C9	21:A:6007:BCR:H373	1.67	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:148:ASP:CB	16:2:152:LEU:HB3	1.64	1.23
17:3:96:ARG:HA	17:3:99:ALA:CB	1.67	1.22
4:D:114:MET:HG3	4:D:115:PRO:O	1.30	1.22
1:A:154:ARG:NE	1:A:384:TYR:CE1	2.08	1.22
15:1:157:ASP:HB2	15:1:178:LYS:CA	1.69	1.22
7:G:98:THR:CB	7:G:101:GLU:OE1	1.86	1.22
5:E:106:ARG:NH2	5:E:107:PHE:HA	1.51	1.22
4:D:80:SER:OG	4:D:126:PRO:HD2	1.06	1.22
16:2:122:ILE:CD1	19:2:2002:CLA:C3B	2.16	1.22
6:F:190:LYS:HZ2	6:F:192:THR:CG2	1.42	1.22
22:3:7003:LMU:C3B	22:3:7005:LMU:H4B	1.68	1.22
7:G:149:TYR:HA	7:G:150:ASP:OD1	1.36	1.22
15:1:78:ARG:HH21	15:1:179:LYS:CD	1.52	1.22
19:A:1237:CLA:H141	12:L:141:LEU:CD2	1.68	1.22
17:3:122:LEU:HD22	19:3:3006:CLA:CHA	1.60	1.22
6:F:107:LYS:O	6:F:108:LEU:HD12	1.05	1.22
2:B:469:LYS:CD	2:B:470:THR:HA	1.70	1.21
2:B:558:PRO:CB	2:B:703:VAL:HG22	1.69	1.21
12:L:72:PRO:O	12:L:73:VAL:HG22	1.36	1.21
16:2:133:ASN:ND2	16:2:134:THR:CB	1.94	1.21
19:A:1122:CLA:CHD	21:A:6007:BCR:H19C	1.68	1.21
18:4:169:ASP:O	18:4:173:LYS:HG2	1.36	1.21
18:4:103:MET:CE	18:4:207:ASN:C	2.09	1.21
19:1:1006:CLA:CAB	19:1:1013:CLA:HBC2	1.70	1.21
16:2:165:GLY:C	16:2:167:ARG:CB	2.09	1.21
6:F:100:LYS:O	6:F:103:GLN:HB3	1.38	1.21
2:B:73:ASN:O	2:B:121:TYR:OH	1.55	1.21
2:B:294:ASN:ND2	7:G:94:GLN:CG	2.02	1.21
4:D:162:GLU:O	4:D:163:VAL:HG23	1.37	1.21
15:1:95:PRO:HA	15:1:98:LEU:HG	1.22	1.21
19:A:1140:CLA:H141	21:A:6011:BCR:C2	1.71	1.21
2:B:398:TYR:O	4:D:197:PRO:HG2	1.37	1.21
22:4:7034:LMU:C9	22:4:7052:LMU:C1'	2.07	1.21
21:I:6021:BCR:C8	21:I:6021:BCR:H313	1.51	1.21
2:B:315:LEU:CD1	2:B:317:ARG:HG2	1.71	1.21
2:B:429:LEU:O	2:B:525:LEU:HD12	1.36	1.21
1:A:250:LEU:HB2	17:3:136:TRP:CZ2	1.73	1.21
2:B:123:TRP:CA	2:B:126:THR:HG22	1.68	1.20
17:3:111:LEU:CG	17:3:112:GLY:H	1.38	1.20
17:3:130:GLN:HB3	17:3:132:THR:N	1.56	1.20
17:3:130:GLN:CB	17:3:132:THR:H	1.55	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:240:ILE:CG2	16:2:263:PHE:HB3	1.70	1.20
17:3:197:SER:CB	17:3:206:PRO:HD3	1.70	1.20
22:4:7034:LMU:H111	22:4:7052:LMU:C3'	1.70	1.20
18:4:159:ASP:OD1	18:4:171:ILE:HD11	1.04	1.20
19:A:1105:CLA:C3B	21:J:6012:BCR:H331	1.71	1.20
17:3:113:ALA:CB	17:3:239:LEU:CD1	2.15	1.20
17:3:150:TYR:CB	17:3:151:TRP:CD1	2.22	1.20
11:K:115:ILE:HG12	11:K:122:LEU:N	1.55	1.20
18:4:103:MET:HE1	18:4:207:ASN:C	1.58	1.20
6:F:99:LEU:O	6:F:102:LEU:HG	1.35	1.20
1:A:702:GLU:OE2	2:B:550:LYS:NZ	1.74	1.20
15:1:190:ASN:HD21	19:1:1002:CLA:C1A	1.53	1.20
2:B:596:TRP:HH2	2:B:612:SER:O	0.94	1.20
18:4:172:PHE:CB	18:4:194:PHE:CE2	1.76	1.20
16:2:96:PRO:CD	17:3:85:ASP:OD2	1.90	1.20
11:K:84:LEU:HG	11:K:85:LYS:HG2	1.24	1.20
18:4:165:SER:O	18:4:168:GLN:HG3	1.06	1.20
18:4:158:GLN:OE1	19:4:1004:CLA:O1D	1.55	1.20
1:A:223:VAL:HG23	1:A:227:LEU:CD1	1.70	1.20
18:4:89:ARG:HD3	18:4:90:TRP:N	1.54	1.20
11:K:113:GLY:O	11:K:116:ILE:HG22	1.41	1.20
4:D:123:ARG:NH2	22:D:7050:LMU:C6B	2.00	1.19
19:B:1235:CLA:CBB	19:B:1235:CLA:H93	1.72	1.19
16:2:118:ALA:O	16:2:121:PHE:CE2	1.96	1.19
5:E:89:SER:CB	5:E:106:ARG:NE	2.06	1.19
11:K:127:ILE:CA	11:K:130:LEU:HG	1.71	1.19
3:C:17:CYS:HB2	3:C:58:CYS:SG	1.83	1.19
11:K:115:ILE:HA	11:K:118:VAL:CG2	1.72	1.19
1:A:575:LEU:HD12	1:A:576:GLY:N	1.56	1.19
18:4:177:LEU:CD1	18:4:178:PRO:HD3	1.69	1.19
2:B:294:ASN:HB2	7:G:94:GLN:CD	1.62	1.19
17:3:185:GLN:HG2	17:3:186:TYR:N	1.45	1.19
14:R:41:UNK:CB	14:R:42:UNK:HA	1.70	1.19
15:1:157:ASP:HB2	15:1:178:LYS:CB	1.73	1.19
2:B:459:PHE:CE2	19:B:1235:CLA:C1D	2.17	1.19
17:3:135:ALA:HB1	17:3:139:THR:OG1	1.40	1.19
12:L:92:ALA:H	12:L:98:ARG:NH1	1.39	1.18
17:3:95:PRO:O	17:3:96:ARG:HG2	1.36	1.18
17:3:192:LYS:HA	17:3:192:LYS:CE	1.66	1.18
15:1:150:HIS:CD2	15:1:151:GLN:HE22	1.61	1.18
1:A:668:TYR:CG	2:B:445:ALA:HB2	1.77	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:58:LEU:HD12	8:H:61:THR:CB	1.73	1.18
17:3:150:TYR:H	17:3:152:ALA:CB	1.56	1.18
14:R:52:UNK:HA	14:R:53:UNK:CB	1.68	1.18
15:1:149:GLU:HG2	15:1:152:ARG:NH1	1.55	1.18
3:C:69:LEU:HD13	3:C:70:TRP:O	1.44	1.18
6:F:185:ILE:O	6:F:186:ARG:HG2	1.44	1.18
1:A:715:LYS:HD2	6:F:230:ASN:ND2	1.58	1.18
1:A:425:THR:CB	1:A:428:TYR:HE1	1.55	1.18
21:B:6020:BCR:C33	19:L:1502:CLA:CHC	2.22	1.18
15:1:177:PRO:HD2	15:1:180:LEU:CB	1.73	1.18
1:A:113:PRO:O	1:A:114:THR:HG22	1.43	1.18
15:1:78:ARG:HD3	19:1:1011:CLA:HMC2	1.25	1.18
1:A:545:HIS:CG	19:A:1135:CLA:HBB2	1.79	1.18
2:B:440:ASN:OD1	2:B:614:THR:CG2	1.91	1.18
4:D:86:SER:O	12:L:67:GLY:HA3	1.42	1.18
1:A:21:LEU:O	1:A:21:LEU:HD12	1.39	1.18
13:N:142:LYS:HE3	13:N:142:LYS:HA	1.18	1.18
12:L:205:TYR:CD1	12:L:207:LEU:CD1	2.25	1.18
2:B:123:TRP:CA	2:B:126:THR:CG2	2.21	1.17
1:A:281:LEU:HD13	19:A:1115:CLA:HED2	1.22	1.17
19:B:1220:CLA:H102	19:B:1220:CLA:H151	1.24	1.17
19:L:1503:CLA:HHD	19:L:1503:CLA:HBC3	1.18	1.17
13:N:103:ASP:CB	13:N:107:LEU:CD1	2.07	1.17
16:2:184:PRO:HD3	16:2:187:LYS:CB	1.74	1.17
13:N:99:LYS:HA	13:N:102:ASN:OD1	1.44	1.17
11:K:81:THR:HG23	11:K:83:GLY:H	1.02	1.17
1:A:351:THR:O	19:A:1123:CLA:H191	1.43	1.17
11:K:49:ILE:C	11:K:52:PRO:CD	2.12	1.17
1:A:281:LEU:CD2	19:A:1115:CLA:HMA2	1.69	1.17
1:A:223:VAL:CG2	1:A:227:LEU:HD12	1.71	1.17
8:H:58:LEU:CD1	8:H:61:THR:HB	1.74	1.17
17:3:98:LEU:HD11	19:3:3012:CLA:C2D	1.75	1.17
16:2:182:ILE:HB	16:2:187:LYS:CB	1.72	1.17
2:B:247:THR:CG2	2:B:248:GLN:H	1.56	1.17
12:L:153:PHE:HA	12:L:179:ALA:HB2	1.24	1.17
22:A:7016:LMU:H21	22:A:7016:LMU:H81	1.24	1.17
6:F:127:LYS:C	6:F:129:ARG:H	1.39	1.17
18:4:159:ASP:OD1	18:4:171:ILE:CD1	1.92	1.17
19:A:1115:CLA:HMC1	19:A:1115:CLA:HBC3	1.25	1.17
1:A:342:GLY:HA3	1:A:430:ASP:CB	1.75	1.17
16:2:229:MET:SD	16:2:230:LEU:HD22	1.85	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:140:LEU:HD21	4:D:144:LEU:HD12	1.26	1.17
19:K:1143:CLA:HAC2	22:K:7001:LMU:O3B	1.39	1.17
19:3:3008:CLA:HBA2	19:3:3008:CLA:CB	1.75	1.17
18:4:158:GLN:CB	19:4:1004:CLA:CMA	2.03	1.16
19:4:4002:CLA:HMA2	19:4:4002:CLA:HBA1	1.20	1.16
19:B:1218:CLA:HHD	19:B:1218:CLA:HBC2	1.27	1.16
15:1:92:LEU:O	15:1:95:PRO:HD2	1.41	1.16
11:K:49:ILE:CA	11:K:52:PRO:HG3	1.73	1.16
1:A:24:ARG:HD2	1:A:24:ARG:N	1.60	1.16
19:A:1124:CLA:H72	19:A:1125:CLA:CED	1.76	1.16
19:A:1122:CLA:C4C	21:A:6007:BCR:H19C	1.75	1.16
9:I:7:LEU:HD12	21:I:6021:BCR:H333	1.17	1.16
16:2:226:ARG:HD2	16:2:230:LEU:HD21	1.19	1.16
15:1:93:ALA:CB	19:1:1006:CLA:CHC	2.22	1.16
3:C:44:ARG:NH2	4:D:181:ARG:CG	2.08	1.16
6:F:127:LYS:O	6:F:129:ARG:N	1.77	1.16
18:4:158:GLN:HE22	19:4:1004:CLA:C1A	1.51	1.16
6:F:200:VAL:HG12	10:J:7:TYR:HB2	1.17	1.16
12:L:92:ALA:H	12:L:98:ARG:CZ	1.58	1.16
2:B:633:ASN:HB2	2:B:636:THR:CB	1.76	1.16
17:3:197:SER:OG	17:3:205:GLY:HA3	1.46	1.16
18:4:228:PRO:HB2	18:4:229:PHE:CD1	1.80	1.16
1:A:423:ASP:HB3	1:A:424:PRO:HG3	1.20	1.16
22:E:7048:LMU:C4B	22:F:7036:LMU:H6E	1.74	1.16
4:D:111:ILE:HG12	4:D:121:ILE:HG22	1.22	1.16
16:2:195:TYR:CD1	16:2:196:PRO:HD2	1.81	1.16
1:A:217:SER:OG	21:A:6002:BCR:H15C	1.42	1.16
2:B:216:LEU:HD23	2:B:218:TYR:O	1.44	1.16
2:B:293:THR:HG22	7:G:94:GLN:CD	1.64	1.16
19:3:3011:CLA:H12	19:3:3011:CLA:HMA2	1.24	1.16
13:N:114:PHE:CG	13:N:117:ALA:HB2	1.80	1.16
15:1:189:LYS:CB	19:1:1007:CLA:HMC2	1.75	1.16
6:F:99:LEU:HA	6:F:102:LEU:HD23	1.28	1.16
19:J:1308:CLA:CBC	19:J:1308:CLA:HHD	1.74	1.16
16:2:125:PHE:CA	16:2:127:THR:HG23	1.76	1.15
16:2:177:VAL:HG12	16:2:178:ASN:HB2	1.18	1.15
15:1:171:LEU:HA	15:1:173:TYR:CE2	1.80	1.15
16:2:269:LYS:HA	16:2:269:LYS:NZ	1.59	1.15
18:4:169:ASP:C	18:4:173:LYS:HA	1.67	1.15
21:I:6021:BCR:HC8	21:I:6021:BCR:C31	1.74	1.15
18:4:177:LEU:CG	18:4:178:PRO:HD3	1.75	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:139:LYS:HA	13:N:142:LYS:NZ	1.62	1.15
17:3:122:LEU:HD21	19:3:3006:CLA:CHA	1.65	1.15
4:D:114:MET:HG3	4:D:115:PRO:C	1.67	1.15
19:K:1143:CLA:CBC	22:K:7001:LMU:O3B	1.95	1.15
11:K:127:ILE:HA	11:K:130:LEU:HG	1.22	1.15
1:A:342:GLY:CA	1:A:430:ASP:CB	2.23	1.15
2:B:470:THR:N	2:B:501:ILE:HB	1.32	1.15
3:C:10:THR:HG23	5:E:101:TYR:CD2	1.82	1.15
8:H:58:LEU:HD12	8:H:62:THR:CG2	1.66	1.15
1:A:249:ILE:CG2	17:3:136:TRP:CZ3	2.18	1.15
16:2:156:GLU:CG	16:2:157:LEU:HD13	1.75	1.15
6:F:124:GLU:HG3	6:F:128:LYS:HD3	1.21	1.15
8:H:116:ALA:HB1	8:H:117:SER:HA	1.26	1.15
15:1:77:GLU:HA	15:1:80:LYS:HG2	1.23	1.15
1:A:451:ILE:HD12	19:A:1131:CLA:HED3	1.28	1.15
5:E:82:TYR:HB3	5:E:83:TRP:CZ3	1.81	1.15
4:D:140:LEU:HD11	4:D:144:LEU:HB2	1.22	1.15
4:D:132:ALA:O	4:D:133:ARG:HD3	1.44	1.15
18:4:174:GLN:O	18:4:194:PHE:CG	1.99	1.15
2:B:620:LEU:HD12	2:B:624:LEU:HD23	1.23	1.15
4:D:201:LYS:HD2	4:D:201:LYS:H	1.02	1.15
13:N:139:LYS:HE3	13:N:142:LYS:CE	1.76	1.15
13:N:139:LYS:HA	13:N:142:LYS:HZ3	0.98	1.15
16:2:184:PRO:HD3	16:2:187:LYS:CG	1.74	1.15
2:B:628:SER:O	2:B:631:LEU:HD23	1.45	1.15
18:4:168:GLN:HB3	18:4:172:PHE:HE1	1.06	1.14
8:H:97:LEU:HG	8:H:98:LEU:HA	1.29	1.14
1:A:336:GLY:CA	1:A:339:THR:OG1	1.94	1.14
2:B:255:LEU:HA	2:B:271:THR:HB	1.16	1.14
8:H:58:LEU:HB3	8:H:61:THR:CG2	1.76	1.14
17:3:111:LEU:HG	17:3:112:GLY:N	1.48	1.14
19:L:1148:CLA:HBC3	19:L:1148:CLA:HHD	1.26	1.14
16:2:182:ILE:CG2	16:2:187:LYS:HG3	1.76	1.14
19:A:1119:CLA:CMD	19:A:1121:CLA:HBB2	1.75	1.14
1:A:150:PHE:O	1:A:151:GLN:HG3	1.46	1.14
16:2:112:TRP:CZ2	16:2:167:ARG:NH2	2.04	1.14
16:2:182:ILE:HG22	16:2:187:LYS:HG3	1.26	1.14
17:3:150:TYR:HB3	17:3:151:TRP:CD1	1.81	1.14
11:K:118:VAL:HG23	11:K:121:VAL:HG22	1.25	1.14
14:R:26:UNK:O	14:R:28:UNK:CB	1.96	1.14
5:E:79:LYS:HG3	5:E:84:TYR:CZ	1.82	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:GLU:CB	2:B:132:ASN:ND2	2.09	1.14
18:4:175:TYR:HD2	18:4:195:ALA:O	1.26	1.14
1:A:443:ILE:CD1	1:A:557:LEU:HD22	1.77	1.14
17:3:141:VAL:HG23	17:3:142:ILE:HG12	1.30	1.14
1:A:575:LEU:HD12	1:A:576:GLY:CA	1.78	1.14
1:A:499:ALA:HB1	19:A:1133:CLA:HED1	1.24	1.13
2:B:329:SER:O	2:B:330:ILE:HG22	1.48	1.13
2:B:569:ASP:OD1	2:B:706:ARG:CZ	1.95	1.13
16:2:171:ILE:HG13	16:2:172:LEU:N	1.60	1.13
16:2:187:LYS:HA	16:2:187:LYS:HE3	1.28	1.13
7:G:149:TYR:HA	7:G:150:ASP:CG	1.66	1.13
1:A:267:THR:HG22	1:A:269:PHE:CE2	1.83	1.13
1:A:281:LEU:CD2	19:A:1115:CLA:HMA3	1.74	1.13
1:A:397:THR:CG2	1:A:613:ILE:HG13	1.78	1.13
22:R:7020:LMU:H5B	22:R:7020:LMU:H6E	1.30	1.13
15:1:177:PRO:CD	15:1:180:LEU:CG	1.86	1.13
18:4:173:LYS:NZ	18:4:201:LYS:HG3	1.64	1.13
2:B:469:LYS:HD2	2:B:470:THR:CA	1.77	1.13
17:3:103:VAL:HG12	17:3:107:ARG:HD3	1.30	1.13
18:4:87:ASN:HB2	18:4:90:TRP:CZ3	1.82	1.13
11:K:111:VAL:O	11:K:114:HIS:HB2	1.46	1.13
16:2:246:PRO:HB3	16:2:247:ILE:HD13	1.13	1.13
19:1:1303:CLA:HBC2	19:1:1303:CLA:HMC1	1.30	1.13
2:B:22:TRP:HE1	19:B:1238:CLA:CBB	1.62	1.13
1:A:152:ILE:HD11	19:A:1127:CLA:O1D	1.45	1.13
2:B:310:PRO:CB	2:B:311:PRO:HD3	1.71	1.13
17:3:109:ALA:CA	17:3:111:LEU:HB3	1.78	1.13
22:3:7003:LMU:C3B	22:3:7005:LMU:C4B	2.25	1.13
22:D:7050:LMU:C2B	22:D:7050:LMU:H6E	1.78	1.13
19:H:1145:CLA:HMC1	19:H:1145:CLA:HBC2	1.30	1.13
17:3:159:VAL:O	17:3:161:GLU:N	1.81	1.13
15:1:92:LEU:C	15:1:95:PRO:HD2	1.68	1.13
7:G:100:PHE:N	7:G:101:GLU:HB2	1.64	1.13
19:A:1124:CLA:HBC2	19:A:1124:CLA:HHD	1.29	1.12
19:A:9022:CLA:H93	19:A:9023:CLA:H91	1.28	1.12
7:G:89:LYS:NZ	7:G:89:LYS:HA	1.63	1.12
11:K:78:ARG:HA	11:K:78:ARG:NE	1.60	1.12
13:N:139:LYS:HB3	13:N:142:LYS:HD3	1.18	1.12
19:1:1014:CLA:HBC3	19:1:1014:CLA:HHD	1.25	1.13
3:C:66:ARG:HG2	3:C:66:ARG:HH21	1.12	1.12
15:1:189:LYS:HG3	19:1:1007:CLA:HMC2	1.19	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:294:ASN:HD22	7:G:94:GLN:CA	1.60	1.12
12:L:141:LEU:HD11	21:L:6019:BCR:H312	1.24	1.12
12:L:60:ILE:HG22	12:L:61:ASN:N	1.52	1.12
16:2:148:ASP:HB3	16:2:152:LEU:CB	1.79	1.12
2:B:247:THR:HA	2:B:250:ALA:HB2	1.25	1.12
17:3:201:ALA:HB1	17:3:202:TYR:CE2	1.83	1.12
22:L:7029:LMU:H1'	22:L:7029:LMU:H31	1.31	1.12
19:A:1141:CLA:H12	19:A:1141:CLA:HMA2	1.23	1.12
7:G:72:LEU:CD2	7:G:124:ILE:HD11	1.78	1.12
18:4:175:TYR:CD2	18:4:195:ALA:O	2.00	1.12
2:B:553:PHE:O	2:B:554:GLY:C	1.85	1.12
19:1:1010:CLA:HBC3	19:1:1010:CLA:HHD	1.26	1.12
22:N:7049:LMU:H12	22:N:7049:LMU:H61	1.19	1.12
2:B:382:ILE:HG22	2:B:383:MET:H	1.09	1.12
18:4:193:ASN:O	18:4:194:PHE:CG	2.03	1.12
1:A:217:SER:OG	21:A:6002:BCR:C15	1.98	1.12
2:B:304:ILE:HD11	19:B:1216:CLA:CED	1.79	1.12
19:J:1308:CLA:HBD	19:J:1308:CLA:HBA2	1.28	1.12
1:A:281:LEU:HD22	19:A:1115:CLA:CED	1.80	1.12
2:B:314:ARG:HH12	15:1:67:LEU:CD2	1.61	1.12
1:A:502:THR:HG22	1:A:504:ALA:H	1.09	1.12
2:B:310:PRO:HB2	2:B:311:PRO:HD3	1.21	1.12
19:B:1235:CLA:H152	21:F:6016:BCR:C31	1.78	1.12
19:1:1014:CLA:H71	19:1:1014:CLA:H41	1.31	1.12
11:K:125:LYS:HB2	11:K:128:GLY:CA	1.80	1.12
22:L:7029:LMU:H5B	22:L:7029:LMU:H4'	1.27	1.12
1:A:669:GLY:N	2:B:445:ALA:HA	1.63	1.12
15:1:97:ILE:HD13	15:1:98:LEU:CB	1.80	1.12
1:A:158:ILE:CG1	1:A:159:THR:H	1.62	1.12
4:D:167:HIS:CE1	4:D:172:VAL:HG11	1.85	1.12
13:N:103:ASP:HB3	13:N:107:LEU:HD12	1.15	1.12
17:3:98:LEU:O	17:3:101:GLY:N	1.81	1.12
17:3:103:VAL:CG1	17:3:107:ARG:CD	2.14	1.12
19:A:1115:CLA:H172	19:A:1115:CLA:H141	1.26	1.11
12:L:96:LEU:H	12:L:96:LEU:HD23	1.13	1.11
1:A:244:LEU:CB	1:A:247:GLU:CG	2.11	1.11
16:2:125:PHE:HA	16:2:127:THR:HG23	1.14	1.11
3:C:62:PHE:CE2	5:E:80:GLU:CG	2.33	1.11
19:1:1014:CLA:H52	19:1:1014:CLA:H102	1.28	1.11
11:K:125:LYS:CA	11:K:126:ASN:HB3	1.79	1.11
1:A:487:VAL:HG13	1:A:489:ALA:N	1.63	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:LEU:HD21	1:A:296:LEU:O	1.48	1.11
2:B:315:LEU:HD12	2:B:317:ARG:HG2	1.13	1.11
15:1:97:ILE:CD1	15:1:98:LEU:HA	1.66	1.11
2:B:230:TRP:N	7:G:63:VAL:HG21	1.62	1.11
6:F:173:TRP:CZ3	6:F:211:PHE:HB2	1.84	1.11
13:N:139:LYS:CE	13:N:142:LYS:HE2	1.78	1.11
13:N:103:ASP:HB2	13:N:107:LEU:HD11	1.22	1.11
17:3:243:ILE:HD11	19:3:3005:CLA:C2C	1.80	1.11
1:A:167:THR:HG22	19:A:1112:CLA:HAA2	1.32	1.11
1:A:472:ARG:NH1	12:L:120:LEU:HD22	1.64	1.11
2:B:123:TRP:HA	2:B:126:THR:CB	1.79	1.11
2:B:89:HIS:O	2:B:113:VAL:HG13	1.45	1.11
19:3:1147:CLA:HBC3	19:3:1147:CLA:CMC	1.77	1.11
19:A:1124:CLA:HED1	19:A:1125:CLA:C2D	1.80	1.11
1:A:492:ILE:HD11	19:A:1133:CLA:HMC3	1.13	1.11
2:B:90:ALA:HA	2:B:113:VAL:HG13	1.33	1.11
13:N:132:THR:HB	13:N:139:LYS:NZ	1.65	1.11
13:N:135:GLN:HA	13:N:136:ASP:O	1.47	1.11
3:C:44:ARG:HB3	4:D:182:GLN:NE2	1.65	1.11
16:2:176:CYS:O	16:2:177:VAL:HG23	1.50	1.11
2:B:53:GLN:NE2	19:B:1201:CLA:HBB1	1.63	1.11
19:B:1202:CLA:O1A	19:B:1202:CLA:H2	1.30	1.11
2:B:174:ARG:HB2	19:B:1210:CLA:HBC2	1.32	1.11
2:B:89:HIS:C	2:B:113:VAL:CG1	1.81	1.11
15:1:157:ASP:CB	15:1:178:LYS:HA	1.79	1.11
19:B:1235:CLA:H152	21:F:6016:BCR:H312	1.18	1.11
12:L:128:GLN:HA	12:L:130:GLY:HA3	1.27	1.11
17:3:135:ALA:CB	17:3:139:THR:HB	1.80	1.11
16:2:166:ARG:N	16:2:167:ARG:CB	2.14	1.11
16:2:186:ASN:CG	16:2:188:LEU:HD11	1.54	1.11
5:E:96:ASP:HB3	5:E:98:ASN:H	1.03	1.11
5:E:125:ILE:HG13	5:E:125:ILE:O	1.40	1.11
13:N:146:LEU:HD11	17:3:142:ILE:O	1.22	1.11
19:4:1304:CLA:CED	19:4:1304:CLA:HAA2	1.79	1.11
2:B:314:ARG:NH1	15:1:67:LEU:CD2	2.14	1.10
1:A:308:ILE:HD12	19:A:1115:CLA:HHC	1.20	1.10
1:A:478:SER:HB2	1:A:644:GLN:NE2	1.65	1.10
6:F:207:LEU:HD13	6:F:208:PHE:H	1.03	1.10
15:1:157:ASP:HB2	15:1:178:LYS:HA	1.24	1.10
19:A:1134:CLA:CGA	19:A:1141:CLA:HBB1	1.80	1.10
21:A:6002:BCR:HC8	21:A:6002:BCR:H311	1.15	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:GLU:O	1:A:76:ARG:N	1.85	1.10
2:B:120:VAL:HG22	2:B:123:TRP:HE1	0.93	1.10
13:N:155:GLU:CA	13:N:157:LYS:HE2	1.81	1.10
8:H:58:LEU:HD12	8:H:61:THR:HB	1.17	1.10
1:A:478:SER:HB2	1:A:644:GLN:HE22	1.06	1.10
15:1:177:PRO:HD3	15:1:180:LEU:HG	1.32	1.10
2:B:25:ILE:O	2:B:25:ILE:HG13	1.50	1.10
2:B:620:LEU:HD12	2:B:624:LEU:CD2	1.81	1.10
6:F:173:TRP:HZ3	6:F:211:PHE:HB2	1.07	1.10
7:G:113:LEU:O	7:G:117:ASN:ND2	1.85	1.10
16:2:184:PRO:CB	16:2:187:LYS:HD2	1.81	1.10
22:3:7003:LMU:C4B	22:3:7005:LMU:H4B	1.81	1.10
4:D:140:LEU:HD13	4:D:144:LEU:HG	1.19	1.10
6:F:107:LYS:O	6:F:108:LEU:CD1	1.99	1.10
6:F:130:PHE:N	6:F:133:TYR:HE1	1.50	1.10
15:1:85:ILE:HG12	15:1:88:ARG:CZ	1.82	1.10
1:A:157:GLY:HA3	1:A:229:ILE:HG21	1.22	1.10
19:B:1220:CLA:HBC3	19:B:1220:CLA:HMC1	1.17	1.10
5:E:111:ASN:ND2	5:E:113:ALA:H	1.50	1.10
1:A:158:ILE:HG13	1:A:159:THR:N	1.56	1.10
8:H:58:LEU:HD11	8:H:62:THR:HG21	1.13	1.10
17:3:108:PHE:HB3	19:3:3013:CLA:C4	1.82	1.10
4:D:84:GLY:O	12:L:64:PRO:HB3	1.50	1.10
15:1:168:PHE:O	15:1:169:ASP:HB2	1.52	1.10
18:4:141:LEU:H	18:4:141:LEU:CD2	1.64	1.10
2:B:459:PHE:HD2	19:B:1235:CLA:CAD	1.63	1.10
2:B:20:ARG:HG3	2:B:20:ARG:HH11	1.02	1.10
2:B:317:ARG:NH2	2:B:410:ARG:CG	2.14	1.10
2:B:429:LEU:C	2:B:525:LEU:HD12	1.70	1.10
8:H:58:LEU:HB3	8:H:61:THR:CB	1.81	1.10
14:R:38:UNK:O	14:R:42:UNK:HA	1.48	1.10
4:D:158:PHE:HB3	4:D:159:PRO:HD2	1.34	1.10
8:H:78:PRO:HD3	19:L:1501:CLA:HMD3	1.14	1.10
1:A:423:ASP:HB3	1:A:424:PRO:CG	1.82	1.10
1:A:316:MET:HB3	1:A:317:TYR:HB2	1.34	1.10
2:B:140:ILE:HG13	2:B:141:PHE:N	1.59	1.10
22:4:7034:LMU:H112	22:4:7052:LMU:H4'	1.29	1.09
21:F:6016:BCR:C8	21:F:6016:BCR:H321	1.62	1.09
6:F:82:LEU:HG	6:F:83:THR:H	1.12	1.09
19:A:1124:CLA:HED1	19:A:1125:CLA:C3D	1.81	1.09
7:G:89:LYS:HE3	7:G:89:LYS:HA	1.32	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:122:ILE:HD13	19:2:2002:CLA:C3B	1.78	1.09
17:3:135:ALA:CB	17:3:139:THR:CB	2.28	1.09
6:F:119:ILE:HG13	6:F:120:LYS:H	1.07	1.09
2:B:131:THR:HG22	2:B:134:ASP:H	1.01	1.09
1:A:435:VAL:O	1:A:438:HIS:O	1.70	1.09
5:E:82:TYR:HB3	5:E:83:TRP:CE3	1.86	1.09
19:B:1235:CLA:H161	21:F:6016:BCR:H313	1.30	1.09
2:B:98:GLN:O	2:B:100:ALA:N	1.86	1.09
12:L:131:SER:HB3	12:L:201:TYR:CE2	1.67	1.09
5:E:127:GLU:HB3	5:E:129:GLU:O	1.49	1.09
5:E:106:ARG:HH21	5:E:107:PHE:CA	1.63	1.09
16:2:168:TRP:CD1	16:2:171:ILE:CG2	2.26	1.09
16:2:184:PRO:HD2	16:2:185:ASN:C	1.72	1.09
4:D:140:LEU:HD12	4:D:140:LEU:C	1.60	1.09
8:H:56:GLU:HG3	8:H:57:ASP:N	1.65	1.09
19:4:1306:CLA:HBC3	19:4:1306:CLA:HMC1	1.21	1.09
19:A:1125:CLA:CBB	19:A:1133:CLA:CMA	1.89	1.09
1:A:56:ASN:O	1:A:57:LEU:HB3	1.37	1.09
19:2:2007:CLA:HBC2	19:3:2009:CLA:HED2	1.13	1.09
4:D:80:SER:OG	4:D:126:PRO:CD	1.99	1.09
19:3:3008:CLA:HBA2	19:3:3008:CLA:HBD	1.15	1.09
14:R:46:UNK:CB	14:R:47:UNK:CB	2.30	1.09
17:3:210:PRO:HG2	17:3:211:LEU:HD12	1.30	1.09
15:1:78:ARG:NH2	15:1:179:LYS:HB3	1.67	1.09
1:A:331:LEU:HD11	1:A:346:LEU:HB3	1.10	1.09
2:B:89:HIS:O	2:B:113:VAL:CB	2.00	1.09
10:J:11:ALA:HB1	10:J:12:PRO:HD2	1.29	1.09
18:4:158:GLN:NE2	19:4:1004:CLA:NA	2.00	1.09
1:A:669:GLY:H	2:B:445:ALA:HA	1.15	1.09
2:B:545:LYS:HD3	2:B:546:LEU:H	1.01	1.09
12:L:73:VAL:O	19:L:1130:CLA:O2A	1.71	1.09
16:2:122:ILE:HD11	19:2:2002:CLA:C3B	1.81	1.09
3:C:44:ARG:CZ	4:D:181:ARG:HD3	1.83	1.09
14:R:34:UNK:CB	14:R:35:UNK:CB	2.30	1.09
16:2:182:ILE:CB	16:2:187:LYS:HG3	1.81	1.09
21:3:6022:BCR:H23C	21:3:6022:BCR:C39	1.82	1.09
1:A:338:PHE:HE1	19:A:1151:CLA:HBB1	0.93	1.09
1:A:145:ILE:HG23	19:A:1106:CLA:OBD	1.50	1.09
21:B:6020:BCR:H331	19:L:1502:CLA:CHC	1.83	1.09
1:A:158:ILE:HG13	1:A:159:THR:H	1.03	1.09
1:A:331:LEU:HD21	1:A:343:HIS:O	1.53	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:141:LEU:HD11	21:L:6019:BCR:C31	1.81	1.09
17:3:185:GLN:CG	17:3:186:TYR:H	1.65	1.09
14:R:41:UNK:CB	14:R:42:UNK:CA	2.30	1.09
19:K:1142:CLA:CED	19:K:1143:CLA:HMB2	1.82	1.09
1:A:24:ARG:HD2	1:A:24:ARG:H	0.92	1.09
21:A:6011:BCR:H23C	21:A:6011:BCR:H393	1.27	1.08
4:D:87:THR:HG23	12:L:69:LEU:HD12	1.11	1.08
18:4:96:LEU:C	18:4:96:LEU:HD12	1.73	1.08
19:A:1102:CLA:H12	19:A:1109:CLA:H61	1.28	1.08
19:A:1101:CLA:H42	19:A:1140:CLA:H61	1.12	1.08
16:2:130:GLY:HA2	16:2:131:ILE:HG12	1.21	1.08
16:2:152:LEU:HD13	16:2:153:PHE:H	0.99	1.08
17:3:150:TYR:CD2	17:3:151:TRP:CE2	2.41	1.08
22:E:7048:LMU:H4B	22:F:7036:LMU:H6E	1.15	1.08
19:J:1308:CLA:HBC2	19:J:1308:CLA:HHD	1.33	1.08
2:B:475:ASP:HB3	2:B:480:SER:HA	1.33	1.08
12:L:171:LYS:C	12:L:173:PRO:CD	2.21	1.08
19:B:1222:CLA:HBC2	19:B:1222:CLA:HHD	1.31	1.08
2:B:225:LEU:CD1	2:B:233:TYR:OH	2.00	1.08
12:L:115:VAL:HG11	12:L:130:GLY:H	1.14	1.08
18:4:103:MET:HE3	18:4:208:GLY:CA	1.71	1.08
7:G:62:LEU:HB3	7:G:65:SER:HB3	1.24	1.08
16:2:125:PHE:HA	16:2:127:THR:CG2	1.80	1.08
3:C:14:CYS:CA	3:C:17:CYS:SG	2.41	1.08
13:N:147:SER:HB3	13:N:151:ASP:HA	1.19	1.08
13:N:143:VAL:HB	13:N:144:PRO:HD2	1.15	1.08
13:N:155:GLU:C	13:N:157:LYS:HE3	1.60	1.08
17:3:96:ARG:HA	17:3:99:ALA:HB3	1.30	1.08
2:B:247:THR:HG23	2:B:248:GLN:H	1.16	1.08
15:1:177:PRO:CD	15:1:180:LEU:CD2	2.30	1.08
1:A:86:LEU:HD13	1:A:178:MET:HE1	1.25	1.08
2:B:558:PRO:HB2	2:B:703:VAL:HG22	1.16	1.08
15:1:70:GLY:O	15:1:73:PRO:HD2	1.51	1.08
2:B:255:LEU:HA	2:B:271:THR:CB	1.82	1.08
3:C:24:ASP:HB2	24:C:8002:SF4:S2	1.92	1.08
18:4:89:ARG:HD3	18:4:90:TRP:H	1.08	1.08
8:H:121:LEU:HB3	8:H:122:PRO:HD2	1.13	1.08
6:F:224:GLY:C	6:F:227:VAL:HG12	1.72	1.08
1:A:425:THR:HB	1:A:428:TYR:HE1	1.04	1.08
6:F:179:ARG:HG2	6:F:183:ILE:HD11	1.25	1.08
22:H:7030:LMU:H52	22:H:7030:LMU:H91	1.32	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:7022:LMU:H21	22:R:7022:LMU:H2'	1.27	1.08
1:A:361:ASN:ND2	19:A:1103:CLA:OBD	1.84	1.08
19:A:1140:CLA:H141	21:A:6011:BCR:HC22	1.20	1.08
21:I:6021:BCR:C8	21:I:6021:BCR:C31	2.28	1.08
16:2:117:ALA:HB3	16:2:230:LEU:HG	1.28	1.08
19:2:2001:CLA:O1A	19:2:2001:CLA:H42	1.53	1.08
6:F:221:LEU:HD23	6:F:222:LEU:CD2	1.82	1.08
18:4:146:PHE:CZ	19:4:4013:CLA:C1C	2.36	1.08
2:B:459:PHE:CE2	19:B:1235:CLA:HMD2	1.87	1.08
1:A:492:ILE:HD11	19:A:1133:CLA:CMC	1.83	1.08
2:B:302:LYS:O	2:B:303:TYR:HB2	1.52	1.08
17:3:96:ARG:HH11	17:3:96:ARG:CG	1.67	1.08
14:R:39:UNK:C	14:R:41:UNK:CB	2.30	1.08
2:B:247:THR:HA	2:B:250:ALA:HB3	1.27	1.08
1:A:567:ARG:NH1	4:D:89:GLY:HA2	1.68	1.08
1:A:71:LEU:HG	1:A:72:GLU:H	1.14	1.08
11:K:97:ASP:HB2	11:K:101:PHE:HE2	1.12	1.08
18:4:146:PHE:CZ	19:4:4013:CLA:C2C	2.37	1.07
1:A:443:ILE:HD11	1:A:557:LEU:HD22	1.14	1.07
2:B:493:TRP:CH2	19:B:1232:CLA:HMA2	1.89	1.07
19:A:1124:CLA:HED1	19:A:1125:CLA:CMD	1.84	1.07
19:A:1141:CLA:H121	19:A:1141:CLA:H71	1.33	1.07
1:A:479:ASP:HA	1:A:536:THR:HG21	1.32	1.07
2:B:551:LYS:O	2:B:552:ASP:OD1	1.72	1.07
2:B:25:ILE:HG21	21:L:6019:BCR:H292	1.28	1.07
16:2:118:ALA:O	16:2:121:PHE:CD2	2.06	1.07
16:2:227:LEU:HD21	19:2:2004:CLA:C1C	1.84	1.07
4:D:140:LEU:HD13	4:D:144:LEU:CG	1.84	1.07
19:3:3008:CLA:HBC2	19:3:3008:CLA:HMC1	1.30	1.07
1:A:567:ARG:NH2	4:D:136:GLN:OE1	1.85	1.07
15:1:77:GLU:O	15:1:80:LYS:HG3	1.55	1.07
1:A:163:GLN:HA	1:A:166:CYS:SG	1.93	1.07
2:B:119:GLY:HA3	19:B:1225:CLA:HED1	1.22	1.07
2:B:294:ASN:ND2	7:G:94:GLN:CA	2.17	1.07
18:4:173:LYS:HZ3	18:4:201:LYS:HG3	1.09	1.07
2:B:527:LEU:HD13	19:B:1236:CLA:HMA2	1.28	1.07
11:K:52:PRO:HD2	11:K:53:THR:H	1.19	1.07
12:L:131:SER:CB	12:L:201:TYR:CE2	2.31	1.07
4:D:87:THR:HG23	12:L:69:LEU:CD1	1.83	1.07
3:C:62:PHE:CZ	5:E:80:GLU:CG	2.37	1.07
5:E:99:THR:HG22	5:E:100:ARG:N	1.65	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:148:ASP:N	13:N:149:ASP:HB2	1.68	1.07
16:2:195:TYR:HD1	16:2:196:PRO:HD2	1.04	1.07
2:B:131:THR:HG22	2:B:134:ASP:N	1.70	1.07
6:F:213:TRP:HB2	6:F:216:ALA:HB2	1.36	1.07
19:3:3016:CLA:HMC1	19:3:3016:CLA:HBC3	1.35	1.07
19:A:1125:CLA:CAB	19:A:1133:CLA:CMA	2.32	1.07
2:B:500:ALA:O	2:B:501:ILE:HG12	1.55	1.07
2:B:551:LYS:HG2	2:B:552:ASP:H	1.17	1.07
15:1:80:LYS:O	15:1:83:GLU:HB3	1.52	1.07
19:A:1122:CLA:HBB2	21:A:6007:BCR:C35	1.85	1.07
2:B:89:HIS:O	2:B:113:VAL:HG12	1.34	1.07
1:A:328:LYS:HD2	1:A:332:GLU:HB2	1.33	1.07
1:A:51:THR:HG21	19:A:1139:CLA:HBB2	1.37	1.07
2:B:11:GLY:HA3	3:C:71:HIS:HD2	1.03	1.07
5:E:107:PHE:CE2	5:E:109:LYS:HE3	1.88	1.07
17:3:139:THR:HG22	17:3:140:GLY:H	0.90	1.07
17:3:139:THR:HG22	17:3:140:GLY:N	1.65	1.07
16:2:148:ASP:HB3	16:2:152:LEU:HB3	1.15	1.07
11:K:81:THR:HG23	11:K:83:GLY:N	1.68	1.07
18:4:165:SER:O	18:4:168:GLN:CG	2.02	1.07
18:4:146:PHE:CZ	19:4:4013:CLA:C3C	2.38	1.07
13:N:139:LYS:HG3	13:N:142:LYS:CD	1.85	1.07
16:2:152:LEU:HD13	16:2:153:PHE:N	1.70	1.07
16:2:184:PRO:HB3	16:2:187:LYS:HD2	1.33	1.07
12:L:209:LEU:HD12	12:L:210:PRO:CD	1.83	1.07
12:L:164:LEU:HB2	12:L:165:THR:HG23	1.36	1.07
1:A:281:LEU:HD21	19:A:1115:CLA:HMA2	1.08	1.06
7:G:84:ARG:HG3	7:G:85:GLU:CB	1.83	1.06
11:K:49:ILE:CA	11:K:52:PRO:CG	2.31	1.06
6:F:207:LEU:HD22	6:F:208:PHE:CA	1.85	1.06
11:K:49:ILE:HA	11:K:52:PRO:HG3	1.11	1.06
16:2:168:TRP:HA	16:2:171:ILE:HG23	1.28	1.06
11:K:127:ILE:HA	11:K:130:LEU:CG	1.85	1.06
17:3:192:LYS:HA	17:3:192:LYS:HE2	1.27	1.06
2:B:110:LEU:HD12	2:B:111:GLY:N	1.71	1.06
1:A:157:GLY:O	1:A:158:ILE:HG23	0.89	1.06
1:A:499:ALA:HB1	19:A:1133:CLA:CED	1.85	1.06
2:B:123:TRP:HA	2:B:126:THR:HG22	1.13	1.06
19:A:1105:CLA:C3B	21:J:6012:BCR:C33	2.33	1.06
7:G:84:ARG:HG3	7:G:85:GLU:N	1.65	1.06
7:G:96:GLY:C	7:G:97:LEU:HG	1.76	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:134:LEU:HA	15:1:137:ILE:HD11	1.10	1.06
3:C:65:VAL:HG22	3:C:66:ARG:H	1.17	1.06
17:3:109:ALA:CA	17:3:111:LEU:CB	2.33	1.06
17:3:113:ALA:HB1	17:3:239:LEU:HD11	1.12	1.06
1:A:478:SER:HB3	1:A:644:GLN:HE22	1.16	1.06
16:2:246:PRO:HB3	16:2:247:ILE:CD1	1.84	1.06
18:4:242:ASN:O	18:4:243:THR:HG22	1.55	1.06
18:4:146:PHE:CZ	19:4:4013:CLA:C4C	2.37	1.06
19:A:1122:CLA:HBB2	21:A:6007:BCR:H351	1.35	1.06
2:B:696:LYS:HG2	3:C:80:ALA:HA	1.38	1.06
18:4:209:ARG:O	18:4:212:LEU:O	1.72	1.06
19:A:1134:CLA:H3A	19:A:1141:CLA:HBB2	1.31	1.06
16:2:118:ALA:CA	16:2:121:PHE:CE2	2.25	1.06
17:3:93:ILE:HG13	17:3:95:PRO:O	1.55	1.06
1:A:478:SER:CB	1:A:644:GLN:NE2	2.18	1.06
11:K:125:LYS:HA	11:K:126:ASN:CB	1.84	1.06
17:3:197:SER:OG	17:3:206:PRO:HD3	1.55	1.06
19:J:1308:CLA:HED3	19:J:1308:CLA:CAD	1.86	1.06
17:3:201:ALA:C	17:3:202:TYR:HD2	1.59	1.06
1:A:316:MET:HG2	1:A:317:TYR:CD1	1.89	1.06
2:B:475:ASP:CB	2:B:480:SER:HA	1.84	1.06
19:A:9012:CLA:H11	2:B:616:LEU:HD13	1.35	1.06
19:A:9012:CLA:C1	2:B:616:LEU:HD13	1.85	1.06
12:L:143:LEU:HD22	12:L:146:THR:HG22	1.31	1.06
5:E:78:ARG:HH22	5:E:125:ILE:HG21	1.14	1.06
17:3:110:MET:O	17:3:113:ALA:HB3	1.54	1.06
4:D:163:VAL:O	4:D:164:GLN:HG3	1.53	1.06
2:B:475:ASP:O	2:B:476:ILE:HG22	1.54	1.06
19:4:1004:CLA:HHD	19:4:1004:CLA:HBC2	1.30	1.06
19:B:1235:CLA:C9	19:B:1235:CLA:HBB2	1.85	1.06
2:B:317:ARG:CZ	2:B:410:ARG:HG2	1.85	1.06
1:A:365:LEU:HD23	19:A:1103:CLA:HED3	1.31	1.06
1:A:707:ILE:HG22	1:A:711:HIS:NE2	1.71	1.06
2:B:122:GLN:O	2:B:126:THR:HB	0.89	1.06
7:G:64:ILE:O	7:G:68:THR:HG23	1.53	1.06
9:I:11:LEU:HD12	21:I:6021:BCR:H10C	1.34	1.06
16:2:119:GLY:O	16:2:123:PRO:CG	2.02	1.06
16:2:117:ALA:HB1	16:2:230:LEU:HG	1.37	1.06
1:A:21:LEU:HA	1:A:22:VAL:HG13	1.33	1.06
13:N:130:ASN:C	13:N:132:THR:HG22	1.75	1.06
13:N:139:LYS:HG3	13:N:142:LYS:HD3	1.37	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1:1014:CLA:H52	19:1:1014:CLA:C10	1.86	1.06
1:A:578:ARG:CZ	1:A:578:ARG:HB2	1.81	1.06
15:1:162:LYS:C	15:1:164:PRO:HD3	1.75	1.06
18:4:172:PHE:HB3	18:4:194:PHE:CE2	1.88	1.05
1:A:163:GLN:HG3	1:A:164:LEU:H	1.18	1.05
1:A:188:LYS:O	1:A:190:ALA:HB2	1.56	1.05
2:B:89:HIS:O	2:B:113:VAL:CG1	0.76	1.05
1:A:397:THR:HG22	1:A:613:ILE:HG13	1.11	1.05
5:E:78:ARG:NH2	5:E:125:ILE:HG21	1.68	1.05
8:H:76:TYR:OH	12:L:90:ARG:HD2	1.53	1.05
12:L:60:ILE:HG22	12:L:61:ASN:H	1.02	1.05
8:H:98:LEU:CD2	12:L:146:THR:HG21	1.86	1.05
19:2:2007:CLA:HAC2	19:3:2009:CLA:HED3	1.38	1.05
6:F:132:ASN:O	6:F:133:TYR:HD1	1.38	1.05
19:2:2014:CLA:C10	19:2:2014:CLA:H152	1.75	1.05
6:F:219:ARG:HH11	6:F:219:ARG:HG2	0.93	1.05
2:B:70:TRP:HB3	2:B:136:TYR:OH	1.56	1.05
1:A:439:ARG:NH1	1:A:565:SER:O	1.90	1.05
1:A:483:GLN:HB3	1:A:485:GLN:NE2	1.71	1.05
1:A:281:LEU:CD2	19:A:1115:CLA:CED	2.33	1.05
7:G:65:SER:O	7:G:68:THR:OG1	1.74	1.05
8:H:58:LEU:HB3	8:H:61:THR:HG21	1.36	1.05
16:2:182:ILE:HB	16:2:187:LYS:HB3	1.05	1.05
22:3:7003:LMU:H3B	22:3:7005:LMU:O5B	1.55	1.05
4:D:102:ILE:HD12	4:D:137:CYS:HB3	1.39	1.05
15:1:189:LYS:CB	19:1:1007:CLA:CMC	2.33	1.05
1:A:425:THR:HB	1:A:428:TYR:CE1	1.90	1.05
10:J:31:ARG:HH22	19:J:1311:CLA:C4B	1.69	1.05
7:G:98:THR:CB	7:G:101:GLU:OE2	2.01	1.05
15:1:78:ARG:HG3	15:1:81:GLU:OE1	1.55	1.05
1:A:279:ASP:O	1:A:281:LEU:CG	2.03	1.05
2:B:87:ILE:HA	2:B:115:ASN:HA	1.38	1.05
2:B:11:GLY:CA	3:C:71:HIS:HD2	1.68	1.05
19:1:1013:CLA:O1D	19:1:1013:CLA:HAA2	1.53	1.05
19:2:2014:CLA:H41	19:2:2014:CLA:H72	1.39	1.05
1:A:259:TYR:HB3	1:A:260:PRO:HD2	1.37	1.05
10:J:37:LEU:O	10:J:38:ILE:HG13	1.56	1.05
1:A:51:THR:CG2	19:A:1139:CLA:HBB2	1.85	1.05
2:B:517:PHE:O	2:B:517:PHE:CD2	2.09	1.05
2:B:11:GLY:HA3	3:C:71:HIS:CD2	1.91	1.05
7:G:131:GLY:HA2	7:G:136:VAL:HG23	1.35	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:103:VAL:HG13	16:2:104:GLN:OE1	1.56	1.05
5:E:127:GLU:O	5:E:128:VAL:HG23	1.55	1.05
6:F:190:LYS:HZ3	6:F:192:THR:HG22	1.17	1.05
1:A:250:LEU:CB	17:3:136:TRP:CH2	2.39	1.05
16:2:160:ILE:HG21	19:2:2012:CLA:CBB	1.81	1.05
4:D:114:MET:SD	4:D:115:PRO:O	2.15	1.05
1:A:715:LYS:CD	6:F:230:ASN:HD21	1.69	1.05
1:A:581:CYS:HB2	1:A:590:CYS:HA	1.38	1.05
22:4:7034:LMU:C9	22:4:7052:LMU:H2'	1.86	1.04
1:A:451:ILE:CD1	19:A:1131:CLA:CED	2.35	1.04
15:1:97:ILE:CD1	15:1:98:LEU:CB	2.34	1.04
1:A:588:GLY:CA	2:B:668:ARG:HD3	1.86	1.04
19:3:2009:CLA:O1A	19:3:2009:CLA:HBD	1.52	1.04
3:C:54:CYS:SG	24:C:8002:SF4:S1	2.54	1.04
16:2:174:PRO:HB2	16:2:194:GLY:HA3	1.37	1.04
8:H:85:GLU:HG3	8:H:86:THR:H	1.10	1.04
22:4:7034:LMU:C8	22:4:7052:LMU:C2'	2.01	1.04
19:1:1001:CLA:HBC3	19:1:1001:CLA:HMC1	1.34	1.04
15:1:78:ARG:HH21	15:1:179:LYS:HD2	1.14	1.04
2:B:319:HIS:CE1	2:B:322:LEU:HD12	1.92	1.04
1:A:120:ALA:H	1:A:145:ILE:HD11	1.15	1.04
1:A:443:ILE:CD1	1:A:557:LEU:CD2	2.33	1.04
3:C:5:VAL:CB	3:C:65:VAL:HG23	1.88	1.04
6:F:190:LYS:HZ3	6:F:192:THR:CG2	1.57	1.04
17:3:150:TYR:C	17:3:152:ALA:N	1.99	1.04
22:D:7050:LMU:H2B	22:D:7050:LMU:H6E	1.05	1.04
12:L:153:PHE:HB2	12:L:155:GLU:OE1	1.55	1.04
21:B:6020:BCR:H333	19:L:1502:CLA:CHC	1.87	1.04
2:B:694:ARG:HG2	2:B:694:ARG:HH21	0.90	1.04
17:3:201:ALA:HB1	17:3:202:TYR:CD2	1.92	1.04
15:1:162:LYS:H	15:1:164:PRO:HG3	1.18	1.04
2:B:213:LEU:HD12	2:B:214:ASP:N	1.72	1.04
1:A:308:ILE:CD1	19:A:1115:CLA:CHC	2.34	1.04
2:B:315:LEU:HD13	2:B:315:LEU:C	1.78	1.04
12:L:131:SER:N	12:L:201:TYR:CE2	2.25	1.04
18:4:169:ASP:HA	18:4:173:LYS:HA	1.35	1.04
16:2:226:ARG:CD	16:2:230:LEU:CD2	2.35	1.04
17:3:113:ALA:HB2	17:3:239:LEU:HD11	1.11	1.04
19:B:1220:CLA:C4	19:B:1220:CLA:NA	2.21	1.04
2:B:202:SER:OG	2:B:270:LEU:HD22	1.57	1.04
19:A:9022:CLA:H151	21:B:6017:BCR:H20C	1.36	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:64:SER:O	3:C:65:VAL:CG1	2.06	1.04
17:3:238:ILE:CD1	19:3:3003:CLA:HMC2	1.88	1.04
19:3:3011:CLA:HAC2	19:3:3012:CLA:C2A	1.88	1.04
16:2:165:GLY:O	16:2:167:ARG:HB3	1.55	1.04
6:F:127:LYS:C	6:F:129:ARG:N	2.07	1.04
22:R:7014:LMU:H11	22:R:7014:LMU:H62	1.34	1.04
1:A:126:ILE:O	1:A:127:VAL:HG22	1.54	1.03
1:A:86:LEU:HD13	1:A:178:MET:CE	1.87	1.03
6:F:170:ILE:HG21	21:F:6014:BCR:C37	1.88	1.03
2:B:294:ASN:HD22	7:G:94:GLN:CB	1.71	1.03
2:B:469:LYS:HG3	2:B:470:THR:HG23	1.35	1.03
12:L:145:LEU:HD11	21:L:6019:BCR:H313	1.39	1.03
13:N:139:LYS:HD2	13:N:142:LYS:HZ3	1.17	1.03
22:3:7003:LMU:C3B	22:3:7005:LMU:C5B	2.35	1.03
17:3:150:TYR:O	17:3:152:ALA:N	1.91	1.03
1:A:575:LEU:HD12	1:A:576:GLY:HA3	1.40	1.03
18:4:158:GLN:HE22	19:4:1004:CLA:CHA	1.72	1.03
1:A:343:HIS:O	1:A:346:LEU:HB2	1.56	1.03
2:B:120:VAL:CA	2:B:123:TRP:CD1	2.39	1.03
2:B:459:PHE:CD2	19:B:1235:CLA:CMD	2.38	1.03
21:F:6016:BCR:HC8	21:F:6016:BCR:H321	1.05	1.03
17:3:122:LEU:HD21	19:3:3006:CLA:C4D	1.87	1.03
16:2:156:GLU:HG2	16:2:157:LEU:HD13	1.08	1.03
17:3:150:TYR:O	17:3:151:TRP:C	1.95	1.03
11:K:97:ASP:CB	11:K:101:PHE:HE2	1.72	1.03
1:A:98:PHE:O	1:A:100:GLY:N	1.90	1.03
16:2:120:ILE:HG13	16:2:121:PHE:N	1.69	1.03
16:2:124:GLU:O	16:2:127:THR:HA	1.59	1.03
13:N:130:ASN:O	13:N:132:THR:CG2	2.06	1.03
12:L:154:ASN:C	12:L:178:THR:HG23	1.79	1.03
16:2:195:TYR:HD1	16:2:196:PRO:CD	1.70	1.03
21:3:6022:BCR:H393	21:3:6022:BCR:H23C	1.04	1.03
1:A:525:ASN:HB3	1:A:526:LYS:HG3	1.40	1.03
19:4:4002:CLA:HAA2	19:4:4002:CLA:CGD	1.86	1.03
7:G:72:LEU:HD22	7:G:124:ILE:HD12	1.37	1.03
2:B:199:ILE:HG23	2:B:270:LEU:HD13	1.05	1.03
6:F:200:VAL:HG12	10:J:7:TYR:CB	1.89	1.03
16:2:229:MET:SD	16:2:230:LEU:HD13	1.98	1.03
8:H:58:LEU:HD12	8:H:62:THR:HG23	1.06	1.03
18:4:141:LEU:H	18:4:141:LEU:HD22	1.19	1.03
12:L:171:LYS:C	12:L:173:PRO:HD2	1.79	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:LEU:H	1:A:484:LEU:CD2	1.71	1.03
15:1:206:SER:O	15:1:209:PRO:HG3	1.59	1.03
18:4:111:LEU:HD12	18:4:112:PRO:CD	1.88	1.03
18:4:103:MET:HE1	18:4:208:GLY:N	1.66	1.03
18:4:210:LEU:O	18:4:214:PHE:HB2	1.59	1.03
19:A:1112:CLA:C3B	21:A:6002:BCR:H19C	1.89	1.03
10:J:2:ARG:HH12	10:J:8:LEU:HD13	1.21	1.03
15:1:85:ILE:HA	15:1:88:ARG:CG	1.89	1.03
2:B:224:PRO:HB2	2:B:227:THR:HB	1.36	1.03
5:E:99:THR:CG2	5:E:100:ARG:H	1.69	1.03
8:H:58:LEU:CG	8:H:61:THR:HB	1.88	1.03
8:H:58:LEU:HD13	8:H:62:THR:HG21	1.41	1.03
19:1:1013:CLA:C6	19:1:1014:CLA:CED	2.35	1.03
3:C:5:VAL:CG2	3:C:65:VAL:CG2	2.36	1.03
19:3:3016:CLA:C10	19:3:3016:CLA:H142	1.89	1.03
2:B:490:ARG:NH1	2:B:490:ARG:HG3	1.61	1.03
18:4:193:ASN:O	18:4:194:PHE:CD1	2.12	1.02
1:A:370:ILE:HG23	1:A:403:GLY:HA3	1.36	1.02
2:B:558:PRO:CG	2:B:703:VAL:HG22	1.88	1.02
7:G:90:GLN:HB3	7:G:91:VAL:O	1.58	1.02
1:A:555:ILE:HD11	19:A:9023:CLA:OBD	1.59	1.02
7:G:64:ILE:O	7:G:68:THR:CG2	2.06	1.02
19:K:1143:CLA:H3A	19:K:1143:CLA:O1A	1.59	1.02
15:1:170:PRO:HD2	15:1:173:TYR:CE2	1.93	1.02
19:R:1150:CLA:HBA2	19:R:1150:CLA:HBD	1.35	1.02
2:B:504:ASN:OD1	2:B:504:ASN:O	1.77	1.02
15:1:97:ILE:HD11	15:1:98:LEU:HA	1.34	1.02
18:4:175:TYR:O	18:4:194:PHE:CZ	2.12	1.02
1:A:64:PHE:CE2	1:A:74:ILE:CG2	2.42	1.02
2:B:199:ILE:HG23	2:B:270:LEU:CD1	1.88	1.02
2:B:459:PHE:CD2	19:B:1235:CLA:CAD	2.40	1.02
19:B:1235:CLA:HBC1	6:F:160:PHE:CZ	1.93	1.02
8:H:97:LEU:CD1	8:H:100:PHE:HB2	1.88	1.02
16:2:130:GLY:HA3	16:2:131:ILE:HG13	1.03	1.02
11:K:125:LYS:HB2	11:K:128:GLY:HA2	1.38	1.02
15:1:162:LYS:N	15:1:164:PRO:HG3	1.73	1.02
1:A:541:VAL:HG11	1:A:615:HIS:CD2	1.93	1.02
7:G:124:ILE:HG12	7:G:128:LEU:CD1	1.89	1.02
2:B:122:GLN:C	2:B:126:THR:HB	1.79	1.02
16:2:133:ASN:HD22	16:2:134:THR:CA	1.71	1.02
8:H:58:LEU:HD12	8:H:61:THR:CA	1.89	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:152:LEU:C	13:N:153:GLU:HG3	1.78	1.02
4:D:140:LEU:HA	4:D:143:ARG:HB2	1.03	1.02
16:2:246:PRO:CB	16:2:247:ILE:HD13	1.89	1.02
20:B:5002:PQN:C16	21:B:6017:BCR:C33	2.37	1.02
2:B:90:ALA:CA	2:B:113:VAL:HG13	1.88	1.02
7:G:98:THR:OG1	7:G:101:GLU:CD	1.98	1.02
19:H:1241:CLA:CAC	21:I:6021:BCR:HC31	1.88	1.02
16:2:122:ILE:O	16:2:126:LEU:HG	1.60	1.02
1:A:249:ILE:C	1:A:251:ASN:H	1.60	1.02
17:3:150:TYR:HD2	17:3:151:TRP:NE1	1.45	1.02
2:B:160:LYS:HD3	2:B:161:TRP:CD2	1.94	1.02
2:B:5:ILE:HG22	2:B:6:PRO:HD3	1.05	1.02
4:D:111:ILE:HG12	4:D:121:ILE:CG2	1.88	1.02
22:R:7020:LMU:C5B	22:R:7020:LMU:H6E	1.89	1.02
1:A:255:LEU:HD13	1:A:280:PHE:HZ	1.20	1.02
19:A:1104:CLA:H43	19:A:1128:CLA:H11	1.38	1.02
12:L:96:LEU:H	12:L:96:LEU:CD2	1.67	1.02
1:A:107:GLU:OE2	1:A:161:GLU:HG3	1.58	1.02
2:B:310:PRO:O	19:B:1301:CLA:CHD	2.07	1.02
12:L:112:GLY:HA3	19:L:1503:CLA:CHC	1.90	1.02
16:2:122:ILE:CD1	19:2:2002:CLA:CAB	2.36	1.02
17:3:135:ALA:HB1	17:3:139:THR:HB	1.34	1.02
1:A:249:ILE:O	1:A:251:ASN:N	1.93	1.02
22:E:7048:LMU:H3'	22:E:7048:LMU:C6B	1.89	1.02
12:L:171:LYS:O	12:L:173:PRO:HD2	1.59	1.02
1:A:149:PHE:O	1:A:150:PHE:HB2	1.54	1.01
1:A:351:THR:O	19:A:1123:CLA:C19	2.07	1.01
1:A:370:ILE:HG22	1:A:400:MET:HA	1.41	1.01
16:2:117:ALA:O	16:2:120:ILE:HG12	1.58	1.01
19:L:1148:CLA:HED1	19:L:1148:CLA:C1	1.90	1.01
6:F:88:SER:OG	6:F:91:PHE:HB3	1.58	1.01
2:B:542:ARG:HH11	2:B:542:ARG:CG	1.71	1.01
18:4:120:ILE:HD12	18:4:226:LYS:HG3	1.40	1.01
1:A:340:GLY:O	1:A:343:HIS:HB2	1.58	1.01
7:G:123:ASN:HA	7:G:126:ASP:OD2	1.58	1.01
12:L:92:ALA:N	12:L:98:ARG:NH1	2.06	1.01
19:3:1147:CLA:CBC	19:3:1147:CLA:CMC	2.30	1.01
18:4:170:PRO:HG3	19:4:4011:CLA:C2D	1.90	1.01
1:A:157:GLY:HA3	1:A:229:ILE:HG22	1.40	1.01
2:B:120:VAL:CG2	2:B:123:TRP:HE1	1.74	1.01
19:H:1241:CLA:HAC2	21:I:6021:BCR:HC31	1.42	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:200:VAL:HG13	10:J:7:TYR:H	1.25	1.01
1:A:21:LEU:CD1	1:A:21:LEU:O	2.08	1.01
13:N:157:LYS:HB3	13:N:159:LYS:N	1.73	1.01
4:D:95:GLN:NE2	4:D:96:VAL:HA	1.76	1.01
19:4:1304:CLA:HAA2	19:4:1304:CLA:HED3	1.03	1.01
15:1:64:PHE:O	15:1:69:LEU:HD13	1.60	1.01
15:1:84:LEU:O	15:1:88:ARG:HG3	1.60	1.01
19:A:1134:CLA:CBC	21:A:6008:BCR:HC31	1.90	1.01
1:A:157:GLY:CA	1:A:229:ILE:HG21	1.89	1.01
19:A:1124:CLA:HED2	19:A:1125:CLA:CAD	1.91	1.01
2:B:120:VAL:HA	2:B:123:TRP:HD1	1.23	1.01
3:C:44:ARG:CA	4:D:182:GLN:OE1	2.08	1.01
22:3:7005:LMU:H51	22:3:7005:LMU:C1	1.88	1.01
17:3:243:ILE:HG12	19:3:3005:CLA:C4C	1.88	1.01
15:1:112:GLN:HG2	15:1:113:GLU:H	1.20	1.01
1:A:328:LYS:CD	1:A:332:GLU:HB2	1.88	1.01
1:A:132:LEU:HD11	1:A:674:ALA:HB2	1.41	1.01
2:B:294:ASN:CG	7:G:94:GLN:HG3	1.81	1.01
15:1:97:ILE:CG1	15:1:98:LEU:N	2.22	1.01
1:A:368:LEU:HD21	19:A:1117:CLA:H93	1.42	1.01
19:1:1010:CLA:HBC3	19:1:1010:CLA:CHD	1.89	1.01
16:2:184:PRO:HG3	16:2:187:LYS:H	1.24	1.01
17:3:150:TYR:CB	17:3:151:TRP:HD1	1.71	1.01
4:D:140:LEU:CD1	4:D:144:LEU:HB2	1.89	1.01
11:K:81:THR:CG2	11:K:83:GLY:H	1.71	1.01
19:B:1223:CLA:HED1	19:B:1231:CLA:HBB2	1.41	1.01
2:B:732:LYS:CG	2:B:733:PHE:C	2.29	1.01
15:1:78:ARG:HD3	19:1:1011:CLA:CMC	1.91	1.01
1:A:227:LEU:CD2	1:A:296:LEU:O	2.09	1.01
19:A:9012:CLA:C1	2:B:616:LEU:CD1	2.39	1.01
15:1:136:THR:O	15:1:140:ILE:HG12	1.61	1.01
1:A:249:ILE:HG23	17:3:136:TRP:HZ3	0.85	1.01
1:A:575:LEU:CD1	1:A:576:GLY:HA3	1.90	1.01
1:A:426:THR:HG22	1:A:428:TYR:CE2	1.96	1.01
15:1:170:PRO:HD2	15:1:173:TYR:CD2	1.96	1.01
15:1:102:ALA:C	15:1:103:LEU:HD23	1.81	1.01
15:1:77:GLU:HG3	15:1:80:LYS:HD2	1.42	1.00
19:A:1124:CLA:HBA2	19:A:1137:CLA:HED1	1.38	1.00
2:B:545:LYS:CD	2:B:546:LEU:H	1.74	1.00
11:K:49:ILE:O	11:K:52:PRO:CD	2.08	1.00
12:L:92:ALA:HB2	12:L:98:ARG:NH2	1.75	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1205:CLA:HBB2	19:B:1205:CLA:H92	1.44	1.00
2:B:457:PRO:HB3	2:B:517:PHE:HB2	1.44	1.00
20:B:5002:PQN:H162	21:B:6017:BCR:H333	1.05	1.00
16:2:125:PHE:C	16:2:127:THR:HG23	1.82	1.00
17:3:95:PRO:O	17:3:96:ARG:CG	2.09	1.00
17:3:122:LEU:HD22	19:3:3006:CLA:C1A	1.90	1.00
15:1:189:LYS:CA	15:1:189:LYS:HE2	1.86	1.00
1:A:487:VAL:HG13	1:A:489:ALA:H	0.89	1.00
18:4:96:LEU:HD11	18:4:100:ARG:CZ	1.90	1.00
2:B:409:ALA:O	2:B:410:ARG:HB2	1.56	1.00
7:G:96:GLY:O	7:G:97:LEU:HG	1.62	1.00
13:N:147:SER:HB3	13:N:151:ASP:CA	1.91	1.00
16:2:254:LEU:C	16:2:254:LEU:CD2	2.30	1.00
15:1:162:LYS:H	15:1:164:PRO:CG	1.73	1.00
22:1:7004:LMU:H3'	22:1:7004:LMU:H12	1.43	1.00
15:1:77:GLU:HA	15:1:80:LYS:CD	1.91	1.00
19:B:1222:CLA:HBB1	19:B:1236:CLA:HBB	1.40	1.00
3:C:69:LEU:CD1	3:C:70:TRP:O	2.09	1.00
12:L:79:ILE:HD11	19:L:1130:CLA:C4	1.90	1.00
1:A:342:GLY:HA2	1:A:430:ASP:CB	1.91	1.00
2:B:120:VAL:HG22	2:B:123:TRP:NE1	1.77	1.00
19:B:1228:CLA:CBC	19:B:1228:CLA:HHD	1.91	1.00
7:G:84:ARG:CG	7:G:85:GLU:N	2.24	1.00
6:F:200:VAL:CG1	10:J:7:TYR:CB	2.39	1.00
15:1:134:LEU:CA	15:1:137:ILE:HD11	1.91	1.00
3:C:44:ARG:HB3	4:D:182:GLN:CD	1.80	1.00
16:2:147:THR:HG22	16:2:148:ASP:OD2	1.61	1.00
8:H:56:GLU:HG3	8:H:57:ASP:CA	1.92	1.00
15:1:157:ASP:HB2	15:1:178:LYS:HB2	1.40	1.00
2:B:638:LEU:O	2:B:639:VAL:HG12	1.60	1.00
2:B:732:LYS:CG	2:B:734:GLY:N	2.23	1.00
15:1:93:ALA:HB1	19:1:1006:CLA:HHC	1.42	1.00
16:2:160:ILE:CG2	19:2:2012:CLA:HBB1	1.91	1.00
4:D:140:LEU:HD21	4:D:144:LEU:CD1	1.90	1.00
1:A:267:THR:CG2	1:A:269:PHE:HE2	1.74	1.00
11:K:99:ALA:O	11:K:103:LEU:HD11	1.60	1.00
4:D:187:ASN:N	4:D:187:ASN:HD22	1.60	1.00
15:1:95:PRO:HA	15:1:98:LEU:CG	1.92	1.00
19:A:1125:CLA:CAB	19:A:1133:CLA:HMA2	1.89	1.00
2:B:50:HIS:HD2	19:B:1202:CLA:HAA2	1.24	1.00
5:E:107:PHE:CD2	5:E:109:LYS:HG3	1.97	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:165:GLY:O	16:2:167:ARG:CB	2.07	1.00
2:B:247:THR:CA	2:B:250:ALA:HB2	1.92	1.00
12:L:164:LEU:HD12	12:L:165:THR:N	1.75	1.00
17:3:176:TRP:O	17:3:178:LYS:HB2	1.62	1.00
1:A:116:ILE:O	1:A:136:VAL:O	1.77	1.00
2:B:353:TYR:CG	2:B:594:TRP:HZ3	1.79	1.00
2:B:560:ASP:HB2	3:C:66:ARG:HE	1.27	1.00
4:D:140:LEU:CA	4:D:143:ARG:HB2	1.90	1.00
22:E:7048:LMU:H6'2	22:E:7048:LMU:H3'	1.44	1.00
12:L:52:PRO:HB2	12:L:55:GLN:O	1.60	1.00
1:A:304:LEU:HG	19:A:1115:CLA:CBB	1.91	1.00
4:D:167:HIS:CD2	4:D:172:VAL:CG2	2.44	1.00
19:4:4006:CLA:HMA1	22:4:7034:LMU:H62	1.40	0.99
15:1:68:GLY:O	15:1:72:VAL:HB	1.61	0.99
15:1:83:GLU:C	15:1:86:HIS:HD2	1.64	0.99
18:4:177:LEU:HD13	18:4:178:PRO:HD3	1.42	0.99
16:2:218:ARG:HB2	16:2:219:THR:CG2	1.91	0.99
3:C:27:GLU:OE1	3:C:39:ILE:O	1.78	0.99
5:E:79:LYS:HA	5:E:84:TYR:CE1	1.97	0.99
4:D:200:VAL:CG2	4:D:206:GLN:HE21	1.74	0.99
22:R:7020:LMU:H5B	22:R:7020:LMU:C6'	1.90	0.99
22:N:7049:LMU:C1	22:N:7049:LMU:H61	1.91	0.99
19:A:1124:CLA:CED	19:A:1125:CLA:CAD	2.40	0.99
1:A:328:LYS:CG	1:A:332:GLU:HB2	1.92	0.99
1:A:531:PRO:O	1:A:532:ILE:HG22	1.63	0.99
19:A:9022:CLA:HBB2	19:A:9023:CLA:C1B	1.92	0.99
2:B:352:MET:HE1	19:B:1225:CLA:OBD	1.62	0.99
2:B:430:GLY:HA2	2:B:525:LEU:HD11	1.41	0.99
16:2:104:GLN:O	16:2:107:LEU:HG	1.62	0.99
18:4:88:LEU:C	18:4:90:TRP:HB3	1.82	0.99
16:2:171:ILE:CG1	16:2:172:LEU:N	2.25	0.99
16:2:172:LEU:HB3	16:2:173:ASN:ND2	1.77	0.99
13:N:114:PHE:HB3	13:N:117:ALA:HB3	1.41	0.99
22:A:7016:LMU:H22	22:A:7016:LMU:H61	1.42	0.99
2:B:58:PHE:CD2	2:B:145:LEU:HD22	1.97	0.99
1:A:246:HIS:CA	1:A:248:PHE:HE2	1.75	0.99
1:A:336:GLY:HA3	1:A:339:THR:OG1	1.62	0.99
19:B:1213:CLA:HBC2	19:B:1213:CLA:HHD	1.44	0.99
4:D:201:LYS:CD	4:D:201:LYS:H	1.66	0.99
16:2:186:ASN:CG	16:2:188:LEU:CD1	2.25	0.99
19:K:1146:CLA:HMA2	19:K:1146:CLA:O1A	1.62	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:131:THR:HG22	2:B:134:ASP:HB2	1.44	0.99
17:3:127:LEU:CB	19:3:1147:CLA:HED1	1.88	0.99
1:A:451:ILE:CD1	19:A:1131:CLA:HED3	1.92	0.99
19:A:1141:CLA:HMA2	19:A:1141:CLA:C1	1.90	0.99
1:A:208:ALA:HA	1:A:310:PHE:O	1.62	0.99
2:B:73:ASN:O	2:B:121:TYR:CZ	2.16	0.99
19:A:1138:CLA:H191	6:F:181:TYR:HB3	1.41	0.99
2:B:58:PHE:CE2	2:B:145:LEU:CD2	2.44	0.99
2:B:58:PHE:HB2	2:B:146:SER:HB3	1.41	0.99
2:B:7:ARG:CG	2:B:7:ARG:HH11	1.75	0.99
18:4:232:LEU:HB2	18:4:236:ILE:HD12	1.41	0.99
19:4:4006:CLA:C10	22:4:7034:LMU:C12	2.40	0.99
15:1:66:PRO:HD2	15:1:67:LEU:H	1.23	0.99
1:A:51:THR:HG21	19:A:1139:CLA:CBB	1.92	0.99
1:A:22:VAL:O	1:A:22:VAL:HG22	1.59	0.99
13:N:130:ASN:HB3	13:N:139:LYS:HG2	1.40	0.99
17:3:173:PHE:HD1	17:3:174:GLN:N	1.59	0.99
1:A:422:TYR:N	1:A:422:TYR:HD1	1.58	0.99
2:B:531:THR:HG22	19:B:1222:CLA:HMC2	1.44	0.99
3:C:80:ALA:O	3:C:81:TYR:HB3	1.62	0.99
2:B:294:ASN:ND2	7:G:94:GLN:N	2.11	0.99
15:1:137:ILE:O	15:1:141:GLU:HG2	1.63	0.99
17:3:109:ALA:HA	17:3:111:LEU:CB	1.91	0.99
16:2:139:THR:HG23	16:2:140:ALA:H	1.21	0.99
22:4:7052:LMU:O1'	22:4:7052:LMU:H61	1.61	0.99
1:A:534:LEU:CD1	1:A:535:GLY:N	2.25	0.99
2:B:694:ARG:HG2	2:B:694:ARG:NH2	1.62	0.99
19:2:2002:CLA:HBC2	19:2:2002:CLA:HHD	1.43	0.99
1:A:249:ILE:O	1:A:252:ARG:HG3	1.62	0.99
4:D:103:THR:HG22	4:D:128:LEU:HG	1.42	0.99
14:R:52:UNK:CA	14:R:53:UNK:CB	2.36	0.99
19:B:1205:CLA:CBB	19:B:1205:CLA:H92	1.93	0.99
2:B:199:ILE:CG2	2:B:270:LEU:HD13	1.92	0.99
17:3:96:ARG:NH1	17:3:96:ARG:HB2	1.77	0.99
4:D:200:VAL:HG21	4:D:206:GLN:HE21	0.84	0.99
15:1:178:LYS:HG3	15:1:179:LYS:H	1.23	0.99
19:A:1124:CLA:CED	19:A:1125:CLA:HMD1	1.92	0.99
19:A:1141:CLA:H121	19:A:1141:CLA:C7	1.91	0.99
19:B:1202:CLA:O1A	19:B:1202:CLA:H62	1.63	0.99
2:B:268:LEU:HD21	19:B:1214:CLA:CMA	1.91	0.99
8:H:97:LEU:CD1	8:H:100:PHE:CB	2.41	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:189:LYS:HB2	19:1:1007:CLA:CMC	1.93	0.99
16:2:237:PHE:HA	16:2:240:ILE:CD1	1.92	0.99
2:B:85:ARG:HH11	2:B:85:ARG:HG2	1.24	0.99
18:4:158:GLN:C	19:4:1004:CLA:HMA2	1.84	0.99
1:A:368:LEU:CD2	19:A:1117:CLA:C9	2.41	0.99
1:A:699:TYR:OH	2:B:533:ILE:HG22	1.61	0.99
21:F:6016:BCR:HC8	21:F:6016:BCR:C32	1.89	0.99
7:G:102:ALA:HA	7:G:104:ASP:CG	1.82	0.99
12:L:79:ILE:CD1	19:L:1130:CLA:H42	1.92	0.99
8:H:77:ASN:CG	8:H:78:PRO:HD2	1.81	0.99
2:B:490:ARG:CG	2:B:490:ARG:HH11	1.75	0.99
18:4:223:VAL:O	18:4:223:VAL:HG12	1.63	0.98
1:A:163:GLN:CG	1:A:164:LEU:H	1.74	0.98
1:A:365:LEU:CD2	19:A:1103:CLA:HED3	1.92	0.98
7:G:90:GLN:HB2	7:G:92:PRO:HD3	1.43	0.98
12:L:60:ILE:CG2	12:L:61:ASN:N	2.12	0.98
12:L:96:LEU:N	12:L:96:LEU:HD23	1.77	0.98
16:2:177:VAL:HG12	16:2:178:ASN:CB	1.93	0.98
15:1:190:ASN:HD21	19:1:1002:CLA:CHA	1.76	0.98
1:A:715:LYS:NZ	6:F:230:ASN:OD1	1.95	0.98
2:B:58:PHE:CB	2:B:146:SER:HB3	1.93	0.98
15:1:161:LYS:HE2	15:1:162:LYS:HB2	1.45	0.98
15:1:129:VAL:HG12	15:1:130:PRO:HD3	1.41	0.98
11:K:63:LEU:N	11:K:63:LEU:HD13	1.75	0.98
1:A:567:ARG:HH12	4:D:89:GLY:HA2	1.21	0.98
17:3:159:VAL:HG13	17:3:160:LEU:N	1.72	0.98
1:A:106:TYR:O	1:A:110:LEU:HD23	1.61	0.98
1:A:120:ALA:N	1:A:145:ILE:CD1	2.26	0.98
1:A:397:THR:HG22	1:A:613:ILE:CG1	1.92	0.98
7:G:84:ARG:HA	19:G:1242:CLA:HMA3	1.41	0.98
15:1:198:PHE:O	15:1:202:CYS:HB3	1.63	0.98
1:A:90:PHE:CE1	19:A:1103:CLA:H91	1.99	0.98
8:H:63:GLY:O	8:H:66:ASP:OD1	1.81	0.98
13:N:146:LEU:CD1	17:3:142:ILE:C	2.31	0.98
4:D:158:PHE:HB3	4:D:159:PRO:O	1.60	0.98
17:3:150:TYR:HD2	17:3:151:TRP:CE2	1.80	0.98
19:J:1308:CLA:C9	19:2:2014:CLA:O1D	2.11	0.98
2:B:476:ILE:CG2	2:B:479:SER:OG	2.11	0.98
19:4:4003:CLA:HBC2	19:4:4003:CLA:HMC1	1.38	0.98
19:A:1125:CLA:HBC2	19:A:1125:CLA:HMC1	1.43	0.98
1:A:605:MET:HA	1:A:608:SER:OG	1.63	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:HIS:CD2	19:A:1139:CLA:HBC1	1.98	0.98
2:B:622:ASP:HB2	2:B:626:LEU:HD12	1.42	0.98
3:C:1:MET:HG2	3:C:4:SER:OG	1.62	0.98
8:H:78:PRO:CD	19:L:1501:CLA:CMD	2.40	0.98
19:4:1304:CLA:H151	19:4:1304:CLA:C20	1.93	0.98
1:A:132:LEU:O	1:A:671:SER:O	1.80	0.98
2:B:189:ALA:HB2	19:B:1225:CLA:H203	1.46	0.98
2:B:429:LEU:O	2:B:525:LEU:CD1	2.11	0.98
13:N:146:LEU:CD2	17:3:142:ILE:O	2.10	0.98
6:F:97:GLN:CD	6:F:98:ALA:H	1.67	0.98
2:B:303:TYR:HA	2:B:306:GLU:HB2	1.45	0.98
8:H:58:LEU:HD13	8:H:62:THR:CG2	1.92	0.98
1:A:249:ILE:HG21	17:3:136:TRP:HZ3	1.24	0.98
19:L:1148:CLA:HHD	19:L:1148:CLA:CBC	1.93	0.98
8:H:89:ALA:HA	8:H:92:THR:HB	1.45	0.98
16:2:237:PHE:CA	16:2:240:ILE:HD12	1.92	0.98
22:E:7048:LMU:H72	22:E:7048:LMU:H111	1.45	0.98
16:2:269:LYS:HZ2	16:2:269:LYS:HA	1.22	0.98
19:A:1119:CLA:HMD3	19:A:1121:CLA:CBB	1.93	0.98
1:A:64:PHE:HZ	1:A:77:LYS:HE2	1.29	0.98
2:B:304:ILE:CD1	19:B:1216:CLA:CED	2.39	0.98
16:2:113:ALA:C	16:2:114:MET:HE3	1.84	0.98
13:N:132:THR:OG1	13:N:137:LEU:O	1.82	0.98
1:A:267:THR:HG22	1:A:269:PHE:HE2	1.18	0.98
1:A:193:LEU:HA	1:A:196:PHE:HE2	1.27	0.98
13:N:139:LYS:CB	13:N:142:LYS:CD	2.41	0.98
1:A:68:THR:CG2	1:A:70:ASP:H	1.76	0.98
18:4:96:LEU:HD11	18:4:100:ARG:NH1	1.77	0.98
19:A:1119:CLA:HMD3	19:A:1121:CLA:HBB2	0.98	0.98
19:A:9022:CLA:C15	21:B:6017:BCR:H20C	1.93	0.98
21:J:6012:BCR:H23C	21:J:6012:BCR:H393	1.46	0.98
6:F:219:ARG:CG	6:F:219:ARG:HH11	1.75	0.98
1:A:217:SER:HG	21:A:6002:BCR:H15C	1.24	0.97
1:A:51:THR:OG1	19:A:1139:CLA:HBB2	1.62	0.97
1:A:89:ILE:O	1:A:92:TRP:O	1.82	0.97
7:G:102:ALA:HA	7:G:104:ASP:OD1	1.63	0.97
8:H:97:LEU:HD11	8:H:100:PHE:CB	1.94	0.97
12:L:154:ASN:O	12:L:178:THR:CG2	2.11	0.97
18:4:172:PHE:HB2	18:4:194:PHE:CD2	1.97	0.97
1:A:454:GLY:H	1:A:457:SER:HB3	1.23	0.97
2:B:268:LEU:CD2	19:B:1214:CLA:HMA2	1.93	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:99:HIS:C	7:G:101:GLU:HB2	1.84	0.97
16:2:119:GLY:O	16:2:123:PRO:HG2	1.63	0.97
18:4:87:ASN:CB	18:4:90:TRP:CE3	2.46	0.97
12:L:155:GLU:HA	12:L:178:THR:CG2	1.93	0.97
2:B:486:LEU:HB2	19:B:1232:CLA:HMD3	1.44	0.97
2:B:732:LYS:HB3	2:B:733:PHE:HA	1.45	0.97
7:G:99:HIS:HA	7:G:100:PHE:HB3	1.46	0.97
12:L:79:ILE:HD11	19:L:1130:CLA:H42	1.00	0.97
16:2:103:VAL:CG1	16:2:104:GLN:OE1	2.12	0.97
19:2:2007:CLA:HBC1	19:3:2009:CLA:HED2	1.00	0.97
19:4:1304:CLA:H151	19:4:1304:CLA:H203	1.45	0.97
22:H:7032:LMU:C1B	22:H:7032:LMU:H31	1.92	0.97
18:4:158:GLN:HB3	19:4:1004:CLA:HMA2	1.43	0.97
1:A:129:GLN:O	1:A:130:GLU:HB3	1.62	0.97
2:B:353:TYR:CD2	2:B:594:TRP:CZ3	2.51	0.97
12:L:73:VAL:HA	19:L:1504:CLA:CMA	1.92	0.97
11:K:127:ILE:HB	11:K:129:ALA:HB1	1.45	0.97
15:1:149:GLU:HG2	15:1:152:ARG:HH12	1.16	0.97
11:K:92:GLY:O	11:K:93:LEU:CG	2.11	0.97
15:1:158:PRO:HA	15:1:175:LYS:HG3	1.46	0.97
1:A:491:TRP:HE1	19:A:1135:CLA:H12	1.27	0.97
1:A:564:ARG:HH21	1:A:564:ARG:HB3	1.29	0.97
2:B:172:GLU:O	2:B:176:ASN:HB2	1.64	0.97
2:B:310:PRO:HG3	19:B:1220:CLA:HMA1	1.47	0.97
2:B:708:VAL:O	2:B:712:HIS:HB2	1.62	0.97
8:H:99:LYS:O	8:H:101:LEU:N	1.97	0.97
13:N:139:LYS:HE3	13:N:142:LYS:HE2	0.98	0.97
11:K:125:LYS:HA	11:K:126:ASN:HB3	0.97	0.97
15:1:171:LEU:HA	15:1:173:TYR:CZ	2.00	0.97
18:4:169:ASP:CA	18:4:173:LYS:HA	1.94	0.97
1:A:296:LEU:HD12	1:A:297:THR:HG22	1.47	0.97
19:A:1122:CLA:C1D	21:A:6007:BCR:H19C	1.93	0.97
2:B:527:LEU:HD13	19:B:1236:CLA:CMA	1.94	0.97
6:F:139:LEU:HD13	6:F:149:ILE:CD1	1.93	0.97
8:H:109:LEU:O	8:H:113:SER:HB2	1.63	0.97
4:D:140:LEU:HA	4:D:143:ARG:CB	1.93	0.97
2:B:213:LEU:HD12	2:B:214:ASP:H	1.29	0.97
15:1:78:ARG:NH2	15:1:179:LYS:HD2	1.80	0.97
15:1:67:LEU:CD1	15:1:68:GLY:N	2.27	0.97
1:A:64:PHE:CE2	1:A:74:ILE:HG21	2.00	0.97
11:K:49:ILE:HA	11:K:52:PRO:CG	1.92	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:126:LEU:HB3	19:2:2006:CLA:H192	1.45	0.97
16:2:237:PHE:HA	16:2:240:ILE:HD12	0.98	0.97
22:H:7030:LMU:C5	22:H:7030:LMU:H91	1.93	0.97
6:F:221:LEU:HD23	6:F:222:LEU:HD23	1.46	0.97
13:N:122:PHE:N	13:N:122:PHE:HD2	1.60	0.97
2:B:666:SER:HB3	2:B:671:TRP:HE1	1.27	0.96
8:H:113:SER:OG	19:H:1207:CLA:H61	1.65	0.96
5:E:99:THR:HG22	5:E:100:ARG:H	0.81	0.96
13:N:136:ASP:O	13:N:137:LEU:HD22	1.64	0.96
11:K:98:PRO:HD2	11:K:99:ALA:H	1.28	0.96
2:B:594:TRP:O	2:B:595:HIS:HB3	1.61	0.96
16:2:160:ILE:HG21	19:2:2012:CLA:HBB1	1.44	0.96
8:H:86:THR:HG22	8:H:87:PHE:O	1.65	0.96
8:H:121:LEU:HB3	8:H:122:PRO:CD	1.95	0.96
22:R:7021:LMU:H31	22:R:7021:LMU:H1'	1.45	0.96
15:1:85:ILE:HA	15:1:88:ARG:HG3	1.47	0.96
18:4:145:GLU:HG3	18:4:146:PHE:HD1	1.20	0.96
2:B:98:GLN:C	2:B:100:ALA:H	1.63	0.96
2:B:256:THR:O	2:B:272:ASP:OD1	1.83	0.96
21:F:6016:BCR:C8	21:F:6016:BCR:C32	2.38	0.96
1:A:426:THR:HA	1:A:428:TYR:CZ	2.00	0.96
17:3:254:GLN:HG3	17:3:255:ASN:H	1.27	0.96
2:B:189:ALA:CB	19:B:1225:CLA:H203	1.96	0.96
11:K:49:ILE:C	11:K:52:PRO:HG2	1.77	0.96
16:2:118:ALA:C	16:2:121:PHE:CE2	2.37	0.96
3:C:44:ARG:H	4:D:182:GLN:HG3	1.27	0.96
17:3:176:TRP:CH2	17:3:199:ASN:OD1	2.15	0.96
18:4:173:LYS:NZ	18:4:201:LYS:CG	2.27	0.96
19:4:4002:CLA:CBA	19:4:4002:CLA:HMA2	1.94	0.96
2:B:225:LEU:HD13	2:B:233:TYR:HH	1.29	0.96
2:B:621:ARG:O	2:B:625:TRP:HB3	1.66	0.96
3:C:72:GLU:HG2	3:C:77:MET:HE2	1.48	0.96
16:2:172:LEU:O	16:2:174:PRO:HD3	1.63	0.96
17:3:176:TRP:O	17:3:178:LYS:CB	2.13	0.96
18:4:159:ASP:CG	18:4:171:ILE:HD11	1.85	0.96
5:E:127:GLU:HB3	5:E:128:VAL:O	1.65	0.96
13:N:157:LYS:HE2	13:N:157:LYS:N	1.80	0.96
3:C:44:ARG:H	4:D:182:GLN:CG	1.77	0.96
6:F:130:PHE:H	6:F:133:TYR:HE1	1.01	0.96
2:B:314:ARG:CZ	15:1:67:LEU:HD21	1.94	0.96
1:A:281:LEU:HD22	19:A:1115:CLA:HED3	1.45	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:TRP:NE1	19:A:1135:CLA:H12	1.79	0.96
5:E:93:VAL:HG23	5:E:103:VAL:HB	1.46	0.96
16:2:167:ARG:HA	16:2:167:ARG:NE	1.77	0.96
18:4:111:LEU:HD12	18:4:112:PRO:N	1.80	0.96
1:A:308:ILE:HD13	19:A:1115:CLA:H102	1.48	0.96
1:A:430:ASP:O	1:A:432:LEU:N	1.98	0.96
2:B:527:LEU:HD22	19:B:1222:CLA:ND	1.80	0.96
16:2:118:ALA:C	16:2:121:PHE:HE2	1.68	0.96
2:B:480:SER:O	2:B:481:THR:HG22	1.63	0.96
8:H:111:TYR:C	8:H:112:LEU:HD23	1.86	0.96
1:A:308:ILE:HD13	19:A:1115:CLA:HHC	1.46	0.96
2:B:422:LEU:HD13	2:B:535:VAL:HG11	1.47	0.96
12:L:138:VAL:O	12:L:142:SER:OG	1.84	0.96
13:N:146:LEU:HD13	17:3:142:ILE:C	1.85	0.96
17:3:96:ARG:HH11	17:3:96:ARG:HG3	1.25	0.96
17:3:197:SER:HB3	17:3:206:PRO:HD3	1.46	0.96
1:A:24:ARG:CD	1:A:24:ARG:H	1.75	0.96
18:4:168:GLN:HB3	18:4:172:PHE:CE1	1.99	0.96
1:A:394:SER:HB2	19:A:1126:CLA:HMA1	1.45	0.96
19:B:1219:CLA:H72	19:B:1219:CLA:HBB2	1.47	0.96
19:F:1305:CLA:H42	19:4:1306:CLA:HAA1	1.45	0.96
21:B:6020:BCR:H333	19:L:1502:CLA:NB	1.81	0.96
4:D:87:THR:CG2	12:L:69:LEU:HD12	1.95	0.96
1:A:252:ARG:HD3	1:A:252:ARG:H	1.30	0.96
19:H:1145:CLA:HMA2	19:H:1145:CLA:C2	1.95	0.96
15:1:177:PRO:HD2	15:1:180:LEU:CD2	1.92	0.95
18:4:175:TYR:HB3	18:4:194:PHE:CD1	2.00	0.95
2:B:569:ASP:OD1	2:B:706:ARG:NH1	1.99	0.95
6:F:207:LEU:HD21	6:F:208:PHE:CD1	2.00	0.95
12:L:141:LEU:CD1	12:L:145:LEU:CD1	2.44	0.95
16:2:103:VAL:O	16:2:106:GLU:N	1.99	0.95
13:N:133:GLY:C	13:N:134:CYS:SG	2.44	0.95
13:N:143:VAL:CB	13:N:144:PRO:HD2	1.95	0.95
17:3:130:GLN:HB3	17:3:132:THR:H	0.79	0.95
4:D:124:GLU:OE1	4:D:125:GLY:HA3	1.66	0.95
4:D:140:LEU:CD1	4:D:144:LEU:CB	2.44	0.95
2:B:131:THR:CG2	2:B:134:ASP:HB2	1.94	0.95
1:A:412:ALA:HB2	1:A:598:VAL:HG11	1.47	0.95
2:B:282:PHE:HZ	19:B:1213:CLA:C1	1.79	0.95
2:B:292:ARG:NH1	2:B:296:GLY:H	1.63	0.95
5:E:111:ASN:HD21	5:E:113:ALA:H	0.96	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:148:LEU:HD12	6:F:148:LEU:O	1.65	0.95
11:K:62:SER:OG	11:K:63:LEU:HD13	1.64	0.95
18:4:228:PRO:HB2	18:4:229:PHE:CE1	2.00	0.95
15:1:200:GLY:O	15:1:203:VAL:HG12	1.66	0.95
18:4:145:GLU:HG3	18:4:146:PHE:CE1	2.00	0.95
2:B:459:PHE:HD2	19:B:1235:CLA:C4D	1.77	0.95
5:E:107:PHE:CE2	5:E:109:LYS:CG	2.48	0.95
1:A:425:THR:O	1:A:427:ARG:HD3	1.66	0.95
15:1:76:LEU:HB3	15:1:77:GLU:OE1	1.66	0.95
3:C:44:ARG:N	4:D:182:GLN:OE1	2.00	0.95
16:2:183:PHE:N	16:2:187:LYS:HG2	1.81	0.95
8:H:78:PRO:CG	19:L:1501:CLA:HMD1	1.95	0.95
8:H:119:ASP:O	8:H:120:ILE:CG2	2.13	0.95
19:3:3008:CLA:CGD	19:3:3008:CLA:HBA2	1.95	0.95
15:1:94:VAL:O	15:1:97:ILE:HG23	1.64	0.95
21:A:6007:BCR:H23C	21:A:6007:BCR:H382	1.44	0.95
2:B:180:SER:HB3	2:B:288:GLY:HA3	1.47	0.95
2:B:382:ILE:CG2	2:B:383:MET:H	1.80	0.95
17:3:181:SER:CB	19:3:2009:CLA:C11	2.40	0.95
5:E:89:SER:HB2	5:E:106:ARG:NH1	1.81	0.95
16:2:240:ILE:HG23	16:2:263:PHE:HB3	1.46	0.95
19:J:1311:CLA:HED3	19:J:1311:CLA:C1A	1.97	0.95
2:B:103:ALA:HB1	2:B:106:ARG:HD2	1.49	0.95
6:F:204:SER:O	6:F:207:LEU:HD12	1.65	0.95
7:G:89:LYS:NZ	7:G:89:LYS:CA	2.29	0.95
16:2:218:ARG:HB2	16:2:219:THR:HG22	1.45	0.95
3:C:62:PHE:CE2	5:E:80:GLU:CD	2.40	0.95
22:R:7022:LMU:C2'	22:R:7022:LMU:H21	1.95	0.95
18:4:187:GLY:O	18:4:188:ILE:HB	1.64	0.95
2:B:478:LEU:HD23	2:B:478:LEU:O	1.65	0.95
15:1:91:MET:O	15:1:95:PRO:CD	2.13	0.95
18:4:172:PHE:CB	18:4:194:PHE:CZ	2.49	0.95
1:A:302:HIS:O	1:A:306:ILE:HG12	1.67	0.95
1:A:714:LEU:HD13	21:F:6016:BCR:H393	1.48	0.95
19:B:1226:CLA:HMC1	19:B:1226:CLA:CBC	1.97	0.95
17:3:139:THR:CG2	17:3:140:GLY:H	1.79	0.95
18:4:124:PRO:HB2	18:4:126:TRP:H	1.31	0.95
1:A:281:LEU:HD11	19:A:1115:CLA:HED1	1.46	0.95
19:A:9022:CLA:C9	19:A:9023:CLA:H91	1.97	0.95
19:L:1503:CLA:HHD	19:L:1503:CLA:CBC	1.96	0.95
15:1:128:PRO:HG2	15:1:131:TRP:CH2	2.00	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:H:7011:LMU:H6E	22:H:7011:LMU:H2B	1.46	0.95
6:F:204:SER:O	6:F:207:LEU:N	2.00	0.95
6:F:207:LEU:CD1	6:F:208:PHE:H	1.78	0.95
7:G:72:LEU:CD2	7:G:124:ILE:HD12	1.90	0.95
2:B:294:ASN:HD22	7:G:94:GLN:N	1.64	0.95
19:2:2001:CLA:CBC	19:2:2001:CLA:HMC1	1.97	0.95
3:C:5:VAL:HG21	3:C:65:VAL:CG2	1.97	0.95
3:C:5:VAL:HB	3:C:65:VAL:HG23	1.47	0.95
14:R:40:UNK:N	14:R:41:UNK:CB	2.30	0.95
4:D:156:ARG:NH2	4:D:158:PHE:CE1	2.35	0.95
8:H:78:PRO:CD	19:L:1501:CLA:HMD3	1.96	0.95
19:K:1143:CLA:HBC1	22:K:7001:LMU:O3B	1.63	0.95
3:C:34:CYS:H	3:C:37:LYS:HB3	1.30	0.95
1:A:190:ALA:HB1	1:A:191:PRO:CD	1.97	0.94
2:B:622:ASP:CB	2:B:626:LEU:CD1	2.44	0.94
12:L:128:GLN:HA	12:L:130:GLY:CA	1.96	0.94
12:L:131:SER:CA	12:L:201:TYR:CE2	2.50	0.94
1:A:586:ARG:HG3	3:C:49:VAL:HG21	1.48	0.94
14:R:34:UNK:N	14:R:36:UNK:CB	2.30	0.94
1:A:73:GLU:HG3	1:A:74:ILE:N	1.82	0.94
2:B:298:GLY:HA2	19:B:1218:CLA:HMD3	1.49	0.94
6:F:150:VAL:HG21	6:F:160:PHE:HB2	1.48	0.94
7:G:99:HIS:CA	7:G:100:PHE:HB3	1.97	0.94
1:A:26:PRO:HB2	1:A:27:ILE:HG13	1.49	0.94
17:3:150:TYR:HB3	17:3:151:TRP:NE1	1.82	0.94
17:3:207:PHE:HD1	17:3:207:PHE:O	1.50	0.94
1:A:102:ARG:C	1:A:103:PHE:HD2	1.70	0.94
19:A:1112:CLA:HMB2	21:A:6002:BCR:C38	1.98	0.94
2:B:293:THR:HG21	19:B:1209:CLA:HMA2	1.49	0.94
19:B:1220:CLA:H43	19:B:1220:CLA:HAA1	1.48	0.94
2:B:20:ARG:CG	2:B:20:ARG:HH11	1.78	0.94
2:B:315:LEU:HD13	2:B:315:LEU:O	1.68	0.94
5:E:76:ILE:HB	5:E:84:TYR:O	1.67	0.94
17:3:103:VAL:O	17:3:107:ARG:HD2	1.67	0.94
6:F:119:ILE:HG13	6:F:120:LYS:N	1.77	0.94
2:B:490:ARG:HG3	2:B:490:ARG:HH11	0.82	0.94
19:A:1126:CLA:H203	21:J:6012:BCR:H17C	1.46	0.94
2:B:294:ASN:HD22	7:G:94:GLN:CG	1.74	0.94
22:D:7050:LMU:C6'	22:D:7050:LMU:H2B	1.97	0.94
16:2:168:TRP:HD1	16:2:171:ILE:HG23	1.32	0.94
2:B:247:THR:CA	2:B:250:ALA:CB	2.45	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:76:TYR:HH	12:L:90:ARG:CD	1.69	0.94
2:B:542:ARG:HH11	2:B:542:ARG:HG3	1.29	0.94
11:K:97:ASP:HB2	11:K:101:PHE:CE2	2.02	0.94
6:F:213:TRP:HB2	6:F:216:ALA:CB	1.97	0.94
15:1:85:ILE:O	15:1:88:ARG:HB2	1.67	0.94
19:A:1124:CLA:C7	19:A:1125:CLA:HED1	1.97	0.94
1:A:248:PHE:H	1:A:248:PHE:HD2	1.11	0.94
1:A:502:THR:HB	1:A:504:ALA:HB3	1.46	0.94
1:A:588:GLY:HA3	2:B:668:ARG:HD3	1.46	0.94
5:E:75:LYS:HA	5:E:87:THR:HG22	1.50	0.94
17:3:96:ARG:CA	17:3:99:ALA:H	1.79	0.94
16:2:160:ILE:HG22	19:2:2012:CLA:HBB2	1.47	0.94
16:2:189:THR:O	16:2:192:ASP:O	1.86	0.94
2:B:7:ARG:HH11	2:B:7:ARG:HG3	1.30	0.94
15:1:80:LYS:O	15:1:83:GLU:CB	2.15	0.94
1:A:338:PHE:HE1	19:A:1151:CLA:CBB	1.61	0.94
2:B:317:ARG:HH22	2:B:410:ARG:CG	1.76	0.94
11:K:127:ILE:HG12	11:K:130:LEU:HD12	1.46	0.94
8:H:112:LEU:N	8:H:112:LEU:HD23	1.78	0.94
18:4:120:ILE:HD11	18:4:226:LYS:CB	1.96	0.94
18:4:226:LYS:CE	18:4:226:LYS:H	1.80	0.94
15:1:95:PRO:O	15:1:98:LEU:HB2	1.66	0.94
2:B:73:ASN:O	2:B:121:TYR:CE1	2.21	0.94
11:K:63:LEU:HD22	11:K:63:LEU:H	1.31	0.94
19:A:1237:CLA:H141	12:L:141:LEU:HD23	1.47	0.94
1:A:331:LEU:CD1	1:A:346:LEU:HB3	1.97	0.94
2:B:454:LEU:HD11	6:F:147:HIS:HA	1.47	0.94
3:C:72:GLU:CG	3:C:77:MET:HE2	1.98	0.94
17:3:96:ARG:HH11	17:3:96:ARG:CB	1.79	0.94
18:4:89:ARG:CD	18:4:90:TRP:H	1.79	0.94
16:2:187:LYS:HE3	16:2:187:LYS:CA	1.97	0.94
16:2:182:ILE:CB	16:2:187:LYS:HB3	1.97	0.94
17:3:150:TYR:O	17:3:152:ALA:CB	2.15	0.94
4:D:141:GLY:H	4:D:144:LEU:H	1.01	0.94
19:2:2014:CLA:C7	19:2:2014:CLA:H41	1.98	0.94
11:K:70:PHE:C	11:K:70:PHE:HD1	1.71	0.94
1:A:523:VAL:HG13	1:A:524:GLY:N	1.80	0.94
15:1:78:ARG:NH2	15:1:179:LYS:CB	2.30	0.94
19:A:1122:CLA:CBB	21:A:6007:BCR:H351	1.98	0.94
11:K:76:ALA:H	11:K:78:ARG:HH12	1.02	0.94
16:2:229:MET:SD	16:2:230:LEU:HA	2.06	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:87:ASN:HB2	18:4:90:TRP:CD2	2.02	0.94
4:D:123:ARG:HH21	22:D:7050:LMU:C4B	1.71	0.94
4:D:140:LEU:CD2	4:D:144:LEU:CD1	2.45	0.94
2:B:394:PHE:O	2:B:542:ARG:NE	2.01	0.94
11:K:115:ILE:HA	11:K:118:VAL:HG22	1.46	0.94
15:1:130:PRO:O	15:1:131:TRP:HE3	1.49	0.94
18:4:169:ASP:O	18:4:173:LYS:CG	2.15	0.94
1:A:157:GLY:CA	1:A:229:ILE:CG2	2.45	0.94
1:A:248:PHE:CD2	1:A:248:PHE:N	2.36	0.94
2:B:493:TRP:CH2	19:B:1214:CLA:H122	2.02	0.94
2:B:622:ASP:HB2	2:B:626:LEU:CD1	1.96	0.94
6:F:82:LEU:HG	6:F:83:THR:N	1.72	0.94
3:C:62:PHE:HZ	5:E:80:GLU:CD	1.60	0.94
16:2:254:LEU:CD2	16:2:255:ALA:N	2.30	0.94
2:B:58:PHE:HB2	2:B:146:SER:CB	1.97	0.94
13:N:96:LYS:HG3	13:N:97:THR:OG1	1.67	0.94
2:B:268:LEU:HD21	19:B:1214:CLA:HMA2	0.98	0.93
2:B:493:TRP:HE1	19:B:1213:CLA:HAC2	1.30	0.93
2:B:685:THR:OG1	19:L:1130:CLA:H3A	1.68	0.93
7:G:84:ARG:NE	7:G:85:GLU:HB3	1.83	0.93
11:K:60:SER:HA	11:K:63:LEU:HD21	1.49	0.93
5:E:78:ARG:NH2	5:E:125:ILE:CG2	2.29	0.93
4:D:100:TYR:CE1	4:D:134:LYS:HG3	2.02	0.93
16:2:237:PHE:HE1	16:2:241:TYR:CZ	1.86	0.93
19:A:9012:CLA:H11	2:B:616:LEU:HD12	1.45	0.93
3:C:1:MET:N	3:C:4:SER:OG	2.01	0.93
2:B:294:ASN:CB	7:G:94:GLN:CD	2.37	0.93
1:A:249:ILE:HG12	1:A:250:LEU:N	1.81	0.93
11:K:118:VAL:O	11:K:121:VAL:HG23	1.69	0.93
11:K:115:ILE:HG12	11:K:122:LEU:H	1.24	0.93
17:3:173:PHE:C	17:3:173:PHE:HD1	1.70	0.93
2:B:130:ARG:HH11	2:B:130:ARG:HG3	1.32	0.93
1:A:382:TYR:OH	19:A:1127:CLA:H42	1.67	0.93
2:B:340:SER:HA	19:B:1223:CLA:H51	1.49	0.93
2:B:560:ASP:HB2	3:C:66:ARG:NE	1.82	0.93
11:K:99:ALA:O	11:K:103:LEU:CD1	2.15	0.93
19:A:1124:CLA:CED	19:A:1125:CLA:CMD	2.45	0.93
1:A:462:ILE:HD11	19:A:9022:CLA:H51	1.50	0.93
7:G:124:ILE:HG12	7:G:128:LEU:HD12	1.48	0.93
3:C:66:ARG:CG	3:C:66:ARG:HH21	1.81	0.93
8:H:85:GLU:HG3	8:H:86:THR:N	1.73	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:131:THR:CG2	2:B:134:ASP:H	1.81	0.93
1:A:127:VAL:HG23	1:A:128:GLY:N	1.83	0.93
1:A:514:THR:O	1:A:531:PRO:HA	1.69	0.93
2:B:620:LEU:HA	2:B:624:LEU:HD23	1.47	0.93
1:A:426:THR:HA	1:A:428:TYR:CE2	2.04	0.93
17:3:201:ALA:C	17:3:202:TYR:CD2	2.42	0.93
1:A:259:TYR:CB	1:A:260:PRO:HD2	1.87	0.93
19:A:1138:CLA:HED3	19:A:1138:CLA:H2A	1.48	0.93
9:I:26:LEU:HA	9:I:29:GLU:O	1.67	0.93
2:B:3:LEU:HD13	9:I:29:GLU:OE1	1.66	0.93
16:2:101:TRP:H	16:2:103:VAL:HB	1.32	0.93
18:4:177:LEU:HD22	18:4:178:PRO:N	1.84	0.93
1:A:127:VAL:HG21	19:A:1107:CLA:CBB	1.99	0.93
2:B:25:ILE:HG22	21:L:6019:BCR:H282	1.51	0.93
21:B:6017:BCR:H382	21:B:6017:BCR:H23C	1.49	0.93
19:B:1235:CLA:C15	21:F:6016:BCR:C31	2.46	0.93
8:H:58:LEU:CD1	8:H:62:THR:HG23	1.76	0.93
13:N:139:LYS:CG	13:N:142:LYS:CD	2.42	0.93
2:B:633:ASN:HB2	2:B:636:THR:HB	0.94	0.93
1:A:606:TYR:O	1:A:610:SER:HB2	1.68	0.93
21:A:6011:BCR:C31	19:A:9013:CLA:H143	1.98	0.93
4:D:115:PRO:O	4:D:116:THR:OG1	1.87	0.93
15:1:91:MET:C	15:1:95:PRO:HD3	1.87	0.93
18:4:153:GLU:OE2	19:4:4012:CLA:C3B	2.16	0.93
1:A:57:LEU:C	1:A:57:LEU:HD23	1.88	0.93
4:D:201:LYS:HD2	4:D:201:LYS:N	1.78	0.93
16:2:212:GLN:HG2	16:2:213:LYS:H	1.31	0.93
19:4:4015:CLA:HBA1	19:4:4015:CLA:HBD	1.50	0.93
19:B:1220:CLA:H43	19:B:1220:CLA:C1A	1.99	0.93
2:B:361:ILE:HG23	2:B:368:GLN:OE1	1.69	0.93
6:F:207:LEU:HD22	6:F:208:PHE:N	1.84	0.93
4:D:140:LEU:CD1	4:D:144:LEU:CG	2.47	0.93
4:D:140:LEU:HD11	4:D:144:LEU:CB	1.99	0.93
17:3:156:THR:O	17:3:158:PHE:C	2.08	0.93
21:A:6002:BCR:H12C	21:A:6002:BCR:H341	1.50	0.92
7:G:125:VAL:HG13	7:G:129:ALA:HB3	1.49	0.92
19:A:1237:CLA:C14	12:L:141:LEU:CD2	2.46	0.92
12:L:73:VAL:HG12	19:L:1504:CLA:HMA3	1.50	0.92
5:E:126:VAL:C	5:E:127:GLU:HG3	1.88	0.92
17:3:109:ALA:HA	17:3:111:LEU:HD22	1.49	0.92
1:A:250:LEU:CB	17:3:136:TRP:CZ2	2.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:187:LYS:HA	16:2:187:LYS:CE	1.83	0.92
12:L:205:TYR:HD1	12:L:207:LEU:HD12	1.18	0.92
18:4:158:GLN:OE1	19:4:1004:CLA:CGD	2.15	0.92
1:A:648:THR:HG23	1:A:651:GLY:H	1.32	0.92
2:B:558:PRO:HB2	2:B:703:VAL:CG2	1.99	0.92
15:1:133:THR:O	15:1:137:ILE:HD13	1.68	0.92
16:2:156:GLU:HG2	16:2:157:LEU:CD1	1.97	0.92
19:3:3016:CLA:H102	19:3:3016:CLA:C14	1.97	0.92
2:B:8:PHE:N	2:B:8:PHE:CD1	2.37	0.92
15:1:89:TRP:O	15:1:92:LEU:HB3	1.69	0.92
18:4:158:GLN:CB	19:4:1004:CLA:HMA2	1.98	0.92
1:A:668:TYR:CD1	2:B:445:ALA:CB	2.51	0.92
2:B:419:ILE:O	2:B:420:SER:OG	1.87	0.92
2:B:696:LYS:HE3	3:C:80:ALA:HB1	1.48	0.92
6:F:139:LEU:HD13	6:F:149:ILE:HD13	1.49	0.92
5:E:79:LYS:HG3	5:E:84:TYR:CE1	2.02	0.92
4:D:140:LEU:CD2	4:D:144:LEU:HD12	1.99	0.92
1:A:388:ASP:OD1	1:A:391:THR:OG1	1.87	0.92
2:B:188:LEU:HD11	19:B:1212:CLA:HBB2	1.51	0.92
19:B:1220:CLA:H2A	19:B:1220:CLA:O2D	1.70	0.92
19:B:1232:CLA:HMB1	21:B:6010:BCR:H292	1.50	0.92
16:2:114:MET:HG2	16:2:227:LEU:HA	1.51	0.92
1:A:267:THR:O	1:A:269:PHE:CD2	2.22	0.92
6:F:219:ARG:HG2	6:F:219:ARG:NH1	1.62	0.92
1:A:120:ALA:H	1:A:145:ILE:HD12	1.34	0.92
1:A:351:THR:O	19:A:1123:CLA:C18	2.17	0.92
19:H:1241:CLA:C4C	21:I:6021:BCR:HC22	2.00	0.92
19:2:2007:CLA:HAC2	19:3:2009:CLA:HED1	1.48	0.92
5:E:78:ARG:N	5:E:78:ARG:HD2	1.83	0.92
3:C:54:CYS:HB2	24:C:8002:SF4:S1	2.08	0.92
16:2:173:ASN:N	16:2:173:ASN:HD22	1.65	0.92
4:D:123:ARG:NH2	22:D:7050:LMU:C5B	2.32	0.92
19:R:1144:CLA:CHA	19:R:1144:CLA:HED3	2.00	0.92
21:A:6011:BCR:C31	19:A:9013:CLA:C14	2.47	0.92
17:3:185:GLN:HG2	17:3:186:TYR:H	0.79	0.92
19:L:1148:CLA:HAA1	19:L:1148:CLA:O2D	1.69	0.92
1:A:451:ILE:CD1	19:A:1131:CLA:HED1	2.00	0.92
1:A:281:LEU:HD23	19:A:1115:CLA:CMA	1.98	0.92
1:A:358:LEU:HD11	1:A:413:HIS:CG	2.05	0.92
1:A:672:LEU:O	1:A:674:ALA:N	2.02	0.92
19:B:1224:CLA:O1D	19:B:1225:CLA:HMA1	1.69	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:694:ARG:CG	2:B:694:ARG:HH21	1.81	0.92
11:K:115:ILE:CG1	11:K:122:LEU:N	2.32	0.92
18:4:120:ILE:HG22	18:4:121:ILE:H	1.33	0.92
19:A:1124:CLA:H72	19:A:1125:CLA:HED2	1.51	0.92
1:A:246:HIS:HA	1:A:248:PHE:HE2	0.79	0.92
5:E:126:VAL:O	5:E:127:GLU:HG3	1.69	0.92
2:B:453:ILE:HG23	2:B:453:ILE:O	1.68	0.92
18:4:146:PHE:CE2	19:4:4013:CLA:C3C	2.52	0.92
18:4:173:LYS:HZ3	18:4:201:LYS:CG	1.81	0.92
1:A:51:THR:CB	19:A:1139:CLA:HBB2	1.99	0.92
1:A:390:ALA:HB2	1:A:754:ILE:HB	1.52	0.92
7:G:72:LEU:HD23	7:G:124:ILE:CG1	2.00	0.92
17:3:197:SER:OG	17:3:205:GLY:CA	2.17	0.92
19:3:3016:CLA:H102	19:3:3016:CLA:H142	1.50	0.92
18:4:222:ASN:O	18:4:223:VAL:HB	1.66	0.92
19:A:9023:CLA:H43	19:A:9023:CLA:HHB	1.52	0.92
2:B:317:ARG:HH22	2:B:410:ARG:HG2	1.18	0.92
23:B:7101:LMG:O3	3:C:70:TRP:CZ2	2.23	0.92
7:G:99:HIS:HA	7:G:100:PHE:CB	1.99	0.92
7:G:84:ARG:HE	7:G:89:LYS:HE2	1.34	0.92
16:2:226:ARG:HH11	16:2:226:ARG:CB	1.82	0.92
3:C:39:ILE:HG23	3:C:40:ALA:N	1.85	0.92
4:D:167:HIS:HD2	4:D:172:VAL:HG21	1.20	0.92
17:3:109:ALA:HA	17:3:111:LEU:CG	1.99	0.92
11:K:125:LYS:HB2	11:K:128:GLY:N	1.84	0.92
21:1:6023:BCR:H313	21:1:6023:BCR:C8	1.74	0.92
1:A:236:GLY:O	1:A:237:VAL:HG13	1.71	0.92
18:4:174:GLN:O	18:4:194:PHE:CB	2.18	0.91
1:A:281:LEU:HD23	19:A:1115:CLA:HMA3	1.49	0.91
19:B:1235:CLA:C16	21:F:6016:BCR:H313	2.00	0.91
6:F:173:TRP:HZ3	6:F:211:PHE:CB	1.83	0.91
8:H:97:LEU:HD11	8:H:100:PHE:HB3	1.50	0.91
9:I:12:VAL:O	9:I:17:PRO:HD3	1.69	0.91
19:L:1148:CLA:HED1	19:L:1148:CLA:H2	0.92	0.91
15:1:189:LYS:HG3	19:1:1007:CLA:CMC	1.99	0.91
15:1:77:GLU:CG	15:1:80:LYS:HD2	1.99	0.91
19:B:1220:CLA:H71	19:B:1220:CLA:C2	1.99	0.91
17:3:133:ALA:HB3	17:3:134:LEU:CD1	1.99	0.91
15:1:190:ASN:ND2	19:1:1002:CLA:C1A	2.33	0.91
1:A:628:ILE:HD12	1:A:629:ASN:H	1.34	0.91
18:4:134:TYR:HB3	18:4:136:ALA:HB2	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1107:CLA:HBB2	19:B:1230:CLA:CMD	2.00	0.91
2:B:457:PRO:HB3	2:B:517:PHE:CD1	2.04	0.91
6:F:207:LEU:HD13	6:F:208:PHE:N	1.85	0.91
21:I:6021:BCR:H391	21:L:6019:BCR:H401	1.47	0.91
3:C:14:CYS:HA	3:C:17:CYS:HG	1.13	0.91
16:2:184:PRO:CD	16:2:187:LYS:HD2	2.00	0.91
16:2:182:ILE:HD13	16:2:190:GLY:HA3	1.51	0.91
19:K:1142:CLA:HED1	19:K:1143:CLA:HMB2	1.50	0.91
2:B:5:ILE:CG2	2:B:6:PRO:HD3	1.98	0.91
15:1:129:VAL:HG12	15:1:130:PRO:CD	1.99	0.91
15:1:129:VAL:CG1	15:1:130:PRO:HD3	2.00	0.91
18:4:226:LYS:H	18:4:226:LYS:CD	1.81	0.91
1:A:336:GLY:N	1:A:339:THR:OG1	2.02	0.91
1:A:368:LEU:HD11	19:A:1125:CLA:H61	1.52	0.91
2:B:443:MET:O	2:B:446:PHE:HB2	1.69	0.91
7:G:116:SER:HA	7:G:119:PRO:HG2	1.52	0.91
11:K:51:SER:N	11:K:52:PRO:CD	2.34	0.91
12:L:102:VAL:HA	19:L:1502:CLA:HED2	1.50	0.91
1:A:425:THR:CB	1:A:428:TYR:CE1	2.48	0.91
1:A:483:GLN:C	1:A:485:GLN:HE22	1.73	0.91
19:A:1107:CLA:HBB2	19:B:1230:CLA:HMD2	1.51	0.91
1:A:328:LYS:NZ	1:A:345:GLY:CA	2.33	0.91
1:A:411:ALA:HB2	21:A:6008:BCR:H392	1.53	0.91
7:G:131:GLY:O	7:G:136:VAL:HB	1.68	0.91
12:L:110:LEU:HB3	12:L:114:PHE:HE1	1.32	0.91
12:L:142:SER:O	12:L:143:LEU:HG	1.70	0.91
16:2:101:TRP:CA	16:2:103:VAL:H	1.82	0.91
19:3:2009:CLA:HBA2	19:3:2009:CLA:CHA	2.00	0.91
3:C:6:LYS:HE2	4:D:191:ILE:HG13	1.49	0.91
15:1:142:PHE:HA	15:1:145:ILE:CD1	2.00	0.91
19:H:1145:CLA:CBC	19:H:1145:CLA:HMC1	1.99	0.91
5:E:96:ASP:OD2	5:E:98:ASN:OD1	1.87	0.91
1:A:564:ARG:NH2	1:A:564:ARG:HB3	1.85	0.91
19:A:1149:CLA:HAA1	19:A:1149:CLA:O1D	1.71	0.91
1:A:365:LEU:HD23	19:A:1103:CLA:CED	1.99	0.91
11:K:118:VAL:CG2	11:K:121:VAL:HG22	2.00	0.91
1:A:484:LEU:H	1:A:484:LEU:HD22	1.36	0.91
19:A:1125:CLA:O1D	19:A:1125:CLA:HBA1	1.69	0.91
19:A:1112:CLA:HHC	21:A:6002:BCR:H17C	1.50	0.91
2:B:103:ALA:HA	2:B:105:THR:N	1.85	0.91
2:B:310:PRO:CG	2:B:311:PRO:HD3	2.00	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:124:ILE:O	7:G:128:LEU:HB2	1.71	0.91
5:E:89:SER:O	5:E:106:ARG:N	2.03	0.91
4:D:95:GLN:HE21	4:D:96:VAL:HA	1.30	0.91
17:3:133:ALA:HB3	17:3:134:LEU:HD11	1.53	0.91
22:4:7034:LMU:H71	22:4:7052:LMU:H11	1.53	0.91
15:1:157:ASP:CG	15:1:178:LYS:HA	1.89	0.91
15:1:177:PRO:HD3	15:1:180:LEU:CD2	2.00	0.91
19:A:1113:CLA:CBB	21:A:6002:BCR:H352	2.01	0.91
1:A:338:PHE:CE1	19:A:1151:CLA:HBB2	2.03	0.91
7:G:125:VAL:HG13	7:G:129:ALA:CB	2.01	0.91
7:G:63:VAL:CG2	7:G:64:ILE:H	1.84	0.91
7:G:94:GLN:O	7:G:97:LEU:HD23	1.70	0.91
12:L:137:LEU:C	12:L:137:LEU:HD23	1.91	0.91
4:D:100:TYR:CD1	4:D:134:LYS:HG3	2.06	0.91
4:D:83:PHE:HB3	4:D:84:GLY:O	1.71	0.91
6:F:132:ASN:O	6:F:133:TYR:CD1	2.23	0.91
1:A:105:ASN:OD1	1:A:118:PRO:HA	1.70	0.91
2:B:270:LEU:HD12	2:B:271:THR:N	1.86	0.91
2:B:574:ASP:HA	2:B:577:TYR:HB3	1.50	0.91
8:H:120:ILE:HG13	8:H:120:ILE:O	1.68	0.91
12:L:174:ASP:OD2	12:L:175:GLN:HG3	1.70	0.91
15:1:177:PRO:HG2	15:1:179:LYS:O	1.70	0.91
19:A:1126:CLA:H203	21:J:6012:BCR:C17	2.01	0.91
19:A:1141:CLA:C7	19:A:1141:CLA:C12	2.48	0.91
2:B:403:ASN:O	2:B:406:ASN:CB	2.19	0.91
2:B:672:GLN:HE22	3:C:79:LEU:HD12	1.35	0.91
4:D:133:ARG:H	4:D:136:GLN:NE2	1.66	0.91
2:B:110:LEU:HD12	2:B:111:GLY:CA	2.01	0.91
4:D:186:GLN:C	4:D:187:ASN:HD22	1.74	0.91
18:4:177:LEU:CD2	18:4:178:PRO:HD3	2.01	0.90
2:B:306:GLU:HG3	2:B:307:ALA:H	1.31	0.90
2:B:257:ILE:O	2:B:497:TRP:HE3	1.38	0.90
16:2:117:ALA:HB1	16:2:230:LEU:CG	2.02	0.90
3:C:62:PHE:CD2	5:E:80:GLU:HG3	2.07	0.90
3:C:52:LYS:HG3	3:C:52:LYS:O	1.71	0.90
17:3:150:TYR:H	17:3:152:ALA:HB2	0.75	0.90
19:H:1145:CLA:C1	19:H:1145:CLA:HMA2	2.01	0.90
8:H:56:GLU:CG	8:H:57:ASP:N	2.34	0.90
1:A:188:LYS:HD2	1:A:188:LYS:C	1.92	0.90
21:A:6002:BCR:C31	21:A:6002:BCR:HC8	2.01	0.90
8:H:58:LEU:HB3	8:H:61:THR:HB	1.48	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1:1014:CLA:HBC3	19:1:1014:CLA:CHD	2.01	0.90
2:B:560:ASP:OD1	2:B:561:GLY:N	2.04	0.90
14:R:33:UNK:C	14:R:36:UNK:CB	2.50	0.90
19:J:1308:CLA:CED	19:J:1308:CLA:CAD	2.50	0.90
5:E:111:ASN:HB3	5:E:116:SER:OG	1.71	0.90
13:N:155:GLU:HB3	13:N:157:LYS:CA	2.01	0.90
16:2:156:GLU:OE2	19:2:2013:CLA:CHD	2.18	0.90
4:D:137:CYS:O	4:D:140:LEU:O	1.89	0.90
15:1:65:ASP:CG	15:1:66:PRO:N	2.24	0.90
1:A:129:GLN:NE2	19:A:1107:CLA:NA	2.19	0.90
19:B:1210:CLA:H151	19:B:1225:CLA:HMD2	1.50	0.90
2:B:558:PRO:HG2	2:B:703:VAL:CG2	2.02	0.90
5:E:103:VAL:HG13	5:E:120:TYR:O	1.72	0.90
5:E:79:LYS:HA	5:E:84:TYR:CD1	2.06	0.90
3:C:5:VAL:HG21	3:C:65:VAL:HG23	1.52	0.90
19:3:3011:CLA:H122	19:3:3011:CLA:H172	1.52	0.90
11:K:128:GLY:N	11:K:129:ALA:HA	1.80	0.90
19:4:4014:CLA:HHD	19:4:4014:CLA:HBC2	1.51	0.90
1:A:733:VAL:O	1:A:733:VAL:HG12	1.72	0.90
19:B:1234:CLA:HBC3	19:B:1234:CLA:HMC1	1.53	0.90
21:B:6006:BCR:C8	21:B:6006:BCR:H331	2.00	0.90
12:L:74:THR:HG22	12:L:75:SER:OG	1.71	0.90
13:N:133:GLY:C	13:N:134:CYS:HG	1.74	0.90
13:N:165:ASN:C	13:N:167:PHE:H	1.75	0.90
6:F:130:PHE:N	6:F:133:TYR:CE1	2.37	0.90
17:3:206:PRO:HG2	17:3:208:PHE:CE2	2.06	0.90
2:B:75:GLU:HB2	2:B:132:ASN:ND2	1.83	0.90
17:3:173:PHE:C	17:3:173:PHE:CD1	2.40	0.90
16:2:137:TRP:O	16:2:139:THR:HG22	1.72	0.90
1:A:62:HIS:O	19:A:1128:CLA:HAA2	1.71	0.90
1:A:64:PHE:CD2	1:A:74:ILE:HG21	2.05	0.90
2:B:459:PHE:HB2	19:B:1235:CLA:CAD	2.01	0.90
8:H:58:LEU:HD12	8:H:61:THR:HA	1.52	0.90
8:H:58:LEU:CB	8:H:61:THR:HB	2.00	0.90
15:1:221:LEU:HD13	19:1:1003:CLA:HAC1	1.51	0.90
13:N:120:VAL:O	13:N:120:VAL:HG12	1.69	0.90
1:A:96:MET:HE3	19:A:1106:CLA:HED2	1.54	0.90
2:B:370:ALA:O	19:B:1224:CLA:HMA1	1.71	0.90
2:B:459:PHE:HE2	19:B:1235:CLA:C2D	1.42	0.90
2:B:457:PRO:HB3	2:B:517:PHE:HD1	1.37	0.90
21:3:6022:BCR:H393	21:3:6022:BCR:C23	1.95	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1141:CLA:H12	19:A:1141:CLA:CMA	2.01	0.90
1:A:126:ILE:HD11	19:A:1107:CLA:CMA	2.02	0.90
1:A:345:GLY:C	1:A:347:TYR:H	1.73	0.90
1:A:342:GLY:HA2	1:A:430:ASP:HB3	1.52	0.90
2:B:224:PRO:HB2	2:B:227:THR:CB	2.01	0.90
2:B:352:MET:CE	19:B:1225:CLA:OBD	2.20	0.90
2:B:229:GLN:O	7:G:63:VAL:HG21	1.70	0.90
12:L:131:SER:HB3	12:L:201:TYR:HE2	1.34	0.90
16:2:131:ILE:O	16:2:131:ILE:HG22	1.71	0.90
17:3:205:GLY:N	17:3:206:PRO:HD2	1.85	0.90
19:J:1308:CLA:CHD	19:J:1308:CLA:CBC	2.48	0.90
17:3:159:VAL:CG1	17:3:160:LEU:N	2.31	0.90
11:K:70:PHE:HB3	11:K:98:PRO:HB3	1.52	0.90
15:1:64:PHE:CD1	15:1:65:ASP:N	2.40	0.90
18:4:169:ASP:OD2	18:4:174:GLN:HB2	1.70	0.90
21:B:6020:BCR:H332	19:L:1502:CLA:C4B	2.00	0.90
17:3:109:ALA:HA	17:3:111:LEU:CD2	2.02	0.90
4:D:140:LEU:CD1	4:D:144:LEU:HG	2.00	0.90
7:G:69:GLY:O	7:G:72:LEU:HG	1.71	0.90
7:G:77:PHE:O	7:G:79:PHE:CB	2.19	0.90
15:1:69:LEU:C	15:1:73:PRO:HD3	1.93	0.89
18:4:146:PHE:CZ	19:4:4013:CLA:NC	2.39	0.89
2:B:120:VAL:CA	2:B:123:TRP:HD1	1.79	0.89
19:B:1222:CLA:CAD	19:B:1234:CLA:HBB1	2.03	0.89
2:B:655:LEU:HD21	19:B:1239:CLA:HBB1	1.53	0.89
2:B:312:GLY:HA3	2:B:315:LEU:CB	2.03	0.89
2:B:269:TRP:HB2	2:B:497:TRP:HH2	1.38	0.89
2:B:545:LYS:HD3	2:B:546:LEU:N	1.87	0.89
2:B:558:PRO:HG2	2:B:703:VAL:HG22	1.53	0.89
6:F:170:ILE:HG21	21:F:6014:BCR:H371	1.52	0.89
13:N:143:VAL:HB	13:N:144:PRO:CD	1.99	0.89
16:2:184:PRO:HD3	16:2:187:LYS:CA	2.02	0.89
1:A:71:LEU:CG	1:A:72:GLU:H	1.84	0.89
22:4:7034:LMU:C11	22:4:7052:LMU:C3'	2.47	0.89
18:4:146:PHE:CE2	19:4:4013:CLA:C2C	2.53	0.89
1:A:281:LEU:HD21	19:A:1115:CLA:CMA	1.85	0.89
2:B:232:LEU:HD13	2:B:235:GLN:HG3	1.50	0.89
18:4:96:LEU:CD1	18:4:100:ARG:CZ	2.50	0.89
18:4:175:TYR:O	18:4:194:PHE:CD1	2.25	0.89
1:A:331:LEU:CD2	1:A:343:HIS:O	2.21	0.89
1:A:499:ALA:CB	19:A:1133:CLA:HED1	2.02	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:6011:BCR:H23C	21:A:6011:BCR:C39	2.01	0.89
1:A:740:LEU:HD21	19:A:1140:CLA:CMA	2.01	0.89
19:A:9022:CLA:H112	21:B:6017:BCR:H19C	1.53	0.89
11:K:48:PHE:O	11:K:52:PRO:HD3	1.72	0.89
16:2:119:GLY:O	16:2:123:PRO:CD	2.20	0.89
4:D:82:ILE:HG13	4:D:82:ILE:O	1.69	0.89
15:1:170:PRO:HG2	15:1:171:LEU:CA	2.02	0.89
12:L:171:LYS:C	12:L:173:PRO:HD3	1.92	0.89
18:4:110:LEU:O	18:4:113:GLU:HG3	1.71	0.89
2:B:244:PHE:CD2	2:B:244:PHE:C	2.46	0.89
19:A:1237:CLA:H201	12:L:110:LEU:HD21	1.52	0.89
12:L:143:LEU:HA	12:L:146:THR:H	1.36	0.89
15:1:134:LEU:HA	15:1:137:ILE:CD1	2.01	0.89
4:D:140:LEU:HD12	4:D:141:GLY:CA	2.02	0.89
6:F:221:LEU:HD23	6:F:222:LEU:HD21	1.52	0.89
13:N:169:LYS:HB3	13:N:170:TRP:CD1	2.06	0.89
1:A:381:PRO:HB2	19:A:1117:CLA:HAA2	1.54	0.89
1:A:78:VAL:O	1:A:82:HIS:CD2	2.26	0.89
1:A:83:PHE:CE1	19:A:1111:CLA:HED1	2.08	0.89
5:E:79:LYS:CA	5:E:84:TYR:CE1	2.54	0.89
13:N:130:ASN:HB2	13:N:139:LYS:CD	2.02	0.89
1:A:250:LEU:HB2	17:3:136:TRP:HH2	1.36	0.89
16:2:237:PHE:HE1	16:2:241:TYR:CE1	1.90	0.89
19:H:1145:CLA:H142	19:H:1145:CLA:H101	1.50	0.89
18:4:173:LYS:HD2	18:4:201:LYS:HE3	1.52	0.89
19:A:1134:CLA:C3A	19:A:1141:CLA:HBB2	2.01	0.89
1:A:163:GLN:HG3	1:A:164:LEU:N	1.86	0.89
1:A:547:PHE:O	1:A:551:VAL:HG13	1.73	0.89
19:B:1211:CLA:HMA1	21:B:6006:BCR:H313	1.53	0.89
16:2:117:ALA:CB	16:2:230:LEU:CG	2.49	0.89
13:N:139:LYS:HB3	13:N:142:LYS:CD	1.99	0.89
16:2:112:TRP:HZ2	16:2:167:ARG:NH2	1.30	0.89
11:K:127:ILE:HG23	11:K:130:LEU:CG	1.95	0.89
11:K:118:VAL:O	11:K:121:VAL:CG2	2.20	0.89
2:B:140:ILE:CG1	2:B:141:PHE:N	2.34	0.89
7:G:145:THR:HG23	7:G:146:SER:N	1.87	0.89
15:1:177:PRO:HD3	15:1:180:LEU:CG	1.92	0.89
5:E:78:ARG:HH22	5:E:125:ILE:CG2	1.86	0.89
13:N:130:ASN:O	13:N:132:THR:HG23	1.72	0.89
13:N:142:LYS:O	13:N:145:PHE:N	2.06	0.89
15:1:189:LYS:HB2	19:1:1007:CLA:HMC1	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3:197:SER:HG	17:3:205:GLY:HA3	1.30	0.89
1:A:715:LYS:HD2	6:F:230:ASN:HD21	0.76	0.89
1:A:426:THR:CG2	1:A:428:TYR:CE2	2.55	0.89
1:A:24:ARG:CD	1:A:24:ARG:N	2.33	0.89
2:B:391:PRO:HB3	2:B:538:ALA:HA	1.51	0.89
17:3:96:ARG:HA	17:3:99:ALA:N	1.87	0.89
1:A:423:ASP:HB3	1:A:424:PRO:CD	2.02	0.89
15:1:171:LEU:CA	15:1:173:TYR:CE2	2.55	0.89
1:A:316:MET:HB3	1:A:317:TYR:CB	2.02	0.89
8:H:57:ASP:O	8:H:59:GLY:N	2.06	0.89
1:A:103:PHE:HE1	19:A:1105:CLA:O1D	1.55	0.89
2:B:244:PHE:C	2:B:244:PHE:HD2	1.76	0.89
5:E:83:TRP:N	5:E:83:TRP:HE3	1.71	0.89
11:K:49:ILE:O	11:K:52:PRO:HD2	1.73	0.89
1:A:244:LEU:HD12	1:A:247:GLU:CD	1.93	0.89
15:1:133:THR:O	15:1:136:THR:HG23	1.73	0.89
4:D:123:ARG:HH22	22:D:7050:LMU:C4B	1.85	0.89
5:E:70:ARG:HG2	5:E:71:GLY:N	1.88	0.89
15:1:97:ILE:C	15:1:97:ILE:HD13	1.94	0.89
18:4:220:GLN:CG	19:4:1306:CLA:HAC2	2.03	0.89
18:4:202:GLU:O	18:4:205:ILE:HG12	1.72	0.89
1:A:204:ASN:O	1:A:205:HIS:HB2	1.73	0.89
19:A:1112:CLA:HMB2	21:A:6002:BCR:H382	1.55	0.89
2:B:459:PHE:CD2	19:B:1235:CLA:C4D	2.54	0.89
2:B:535:VAL:O	2:B:539:LEU:HD23	1.72	0.89
19:B:1235:CLA:C15	21:F:6016:BCR:H312	2.03	0.89
12:L:92:ALA:N	12:L:98:ARG:HH12	1.71	0.89
13:N:139:LYS:O	13:N:142:LYS:HD2	1.72	0.89
16:2:148:ASP:CG	16:2:152:LEU:HB3	1.92	0.89
4:D:203:THR:HG22	4:D:205:LYS:H	1.37	0.89
4:D:73:GLU:O	4:D:76:PRO:HD2	1.73	0.89
1:A:207:LEU:CD2	19:A:1119:CLA:HBB2	2.03	0.88
1:A:127:VAL:HG23	1:A:128:GLY:H	1.34	0.88
1:A:502:THR:CG2	1:A:504:ALA:H	1.86	0.88
1:A:599:PHE:CE2	1:A:731:ARG:HB3	2.06	0.88
19:B:1202:CLA:C2	19:B:1202:CLA:O1A	2.20	0.88
2:B:232:LEU:CD1	2:B:235:GLN:CG	2.50	0.88
2:B:521:HIS:HE1	19:B:1235:CLA:NA	1.69	0.88
7:G:98:THR:OG1	7:G:101:GLU:HB2	1.71	0.88
11:K:52:PRO:CD	11:K:53:THR:H	1.81	0.88
13:N:146:LEU:CG	17:3:142:ILE:O	2.21	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3:96:ARG:CA	17:3:99:ALA:CB	2.50	0.88
18:4:90:TRP:CG	18:4:91:PHE:N	2.36	0.88
17:3:157:LEU:O	17:3:160:LEU:N	2.06	0.88
1:A:71:LEU:CG	1:A:72:GLU:N	2.36	0.88
19:A:1123:CLA:OBD	19:A:1123:CLA:H92	1.72	0.88
2:B:319:HIS:HE1	2:B:322:LEU:CD1	1.85	0.88
15:1:142:PHE:HA	15:1:145:ILE:HD11	1.54	0.88
13:N:114:PHE:HB3	13:N:117:ALA:CB	2.02	0.88
1:A:316:MET:CB	1:A:317:TYR:CD1	2.57	0.88
16:2:211:PRO:HD2	16:2:212:GLN:H	1.36	0.88
1:A:453:LEU:HB3	1:A:547:PHE:HB2	1.55	0.88
19:A:1122:CLA:CBB	21:A:6007:BCR:C35	2.51	0.88
19:B:1235:CLA:HBB2	19:B:1235:CLA:H93	0.92	0.88
2:B:382:ILE:HG22	2:B:383:MET:N	1.89	0.88
7:G:72:LEU:HD23	7:G:124:ILE:HD11	1.34	0.88
17:3:96:ARG:CA	17:3:99:ALA:HB3	2.04	0.88
17:3:108:PHE:HB3	19:3:3013:CLA:H42	1.54	0.88
5:E:96:ASP:HB3	5:E:98:ASN:N	1.88	0.88
4:D:146:SER:O	4:D:147:LYS:HG3	1.72	0.88
7:G:141:ILE:O	7:G:142:LEU:HB2	1.71	0.88
15:1:88:ARG:O	15:1:92:LEU:CB	2.20	0.88
19:A:1138:CLA:H61	21:F:6014:BCR:H12C	1.52	0.88
19:A:1131:CLA:H161	21:L:6019:BCR:H361	1.53	0.88
14:R:39:UNK:HA	14:R:42:UNK:CB	2.04	0.88
16:2:184:PRO:HG3	16:2:187:LYS:N	1.89	0.88
11:K:84:LEU:CG	11:K:85:LYS:HG2	2.03	0.88
18:4:198:LEU:HG	18:4:199:GLU:N	1.88	0.88
19:B:1220:CLA:CBC	19:B:1220:CLA:HMC1	2.03	0.88
17:3:93:ILE:CG1	17:3:95:PRO:O	2.20	0.88
16:2:182:ILE:HB	16:2:187:LYS:CG	2.02	0.88
19:K:1142:CLA:HMD1	19:K:1143:CLA:NA	1.87	0.88
1:A:426:THR:HG22	1:A:428:TYR:HE2	1.32	0.88
1:A:23:ASP:CG	1:A:33:GLN:HG2	1.92	0.88
17:3:159:VAL:O	17:3:162:MET:N	2.05	0.88
1:A:289:PRO:O	1:A:290:LEU:HB3	1.73	0.88
2:B:222:LEU:HD12	2:B:223:GLY:O	1.74	0.88
2:B:268:LEU:HD22	2:B:273:VAL:HG12	1.54	0.88
21:B:6010:BCR:H23C	21:B:6010:BCR:H382	1.53	0.88
11:K:56:ILE:HA	11:K:59:THR:CG2	2.02	0.88
3:C:65:VAL:O	3:C:66:ARG:HB3	1.71	0.88
17:3:135:ALA:CB	17:3:139:THR:OG1	2.20	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:95:GLN:HE21	4:D:96:VAL:CA	1.86	0.88
16:2:254:LEU:C	16:2:254:LEU:HD22	1.89	0.88
2:B:398:TYR:O	4:D:197:PRO:CG	2.20	0.88
18:4:143:VAL:O	18:4:147:ILE:HD12	1.73	0.88
2:B:87:ILE:HA	2:B:115:ASN:CA	2.04	0.88
2:B:293:THR:HG21	19:B:1209:CLA:CMA	2.04	0.88
19:B:1214:CLA:CBD	19:B:1223:CLA:HBB2	2.04	0.88
20:B:5002:PQN:C16	21:B:6017:BCR:H333	2.00	0.88
2:B:693:TRP:CD1	19:B:1238:CLA:C2D	2.56	0.88
6:F:200:VAL:HG11	10:J:7:TYR:HB2	1.54	0.88
12:L:102:VAL:HA	19:L:1502:CLA:CED	2.04	0.88
5:E:129:GLU:C	5:E:129:GLU:CD	2.30	0.88
3:C:62:PHE:CZ	5:E:80:GLU:OE2	2.24	0.88
17:3:238:ILE:HD11	19:3:3003:CLA:HMC2	1.55	0.88
7:G:149:TYR:CA	7:G:150:ASP:OD1	2.20	0.88
12:L:51:LYS:HA	12:L:51:LYS:HE2	1.54	0.88
21:A:6011:BCR:C8	21:A:6011:BCR:H311	2.04	0.88
19:B:1228:CLA:H12	19:B:1228:CLA:HMA2	1.54	0.88
19:3:2009:CLA:CGA	19:3:2009:CLA:CBD	2.49	0.88
17:3:122:LEU:HD21	19:3:3006:CLA:C3D	2.02	0.88
19:2:4009:CLA:H152	19:2:4009:CLA:H192	1.54	0.88
3:C:31:TRP:HD1	3:C:32:GLY:N	1.72	0.88
19:A:9022:CLA:HBB2	19:A:9023:CLA:CHB	2.03	0.88
2:B:442:VAL:HG21	19:B:1230:CLA:HAC2	1.55	0.88
2:B:299:HIS:CE1	19:B:1219:CLA:HMD1	2.08	0.88
7:G:72:LEU:HD12	7:G:73:PHE:CE2	2.09	0.88
5:E:107:PHE:HE2	5:E:109:LYS:HG3	1.19	0.88
3:C:65:VAL:HG22	3:C:66:ARG:N	1.84	0.88
8:H:119:ASP:OD2	8:H:121:LEU:HG	1.72	0.88
17:3:207:PHE:CD1	17:3:207:PHE:C	2.45	0.88
16:2:195:TYR:CD2	16:2:198:GLY:HA3	2.08	0.88
16:2:261:THR:HG22	16:2:262:ILE:H	1.38	0.88
18:4:103:MET:HE3	18:4:208:GLY:N	1.71	0.88
2:B:493:TRP:HH2	19:B:1214:CLA:H122	1.36	0.88
2:B:469:LYS:HG3	2:B:470:THR:CG2	2.03	0.88
2:B:470:THR:H	2:B:501:ILE:HB	1.29	0.88
21:B:6020:BCR:H331	21:B:6020:BCR:HC8	1.55	0.88
5:E:81:SER:OG	5:E:120:TYR:OH	1.64	0.88
1:A:252:ARG:CD	1:A:252:ARG:H	1.82	0.88
19:H:1145:CLA:H143	19:H:1145:CLA:H193	1.55	0.88
1:A:154:ARG:HE	1:A:384:TYR:HE1	0.92	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:GLU:HA	1:A:76:ARG:HD2	1.54	0.87
19:B:1228:CLA:HHD	19:B:1228:CLA:HBC2	1.56	0.87
2:B:693:TRP:HD1	19:B:1238:CLA:C2D	1.87	0.87
2:B:294:ASN:ND2	7:G:94:GLN:HA	1.88	0.87
16:2:184:PRO:CD	16:2:187:LYS:CG	2.52	0.87
1:A:71:LEU:HD12	1:A:72:GLU:N	1.87	0.87
19:A:1133:CLA:HBC2	19:A:1133:CLA:HMC1	1.55	0.87
19:A:1136:CLA:H192	19:L:1130:CLA:HBB1	1.54	0.87
12:L:142:SER:O	12:L:143:LEU:CG	2.23	0.87
12:L:141:LEU:HD13	12:L:145:LEU:HD12	1.57	0.87
16:2:120:ILE:O	16:2:123:PRO:HD2	1.73	0.87
4:D:100:TYR:CE1	4:D:134:LYS:CG	2.57	0.87
12:L:209:LEU:HD12	12:L:210:PRO:HD2	0.89	0.87
1:A:566:SER:OG	2:B:673:GLU:OE2	1.90	0.87
19:3:1147:CLA:HMC1	19:3:1147:CLA:HBC3	0.87	0.87
18:4:172:PHE:HB3	18:4:194:PHE:CZ	2.09	0.87
1:A:368:LEU:CD2	19:A:1117:CLA:H92	2.03	0.87
1:A:207:LEU:HA	1:A:211:LEU:HG	1.55	0.87
21:A:6002:BCR:C8	21:A:6002:BCR:H311	2.01	0.87
1:A:668:TYR:CG	2:B:445:ALA:CB	2.58	0.87
3:C:43:PRO:HA	4:D:182:GLN:HB3	1.56	0.87
3:C:52:LYS:HZ1	3:C:64:SER:HB2	1.39	0.87
3:C:44:ARG:N	4:D:182:GLN:CD	2.27	0.87
19:L:1148:CLA:C2	19:L:1148:CLA:CED	2.31	0.87
17:3:197:SER:CB	17:3:206:PRO:CD	2.52	0.87
2:B:475:ASP:OD1	2:B:480:SER:O	1.92	0.87
15:1:85:ILE:HA	15:1:88:ARG:CD	2.03	0.87
1:A:150:PHE:H	1:A:153:TRP:HB2	1.39	0.87
19:A:9012:CLA:HMB3	19:B:9010:CLA:H18	1.55	0.87
2:B:319:HIS:HE1	2:B:322:LEU:HD12	1.32	0.87
16:2:103:VAL:O	16:2:105:ALA:N	2.08	0.87
4:D:100:TYR:CE1	4:D:134:LYS:HE3	2.09	0.87
19:3:1147:CLA:HMC1	19:3:1147:CLA:HBC2	1.55	0.87
19:A:1124:CLA:C7	19:A:1125:CLA:CED	2.51	0.87
19:A:1140:CLA:H141	21:A:6011:BCR:HC21	1.55	0.87
1:A:160:SER:O	1:A:163:GLN:HG2	1.74	0.87
1:A:85:GLN:O	1:A:87:SER:O	1.91	0.87
1:A:92:TRP:O	1:A:93:LEU:CD2	2.23	0.87
2:B:303:TYR:CA	2:B:306:GLU:HB2	2.03	0.87
2:B:312:GLY:HA3	2:B:315:LEU:HB2	1.55	0.87
2:B:697:PRO:O	3:C:79:LEU:HD13	1.73	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:L:1503:CLA:HBC3	19:L:1503:CLA:CHD	2.05	0.87
13:N:155:GLU:CA	13:N:157:LYS:CE	2.31	0.87
15:1:141:GLU:O	15:1:145:ILE:HG13	1.74	0.87
17:3:96:ARG:HH11	17:3:96:ARG:HB2	1.36	0.87
4:D:80:SER:HG	4:D:126:PRO:HD2	1.07	0.87
1:A:71:LEU:HG	1:A:72:GLU:N	1.86	0.87
4:D:150:ILE:O	4:D:151:LYS:HG2	1.73	0.87
1:A:281:LEU:CG	19:A:1115:CLA:CED	2.53	0.87
1:A:470:LEU:CD1	2:B:95:HIS:HB3	2.03	0.87
19:B:1214:CLA:H52	19:B:1223:CLA:HMB1	1.53	0.87
21:B:6020:BCR:H331	21:B:6020:BCR:C8	2.03	0.87
1:A:261:SER:O	1:A:262:PHE:CD1	2.28	0.87
17:3:201:ALA:CB	17:3:202:TYR:CD2	2.58	0.87
5:E:96:ASP:OD2	5:E:98:ASN:CG	2.11	0.87
1:A:316:MET:CG	1:A:317:TYR:CD1	2.58	0.87
22:4:7053:LMU:H5'	22:4:7053:LMU:H11	1.56	0.87
1:A:723:ARG:H	19:A:1139:CLA:HBB1	1.37	0.87
19:A:1237:CLA:H141	12:L:141:LEU:HD21	1.56	0.87
1:A:89:ILE:O	1:A:92:TRP:HB3	1.75	0.87
12:L:143:LEU:HD22	12:L:146:THR:CG2	2.04	0.87
10:J:5:LYS:HG3	16:2:178:ASN:OD1	1.75	0.87
15:1:189:LYS:HE2	15:1:189:LYS:HA	1.56	0.87
11:K:127:ILE:CG2	11:K:130:LEU:HG	2.04	0.87
22:H:7043:LMU:H102	22:H:7043:LMU:H62	1.55	0.87
2:B:622:ASP:CB	2:B:626:LEU:HD12	2.03	0.87
6:F:200:VAL:CG1	10:J:7:TYR:H	1.86	0.87
12:L:70:GLU:HG2	12:L:74:THR:HG21	1.57	0.87
12:L:153:PHE:O	12:L:179:ALA:N	2.08	0.87
17:3:205:GLY:N	17:3:206:PRO:CD	2.34	0.87
2:B:482:ASN:OD1	2:B:485:ALA:HB2	1.75	0.87
1:A:308:ILE:HD12	19:A:1115:CLA:CHC	2.03	0.87
19:A:1125:CLA:CAB	19:A:1133:CLA:HMA1	2.02	0.87
1:A:491:TRP:HE1	19:A:1135:CLA:C1	1.87	0.87
1:A:246:HIS:O	1:A:248:PHE:HD2	1.57	0.87
19:A:1134:CLA:HBC1	21:A:6008:BCR:HC31	1.54	0.87
1:A:659:ALA:O	1:A:662:SER:OG	1.93	0.87
2:B:50:HIS:CD2	19:B:1202:CLA:HAA2	2.09	0.87
8:H:109:LEU:CD2	19:H:1207:CLA:H52	2.05	0.87
13:N:114:PHE:CD1	13:N:117:ALA:CB	2.53	0.87
22:4:7053:LMU:H1B	22:4:7053:LMU:H6E	1.54	0.87
15:1:193:LEU:HD23	15:1:193:LEU:C	1.96	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1214:CLA:CAD	19:B:1223:CLA:HBB2	2.05	0.86
22:H:7032:LMU:H1B	22:H:7032:LMU:H31	1.56	0.86
22:H:7032:LMU:H3'	22:H:7032:LMU:O5B	1.75	0.86
1:A:387:THR:HG22	1:A:523:VAL:HG11	1.54	0.86
1:A:40:PHE:O	1:A:41:SER:O	1.93	0.86
1:A:502:THR:HG22	1:A:504:ALA:N	1.90	0.86
2:B:469:LYS:HE3	2:B:470:THR:HG23	1.56	0.86
3:C:62:PHE:CZ	5:E:80:GLU:OE1	2.28	0.86
5:E:89:SER:HB2	5:E:106:ARG:NH2	1.90	0.86
4:D:100:TYR:CE1	4:D:134:LYS:CE	2.57	0.86
16:2:184:PRO:CG	16:2:187:LYS:HD2	2.04	0.86
4:D:103:THR:HG22	4:D:128:LEU:CG	2.05	0.86
22:D:7050:LMU:H4'	22:D:7050:LMU:O2B	1.73	0.86
2:B:393:PHE:HD2	2:B:397:ASP:OD1	1.59	0.86
19:4:1304:CLA:CAA	19:4:1304:CLA:HED3	1.98	0.86
1:A:316:MET:HB3	1:A:317:TYR:CD1	2.10	0.86
15:1:177:PRO:N	15:1:180:LEU:HG	1.89	0.86
1:A:443:ILE:HD11	1:A:557:LEU:HD23	1.57	0.86
15:1:190:ASN:ND2	19:1:1002:CLA:NA	2.23	0.86
17:3:202:TYR:HB3	17:3:203:PRO:CD	2.04	0.86
22:4:7034:LMU:C9	22:4:7052:LMU:C2'	2.42	0.86
19:1:1001:CLA:CMC	19:1:1001:CLA:HBC3	2.03	0.86
15:1:64:PHE:CG	15:1:65:ASP:N	2.44	0.86
15:1:66:PRO:HD2	15:1:67:LEU:N	1.91	0.86
19:A:1111:CLA:HBA1	19:A:1123:CLA:H41	1.55	0.86
1:A:331:LEU:HD11	1:A:346:LEU:CB	2.03	0.86
2:B:353:TYR:CG	2:B:594:TRP:CZ3	2.63	0.86
19:2:2001:CLA:CGA	19:2:2001:CLA:H42	2.04	0.86
3:C:14:CYS:SG	3:C:18:VAL:O	2.32	0.86
19:2:2013:CLA:HBC3	19:2:2013:CLA:HMC1	1.57	0.86
17:3:151:TRP:CD1	17:3:152:ALA:N	2.41	0.86
4:D:82:ILE:HG23	4:D:121:ILE:O	1.74	0.86
1:A:316:MET:CB	1:A:317:TYR:HB2	2.03	0.86
2:B:254:ILE:HB	2:B:255:LEU:HD23	1.56	0.86
3:C:7:ILE:O	3:C:8:TYR:O	1.92	0.86
16:2:182:ILE:C	16:2:187:LYS:CG	2.44	0.86
2:B:247:THR:CG2	2:B:248:GLN:N	2.33	0.86
2:B:382:ILE:O	2:B:384:THR:N	2.08	0.86
8:H:61:THR:CB	8:H:62:THR:HG23	2.05	0.86
17:3:103:VAL:O	17:3:107:ARG:HB2	1.74	0.86
17:3:150:TYR:O	17:3:152:ALA:HB3	1.73	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:96:LYS:O	6:F:100:LYS:HB2	1.74	0.86
2:B:140:ILE:HG13	2:B:141:PHE:H	1.36	0.86
2:B:58:PHE:CD2	2:B:145:LEU:CD2	2.57	0.86
18:4:169:ASP:CG	18:4:174:GLN:HB2	1.95	0.86
1:A:402:ILE:HG13	19:A:1127:CLA:HBB2	1.56	0.86
19:B:1222:CLA:CBB	19:B:1236:CLA:HMB3	2.05	0.86
2:B:310:PRO:CB	2:B:311:PRO:CD	2.54	0.86
19:A:1138:CLA:HMD3	21:F:6014:BCR:HC41	1.57	0.86
7:G:84:ARG:HG3	7:G:85:GLU:CA	2.05	0.86
8:H:99:LYS:O	8:H:100:PHE:C	2.14	0.86
12:L:150:ILE:C	12:L:150:ILE:HD12	1.95	0.86
2:B:561:GLY:HA3	3:C:52:LYS:HG2	1.56	0.86
13:N:114:PHE:CG	13:N:117:ALA:CB	2.59	0.86
16:2:237:PHE:CE1	16:2:241:TYR:CZ	2.64	0.86
11:K:97:ASP:CB	11:K:101:PHE:CE2	2.50	0.86
18:4:243:THR:HG23	18:4:244:ILE:O	1.74	0.86
18:4:207:ASN:ND2	19:4:4002:CLA:NA	2.23	0.86
1:A:103:PHE:N	1:A:103:PHE:HD2	1.71	0.86
1:A:401:TRP:CD1	19:A:1126:CLA:HHC	2.11	0.86
1:A:240:LYS:N	1:A:243:PRO:HD2	1.89	0.86
1:A:248:PHE:HD2	1:A:248:PHE:N	1.73	0.86
1:A:308:ILE:HD11	19:A:1115:CLA:CBB	2.04	0.86
1:A:64:PHE:CE2	1:A:74:ILE:HG23	2.09	0.86
2:B:444:LEU:CD2	2:B:452:GLN:HE22	1.87	0.86
19:B:1223:CLA:H122	21:B:6010:BCR:C14	2.05	0.86
7:G:131:GLY:HA2	7:G:136:VAL:CG2	2.06	0.86
19:A:1105:CLA:C2B	21:J:6012:BCR:H331	2.05	0.86
16:2:148:ASP:HB3	16:2:152:LEU:CG	2.04	0.86
6:F:89:LYS:HG2	6:F:90:GLN:N	1.90	0.86
1:A:23:ASP:HB3	1:A:33:GLN:CD	1.95	0.86
10:J:31:ARG:NH2	19:J:1311:CLA:C4B	2.39	0.86
1:A:267:THR:O	1:A:269:PHE:HD2	1.56	0.86
1:A:207:LEU:HD11	1:A:314:GLY:CA	2.05	0.86
19:B:1226:CLA:HMC1	19:B:1226:CLA:HBC2	1.56	0.86
2:B:421:HIS:NE2	19:B:1228:CLA:ND	2.23	0.86
2:B:123:TRP:CB	2:B:126:THR:HG21	2.06	0.86
2:B:304:ILE:O	2:B:308:HIS:HB2	1.76	0.86
21:B:6020:BCR:C33	19:L:1502:CLA:C3B	2.54	0.86
15:1:137:ILE:HG22	19:1:1013:CLA:HBB2	1.58	0.86
17:3:151:TRP:HD1	17:3:152:ALA:H	1.21	0.86
18:4:177:LEU:HD13	18:4:178:PRO:CD	2.05	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:LEU:O	1:A:331:LEU:HD23	1.75	0.86
2:B:131:THR:CB	2:B:134:ASP:HB2	2.06	0.86
15:1:158:PRO:HG2	15:1:159:GLU:H	1.38	0.85
19:A:1137:CLA:HMC1	19:A:1137:CLA:HBC3	1.55	0.85
1:A:120:ALA:N	1:A:145:ILE:HD11	1.89	0.85
1:A:472:ARG:HH12	12:L:120:LEU:HD22	1.37	0.85
12:L:85:ASN:O	12:L:92:ALA:HB2	1.76	0.85
5:E:78:ARG:CZ	5:E:125:ILE:HG21	2.05	0.85
16:2:186:ASN:OD1	16:2:188:LEU:CD1	2.19	0.85
12:L:104:LEU:HD21	12:L:199:TRP:HZ2	1.41	0.85
18:4:122:ASN:O	18:4:123:VAL:HG12	1.76	0.85
1:A:195:TRP:CZ2	19:A:1108:CLA:HMA1	2.10	0.85
1:A:190:ALA:HB1	1:A:191:PRO:HD3	1.57	0.85
19:A:1131:CLA:H52	21:B:6017:BCR:H343	1.58	0.85
12:L:78:LEU:HD12	12:L:79:ILE:N	1.91	0.85
4:D:159:PRO:HD2	4:D:159:PRO:O	1.75	0.85
16:2:182:ILE:CB	16:2:187:LYS:CG	2.54	0.85
4:D:140:LEU:HD12	4:D:141:GLY:H	1.06	0.85
15:1:150:HIS:CD2	15:1:151:GLN:NE2	2.43	0.85
16:2:139:THR:HG23	16:2:140:ALA:N	1.85	0.85
22:R:7021:LMU:H22	22:R:7021:LMU:H62	1.57	0.85
18:4:103:MET:HE2	18:4:208:GLY:HA2	0.87	0.85
19:4:1306:CLA:HMC1	19:4:1306:CLA:CBC	2.04	0.85
18:4:172:PHE:HD1	18:4:173:LYS:O	1.57	0.85
19:B:1239:CLA:HBC2	19:B:1239:CLA:HMC1	1.56	0.85
19:2:2007:CLA:HBC1	19:3:2009:CLA:CED	1.81	0.85
11:K:115:ILE:CA	11:K:118:VAL:HG22	2.05	0.85
17:3:154:ASN:C	17:3:155:TYR:CD2	2.49	0.85
15:1:67:LEU:HD12	15:1:68:GLY:CA	2.06	0.85
18:4:167:ASN:CG	19:4:4014:CLA:C2	2.45	0.85
1:A:207:LEU:HD11	1:A:314:GLY:N	1.91	0.85
2:B:329:SER:O	2:B:330:ILE:CG2	2.23	0.85
2:B:596:TRP:CZ3	2:B:612:SER:O	2.30	0.85
13:N:155:GLU:CB	13:N:157:LYS:HE2	2.06	0.85
4:D:139:ALA:O	4:D:142:THR:HG22	1.76	0.85
6:F:124:GLU:HG3	6:F:128:LYS:CD	2.06	0.85
22:E:7048:LMU:C7	22:E:7048:LMU:H111	2.04	0.85
21:1:6023:BCR:C31	21:1:6023:BCR:C8	2.54	0.85
1:A:64:PHE:CZ	1:A:77:LYS:HE2	2.11	0.85
19:B:1203:CLA:HHB	19:B:1226:CLA:HBB2	1.57	0.85
2:B:551:LYS:HG2	2:B:552:ASP:N	1.91	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:L:1503:CLA:HAA1	19:L:1503:CLA:CGD	2.05	0.85
13:N:142:LYS:CE	13:N:142:LYS:HA	2.00	0.85
17:3:101:GLY:HA2	17:3:104:ILE:HD12	1.57	0.85
16:2:168:TRP:HD1	16:2:171:ILE:HG21	0.91	0.85
10:J:5:LYS:HD2	16:2:178:ASN:HA	1.56	0.85
16:2:251:PHE:O	16:2:251:PHE:CD1	2.29	0.85
2:B:471:THR:O	2:B:472:TYR:CD1	2.29	0.85
2:B:672:GLN:NE2	3:C:79:LEU:HD12	1.91	0.85
19:I:1204:CLA:H142	21:I:6018:BCR:H392	1.59	0.85
12:L:79:ILE:CG2	12:L:80:ALA:N	2.39	0.85
4:D:156:ARG:CZ	4:D:158:PHE:CE1	2.35	0.85
4:D:157:VAL:HG12	4:D:158:PHE:O	1.77	0.85
16:2:184:PRO:HB3	16:2:187:LYS:CD	2.06	0.85
15:1:206:SER:O	15:1:209:PRO:CG	2.25	0.85
1:A:308:ILE:CD1	19:A:1115:CLA:CAB	2.51	0.85
1:A:308:ILE:HD11	19:A:1115:CLA:C3B	2.06	0.85
1:A:723:ARG:HH11	1:A:723:ARG:CG	1.89	0.85
2:B:200:PRO:O	2:B:204:GLY:HA3	1.77	0.85
2:B:25:ILE:HG21	21:L:6019:BCR:C29	2.06	0.85
6:F:150:VAL:HG13	6:F:150:VAL:O	1.75	0.85
11:K:56:ILE:HG23	11:K:59:THR:HG23	1.58	0.85
12:L:125:ILE:HG21	12:L:128:GLN:OE1	1.77	0.85
13:N:130:ASN:C	13:N:132:THR:CG2	2.43	0.85
13:N:139:LYS:CD	13:N:142:LYS:HZ3	1.89	0.85
2:B:600:THR:O	2:B:604:GLY:CA	2.25	0.85
22:A:7023:LMU:H21	22:A:7023:LMU:H91	1.59	0.85
1:A:167:THR:CG2	19:A:1112:CLA:HAA2	2.04	0.85
1:A:558:LYS:NZ	2:B:674:LEU:HB2	1.92	0.85
2:B:351:HIS:HB3	19:B:1214:CLA:HED1	1.58	0.85
19:B:1220:CLA:C4A	19:B:1220:CLA:C4	2.55	0.85
7:G:77:PHE:O	7:G:79:PHE:HB2	1.76	0.85
7:G:84:ARG:HE	7:G:89:LYS:CE	1.87	0.85
11:K:63:LEU:HD22	11:K:63:LEU:N	1.89	0.85
13:N:132:THR:HB	13:N:139:LYS:HZ2	1.35	0.85
22:A:7016:LMU:C2	22:A:7016:LMU:H81	2.04	0.85
19:J:1308:CLA:HBC3	19:J:1308:CLA:HHD	1.56	0.85
2:B:58:PHE:HE2	2:B:145:LEU:HD21	1.42	0.85
1:A:71:LEU:CD1	1:A:72:GLU:N	2.39	0.85
1:A:259:TYR:HB3	1:A:260:PRO:CD	2.07	0.85
2:B:44:GLN:CD	2:B:163:PRO:HB2	1.97	0.85
15:1:92:LEU:HA	15:1:95:PRO:HG2	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:173:LYS:HB2	18:4:194:PHE:HD2	1.40	0.85
19:A:1134:CLA:HBC2	21:A:6008:BCR:HC31	1.58	0.85
1:A:157:GLY:C	1:A:158:ILE:HG23	1.96	0.85
1:A:600:LEU:HD21	2:B:665:ILE:O	1.76	0.85
13:N:133:GLY:HA3	13:N:134:CYS:O	1.77	0.85
3:C:44:ARG:CB	4:D:182:GLN:CD	2.45	0.85
4:D:171:GLY:O	4:D:172:VAL:HG23	1.77	0.85
1:A:249:ILE:H	17:3:137:PHE:HZ	1.24	0.85
6:F:185:ILE:C	6:F:186:ARG:HG2	1.97	0.85
11:K:70:PHE:CD1	11:K:70:PHE:C	2.46	0.85
1:A:661:ALA:O	1:A:664:VAL:HG22	1.77	0.85
2:B:98:GLN:O	2:B:101:VAL:N	2.08	0.85
12:L:71:THR:O	12:L:74:THR:HB	1.76	0.85
12:L:94:SER:O	12:L:96:LEU:HD23	1.76	0.85
12:L:92:ALA:H	12:L:98:ARG:NH2	1.72	0.85
4:D:103:THR:HG21	4:D:128:LEU:HD12	1.55	0.85
19:2:2014:CLA:H102	19:2:2014:CLA:H152	1.58	0.85
1:A:78:VAL:HG11	19:A:1103:CLA:HBC3	1.59	0.84
2:B:222:LEU:HA	19:B:1212:CLA:HMD1	1.59	0.84
2:B:469:LYS:CG	2:B:470:THR:HG23	2.07	0.84
6:F:170:ILE:O	6:F:173:TRP:HD1	1.60	0.84
12:L:79:ILE:HG23	12:L:80:ALA:CA	2.07	0.84
4:D:191:ILE:HD12	4:D:191:ILE:H	1.40	0.84
8:H:78:PRO:CD	19:L:1501:CLA:HMD1	2.07	0.84
17:3:164:LEU:HD12	17:3:165:MET:N	1.90	0.84
22:L:7029:LMU:H51	22:L:7029:LMU:H6D	1.56	0.84
1:A:51:THR:OG1	19:A:1139:CLA:CBB	2.24	0.84
5:E:82:TYR:HB3	5:E:83:TRP:HZ3	1.40	0.84
9:I:11:LEU:CD1	21:I:6021:BCR:H10C	2.08	0.84
12:L:92:ALA:N	12:L:98:ARG:CZ	2.40	0.84
5:E:78:ARG:NH1	5:E:125:ILE:CG2	2.41	0.84
17:3:108:PHE:HB3	19:3:3013:CLA:H43	1.58	0.84
17:3:131:GLU:CB	17:3:148:TYR:CD2	2.60	0.84
2:B:542:ARG:HH11	2:B:542:ARG:CB	1.90	0.84
19:J:1308:CLA:HBD	19:J:1308:CLA:CBA	2.06	0.84
15:1:125:LEU:H	15:1:125:LEU:HD22	1.40	0.84
19:A:1115:CLA:C14	19:A:1115:CLA:H172	2.04	0.84
21:A:6011:BCR:HC8	21:A:6011:BCR:H311	1.58	0.84
2:B:119:GLY:CA	19:B:1225:CLA:HED1	2.04	0.84
2:B:20:ARG:HG3	2:B:20:ARG:NH1	1.86	0.84
2:B:275:HIS:O	2:B:279:ALA:N	2.09	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:552:ASP:OD1	2:B:553:PHE:CD2	2.30	0.84
19:A:9023:CLA:CMC	2:B:661:PHE:HB2	2.06	0.84
19:H:1241:CLA:CAC	21:I:6021:BCR:C3	2.55	0.84
1:A:244:LEU:CD1	1:A:247:GLU:CD	2.46	0.84
19:2:2001:CLA:HBC3	19:2:2001:CLA:HMC1	1.57	0.84
4:D:99:PHE:N	4:D:157:VAL:O	2.10	0.84
15:1:85:ILE:CA	15:1:88:ARG:HG3	2.07	0.84
18:4:146:PHE:HZ	19:4:4013:CLA:NC	1.73	0.84
1:A:397:THR:CG2	1:A:613:ILE:CG1	2.50	0.84
7:G:90:GLN:HB3	7:G:91:VAL:C	1.97	0.84
11:K:78:ARG:CA	11:K:78:ARG:NE	2.39	0.84
8:H:65:TRP:N	8:H:66:ASP:HA	1.92	0.84
19:L:1148:CLA:CAA	19:L:1148:CLA:CGD	2.51	0.84
1:A:423:ASP:N	1:A:424:PRO:HD3	1.92	0.84
19:J:1308:CLA:CMA	19:2:2014:CLA:HED2	2.06	0.84
17:3:171:ARG:HG2	17:3:175:ASP:OD1	1.77	0.84
15:1:183:LEU:C	15:1:184:LYS:HG2	1.96	0.84
19:A:1126:CLA:H43	19:A:1126:CLA:HBA1	1.60	0.84
1:A:596:ASP:HA	1:A:599:PHE:HB3	1.60	0.84
19:A:1112:CLA:C4B	21:A:6002:BCR:C19	2.55	0.84
2:B:460:ALA:O	2:B:463:ILE:O	1.95	0.84
19:B:1202:CLA:H43	21:B:6005:BCR:H313	1.58	0.84
5:E:106:ARG:HH21	5:E:107:PHE:HA	0.72	0.84
15:1:170:PRO:C	15:1:173:TYR:HE2	1.80	0.84
16:2:246:PRO:CB	16:2:247:ILE:CD1	2.52	0.84
2:B:98:GLN:C	2:B:100:ALA:N	2.26	0.84
21:I:6021:BCR:H322	21:I:6021:BCR:C4	2.06	0.84
16:2:229:MET:SD	16:2:230:LEU:CD2	2.66	0.84
13:N:157:LYS:HB3	13:N:159:LYS:H	1.39	0.84
11:K:124:LEU:HD12	11:K:124:LEU:O	1.77	0.84
12:L:172:GLU:N	12:L:173:PRO:HD3	1.91	0.84
15:1:77:GLU:CA	15:1:80:LYS:HG2	2.06	0.84
15:1:92:LEU:CA	15:1:95:PRO:CD	2.55	0.84
6:F:170:ILE:CG2	21:F:6014:BCR:C37	2.56	0.84
19:H:1241:CLA:C3C	21:I:6021:BCR:HC22	2.07	0.84
11:K:51:SER:N	11:K:52:PRO:HD3	1.92	0.84
3:C:44:ARG:HE	4:D:182:GLN:HE21	1.21	0.84
18:4:88:LEU:O	18:4:90:TRP:HB3	1.77	0.84
8:H:70:SER:O	8:H:73:PRO:HD3	1.78	0.84
18:4:205:ILE:CG1	18:4:206:ALA:N	2.40	0.84
12:L:153:PHE:CD2	12:L:153:PHE:N	2.45	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:99:LEU:HA	6:F:102:LEU:CD2	2.07	0.84
19:A:1149:CLA:HMC1	19:A:1149:CLA:HBC2	1.57	0.84
15:1:64:PHE:O	15:1:69:LEU:CD1	2.25	0.84
12:L:60:ILE:HG23	12:L:61:ASN:H	1.39	0.84
1:A:527:VAL:HB	1:A:626:GLY:HA3	1.58	0.84
15:1:90:ALA:O	15:1:94:VAL:HG23	1.77	0.84
1:A:284:ARG:HA	1:A:284:ARG:HH11	1.20	0.84
2:B:319:HIS:CE1	2:B:322:LEU:CD1	2.60	0.84
5:E:93:VAL:CG2	5:E:103:VAL:HB	2.08	0.84
2:B:454:LEU:CD1	6:F:147:HIS:HA	2.07	0.84
19:B:1235:CLA:C20	21:F:6016:BCR:HC41	2.08	0.84
7:G:124:ILE:CG1	7:G:128:LEU:HD12	2.06	0.84
16:2:134:THR:HG1	16:2:135:PRO:HD2	0.99	0.84
15:1:93:ALA:HB1	19:1:1006:CLA:C1C	2.07	0.84
2:B:542:ARG:HG3	2:B:542:ARG:NH1	1.86	0.84
3:C:44:ARG:N	4:D:182:GLN:HG3	1.93	0.83
17:3:122:LEU:CD2	19:3:3006:CLA:C4D	2.52	0.83
2:B:75:GLU:CB	2:B:132:ASN:HD22	1.86	0.83
19:R:1144:CLA:HED3	19:R:1144:CLA:C1A	2.07	0.83
22:K:7042:LMU:H5'	22:K:7042:LMU:O2B	1.78	0.83
18:4:158:GLN:CA	19:4:1004:CLA:HMA2	2.08	0.83
18:4:169:ASP:O	18:4:173:LYS:HA	1.77	0.83
19:A:1112:CLA:HMC2	21:A:6002:BCR:C16	2.08	0.83
1:A:733:VAL:HG21	19:A:1140:CLA:C2D	2.08	0.83
16:2:101:TRP:H	16:2:103:VAL:CB	1.90	0.83
3:C:54:CYS:CB	24:C:8002:SF4:S1	2.66	0.83
2:B:633:ASN:HB3	2:B:636:THR:HB	1.60	0.83
8:H:78:PRO:CB	19:L:1501:CLA:HMD1	2.08	0.83
1:A:356:ALA:O	1:A:360:ILE:HG22	1.77	0.83
19:B:1220:CLA:HMD2	19:B:1221:CLA:CBB	2.09	0.83
2:B:308:HIS:CG	2:B:309:ILE:H	1.93	0.83
19:A:9022:CLA:H151	21:B:6017:BCR:C20	2.09	0.83
11:K:49:ILE:C	11:K:52:PRO:HD2	1.98	0.83
13:N:164:SER:HA	13:N:165:ASN:C	1.98	0.83
3:C:67:VAL:HG13	3:C:68:TYR:CA	2.08	0.83
3:C:72:GLU:CD	3:C:77:MET:CE	2.46	0.83
17:3:96:ARG:HA	17:3:99:ALA:CA	2.08	0.83
19:4:1004:CLA:CBC	19:4:1004:CLA:HHD	2.07	0.83
1:A:281:LEU:HD22	19:A:1115:CLA:HMA3	1.59	0.83
2:B:230:TRP:HB3	19:B:1213:CLA:HED3	1.57	0.83
2:B:374:HIS:HB2	19:B:1224:CLA:C1B	2.08	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:302:LYS:HD3	7:G:105:THR:HA	1.60	0.83
5:E:78:ARG:NH2	5:E:123:ASP:O	2.10	0.83
13:N:104:LYS:O	13:N:107:LEU:HB2	1.77	0.83
22:A:7016:LMU:H1'	22:A:7016:LMU:H31	1.58	0.83
17:3:158:PHE:N	17:3:158:PHE:CD1	2.37	0.83
18:4:120:ILE:CD1	18:4:226:LYS:CG	2.07	0.83
1:A:210:LEU:CD1	19:A:1111:CLA:HMB2	2.08	0.83
19:B:1220:CLA:C10	19:B:1220:CLA:H151	1.97	0.83
5:E:83:TRP:HH2	5:E:116:SER:HB2	1.43	0.83
22:3:7003:LMU:C4B	22:3:7005:LMU:C4B	2.54	0.83
22:3:7003:LMU:H4B	22:3:7005:LMU:H4B	1.59	0.83
4:D:111:ILE:CG1	4:D:121:ILE:HG22	2.07	0.83
1:A:525:ASN:CB	1:A:526:LYS:HG3	2.08	0.83
7:G:130:TRP:O	7:G:134:GLY:HA3	1.76	0.83
19:A:1133:CLA:OBD	19:A:1134:CLA:HAC1	1.79	0.83
1:A:203:LEU:HD22	19:A:1123:CLA:CED	2.07	0.83
1:A:328:LYS:HG3	1:A:332:GLU:HB2	1.57	0.83
1:A:443:ILE:HD11	1:A:557:LEU:HD21	1.55	0.83
2:B:586:THR:O	2:B:588:GLY:N	2.11	0.83
8:H:63:GLY:C	8:H:66:ASP:OD1	2.08	0.83
1:A:249:ILE:HG21	17:3:136:TRP:CZ3	2.01	0.83
4:D:157:VAL:CG1	4:D:158:PHE:O	2.26	0.83
18:4:122:ASN:HB3	18:4:124:PRO:HD3	1.59	0.83
15:1:178:LYS:HG3	15:1:179:LYS:N	1.87	0.83
1:A:545:HIS:CB	19:A:1135:CLA:HBB2	2.08	0.83
2:B:269:TRP:HB2	2:B:497:TRP:CH2	2.14	0.83
8:H:113:SER:OG	19:H:1207:CLA:C6	2.26	0.83
17:3:181:SER:HB2	19:3:2009:CLA:C11	2.07	0.83
5:E:107:PHE:HE2	5:E:109:LYS:CG	1.85	0.83
13:N:132:THR:HB	13:N:139:LYS:HZ3	1.42	0.83
8:H:56:GLU:HG3	8:H:57:ASP:HA	1.59	0.83
1:A:628:ILE:CD1	1:A:632:GLY:HA2	2.08	0.83
22:4:7053:LMU:C5'	22:4:7053:LMU:H11	2.08	0.83
12:L:100:ILE:HG22	12:L:191:PHE:O	1.79	0.83
1:A:274:TRP:NE1	1:A:277:TYR:CE2	2.47	0.83
2:B:470:THR:N	2:B:501:ILE:CB	2.27	0.83
12:L:145:LEU:HD11	21:L:6019:BCR:C31	2.08	0.83
17:3:243:ILE:CD1	19:3:3005:CLA:C2C	2.57	0.83
19:A:1106:CLA:CHC	19:A:1107:CLA:HMD2	2.09	0.83
1:A:92:TRP:O	1:A:93:LEU:HD23	1.76	0.83
19:B:1223:CLA:H8	21:B:6010:BCR:H12C	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:123:TRP:C	2:B:126:THR:HG22	1.99	0.83
21:B:6020:BCR:H332	19:L:1502:CLA:C3B	2.08	0.83
12:L:79:ILE:HG23	12:L:80:ALA:N	1.92	0.83
1:A:244:LEU:HB3	1:A:247:GLU:CG	2.07	0.83
3:C:44:ARG:H	4:D:182:GLN:CD	1.79	0.83
11:K:125:LYS:CA	11:K:126:ASN:CB	2.51	0.83
17:3:156:THR:O	17:3:159:VAL:N	2.11	0.83
1:A:316:MET:CB	1:A:317:TYR:HD1	1.92	0.83
17:3:210:PRO:CG	17:3:211:LEU:HD12	2.07	0.83
6:F:179:ARG:CG	6:F:183:ILE:HD11	2.09	0.83
16:2:158:VAL:HG22	16:2:159:PHE:N	1.92	0.83
18:4:173:LYS:C	18:4:194:PHE:CD2	2.52	0.83
2:B:174:ARG:HB2	19:B:1210:CLA:CBC	2.08	0.83
19:B:1222:CLA:CED	19:B:1223:CLA:HMD1	2.08	0.83
17:3:111:LEU:CG	17:3:112:GLY:N	2.19	0.83
17:3:108:PHE:CB	19:3:3013:CLA:C4	2.57	0.83
16:2:236:TRP:O	16:2:240:ILE:HG13	1.79	0.83
6:F:228:ASP:O	6:F:231:PHE:HB3	1.79	0.83
2:B:131:THR:HG22	2:B:134:ASP:CB	2.09	0.83
2:B:7:ARG:NH1	2:B:7:ARG:HG3	1.89	0.83
16:2:266:PHE:CD1	16:2:267:THR:N	2.47	0.83
15:1:97:ILE:CD1	15:1:98:LEU:HD23	2.09	0.82
1:A:207:LEU:O	1:A:310:PHE:HB3	1.77	0.82
2:B:257:ILE:O	2:B:497:TRP:HZ3	1.55	0.82
2:B:588:GLY:O	2:B:592:PHE:HB2	1.77	0.82
19:A:1115:CLA:C19	11:K:64:MET:HE3	2.09	0.82
16:2:124:GLU:O	16:2:127:THR:CA	2.27	0.82
13:N:132:THR:HG1	13:N:138:ALA:C	1.82	0.82
14:R:41:UNK:CB	14:R:42:UNK:CB	2.56	0.82
1:A:249:ILE:HG12	1:A:250:LEU:H	1.41	0.82
13:N:99:LYS:HB3	13:N:102:ASN:HD21	1.41	0.82
19:H:1145:CLA:HMA2	19:H:1145:CLA:O2A	1.79	0.82
2:B:7:ARG:HH11	2:B:7:ARG:CB	1.91	0.82
15:1:77:GLU:CA	15:1:80:LYS:CG	2.53	0.82
1:A:488:PHE:CE2	1:A:533:PRO:HB2	2.14	0.82
2:B:732:LYS:HB3	2:B:733:PHE:CA	2.08	0.82
9:I:24:LEU:C	9:I:26:LEU:H	1.80	0.82
11:K:57:MET:SD	11:K:61:THR:OG1	2.36	0.82
12:L:83:LEU:HD12	12:L:83:LEU:O	1.78	0.82
12:L:92:ALA:CB	12:L:98:ARG:NH2	2.41	0.82
8:H:64:GLN:HB2	8:H:67:SER:H	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:K:1143:CLA:CGA	19:K:1143:CLA:H3A	2.09	0.82
19:J:1308:CLA:HMA3	19:2:2014:CLA:HED2	1.61	0.82
1:A:236:GLY:O	1:A:237:VAL:HG22	1.78	0.82
2:B:715:VAL:HG13	2:B:719:PHE:CD2	2.13	0.82
3:C:20:ALA:O	3:C:21:CYS:HB2	1.76	0.82
1:A:668:TYR:OH	2:B:441:ASP:OD1	1.96	0.82
8:H:109:LEU:O	8:H:113:SER:CB	2.27	0.82
24:A:8001:SF4:S4	2:B:560:ASP:O	2.37	0.82
8:H:78:PRO:HD3	19:L:1501:CLA:HMD1	1.60	0.82
19:J:1308:CLA:H92	19:2:2014:CLA:CGD	2.10	0.82
19:2:2014:CLA:H152	19:2:2014:CLA:C8	2.10	0.82
12:L:51:LYS:CA	12:L:51:LYS:HE2	2.07	0.82
2:B:515:GLY:HA3	2:B:613:SER:HB2	1.60	0.82
1:A:103:PHE:N	1:A:103:PHE:CD2	2.44	0.82
19:A:1113:CLA:HBC3	19:A:1113:CLA:HMC1	1.62	0.82
2:B:493:TRP:NE1	19:B:1213:CLA:HAC2	1.93	0.82
2:B:618:GLY:HA2	2:B:621:ARG:HB3	1.61	0.82
23:B:7101:LMG:O3	3:C:70:TRP:CE2	2.31	0.82
6:F:200:VAL:CG1	10:J:7:TYR:N	2.42	0.82
13:N:157:LYS:H	13:N:157:LYS:HE2	1.42	0.82
16:2:177:VAL:CG1	16:2:178:ASN:HB2	2.05	0.82
6:F:103:GLN:CG	6:F:104:ALA:H	1.91	0.82
2:B:7:ARG:HG2	2:B:7:ARG:O	1.79	0.82
18:4:195:ALA:HB3	18:4:197:THR:O	1.79	0.82
1:A:207:LEU:HD22	19:A:1119:CLA:HBB2	1.59	0.82
19:A:1138:CLA:HBC2	19:A:1139:CLA:C1C	2.10	0.82
19:A:9023:CLA:HMC3	2:B:661:PHE:HB2	1.61	0.82
19:B:1210:CLA:H141	19:B:1215:CLA:H2	1.61	0.82
4:D:86:SER:O	12:L:67:GLY:CA	2.27	0.82
4:D:163:VAL:O	4:D:164:GLN:CG	2.27	0.82
15:1:208:TYR:N	15:1:209:PRO:HD3	1.94	0.82
4:D:185:GLY:O	4:D:186:GLN:HG3	1.79	0.82
19:3:3017:CLA:O1A	19:3:3017:CLA:HMA2	1.78	0.82
1:A:93:LEU:CA	1:A:96:MET:H	1.91	0.82
19:B:1218:CLA:HBC2	19:B:1218:CLA:CHD	2.07	0.82
2:B:268:LEU:HD22	2:B:273:VAL:CG1	2.10	0.82
12:L:72:PRO:O	12:L:73:VAL:CG2	2.26	0.82
16:2:229:MET:SD	16:2:230:LEU:CA	2.67	0.82
13:N:114:PHE:CB	13:N:117:ALA:HB3	2.09	0.82
6:F:132:ASN:C	6:F:133:TYR:HD1	1.82	0.82
4:D:132:ALA:HB3	4:D:136:GLN:HE22	1.43	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3:159:VAL:O	17:3:160:LEU:C	2.14	0.82
18:4:96:LEU:HD12	18:4:97:VAL:N	1.95	0.82
19:A:1134:CLA:CGA	19:A:1141:CLA:CBB	2.56	0.82
11:K:63:LEU:H	11:K:63:LEU:HD13	1.42	0.82
19:L:1130:CLA:H52	19:L:1504:CLA:HHB	1.61	0.82
19:4:1306:CLA:H2	19:4:1306:CLA:HED1	1.60	0.82
2:B:279:ALA:O	19:B:1213:CLA:HMB3	1.80	0.82
2:B:315:LEU:HD12	2:B:317:ARG:CG	2.04	0.82
6:F:177:VAL:HA	6:F:180:SER:OG	1.78	0.82
16:2:128:LYS:HB3	16:2:131:ILE:HG12	1.59	0.82
17:3:150:TYR:CD2	17:3:151:TRP:CG	2.67	0.82
19:2:2014:CLA:C15	19:2:2014:CLA:H91	2.09	0.82
15:1:92:LEU:C	15:1:95:PRO:CD	2.47	0.82
5:E:90:VAL:HG12	5:E:91:VAL:N	1.95	0.82
7:G:124:ILE:HG12	7:G:128:LEU:HD13	1.62	0.82
16:2:165:GLY:CA	16:2:167:ARG:HG2	2.08	0.82
19:1:1007:CLA:HHD	19:1:1007:CLA:CBC	2.09	0.82
17:3:156:THR:O	17:3:156:THR:CG2	2.26	0.82
15:1:114:TRP:CH2	15:1:121:GLN:HG3	2.15	0.82
1:A:246:HIS:CD2	19:3:1147:CLA:O1D	2.33	0.82
19:B:1220:CLA:CMC	19:B:1220:CLA:HBC3	2.04	0.82
19:B:1235:CLA:H161	21:F:6016:BCR:C31	2.08	0.82
2:B:123:TRP:CB	2:B:126:THR:CG2	2.57	0.82
2:B:440:ASN:OD1	2:B:614:THR:HG21	1.77	0.82
2:B:440:ASN:OD1	2:B:614:THR:HG22	1.76	0.82
11:K:78:ARG:CZ	11:K:78:ARG:HA	2.09	0.82
17:3:187:PHE:CD1	17:3:187:PHE:C	2.54	0.82
3:C:63:LEU:CD2	3:C:65:VAL:H	1.92	0.82
17:3:131:GLU:CB	17:3:148:TYR:CE2	2.62	0.82
18:4:220:GLN:HG3	19:4:1306:CLA:HAC2	1.61	0.81
1:A:281:LEU:CG	19:A:1115:CLA:HED1	2.09	0.81
2:B:31:PHE:O	2:B:37:ILE:HG21	1.80	0.81
5:E:78:ARG:CZ	5:E:125:ILE:CG2	2.57	0.81
3:C:72:GLU:CD	3:C:77:MET:HE1	1.99	0.81
17:3:98:LEU:CD1	19:3:3012:CLA:C2D	2.57	0.81
1:A:162:LEU:O	1:A:165:TYR:CB	2.25	0.81
18:4:111:LEU:HD12	18:4:112:PRO:CG	2.10	0.81
19:A:1122:CLA:C4C	21:A:6007:BCR:C19	2.59	0.81
1:A:79:PHE:CD1	19:A:1111:CLA:HED3	2.16	0.81
2:B:224:PRO:CB	2:B:227:THR:HB	2.10	0.81
2:B:679:ALA:O	2:B:683:GLU:OE1	1.97	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:100:PHE:N	7:G:101:GLU:CB	2.43	0.81
8:H:97:LEU:HG	8:H:98:LEU:CA	2.10	0.81
12:L:115:VAL:CG1	12:L:130:GLY:H	1.91	0.81
21:I:6021:BCR:C39	21:L:6019:BCR:H401	2.09	0.81
12:L:73:VAL:CG2	19:L:1130:CLA:OBD	2.28	0.81
19:2:2014:CLA:OBD	19:2:2014:CLA:HED3	1.79	0.81
15:1:224:PRO:CA	15:1:225:TRP:HB2	2.10	0.81
1:A:129:GLN:NE2	19:A:1107:CLA:MG	1.36	0.81
2:B:556:SER:C	2:B:558:PRO:HD2	2.00	0.81
8:H:98:LEU:HD23	12:L:146:THR:HG21	1.61	0.81
18:4:169:ASP:HA	18:4:173:LYS:CA	2.10	0.81
18:4:96:LEU:C	18:4:96:LEU:CD1	2.48	0.81
1:A:284:ARG:NH2	1:A:507:ALA:O	2.11	0.81
2:B:293:THR:HG22	7:G:94:GLN:CG	2.10	0.81
5:E:107:PHE:CD2	5:E:109:LYS:CG	2.63	0.81
2:B:633:ASN:CB	2:B:636:THR:CB	2.44	0.81
22:3:7005:LMU:H11	22:3:7005:LMU:H51	1.61	0.81
13:N:118:TYR:O	13:N:119:THR:HG23	1.80	0.81
6:F:97:GLN:CD	6:F:98:ALA:N	2.33	0.81
17:3:204:GLY:HA3	17:3:206:PRO:O	1.80	0.81
15:1:149:GLU:CG	15:1:152:ARG:HH12	1.93	0.81
1:A:426:THR:HG23	1:A:428:TYR:OH	1.79	0.81
2:B:79:GLN:O	2:B:80:ASP:HB3	1.79	0.81
17:3:161:GLU:HA	17:3:164:LEU:HG	1.61	0.81
4:D:185:GLY:O	4:D:186:GLN:CG	2.28	0.81
2:B:600:THR:O	2:B:604:GLY:HA3	1.81	0.81
15:1:77:GLU:CB	15:1:80:LYS:HD2	2.11	0.81
19:B:1205:CLA:HMC2	21:B:6017:BCR:H281	1.61	0.81
9:I:8:PHE:HB2	19:I:1204:CLA:OBD	1.80	0.81
11:K:56:ILE:HA	11:K:59:THR:HG22	1.62	0.81
11:K:76:ALA:H	11:K:78:ARG:NH1	1.78	0.81
12:L:141:LEU:HD13	12:L:145:LEU:CD1	2.09	0.81
3:C:52:LYS:HZ1	3:C:64:SER:CB	1.93	0.81
17:3:96:ARG:NH1	17:3:96:ARG:CB	2.41	0.81
17:3:136:TRP:N	17:3:139:THR:OG1	2.13	0.81
15:1:172:GLY:HA2	15:1:173:TYR:CD2	2.14	0.81
15:1:114:TRP:CH2	15:1:121:GLN:HA	2.14	0.81
4:D:101:VAL:HG12	4:D:130:LYS:HB2	1.62	0.81
18:4:131:LYS:H	18:4:131:LYS:HD2	1.45	0.81
19:A:1112:CLA:C4B	21:A:6002:BCR:H19C	2.10	0.81
1:A:158:ILE:HD13	19:A:1112:CLA:HED3	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:124:ILE:HG23	7:G:125:VAL:N	1.96	0.81
4:D:138:LEU:O	4:D:140:LEU:O	1.98	0.81
1:A:129:GLN:NE2	19:A:1107:CLA:ND	2.29	0.81
2:B:172:GLU:O	2:B:176:ASN:CB	2.28	0.81
2:B:229:GLN:C	7:G:63:VAL:CG2	2.46	0.81
2:B:315:LEU:CD1	2:B:317:ARG:CG	2.57	0.81
2:B:353:TYR:CD2	2:B:594:TRP:HZ3	1.96	0.81
3:C:69:LEU:HD12	3:C:70:TRP:N	1.95	0.81
19:A:1105:CLA:HMB1	21:J:6012:BCR:HC7	1.62	0.81
19:A:1115:CLA:C19	11:K:64:MET:CE	2.59	0.81
12:L:141:LEU:CD1	12:L:145:LEU:HD11	2.08	0.81
24:A:8001:SF4:S2	2:B:702:ILE:HD11	2.21	0.81
16:2:184:PRO:CD	16:2:187:LYS:N	2.44	0.81
19:J:1308:CLA:CHD	19:J:1308:CLA:HBC2	2.10	0.81
15:1:117:LEU:HD13	15:1:117:LEU:N	1.96	0.81
1:A:126:ILE:HD11	19:A:1107:CLA:HMA1	1.63	0.81
19:A:1115:CLA:H193	11:K:64:MET:CE	2.10	0.81
1:A:98:PHE:CZ	19:A:1105:CLA:HMD3	2.16	0.81
2:B:232:LEU:HD11	2:B:235:GLN:HG3	1.59	0.81
5:E:127:GLU:CA	5:E:128:VAL:O	2.29	0.81
4:D:93:LYS:HG3	4:D:96:VAL:CG1	2.10	0.81
12:L:210:PRO:C	12:L:211:TYR:CG	2.53	0.81
1:A:23:ASP:OD1	1:A:24:ARG:HD2	1.80	0.81
17:3:201:ALA:HB1	17:3:202:TYR:HE2	1.39	0.81
2:B:140:ILE:CG1	2:B:141:PHE:H	1.92	0.81
12:L:164:LEU:HD12	12:L:165:THR:H	1.42	0.81
1:A:483:GLN:HB3	1:A:485:GLN:CD	2.01	0.81
15:1:158:PRO:CG	15:1:159:GLU:H	1.92	0.81
15:1:97:ILE:HD12	15:1:98:LEU:HD23	1.63	0.81
2:B:294:ASN:CB	7:G:94:GLN:OE1	2.25	0.81
16:2:129:LEU:O	16:2:130:GLY:C	2.19	0.81
16:2:128:LYS:HB3	16:2:131:ILE:HG23	1.62	0.81
5:E:127:GLU:CB	5:E:128:VAL:O	2.28	0.81
5:E:127:GLU:CB	5:E:129:GLU:O	2.29	0.81
15:1:137:ILE:HG12	15:1:138:LEU:N	1.96	0.81
8:H:116:ALA:HB1	8:H:117:SER:CA	2.06	0.81
1:A:195:TRP:CZ2	19:A:1108:CLA:CMA	2.63	0.81
1:A:415:ALA:O	1:A:419:VAL:HG23	1.80	0.81
2:B:233:TYR:HD1	2:B:254:ILE:HG13	1.44	0.81
2:B:298:GLY:CA	19:B:1218:CLA:HMD3	2.10	0.81
7:G:69:GLY:O	7:G:72:LEU:CG	2.29	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:124:GLU:O	16:2:127:THR:HG22	1.81	0.81
5:E:107:PHE:CD2	5:E:109:LYS:CD	2.64	0.81
1:A:249:ILE:C	1:A:251:ASN:N	2.31	0.81
13:N:114:PHE:O	13:N:117:ALA:HB3	1.80	0.81
19:1:1007:CLA:HHD	19:1:1007:CLA:HBC2	1.63	0.81
6:F:103:GLN:CG	6:F:104:ALA:N	2.44	0.81
22:E:7048:LMU:H4B	22:F:7036:LMU:C6'	2.07	0.81
4:D:198:ILE:O	4:D:198:ILE:HG13	1.75	0.81
15:1:83:GLU:C	15:1:86:HIS:CD2	2.53	0.81
1:A:227:LEU:HD22	1:A:296:LEU:HD13	1.61	0.81
2:B:656:VAL:HG22	19:B:1239:CLA:HMB3	1.63	0.81
2:B:571:SER:OG	2:B:574:ASP:OD1	1.99	0.81
6:F:200:VAL:HG23	6:F:204:SER:H	1.46	0.81
5:E:78:ARG:NH1	5:E:125:ILE:HG21	1.95	0.81
4:D:123:ARG:HH22	22:D:7050:LMU:H4B	1.45	0.81
19:2:2014:CLA:C15	19:2:2014:CLA:C10	2.59	0.81
2:B:314:ARG:HH12	15:1:67:LEU:HD21	0.98	0.80
19:B:1203:CLA:H2A	19:B:1203:CLA:O1D	1.81	0.80
2:B:388:ALA:C	2:B:391:PRO:HD2	2.00	0.80
7:G:73:PHE:O	7:G:76:ARG:HB2	1.80	0.80
16:2:182:ILE:HG22	16:2:187:LYS:CG	2.09	0.80
2:B:542:ARG:NH2	4:D:195:VAL:O	2.14	0.80
17:3:125:VAL:HB	17:3:126:GLY:HA2	1.61	0.80
12:L:174:ASP:CG	12:L:175:GLN:H	1.84	0.80
1:A:68:THR:HG22	1:A:70:ASP:H	1.42	0.80
15:1:116:ALA:C	15:1:117:LEU:HD22	2.00	0.80
18:4:174:GLN:O	18:4:194:PHE:HB3	1.80	0.80
18:4:215:LEU:O	18:4:216:GLY:C	2.17	0.80
19:A:1126:CLA:H172	21:J:6012:BCR:H17C	1.62	0.80
2:B:224:PRO:CB	2:B:227:THR:CB	2.60	0.80
2:B:304:ILE:HD11	19:B:1216:CLA:HED2	0.83	0.80
2:B:625:TRP:C	2:B:625:TRP:CE3	2.55	0.80
19:B:1235:CLA:C16	21:F:6016:BCR:C31	2.59	0.80
7:G:79:PHE:CG	7:G:80:PHE:N	2.50	0.80
15:1:137:ILE:HG12	15:1:138:LEU:H	1.46	0.80
14:R:33:UNK:O	14:R:36:UNK:CB	2.30	0.80
2:B:58:PHE:CE2	2:B:145:LEU:HD21	2.14	0.80
15:1:85:ILE:HG12	15:1:88:ARG:NH2	1.97	0.80
1:A:352:THR:HA	19:A:1123:CLA:H201	1.61	0.80
19:B:1235:CLA:HBC1	6:F:160:PHE:HZ	1.41	0.80
2:B:378:ILE:O	2:B:380:GLY:N	2.14	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1237:CLA:HMD3	21:B:6017:BCR:HC31	1.63	0.80
3:C:29:ILE:HG12	4:D:180:GLY:HA2	1.63	0.80
17:3:113:ALA:HB1	17:3:239:LEU:CD1	1.98	0.80
15:1:170:PRO:C	15:1:173:TYR:CE2	2.54	0.80
2:B:131:THR:O	2:B:135:LEU:HD23	1.82	0.80
9:I:1:MET:O	9:I:2:ILE:HG22	1.80	0.80
15:1:92:LEU:HA	15:1:95:PRO:CD	2.11	0.80
18:4:103:MET:HE2	18:4:208:GLY:N	1.62	0.80
18:4:211:MET:HG3	19:4:4002:CLA:CBB	2.12	0.80
1:A:279:ASP:O	1:A:281:LEU:CD1	2.29	0.80
1:A:370:ILE:CG2	1:A:400:MET:HA	2.11	0.80
1:A:445:HIS:O	1:A:446:LEU:HB3	1.80	0.80
7:G:62:LEU:CB	7:G:65:SER:HB3	2.09	0.80
11:K:47:ASP:HA	11:K:51:SER:HB2	1.64	0.80
12:L:73:VAL:HA	19:L:1504:CLA:HMA3	1.64	0.80
16:2:177:VAL:CG1	16:2:178:ASN:CB	2.58	0.80
6:F:103:GLN:HG3	6:F:104:ALA:H	1.47	0.80
11:K:115:ILE:CG1	11:K:122:LEU:H	1.92	0.80
15:1:171:LEU:CA	15:1:173:TYR:CZ	2.63	0.80
2:B:58:PHE:CE2	2:B:145:LEU:HD22	2.09	0.80
1:A:281:LEU:CD2	19:A:1115:CLA:HED1	2.03	0.80
1:A:328:LYS:HZ3	1:A:345:GLY:HA2	1.44	0.80
1:A:356:ALA:HB2	1:A:417:PHE:CD2	2.17	0.80
19:A:9013:CLA:HMD1	2:B:533:ILE:HG21	1.63	0.80
2:B:432:HIS:HE1	19:B:1229:CLA:NB	1.80	0.80
2:B:459:PHE:HE2	19:B:1235:CLA:CHD	1.95	0.80
16:2:160:ILE:HG22	19:2:2012:CLA:CAB	2.12	0.80
22:D:7050:LMU:C6'	22:D:7050:LMU:C2B	2.57	0.80
1:A:423:ASP:CB	1:A:424:PRO:HD3	2.11	0.80
2:B:628:SER:O	2:B:631:LEU:CD2	2.29	0.80
1:A:255:LEU:CD1	1:A:280:PHE:HZ	1.93	0.80
1:A:123:VAL:O	19:A:1107:CLA:O1D	1.97	0.80
1:A:353:SER:O	1:A:354:TRP:HB2	1.82	0.80
1:A:76:ARG:NH1	1:A:193:LEU:HD22	1.96	0.80
2:B:119:GLY:HA3	19:B:1225:CLA:CED	2.09	0.80
19:B:1213:CLA:CBC	19:B:1213:CLA:HHD	2.12	0.80
2:B:457:PRO:CB	2:B:517:PHE:HB2	2.12	0.80
19:L:1148:CLA:CHD	19:L:1148:CLA:HBC3	2.09	0.80
16:2:184:PRO:HD3	16:2:187:LYS:CD	2.12	0.80
13:N:110:THR:HG22	13:N:111:GLY:H	1.46	0.80
16:2:237:PHE:C	16:2:237:PHE:CD1	2.54	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:131:LYS:H	18:4:131:LYS:CD	1.95	0.80
1:A:50:THR:CG2	1:A:51:THR:N	2.44	0.80
21:A:6011:BCR:H312	19:A:9013:CLA:H143	1.62	0.80
19:A:1138:CLA:C19	6:F:181:TYR:HB3	2.10	0.80
19:A:1131:CLA:H161	21:L:6019:BCR:C36	2.12	0.80
1:A:244:LEU:HD12	1:A:247:GLU:OE1	1.81	0.80
8:H:78:PRO:HB3	19:L:1501:CLA:HMD1	1.63	0.80
22:1:7004:LMU:H1B	22:1:7004:LMU:O6B	1.80	0.80
1:A:355:HIS:ND1	1:A:416:ILE:HG21	1.97	0.80
1:A:446:LEU:HD21	1:A:554:LEU:HA	1.62	0.80
2:B:462:TRP:CZ3	19:B:1231:CLA:CBC	2.65	0.80
2:B:282:PHE:CZ	19:B:1213:CLA:C1	2.64	0.80
5:E:126:VAL:O	5:E:127:GLU:CB	2.30	0.80
14:R:34:UNK:O	14:R:38:UNK:CB	2.30	0.80
4:D:102:ILE:HG13	4:D:154:PHE:HB3	1.64	0.80
18:4:112:PRO:HD2	18:4:113:GLU:HG3	1.62	0.80
1:A:442:ILE:HG23	19:A:1129:CLA:HMC3	1.64	0.80
19:B:1220:CLA:C4A	19:B:1220:CLA:H42	2.11	0.80
2:B:527:LEU:CD1	19:B:1236:CLA:CMA	2.60	0.80
2:B:469:LYS:HD2	2:B:470:THR:HA	0.86	0.80
16:2:120:ILE:HG13	16:2:121:PHE:H	1.47	0.80
16:2:134:THR:HG1	16:2:135:PRO:CD	1.74	0.80
5:E:107:PHE:CE2	5:E:109:LYS:CE	2.65	0.80
13:N:132:THR:OG1	13:N:138:ALA:O	1.98	0.80
4:D:174:PRO:O	4:D:175:GLU:HG2	1.82	0.80
17:3:104:ILE:HG21	19:3:3004:CLA:C1D	2.11	0.80
14:R:35:UNK:O	14:R:38:UNK:CB	2.29	0.80
16:2:156:GLU:CG	16:2:157:LEU:CD1	2.57	0.80
19:J:1311:CLA:HED3	19:J:1311:CLA:CHA	2.10	0.80
22:H:7011:LMU:C10	22:H:7011:LMU:H61	2.12	0.80
19:A:1149:CLA:HAA1	19:A:1149:CLA:CGD	2.12	0.80
16:2:204:LEU:HD12	16:2:210:SER:O	1.82	0.80
22:4:7034:LMU:H111	22:4:7052:LMU:C2'	1.99	0.80
1:A:284:ARG:HG3	1:A:295:TRP:CD1	2.17	0.80
19:B:1219:CLA:HBC2	19:B:1220:CLA:HBA1	1.62	0.80
2:B:199:ILE:CG2	2:B:270:LEU:CD1	2.55	0.80
2:B:456:GLU:HA	2:B:514:PRO:HD3	1.62	0.80
19:2:2007:CLA:CAC	19:3:2009:CLA:HED3	2.00	0.80
5:E:126:VAL:O	5:E:127:GLU:CG	2.29	0.80
11:K:122:LEU:HD22	11:K:122:LEU:O	1.82	0.80
15:1:151:GLN:N	15:1:151:GLN:HE21	1.79	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:177:LEU:HD22	18:4:178:PRO:CD	2.12	0.79
1:A:342:GLY:HA3	1:A:430:ASP:HB2	0.81	0.79
2:B:102:GLU:O	2:B:104:PHE:HB2	1.82	0.79
2:B:462:TRP:HZ3	19:B:1231:CLA:HBC2	1.47	0.79
2:B:293:THR:CG2	7:G:94:GLN:HG2	2.12	0.79
19:H:1207:CLA:HMA2	19:H:1207:CLA:O2A	1.82	0.79
21:I:6021:BCR:HC8	21:I:6021:BCR:H313	0.81	0.79
17:3:141:VAL:HG23	17:3:142:ILE:CG1	2.10	0.79
14:R:36:UNK:O	14:R:38:UNK:CB	2.30	0.79
16:2:166:ARG:CA	16:2:167:ARG:HB2	2.11	0.79
22:2:7006:LMU:H5'	22:2:7006:LMU:O5B	1.79	0.79
17:3:153:ASP:HB2	17:3:154:ASN:OD1	1.81	0.79
6:F:214:PRO:O	6:F:215:VAL:HB	1.78	0.79
1:A:389:TYR:CE1	1:A:625:TRP:CD1	2.70	0.79
22:H:7011:LMU:H101	22:H:7011:LMU:H61	1.61	0.79
13:N:169:LYS:CB	13:N:170:TRP:HD1	1.95	0.79
11:K:89:ARG:NH1	11:K:89:ARG:HG3	1.97	0.79
18:4:142:PHE:HA	18:4:145:GLU:OE1	1.82	0.79
19:A:1105:CLA:CBA	19:A:1107:CLA:H12	2.12	0.79
19:A:1115:CLA:HMC1	19:A:1115:CLA:CBC	2.09	0.79
19:A:1124:CLA:HBC2	19:A:1124:CLA:CHD	2.10	0.79
1:A:152:ILE:CD1	19:A:1127:CLA:O1D	2.29	0.79
19:B:1220:CLA:H41	19:B:1220:CLA:NA	1.95	0.79
2:B:306:GLU:HG3	2:B:307:ALA:N	1.97	0.79
12:L:78:LEU:HD22	19:L:1504:CLA:HED1	1.62	0.79
16:2:101:TRP:N	16:2:103:VAL:H	1.81	0.79
13:N:130:ASN:CB	13:N:139:LYS:CG	2.29	0.79
13:N:142:LYS:N	13:N:145:PHE:O	2.14	0.79
3:C:44:ARG:N	4:D:182:GLN:CG	2.46	0.79
14:R:38:UNK:O	14:R:42:UNK:CA	2.29	0.79
11:K:125:LYS:CB	11:K:128:GLY:HA2	2.13	0.79
15:1:190:ASN:ND2	19:1:1002:CLA:C4D	2.44	0.79
16:2:201:PHE:CD1	16:2:202:ASP:N	2.50	0.79
1:A:316:MET:HG2	1:A:317:TYR:HD1	1.44	0.79
2:B:626:LEU:O	2:B:627:ASN:HB2	1.82	0.79
7:G:128:LEU:HD23	7:G:128:LEU:C	2.03	0.79
12:L:145:LEU:HG	21:L:6019:BCR:HC7	1.62	0.79
13:N:130:ASN:HB2	13:N:139:LYS:HG2	0.80	0.79
13:N:148:ASP:HA	13:N:149:ASP:O	1.83	0.79
17:3:111:LEU:O	17:3:114:VAL:CA	2.30	0.79
6:F:100:LYS:HD2	6:F:100:LYS:O	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:112:GLN:CG	15:1:113:GLU:H	1.92	0.79
17:3:252:PRO:HB3	17:3:254:GLN:HE21	1.47	0.79
18:4:205:ILE:HG12	18:4:206:ALA:N	1.98	0.79
1:A:50:THR:HG22	1:A:51:THR:N	1.98	0.79
1:A:64:PHE:HZ	1:A:77:LYS:CE	1.95	0.79
18:4:87:ASN:CG	18:4:90:TRP:CE2	2.54	0.79
1:A:162:LEU:C	1:A:165:TYR:HB3	2.03	0.79
22:E:7048:LMU:C4B	22:F:7036:LMU:C6'	2.60	0.79
1:A:267:THR:O	1:A:267:THR:HG22	1.81	0.79
18:4:120:ILE:HG22	18:4:121:ILE:N	1.96	0.79
1:A:534:LEU:HD12	1:A:535:GLY:H	0.98	0.79
2:B:594:TRP:O	2:B:595:HIS:CB	2.31	0.79
6:F:200:VAL:HG23	6:F:204:SER:N	1.98	0.79
11:K:59:THR:O	11:K:63:LEU:HD21	1.83	0.79
16:2:101:TRP:N	16:2:103:VAL:HB	1.96	0.79
16:2:131:ILE:O	16:2:132:LEU:HB2	1.82	0.79
16:2:227:LEU:HD21	19:2:2004:CLA:CHC	2.13	0.79
3:C:12:ILE:HG13	24:C:8003:SF4:S1	2.23	0.79
13:N:114:PHE:CB	13:N:117:ALA:CB	2.60	0.79
2:B:160:LYS:NZ	2:B:161:TRP:CE3	2.49	0.79
11:K:127:ILE:C	11:K:130:LEU:HG	2.02	0.79
1:A:579:PHE:N	1:A:579:PHE:HD1	1.81	0.79
17:3:243:ILE:CD1	19:3:3005:CLA:C1C	2.59	0.79
18:4:94:ALA:O	18:4:98:ASN:OD1	2.01	0.79
1:A:388:ASP:CG	1:A:391:THR:OG1	2.21	0.79
2:B:469:LYS:NZ	2:B:471:THR:H	1.80	0.79
2:B:257:ILE:C	2:B:497:TRP:HZ3	1.86	0.79
2:B:527:LEU:O	2:B:527:LEU:HD12	1.82	0.79
9:I:7:LEU:CD1	21:I:6021:BCR:H333	2.08	0.79
1:A:22:VAL:O	1:A:22:VAL:CG2	2.28	0.79
5:E:127:GLU:O	5:E:128:VAL:CG2	2.29	0.79
5:E:79:LYS:HE3	5:E:84:TYR:OH	1.81	0.79
13:N:138:ALA:HB3	13:N:140:GLN:HG3	1.65	0.79
8:H:119:ASP:CG	8:H:121:LEU:HG	2.03	0.79
22:L:7029:LMU:C4'	22:L:7029:LMU:H5B	2.09	0.79
22:L:7029:LMU:H6E	22:L:7029:LMU:O2B	1.82	0.79
15:1:182:GLU:OE1	19:1:1001:CLA:C1D	2.31	0.79
15:1:77:GLU:HG3	15:1:80:LYS:CD	2.13	0.79
21:A:6011:BCR:H313	19:A:9013:CLA:C14	2.11	0.79
1:A:684:PHE:C	1:A:684:PHE:CD2	2.56	0.79
2:B:334:LEU:HG	2:B:334:LEU:O	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:76:ARG:NH2	7:G:117:ASN:O	2.14	0.79
7:G:131:GLY:CA	7:G:136:VAL:HG23	2.13	0.79
22:G:7026:LMU:H2B	22:G:7026:LMU:O3'	1.83	0.79
7:G:90:GLN:CB	7:G:91:VAL:C	2.51	0.79
12:L:91:THR:HA	12:L:98:ARG:HH12	1.47	0.79
16:2:224:ASN:OD1	16:2:227:LEU:HD22	1.82	0.79
19:J:1308:CLA:H2A	19:J:1308:CLA:O2A	1.80	0.79
15:1:170:PRO:CD	15:1:173:TYR:CE2	2.66	0.79
17:3:201:ALA:CB	17:3:202:TYR:HD2	1.94	0.79
2:B:475:ASP:O	2:B:476:ILE:CG2	2.30	0.79
2:B:93:ASP:OD1	2:B:96:PHE:CD1	2.35	0.79
15:1:78:ARG:NH2	15:1:179:LYS:CD	2.37	0.79
1:A:77:LYS:O	1:A:80:SER:OG	2.00	0.79
19:B:1223:CLA:CED	19:B:1231:CLA:HBB2	2.11	0.79
2:B:363:GLN:H	2:B:365:PHE:HB3	1.46	0.79
20:B:5002:PQN:H142	20:B:5002:PQN:H2M1	1.64	0.79
3:C:1:MET:H1	3:C:4:SER:N	1.79	0.79
16:2:229:MET:SD	16:2:230:LEU:N	2.55	0.79
19:1:1014:CLA:C7	19:1:1014:CLA:H41	2.04	0.79
4:D:167:HIS:N	4:D:168:PRO:CD	2.45	0.79
22:3:7003:LMU:C3B	22:3:7005:LMU:O5B	2.30	0.79
17:3:148:TYR:N	17:3:149:ASN:ND2	2.30	0.79
15:1:172:GLY:HA2	15:1:173:TYR:CG	2.17	0.79
1:A:567:ARG:NH1	4:D:89:GLY:CA	2.45	0.79
15:1:162:LYS:O	15:1:164:PRO:HD3	1.83	0.79
1:A:484:LEU:HD22	1:A:484:LEU:N	1.96	0.79
15:1:92:LEU:HA	15:1:95:PRO:CG	2.12	0.79
15:1:97:ILE:CD1	15:1:98:LEU:HB2	2.12	0.79
1:A:452:PHE:CE1	19:A:1136:CLA:CBB	2.66	0.79
2:B:53:GLN:HG3	19:B:1202:CLA:HHB	1.65	0.79
2:B:25:ILE:O	2:B:25:ILE:CG1	2.27	0.79
2:B:310:PRO:CG	2:B:311:PRO:CD	2.61	0.79
2:B:454:LEU:O	2:B:454:LEU:HD12	1.82	0.79
7:G:69:GLY:HA2	7:G:72:LEU:HG	1.65	0.79
13:N:148:ASP:N	13:N:149:ASP:CB	2.45	0.79
4:D:156:ARG:NE	4:D:164:GLN:HB2	1.98	0.79
1:A:255:LEU:HD13	1:A:280:PHE:CZ	2.12	0.79
7:G:134:GLY:O	7:G:135:HIS:CG	2.36	0.79
18:4:123:VAL:N	18:4:124:PRO:HD3	1.98	0.79
2:B:557:PHE:N	2:B:558:PRO:CD	2.46	0.79
23:B:7101:LMG:O3	3:C:70:TRP:NE1	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:115:LEU:O	16:2:118:ALA:HB3	1.82	0.79
8:H:61:THR:HA	8:H:62:THR:HG22	1.64	0.79
13:N:130:ASN:O	13:N:132:THR:HG22	1.78	0.79
4:D:99:PHE:CB	4:D:157:VAL:HG12	2.13	0.79
16:2:269:LYS:HA	16:2:269:LYS:CE	2.12	0.79
1:A:316:MET:HB3	1:A:317:TYR:CG	2.18	0.79
1:A:68:THR:HG23	1:A:70:ASP:H	1.47	0.79
18:4:232:LEU:CB	18:4:236:ILE:HD12	2.12	0.79
15:1:97:ILE:CD1	15:1:98:LEU:CD2	2.61	0.78
1:A:207:LEU:CB	19:A:1119:CLA:HBB2	2.13	0.78
19:A:1124:CLA:H72	19:A:1125:CLA:HED1	1.54	0.78
1:A:158:ILE:CG1	1:A:159:THR:N	2.28	0.78
2:B:87:ILE:CA	2:B:115:ASN:HA	2.12	0.78
17:3:96:ARG:HG3	17:3:96:ARG:NH1	1.98	0.78
11:K:115:ILE:HA	11:K:118:VAL:HG21	1.63	0.78
17:3:254:GLN:HG3	17:3:255:ASN:N	1.98	0.78
19:B:1218:CLA:HHD	19:B:1218:CLA:CBC	2.13	0.78
2:B:232:LEU:HD11	2:B:235:GLN:CG	2.14	0.78
15:1:190:ASN:HD21	19:1:1002:CLA:C4D	1.97	0.78
22:A:7016:LMU:H22	22:A:7016:LMU:C6	2.02	0.78
19:3:3016:CLA:HMC1	19:3:3016:CLA:CBC	2.13	0.78
18:4:173:LYS:O	18:4:194:PHE:CD2	2.36	0.78
19:A:1124:CLA:H2	19:A:1124:CLA:O1A	1.80	0.78
1:A:545:HIS:O	1:A:549:ILE:HG13	1.82	0.78
2:B:317:ARG:NH1	2:B:410:ARG:HG2	1.98	0.78
2:B:462:TRP:CZ3	19:B:1231:CLA:HBC2	2.19	0.78
17:3:187:PHE:HD1	17:3:187:PHE:C	1.86	0.78
16:2:148:ASP:O	16:2:149:THR:OG1	2.00	0.78
15:1:190:ASN:ND2	19:1:1002:CLA:CHA	2.46	0.78
1:A:628:ILE:HD12	1:A:632:GLY:HA2	1.64	0.78
22:1:7013:LMU:H1B	22:1:7013:LMU:O6B	1.82	0.78
22:4:7034:LMU:H101	22:4:7052:LMU:O3'	1.83	0.78
19:A:1112:CLA:CHC	21:A:6002:BCR:C19	2.61	0.78
19:A:1123:CLA:H142	19:A:1123:CLA:HMD2	1.65	0.78
1:A:492:ILE:CD1	19:A:1133:CLA:HMC3	2.06	0.78
1:A:148:GLY:O	1:A:152:ILE:HD12	1.84	0.78
19:H:1241:CLA:HAC1	21:I:6021:BCR:C3	2.13	0.78
12:L:79:ILE:HG23	12:L:80:ALA:HA	1.65	0.78
12:L:95:PRO:O	12:L:98:ARG:N	2.16	0.78
3:C:62:PHE:CE1	5:E:80:GLU:HB3	2.17	0.78
5:E:89:SER:OG	5:E:106:ARG:CG	2.30	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:99:PHE:HB2	4:D:157:VAL:HG12	1.64	0.78
1:A:578:ARG:CZ	1:A:578:ARG:CB	2.61	0.78
12:L:168:GLY:C	12:L:170:LYS:H	1.87	0.78
19:A:1121:CLA:HAA1	11:K:78:ARG:CZ	2.12	0.78
1:A:555:ILE:CD1	19:A:9023:CLA:OBD	2.31	0.78
2:B:645:VAL:HG11	19:B:1205:CLA:HAC1	1.65	0.78
3:C:44:ARG:HB3	4:D:182:GLN:HE22	1.47	0.78
17:3:111:LEU:HG	17:3:112:GLY:H	0.63	0.78
19:K:1142:CLA:CED	19:K:1143:CLA:CMB	2.62	0.78
18:4:110:LEU:O	18:4:113:GLU:CG	2.30	0.78
18:4:173:LYS:O	18:4:194:PHE:CE2	2.36	0.78
19:A:1124:CLA:O1A	19:A:1125:CLA:HED3	1.84	0.78
1:A:203:LEU:HD22	19:A:1123:CLA:HED1	1.63	0.78
1:A:201:SER:O	1:A:204:ASN:HB2	1.84	0.78
6:F:220:GLU:OE1	6:F:225:GLU:HB2	1.83	0.78
19:3:3008:CLA:CBA	19:3:3008:CLA:HBD	2.06	0.78
19:2:2014:CLA:C4	19:2:2014:CLA:H72	2.12	0.78
5:E:111:ASN:HD21	5:E:113:ALA:N	1.80	0.78
3:C:52:LYS:NZ	3:C:64:SER:CB	2.47	0.78
17:3:103:VAL:O	17:3:107:ARG:CD	2.31	0.78
6:F:190:LYS:HG3	6:F:192:THR:HG23	1.66	0.78
16:2:171:ILE:HG13	16:2:172:LEU:CB	2.14	0.78
15:1:128:PRO:HG2	15:1:131:TRP:CZ3	2.18	0.78
19:A:1149:CLA:CAA	19:A:1149:CLA:O1D	2.31	0.78
16:2:261:THR:CG2	16:2:262:ILE:H	1.96	0.78
15:1:176:ASP:HB3	15:1:180:LEU:HD12	0.79	0.78
1:A:492:ILE:HD11	19:A:1133:CLA:C2C	2.12	0.78
2:B:216:LEU:HG	2:B:218:TYR:H	1.48	0.78
7:G:90:GLN:HB2	7:G:92:PRO:CD	2.13	0.78
9:I:7:LEU:HD12	21:I:6021:BCR:C33	2.09	0.78
19:2:2007:CLA:HMD2	19:3:2009:CLA:HMD3	1.65	0.78
1:A:27:ILE:O	1:A:27:ILE:HG22	1.83	0.78
13:N:148:ASP:H	13:N:149:ASP:C	1.87	0.78
16:2:172:LEU:CA	16:2:173:ASN:HD22	1.96	0.78
12:L:210:PRO:C	12:L:211:TYR:CD2	2.57	0.78
22:L:7029:LMU:C5B	22:L:7029:LMU:H4'	2.11	0.78
1:A:421:ASP:OD1	1:A:422:TYR:CE1	2.36	0.78
1:A:603:PHE:HZ	1:A:693:LEU:HD21	1.49	0.78
17:3:151:TRP:CD1	17:3:151:TRP:N	2.48	0.78
17:3:125:VAL:HG21	19:3:3010:CLA:C2C	2.13	0.78
22:H:7011:LMU:H82	22:H:7011:LMU:H122	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:205:ILE:HG12	18:4:206:ALA:H	1.47	0.78
1:A:502:THR:HB	1:A:504:ALA:CB	2.13	0.78
2:B:36:ASP:O	2:B:41:ARG:NE	2.17	0.78
19:2:2002:CLA:H93	19:2:2002:CLA:H51	1.65	0.78
13:N:165:ASN:OD1	13:N:167:PHE:HA	1.84	0.78
18:4:87:ASN:CB	18:4:90:TRP:CD2	2.67	0.78
16:2:254:LEU:HD22	16:2:255:ALA:H	1.49	0.78
15:1:150:HIS:CG	15:1:151:GLN:HE22	2.00	0.78
1:A:425:THR:O	1:A:427:ARG:CD	2.31	0.78
15:1:78:ARG:CG	15:1:81:GLU:OE1	2.32	0.77
1:A:190:ALA:CB	1:A:191:PRO:HD3	2.11	0.77
1:A:328:LYS:HZ3	1:A:345:GLY:CA	1.94	0.77
2:B:242:HIS:ND1	2:B:244:PHE:HA	1.99	0.77
2:B:303:TYR:HA	2:B:306:GLU:CB	2.13	0.77
20:B:5002:PQN:C16	21:B:6017:BCR:H331	2.10	0.77
2:B:648:TRP:CZ3	21:B:6017:BCR:H392	2.19	0.77
7:G:123:ASN:CA	7:G:126:ASP:OD2	2.33	0.77
4:D:167:HIS:N	4:D:168:PRO:HD2	2.00	0.77
18:4:90:TRP:C	18:4:91:PHE:HD1	1.87	0.77
1:A:484:LEU:CD2	1:A:484:LEU:N	2.47	0.77
15:1:206:SER:O	15:1:209:PRO:CD	2.32	0.77
15:1:207:ALA:C	15:1:209:PRO:HD3	2.05	0.77
22:R:7021:LMU:H31	22:R:7021:LMU:C1'	2.13	0.77
18:4:211:MET:SD	19:4:4002:CLA:CBB	2.73	0.77
1:A:291:THR:O	1:A:291:THR:HG22	1.83	0.77
19:B:1222:CLA:HED1	19:B:1223:CLA:HMD1	1.65	0.77
16:2:112:TRP:CZ3	16:2:164:GLU:HG3	2.19	0.77
1:A:40:PHE:H	1:A:44:ILE:CG2	1.97	0.77
18:4:226:LYS:N	18:4:226:LYS:CD	2.47	0.77
15:1:177:PRO:HG2	15:1:179:LYS:C	2.04	0.77
15:1:87:CYS:SG	15:1:88:ARG:N	2.58	0.77
19:B:1226:CLA:H72	23:B:7101:LMG:H311	1.66	0.77
2:B:255:LEU:CA	2:B:271:THR:HB	2.06	0.77
2:B:664:LEU:C	2:B:667:TRP:HZ3	1.87	0.77
5:E:83:TRP:N	5:E:83:TRP:CE3	2.51	0.77
16:2:222:ILE:O	16:2:226:ARG:HB2	1.83	0.77
13:N:132:THR:OG1	13:N:138:ALA:C	2.22	0.77
16:2:184:PRO:HD3	16:2:187:LYS:HG2	1.66	0.77
8:H:77:ASN:ND2	8:H:78:PRO:HG2	1.98	0.77
14:R:27:UNK:O	14:R:29:UNK:O	2.03	0.77
15:1:177:PRO:HD2	15:1:180:LEU:CA	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:183:LEU:O	15:1:184:LYS:HG2	1.85	0.77
15:1:73:PRO:O	15:1:77:GLU:HB2	1.84	0.77
19:A:1122:CLA:CHD	21:A:6007:BCR:C19	2.58	0.77
1:A:360:ILE:HD13	21:A:6007:BCR:H371	1.67	0.77
2:B:123:TRP:O	2:B:126:THR:HG22	1.84	0.77
2:B:455:ILE:HG23	6:F:148:LEU:HD11	1.67	0.77
6:F:83:THR:HB	6:F:84:PRO:HD2	1.67	0.77
7:G:84:ARG:HG3	7:G:85:GLU:HB3	1.63	0.77
19:H:1241:CLA:C3C	21:I:6021:BCR:C2	2.62	0.77
19:B:1239:CLA:H102	9:I:21:MET:SD	2.25	0.77
16:2:125:PHE:O	16:2:127:THR:HG23	1.83	0.77
13:N:150:LEU:HB2	13:N:152:LEU:HD23	1.67	0.77
2:B:154:TRP:O	2:B:157:LEU:HB3	1.84	0.77
11:K:118:VAL:HG23	11:K:121:VAL:CG2	2.11	0.77
16:2:243:GLY:C	16:2:244:THR:HG23	2.05	0.77
1:A:624:VAL:O	1:A:636:HIS:CD2	2.37	0.77
18:4:123:VAL:HG13	18:4:123:VAL:O	1.82	0.77
1:A:726:SER:O	1:A:728:VAL:N	2.18	0.77
1:A:85:GLN:C	1:A:87:SER:O	2.22	0.77
2:B:103:ALA:HB1	2:B:106:ARG:CD	2.14	0.77
19:B:1228:CLA:HBC3	19:B:1228:CLA:HHD	1.66	0.77
2:B:374:HIS:O	2:B:374:HIS:CG	2.38	0.77
19:A:9022:CLA:C11	21:B:6017:BCR:H19C	2.14	0.77
7:G:99:HIS:O	7:G:101:GLU:HB2	1.83	0.77
7:G:72:LEU:HD23	7:G:124:ILE:HG13	1.67	0.77
17:3:111:LEU:O	17:3:115:GLY:N	2.17	0.77
19:3:3011:CLA:HMA2	19:3:3011:CLA:C1	2.12	0.77
4:D:93:LYS:CG	4:D:96:VAL:HG13	2.14	0.77
10:J:5:LYS:CD	16:2:178:ASN:OD1	2.32	0.77
22:3:7003:LMU:C3B	22:3:7005:LMU:C6B	2.62	0.77
2:B:247:THR:HG22	2:B:248:GLN:H	1.49	0.77
12:L:153:PHE:CD1	12:L:155:GLU:OE1	2.38	0.77
14:R:3:UNK:O	14:R:4:UNK:CB	2.33	0.77
22:A:7010:LMU:O2B	22:A:7010:LMU:H3'	1.85	0.77
18:4:177:LEU:CG	18:4:178:PRO:CD	2.59	0.77
1:A:51:THR:CB	19:A:1139:CLA:CBB	2.63	0.77
1:A:202:MET:HG3	19:A:1111:CLA:HBC2	1.65	0.77
1:A:508:THR:O	1:A:509:ALA:CB	2.30	0.77
2:B:732:LYS:CB	2:B:733:PHE:CA	2.62	0.77
7:G:99:HIS:C	7:G:101:GLU:N	2.37	0.77
10:J:9:SER:O	10:J:10:VAL:HB	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:58:LEU:CB	8:H:61:THR:CG2	2.51	0.77
6:F:103:GLN:CD	6:F:104:ALA:H	1.87	0.77
19:J:1311:CLA:HHD	19:J:1311:CLA:HBC3	1.65	0.77
17:3:243:ILE:HG12	19:3:3005:CLA:C3C	2.14	0.77
19:4:4002:CLA:CMA	19:4:4002:CLA:HBA1	1.94	0.77
19:4:4014:CLA:CBC	19:4:4014:CLA:HHD	2.14	0.77
19:A:1103:CLA:H151	21:A:6002:BCR:H393	1.66	0.77
1:A:669:GLY:H	2:B:445:ALA:CA	1.95	0.77
2:B:174:ARG:CB	19:B:1210:CLA:HBC2	2.11	0.77
2:B:615:TYR:HD1	2:B:615:TYR:H	1.32	0.77
17:3:98:LEU:O	17:3:101:GLY:CA	2.33	0.77
18:4:87:ASN:CB	18:4:90:TRP:CZ3	2.66	0.77
15:1:170:PRO:O	15:1:173:TYR:CE2	2.38	0.77
12:L:168:GLY:C	12:L:170:LYS:N	2.35	0.77
1:A:581:CYS:CB	1:A:590:CYS:HA	2.14	0.77
19:K:3009:CLA:HBA1	19:K:3009:CLA:O2D	1.84	0.77
1:A:472:ARG:HE	1:A:474:GLN:HG3	1.49	0.77
13:N:156:GLY:HA2	13:N:157:LYS:HD2	1.64	0.77
3:C:42:ALA:HB1	3:C:43:PRO:HD2	1.65	0.77
17:3:135:ALA:HB1	17:3:139:THR:CG2	2.14	0.77
6:F:119:ILE:CG1	6:F:120:LYS:H	1.94	0.77
13:N:122:PHE:H	13:N:122:PHE:HD2	1.32	0.77
15:1:114:TRP:CZ3	15:1:121:GLN:HA	2.19	0.77
19:A:1108:CLA:HBB2	19:A:1111:CLA:HMA3	1.65	0.77
19:A:1119:CLA:C3C	19:A:1125:CLA:H172	2.15	0.77
19:B:1209:CLA:HAC2	19:B:1210:CLA:HBB2	0.81	0.77
2:B:586:THR:C	2:B:588:GLY:H	1.87	0.77
5:E:83:TRP:HE3	5:E:83:TRP:H	1.29	0.77
16:2:224:ASN:O	16:2:227:LEU:HB3	1.85	0.77
18:4:103:MET:HE3	18:4:208:GLY:HA3	1.63	0.77
19:B:1222:CLA:HED1	19:B:1223:CLA:CMD	2.15	0.77
2:B:261:PHE:HE2	2:B:499:ASN:C	1.87	0.77
2:B:374:HIS:HB2	19:B:1224:CLA:NB	2.00	0.77
3:C:8:TYR:O	3:C:60:THR:HA	1.85	0.77
17:3:134:LEU:N	17:3:134:LEU:HD12	2.00	0.77
19:K:1142:CLA:CMD	19:K:1143:CLA:NA	2.47	0.77
2:B:160:LYS:HD3	2:B:161:TRP:CZ2	2.20	0.77
17:3:207:PHE:HD1	17:3:207:PHE:C	1.84	0.77
3:C:33:GLY:HA2	3:C:37:LYS:HE2	1.67	0.77
2:B:130:ARG:NH1	2:B:130:ARG:HG3	1.99	0.77
11:K:89:ARG:CG	11:K:89:ARG:HH11	1.98	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:314:ARG:HH12	15:1:67:LEU:CG	1.98	0.76
19:4:1306:CLA:HBC3	19:4:1306:CLA:CMC	2.12	0.76
19:A:1124:CLA:CED	19:A:1125:CLA:C3D	2.58	0.76
19:A:9023:CLA:CBC	19:A:9023:CLA:HMC1	2.16	0.76
2:B:267:SER:HB2	2:B:356:PRO:O	1.84	0.76
19:A:9022:CLA:H101	21:B:6017:BCR:H17C	1.68	0.76
2:B:732:LYS:CB	2:B:733:PHE:HA	2.14	0.76
7:G:120:VAL:HG12	7:G:120:VAL:O	1.84	0.76
11:K:47:ASP:CA	11:K:51:SER:HB2	2.15	0.76
5:E:79:LYS:CA	5:E:84:TYR:HE1	1.99	0.76
4:D:158:PHE:HB3	4:D:159:PRO:CD	2.08	0.76
4:D:156:ARG:NH2	4:D:163:VAL:O	2.18	0.76
19:1:1303:CLA:HMC1	19:4:1304:CLA:HMB3	1.66	0.76
19:A:1125:CLA:CBC	19:A:1125:CLA:HMC1	2.15	0.76
1:A:284:ARG:HA	1:A:284:ARG:CZ	2.14	0.76
1:A:295:TRP:O	1:A:298:ASP:OD2	2.03	0.76
2:B:293:THR:O	2:B:295:PHE:CD2	2.38	0.76
2:B:87:ILE:HA	2:B:115:ASN:HB2	1.66	0.76
1:A:714:LEU:HD13	21:F:6016:BCR:C39	2.15	0.76
21:J:6012:BCR:C23	21:J:6012:BCR:H393	2.14	0.76
16:2:107:LEU:HD12	16:2:108:VAL:N	1.99	0.76
13:N:143:VAL:CB	13:N:144:PRO:CD	2.62	0.76
16:2:182:ILE:C	16:2:187:LYS:HG3	2.05	0.76
2:B:247:THR:HG23	2:B:248:GLN:N	1.94	0.76
4:D:103:THR:CG2	4:D:128:LEU:HG	2.15	0.76
16:2:195:TYR:CE2	16:2:198:GLY:HA3	2.20	0.76
19:3:3016:CLA:H142	19:3:3016:CLA:H101	1.64	0.76
19:A:1117:CLA:H8	19:A:1117:CLA:HBB2	1.65	0.76
19:A:1134:CLA:O1A	19:A:1141:CLA:HBB1	1.84	0.76
1:A:534:LEU:CD1	1:A:535:GLY:H	1.90	0.76
1:A:56:ASN:O	1:A:57:LEU:CB	2.24	0.76
2:B:174:ARG:O	2:B:175:LEU:HB3	1.85	0.76
7:G:124:ILE:CG1	7:G:128:LEU:CD1	2.62	0.76
7:G:64:ILE:O	7:G:64:ILE:HG13	1.83	0.76
6:F:200:VAL:HG11	10:J:7:TYR:CB	2.11	0.76
11:K:50:GLY:C	11:K:52:PRO:HD2	2.06	0.76
12:L:115:VAL:HG11	12:L:130:GLY:N	1.95	0.76
19:L:1148:CLA:CHD	19:L:1148:CLA:CBC	2.62	0.76
16:2:172:LEU:CB	16:2:173:ASN:ND2	2.48	0.76
1:A:426:THR:CA	1:A:428:TYR:CZ	2.69	0.76
1:A:525:ASN:HD22	1:A:526:LYS:HE3	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:7023:LMU:H6'2	22:A:7023:LMU:H2B	1.68	0.76
15:1:177:PRO:CD	15:1:180:LEU:HD23	2.15	0.76
1:A:127:VAL:CG2	19:A:1107:CLA:CBB	2.63	0.76
1:A:368:LEU:CD1	19:A:1125:CLA:H61	2.15	0.76
1:A:150:PHE:N	1:A:153:TRP:HB2	2.01	0.76
1:A:343:HIS:O	1:A:346:LEU:CB	2.33	0.76
1:A:411:ALA:HB2	21:A:6008:BCR:C39	2.16	0.76
1:A:746:THR:HA	1:A:749:PHE:HB3	1.66	0.76
4:D:100:TYR:CD1	4:D:134:LYS:CG	2.66	0.76
17:3:161:GLU:OE1	17:3:162:MET:HA	1.84	0.76
12:L:54:TYR:CE1	12:L:57:ILE:HG23	2.19	0.76
1:A:351:THR:C	19:A:1123:CLA:H191	2.05	0.76
21:A:6002:BCR:C12	21:A:6002:BCR:H341	2.15	0.76
2:B:655:LEU:CD2	19:B:1239:CLA:HBB1	2.15	0.76
6:F:139:LEU:CD1	6:F:149:ILE:HD13	2.15	0.76
10:J:23:ALA:O	10:J:26:LEU:HB3	1.85	0.76
17:3:109:ALA:O	17:3:111:LEU:HB3	1.86	0.76
19:3:3011:CLA:CBC	19:3:3012:CLA:CHA	2.63	0.76
14:R:34:UNK:H	14:R:36:UNK:CB	1.99	0.76
13:N:110:THR:CG2	13:N:111:GLY:N	2.47	0.76
22:K:7001:LMU:H81	22:K:7001:LMU:H42	1.67	0.76
12:L:153:PHE:CA	12:L:179:ALA:HB2	2.10	0.76
1:A:23:ASP:CG	1:A:33:GLN:CG	2.54	0.76
16:2:261:THR:HG22	16:2:262:ILE:N	1.98	0.76
4:D:101:VAL:HG12	4:D:130:LYS:CB	2.16	0.76
15:1:73:PRO:CG	15:1:74:ALA:N	2.49	0.76
1:A:193:LEU:HA	1:A:196:PHE:CE2	2.18	0.76
1:A:279:ASP:C	1:A:281:LEU:HG	2.06	0.76
2:B:292:ARG:NH2	2:B:297:ILE:N	2.33	0.76
2:B:353:TYR:O	2:B:354:SER:HB2	1.84	0.76
2:B:517:PHE:O	2:B:517:PHE:HD2	1.66	0.76
2:B:732:LYS:HG2	2:B:733:PHE:CA	2.15	0.76
7:G:88:ALA:HB3	7:G:90:GLN:O	1.86	0.76
19:1:1010:CLA:HBA2	19:1:1010:CLA:HMA2	1.65	0.76
14:R:37:UNK:O	14:R:42:UNK:C	2.34	0.76
4:D:140:LEU:HD13	4:D:144:LEU:CB	2.11	0.76
17:3:125:VAL:HG11	19:3:3010:CLA:CHC	2.16	0.76
17:3:177:ALA:O	17:3:178:LYS:HB2	1.84	0.76
18:4:246:GLN:HG2	18:4:246:GLN:O	1.84	0.76
1:A:270:PHE:CE1	19:A:1141:CLA:H2	2.21	0.76
2:B:203:ARG:HH22	2:B:254:ILE:HG22	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:697:ARG:NH2	2:B:566:GLY:O	2.17	0.76
7:G:63:VAL:CG2	7:G:64:ILE:N	2.45	0.76
11:K:76:ALA:N	11:K:78:ARG:HH12	1.81	0.76
12:L:129:ALA:O	12:L:201:TYR:CB	2.25	0.76
16:2:128:LYS:CB	16:2:131:ILE:HG12	2.16	0.76
5:E:89:SER:O	5:E:105:VAL:HB	1.86	0.76
19:1:1010:CLA:CHD	19:1:1010:CLA:CBC	2.63	0.76
2:B:69:ALA:HB1	2:B:135:LEU:HD12	1.65	0.76
1:A:389:TYR:HE1	1:A:625:TRP:CD1	2.03	0.76
15:1:157:ASP:OD1	15:1:175:LYS:HE3	1.86	0.76
1:A:431:LEU:O	1:A:435:VAL:HG12	1.85	0.76
1:A:457:SER:O	1:A:544:ILE:HD13	1.85	0.76
2:B:493:TRP:HE1	19:B:1213:CLA:CAC	1.99	0.76
19:A:1237:CLA:HMC2	19:B:1238:CLA:H11	1.68	0.76
2:B:233:TYR:CD1	2:B:254:ILE:HG13	2.20	0.76
2:B:387:PHE:O	2:B:391:PRO:HD3	1.86	0.76
5:E:90:VAL:O	5:E:91:VAL:CG2	2.34	0.76
8:H:109:LEU:HD23	19:H:1207:CLA:C7	2.14	0.76
6:F:200:VAL:HG12	10:J:7:TYR:CA	2.15	0.76
4:D:156:ARG:HB2	4:D:166:LEU:CD1	2.15	0.76
16:2:184:PRO:CG	16:2:187:LYS:N	2.49	0.76
2:B:160:LYS:NZ	2:B:161:TRP:CD2	2.54	0.76
1:A:23:ASP:HB3	1:A:33:GLN:OE1	1.84	0.76
4:D:147:LYS:C	4:D:148:TYR:CG	2.57	0.76
15:1:78:ARG:CD	19:1:1011:CLA:CMC	2.64	0.76
18:4:173:LYS:CB	18:4:194:PHE:HD2	1.97	0.76
19:A:1105:CLA:CMB	21:J:6012:BCR:HC7	2.15	0.76
1:A:92:TRP:CD1	19:A:1105:CLA:HBB2	2.20	0.76
1:A:98:PHE:O	1:A:99:HIS:C	2.24	0.76
2:B:229:GLN:O	7:G:63:VAL:CG2	2.34	0.76
5:E:111:ASN:ND2	5:E:113:ALA:N	2.31	0.76
9:I:11:LEU:HD12	21:I:6021:BCR:C10	2.15	0.76
5:E:89:SER:OG	5:E:106:ARG:NE	2.15	0.76
4:D:128:LEU:HD23	4:D:128:LEU:O	1.85	0.76
19:1:1303:CLA:HMC1	19:1:1303:CLA:CBC	2.14	0.76
2:B:69:ALA:CB	2:B:135:LEU:HD12	2.15	0.76
15:1:69:LEU:CA	15:1:73:PRO:HD3	2.16	0.76
1:A:170:GLY:O	1:A:173:VAL:HG22	1.86	0.76
1:A:281:LEU:HD22	19:A:1115:CLA:CMA	2.11	0.76
1:A:217:SER:OG	21:A:6002:BCR:C17	2.34	0.76
1:A:661:ALA:HA	1:A:664:VAL:HG13	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:603:PHE:CZ	1:A:735:VAL:HG22	2.21	0.76
2:B:469:LYS:HB3	2:B:470:THR:OG1	1.86	0.76
2:B:500:ALA:O	2:B:501:ILE:CG1	2.31	0.76
2:B:510:LEU:HD11	2:B:597:LYS:NZ	2.00	0.76
21:B:6006:BCR:HC8	21:B:6006:BCR:H331	1.66	0.76
6:F:207:LEU:HD21	6:F:208:PHE:HD1	1.48	0.76
5:E:89:SER:CB	5:E:106:ARG:CD	2.61	0.76
4:D:99:PHE:HB3	4:D:157:VAL:HB	1.67	0.76
16:2:160:ILE:CB	19:2:2012:CLA:CBB	2.64	0.76
10:J:5:LYS:HD2	16:2:178:ASN:CA	2.15	0.76
22:1:7004:LMU:O2'	22:1:7004:LMU:H11	1.84	0.76
13:N:122:PHE:N	13:N:122:PHE:CD2	2.36	0.76
15:1:84:LEU:O	15:1:87:CYS:SG	2.44	0.75
1:A:163:GLN:CG	1:A:164:LEU:N	2.37	0.75
1:A:187:HIS:HE1	19:A:1109:CLA:C4D	1.86	0.75
2:B:200:PRO:O	2:B:204:GLY:CA	2.33	0.75
2:B:545:LYS:CG	2:B:546:LEU:N	2.48	0.75
1:A:475:ASP:OD2	12:L:120:LEU:HA	1.85	0.75
4:D:138:LEU:C	4:D:140:LEU:O	2.25	0.75
11:K:127:ILE:O	11:K:130:LEU:HD23	1.86	0.75
6:F:129:ARG:HB3	6:F:133:TYR:CZ	2.21	0.75
6:F:225:GLU:N	6:F:227:VAL:HG12	2.01	0.75
19:A:1105:CLA:HBA2	19:A:1107:CLA:H12	1.68	0.75
19:A:1106:CLA:HMB1	19:A:1107:CLA:H11	1.68	0.75
1:A:127:VAL:HG21	19:A:1107:CLA:HBB2	1.69	0.75
19:A:9022:CLA:H93	19:A:9023:CLA:C9	2.11	0.75
2:B:459:PHE:CB	19:B:1235:CLA:CAD	2.64	0.75
6:F:160:PHE:O	6:F:164:GLY:HA3	1.86	0.75
6:F:173:TRP:CE3	6:F:211:PHE:N	2.54	0.75
19:3:3008:CLA:HMC1	19:3:3008:CLA:CBC	2.13	0.75
19:2:2014:CLA:C15	19:2:2014:CLA:H102	2.15	0.75
12:L:175:GLN:O	12:L:176:LEU:HB2	1.86	0.75
19:A:1136:CLA:H171	19:L:1504:CLA:HBB2	1.67	0.75
1:A:701:GLN:OE1	5:E:112:TYR:OH	2.01	0.75
2:B:257:ILE:C	2:B:497:TRP:CZ3	2.57	0.75
2:B:709:GLY:O	2:B:710:LEU:HB2	1.84	0.75
8:H:98:LEU:HD22	12:L:146:THR:HG21	1.69	0.75
19:2:2007:CLA:HBC2	19:3:2009:CLA:CED	1.89	0.75
13:N:146:LEU:HD21	17:3:142:ILE:O	1.84	0.75
13:N:157:LYS:CB	13:N:159:LYS:H	1.98	0.75
16:2:184:PRO:CD	16:2:187:LYS:CD	2.63	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:115:ILE:HG12	11:K:121:VAL:C	2.06	0.75
1:A:425:THR:C	1:A:428:TYR:CE1	2.60	0.75
19:J:1311:CLA:O1A	19:J:1311:CLA:H143	1.86	0.75
1:A:624:VAL:O	1:A:636:HIS:HD2	1.69	0.75
12:L:55:GLN:C	12:L:57:ILE:H	1.90	0.75
1:A:422:TYR:H	1:A:422:TYR:HD1	0.82	0.75
1:A:523:VAL:HG13	1:A:524:GLY:H	1.49	0.75
22:4:7034:LMU:C8	22:4:7052:LMU:C1'	2.58	0.75
18:4:177:LEU:CD2	18:4:178:PRO:CD	2.64	0.75
2:B:679:ALA:O	2:B:683:GLU:CD	2.25	0.75
5:E:74:VAL:HG22	5:E:90:VAL:HG22	1.67	0.75
6:F:207:LEU:CD2	6:F:208:PHE:CD1	2.69	0.75
7:G:102:ALA:HA	7:G:104:ASP:OD2	1.85	0.75
7:G:84:ARG:HA	19:G:1242:CLA:CMA	2.16	0.75
8:H:97:LEU:CD1	8:H:100:PHE:HB3	2.13	0.75
11:K:63:LEU:H	11:K:63:LEU:CD2	1.90	0.75
11:K:84:LEU:HG	11:K:85:LYS:CG	2.10	0.75
19:3:3008:CLA:CGD	19:3:3008:CLA:CBA	2.64	0.75
19:4:4015:CLA:HHD	19:4:4015:CLA:HBC3	1.68	0.75
19:A:1124:CLA:C6	19:A:1125:CLA:HED1	2.15	0.75
19:A:1124:CLA:HBA2	19:A:1137:CLA:CED	2.16	0.75
1:A:196:PHE:HD2	1:A:196:PHE:H	1.33	0.75
1:A:349:ILE:HG22	1:A:350:LEU:CA	2.16	0.75
1:A:154:ARG:CZ	1:A:384:TYR:CE1	2.68	0.75
2:B:88:ALA:H	2:B:115:ASN:HA	1.50	0.75
2:B:323:TYR:O	2:B:327:ASN:HB2	1.86	0.75
1:A:128:GLY:HA3	2:B:446:PHE:CD2	2.21	0.75
20:B:5002:PQN:H162	21:B:6017:BCR:H331	1.62	0.75
5:E:91:VAL:HG12	5:E:92:ALA:H	1.51	0.75
2:B:694:ARG:HD3	9:I:28:VAL:HG13	1.67	0.75
15:1:134:LEU:N	15:1:135:PRO:HD3	2.00	0.75
4:D:103:THR:HG21	4:D:128:LEU:CD1	2.16	0.75
12:L:153:PHE:HD1	12:L:155:GLU:OE1	1.70	0.75
11:K:127:ILE:HB	11:K:129:ALA:CB	2.16	0.75
2:B:628:SER:O	2:B:629:SER:C	2.24	0.75
19:4:4003:CLA:HMC1	19:4:4003:CLA:CBC	2.14	0.75
1:A:163:GLN:O	1:A:166:CYS:N	2.07	0.75
2:B:53:GLN:C	2:B:55:ALA:H	1.90	0.75
9:I:8:PHE:CB	19:I:1204:CLA:OBD	2.34	0.75
2:B:694:ARG:HD3	9:I:28:VAL:CG1	2.17	0.75
1:A:485:GLN:N	1:A:485:GLN:CD	2.40	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:77:GLU:HA	15:1:80:LYS:HD2	1.69	0.75
18:4:172:PHE:CD1	18:4:173:LYS:O	2.40	0.75
19:A:1124:CLA:H43	19:A:1136:CLA:HBA1	1.67	0.75
1:A:240:LYS:H	1:A:243:PRO:HD2	1.48	0.75
1:A:308:ILE:O	1:A:312:ILE:N	2.16	0.75
1:A:349:ILE:HG22	1:A:350:LEU:HA	1.67	0.75
19:A:9012:CLA:HED2	19:A:9012:CLA:CAD	2.16	0.75
1:A:470:LEU:HD11	2:B:95:HIS:HB3	1.68	0.75
13:N:156:GLY:N	13:N:157:LYS:HE2	2.02	0.75
3:C:25:VAL:HA	3:C:43:PRO:CG	2.17	0.75
13:N:104:LYS:N	13:N:107:LEU:HD13	2.02	0.75
16:2:182:ILE:C	16:2:187:LYS:HG2	2.07	0.75
11:K:115:ILE:CA	11:K:118:VAL:CG2	2.59	0.75
1:A:555:ILE:HD13	19:A:9023:CLA:CMD	2.17	0.75
1:A:700:TRP:O	1:A:704:ILE:HB	1.87	0.75
19:B:1222:CLA:H52	19:B:1236:CLA:CAD	2.17	0.75
19:B:1222:CLA:HBC2	19:B:1222:CLA:CHD	2.12	0.75
2:B:625:TRP:HE3	2:B:626:LEU:N	1.85	0.75
22:G:7026:LMU:H82	22:G:7026:LMU:H41	1.69	0.75
16:2:229:MET:SD	16:2:230:LEU:CD1	2.75	0.75
4:D:93:LYS:HG2	4:D:96:VAL:HG13	1.67	0.75
16:2:184:PRO:CD	16:2:187:LYS:HG2	2.16	0.75
19:2:2013:CLA:HMC1	19:2:2013:CLA:CBC	2.17	0.75
12:L:211:TYR:CD2	12:L:211:TYR:N	2.49	0.75
19:A:1117:CLA:H121	19:A:1117:CLA:HBB2	1.68	0.75
1:A:93:LEU:HA	1:A:96:MET:HB2	1.69	0.75
19:B:1205:CLA:HBA1	19:B:1224:CLA:OBD	1.87	0.75
7:G:63:VAL:HG23	7:G:64:ILE:N	2.01	0.75
6:F:88:SER:OG	6:F:91:PHE:CB	2.35	0.75
19:A:1126:CLA:C20	21:J:6012:BCR:H17C	2.17	0.74
1:A:284:ARG:HB3	1:A:295:TRP:CD1	2.22	0.74
1:A:336:GLY:HA3	19:A:1151:CLA:HMC2	1.69	0.74
1:A:514:THR:O	1:A:531:PRO:O	2.05	0.74
1:A:711:HIS:HB3	1:A:717:ALA:HB2	1.66	0.74
21:A:6011:BCR:C31	19:A:9013:CLA:H142	2.17	0.74
2:B:87:ILE:HA	2:B:115:ASN:CB	2.15	0.74
2:B:308:HIS:ND1	2:B:309:ILE:N	2.32	0.74
2:B:461:GLN:O	2:B:464:GLN:HG2	1.86	0.74
12:L:128:GLN:CA	12:L:130:GLY:HA3	2.14	0.74
12:L:67:GLY:O	12:L:68:SER:HB3	1.86	0.74
13:N:132:THR:HA	13:N:136:ASP:OD1	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:73:THR:OG1	3:C:76:SER:N	2.20	0.74
18:4:87:ASN:CG	18:4:90:TRP:CD2	2.59	0.74
17:3:156:THR:C	17:3:158:PHE:O	2.25	0.74
19:R:1150:CLA:HBA2	19:R:1150:CLA:CBD	2.16	0.74
1:A:168:ALA:O	1:A:171:ALA:HB3	1.86	0.74
19:A:1124:CLA:C4B	21:A:6008:BCR:H373	2.17	0.74
19:A:1124:CLA:HED3	19:A:1125:CLA:HMD1	1.68	0.74
1:A:209:GLY:HA2	1:A:213:LEU:HD13	1.68	0.74
19:B:1203:CLA:HBB2	19:B:1225:CLA:HHC	1.68	0.74
3:C:52:LYS:HE3	3:C:64:SER:HB3	1.69	0.74
22:3:7003:LMU:C3B	22:3:7005:LMU:H6'1	2.09	0.74
22:B:7040:LMU:H1B	22:B:7040:LMU:O3'	1.87	0.74
1:A:63:ASP:HB2	19:A:1128:CLA:HED3	1.69	0.74
1:A:129:GLN:O	1:A:130:GLU:CB	2.35	0.74
6:F:180:SER:C	6:F:182:LEU:H	1.91	0.74
6:F:207:LEU:CD2	6:F:208:PHE:N	2.50	0.74
16:2:117:ALA:HB1	16:2:230:LEU:CD1	2.17	0.74
4:D:159:PRO:O	4:D:159:PRO:CD	2.34	0.74
17:3:191:GLU:O	17:3:191:GLU:HG2	1.85	0.74
12:L:172:GLU:O	12:L:173:PRO:C	2.24	0.74
19:R:1144:CLA:CHA	19:R:1144:CLA:CED	2.65	0.74
7:G:145:THR:HG23	7:G:146:SER:H	1.50	0.74
14:R:44:UNK:O	14:R:45:UNK:C	2.35	0.74
15:1:178:LYS:C	15:1:178:LYS:HD2	2.08	0.74
15:1:97:ILE:HD12	15:1:98:LEU:CB	2.17	0.74
18:4:159:ASP:OD2	18:4:163:PRO:HA	1.86	0.74
1:A:284:ARG:CZ	1:A:284:ARG:C	2.56	0.74
21:A:6008:BCR:C33	21:A:6008:BCR:HC8	2.15	0.74
1:A:25:ASP:OD1	1:A:26:PRO:HG3	1.87	0.74
3:C:62:PHE:CD1	4:D:191:ILE:HG22	2.21	0.74
13:N:155:GLU:HB3	13:N:157:LYS:HE2	1.67	0.74
4:D:156:ARG:NH1	4:D:158:PHE:CD1	2.37	0.74
16:2:153:PHE:CE2	16:2:157:LEU:CD2	2.70	0.74
17:3:150:TYR:CD1	17:3:151:TRP:N	2.54	0.74
14:R:24:UNK:O	14:R:27:UNK:CB	2.35	0.74
1:A:479:ASP:HA	1:A:536:THR:CG2	2.15	0.74
21:A:6011:BCR:C23	21:A:6011:BCR:H393	2.15	0.74
2:B:314:ARG:HH22	15:1:67:LEU:HG	1.51	0.74
2:B:500:ALA:HB1	2:B:503:GLU:OE2	1.87	0.74
13:N:147:SER:HB2	13:N:151:ASP:OD1	1.88	0.74
3:C:24:ASP:CB	24:C:8002:SF4:S2	2.73	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:K:7042:LMU:H32	22:K:7042:LMU:C6'	2.18	0.74
1:A:513:LEU:O	1:A:513:LEU:HD12	1.86	0.74
18:4:201:LYS:HG2	18:4:201:LYS:O	1.86	0.74
19:A:1102:CLA:C1	19:A:1109:CLA:H61	2.12	0.74
19:A:1133:CLA:CBC	19:A:1133:CLA:HMC1	2.17	0.74
1:A:452:PHE:HE1	19:A:1136:CLA:CBB	1.99	0.74
2:B:310:PRO:O	19:B:1301:CLA:HHD	1.86	0.74
2:B:295:PHE:N	2:B:295:PHE:HD2	1.85	0.74
2:B:390:GLY:O	21:B:6010:BCR:HC42	1.86	0.74
7:G:89:LYS:N	7:G:89:LYS:HZ2	1.84	0.74
16:2:218:ARG:HB2	16:2:219:THR:HG23	1.68	0.74
17:3:96:ARG:NH1	17:3:100:TYR:CZ	2.47	0.74
6:F:103:GLN:HG3	6:F:104:ALA:N	1.99	0.74
6:F:89:LYS:HG2	6:F:90:GLN:H	1.51	0.74
15:1:147:PHE:C	15:1:147:PHE:CD1	2.60	0.74
1:A:423:ASP:CB	1:A:424:PRO:CD	2.63	0.74
1:A:523:VAL:CG1	1:A:524:GLY:N	2.51	0.74
14:R:7:UNK:O	14:R:11:UNK:N	2.20	0.74
15:1:123:THR:HG22	15:1:124:TYR:O	1.86	0.74
1:A:163:GLN:HA	1:A:166:CYS:HG	1.52	0.74
1:A:283:PHE:O	1:A:284:ARG:NH1	2.19	0.74
1:A:328:LYS:HZ2	1:A:345:GLY:CA	1.99	0.74
1:A:693:LEU:HD21	1:A:735:VAL:H	1.51	0.74
2:B:216:LEU:CD2	2:B:218:TYR:O	2.31	0.74
2:B:295:PHE:HE2	7:G:94:GLN:HE22	1.35	0.74
2:B:317:ARG:NE	2:B:317:ARG:HA	2.02	0.74
5:E:74:VAL:HG22	5:E:90:VAL:CG2	2.17	0.74
2:B:230:TRP:CH2	7:G:67:SER:HB2	2.21	0.74
22:2:7006:LMU:C2'	22:2:7006:LMU:H22	2.18	0.74
8:H:77:ASN:CG	8:H:78:PRO:CD	2.55	0.74
2:B:160:LYS:CE	2:B:161:TRP:CE3	2.71	0.74
11:K:115:ILE:C	11:K:118:VAL:HG22	2.08	0.74
8:H:112:LEU:N	8:H:112:LEU:CD2	2.51	0.74
15:1:83:GLU:HA	15:1:83:GLU:OE2	1.87	0.74
1:A:336:GLY:HA2	19:A:1151:CLA:CMC	2.18	0.74
1:A:336:GLY:CA	19:A:1151:CLA:HMC2	2.18	0.74
1:A:208:ALA:HB2	1:A:314:GLY:HA3	1.68	0.74
1:A:349:ILE:O	1:A:352:THR:N	2.21	0.74
1:A:470:LEU:HD13	2:B:95:HIS:HB3	1.68	0.74
1:A:542:HIS:HA	1:A:545:HIS:HD2	1.53	0.74
1:A:733:VAL:HG21	19:A:1140:CLA:CMD	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:10:GLN:O	2:B:14:GLN:NE2	2.20	0.74
2:B:25:ILE:CG2	21:L:6019:BCR:H282	2.18	0.74
8:H:67:SER:O	8:H:68:TYR:CG	2.41	0.74
8:H:77:ASN:HD21	8:H:78:PRO:HG2	1.51	0.74
22:F:7036:LMU:O2B	22:F:7036:LMU:H4'	1.87	0.74
16:2:246:PRO:HB2	16:2:247:ILE:HG12	1.70	0.74
12:L:164:LEU:CB	12:L:165:THR:HG23	2.16	0.74
1:A:41:SER:O	1:A:44:ILE:HA	1.88	0.74
15:1:73:PRO:HG2	15:1:74:ALA:N	2.03	0.74
19:A:1101:CLA:H42	19:A:1140:CLA:C6	2.07	0.74
1:A:281:LEU:CD1	19:A:1115:CLA:HED2	1.94	0.74
1:A:296:LEU:HD12	1:A:296:LEU:C	2.08	0.74
2:B:53:GLN:HE21	19:B:1201:CLA:HBB1	1.50	0.74
2:B:330:ILE:HD11	19:B:1202:CLA:C19	2.18	0.74
2:B:527:LEU:CD2	19:B:1222:CLA:ND	2.50	0.74
2:B:469:LYS:HZ3	2:B:471:THR:H	1.34	0.74
2:B:504:ASN:CG	2:B:504:ASN:O	2.25	0.74
2:B:429:LEU:C	2:B:525:LEU:CD1	2.53	0.74
12:L:141:LEU:CD1	21:L:6019:BCR:C31	2.65	0.74
12:L:190:PHE:CZ	12:L:194:ILE:HD12	2.21	0.74
16:2:220:LYS:NZ	19:2:2004:CLA:OBD	2.15	0.74
4:D:167:HIS:NE2	4:D:172:VAL:CG2	2.50	0.74
17:3:101:GLY:HA2	17:3:104:ILE:CD1	2.18	0.74
16:2:184:PRO:CD	16:2:185:ASN:C	2.53	0.74
18:4:141:LEU:N	18:4:141:LEU:CD2	2.48	0.74
22:H:7030:LMU:H52	22:H:7030:LMU:C9	2.16	0.74
19:3:3016:CLA:C10	19:3:3016:CLA:C14	2.57	0.74
2:B:70:TRP:CD1	2:B:71:GLN:OE1	2.40	0.74
18:4:123:VAL:N	18:4:124:PRO:CD	2.51	0.74
15:1:225:TRP:HD1	15:1:226:HIS:CE1	2.06	0.74
1:A:692:PHE:CE2	19:A:1140:CLA:HBC3	2.23	0.74
19:A:1140:CLA:C14	21:A:6011:BCR:C2	2.62	0.74
19:B:1220:CLA:H102	19:B:1220:CLA:C15	2.12	0.74
2:B:32:GLU:HG2	2:B:42:LEU:CD2	2.18	0.74
6:F:173:TRP:HE3	6:F:211:PHE:N	1.86	0.74
13:N:165:ASN:C	13:N:167:PHE:N	2.39	0.74
17:3:197:SER:OG	17:3:206:PRO:CD	2.35	0.74
1:A:316:MET:HG2	1:A:317:TYR:CE1	2.21	0.74
15:1:78:ARG:HG2	19:1:1011:CLA:HMC1	1.69	0.73
2:B:90:ALA:HA	2:B:113:VAL:CG1	2.02	0.73
7:G:128:LEU:HD23	7:G:128:LEU:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:139:LYS:CE	13:N:142:LYS:CE	2.51	0.73
3:C:26:LEU:H	3:C:43:PRO:HG3	1.53	0.73
3:C:73:THR:HG23	3:C:76:SER:OG	1.87	0.73
4:D:100:TYR:HE1	4:D:134:LYS:CG	2.01	0.73
16:2:254:LEU:C	16:2:254:LEU:HD23	2.05	0.73
22:E:7037:LMU:H51	22:E:7037:LMU:H12	1.69	0.73
19:A:1136:CLA:H192	19:L:1130:CLA:CBB	2.18	0.73
21:A:6002:BCR:C34	21:A:6002:BCR:H12C	2.17	0.73
2:B:349:ALA:HB2	2:B:375:HIS:HB3	1.69	0.73
2:B:711:VAL:HG12	2:B:711:VAL:O	1.85	0.73
7:G:98:THR:OG1	7:G:101:GLU:CB	2.35	0.73
17:3:111:LEU:C	17:3:114:VAL:H	1.91	0.73
14:R:35:UNK:O	14:R:36:UNK:C	2.35	0.73
12:L:155:GLU:HA	12:L:178:THR:HG21	1.68	0.73
4:D:148:TYR:O	4:D:149:LYS:HG2	1.89	0.73
8:H:70:SER:O	8:H:73:PRO:CD	2.37	0.73
2:B:516:ASP:O	2:B:520:HIS:HB2	1.88	0.73
1:A:591:GLN:HA	1:A:591:GLN:HE21	1.53	0.73
18:4:100:ARG:O	18:4:104:LEU:HD12	1.89	0.73
19:A:1124:CLA:CBC	19:A:1124:CLA:HHD	2.15	0.73
1:A:218:TRP:O	1:A:222:GLN:HB2	1.87	0.73
22:G:7026:LMU:C5	22:G:7026:LMU:H12	2.17	0.73
19:L:1130:CLA:HAC2	19:L:1504:CLA:HMC3	1.70	0.73
5:E:78:ARG:HH12	5:E:125:ILE:HG21	1.51	0.73
13:N:157:LYS:HB3	13:N:158:ASP:CA	2.18	0.73
3:C:44:ARG:CB	4:D:182:GLN:OE1	2.37	0.73
3:C:67:VAL:HG13	3:C:68:TYR:HA	1.70	0.73
4:D:167:HIS:NE2	4:D:172:VAL:HG21	2.02	0.73
3:C:42:ALA:O	4:D:183:GLY:HA3	1.88	0.73
17:3:96:ARG:HA	17:3:99:ALA:H	1.41	0.73
19:3:3013:CLA:O1D	19:3:3013:CLA:H2A	1.88	0.73
2:B:550:LYS:HG2	2:B:550:LYS:O	1.87	0.73
18:4:232:LEU:HD12	18:4:234:GLN:HA	1.69	0.73
16:2:139:THR:CG2	16:2:140:ALA:N	2.51	0.73
16:2:212:GLN:HG2	16:2:213:LYS:HG2	1.71	0.73
18:4:211:MET:CG	19:4:4002:CLA:CBB	2.65	0.73
19:A:1107:CLA:CBB	19:B:1230:CLA:HMD2	2.18	0.73
1:A:150:PHE:N	1:A:153:TRP:HE3	1.86	0.73
1:A:284:ARG:CZ	1:A:284:ARG:O	2.35	0.73
4:D:167:HIS:CE1	4:D:172:VAL:CG1	2.58	0.73
14:R:38:UNK:O	14:R:41:UNK:CB	2.36	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:170:PRO:HD2	15:1:173:TYR:HE2	1.49	0.73
2:B:75:GLU:HB2	2:B:132:ASN:CB	2.19	0.73
17:3:201:ALA:CA	17:3:202:TYR:HD2	2.02	0.73
17:3:210:PRO:CD	17:3:211:LEU:H	2.02	0.73
18:4:173:LYS:HB2	18:4:194:PHE:CD2	2.22	0.73
18:4:201:LYS:N	18:4:201:LYS:HD3	2.03	0.73
1:A:217:SER:HA	21:A:6002:BCR:H351	1.68	0.73
1:A:73:GLU:OE1	1:A:186:TYR:OH	2.07	0.73
1:A:89:ILE:O	1:A:93:LEU:HD22	1.89	0.73
19:A:9023:CLA:O2A	19:A:9023:CLA:H3A	1.87	0.73
7:G:137:VAL:O	7:G:137:VAL:HG23	1.87	0.73
4:D:174:PRO:C	4:D:175:GLU:HG2	2.08	0.73
19:1:1002:CLA:HMC1	19:1:1002:CLA:HBC3	1.71	0.73
19:J:1308:CLA:H91	19:2:2014:CLA:O1D	1.87	0.73
1:A:258:LEU:O	1:A:259:TYR:HB2	1.87	0.73
1:A:29:THR:HG23	1:A:29:THR:O	1.89	0.73
19:A:1119:CLA:CBA	19:A:1123:CLA:HBB2	2.18	0.73
19:A:1125:CLA:HBB2	19:A:1133:CLA:C3A	2.14	0.73
1:A:293:GLY:O	1:A:294:LEU:CB	2.37	0.73
1:A:328:LYS:NZ	1:A:345:GLY:HA3	2.01	0.73
21:A:6002:BCR:H373	19:3:1147:CLA:HBC1	1.68	0.73
19:A:9012:CLA:C3B	2:B:589:TRP:HH2	2.02	0.73
2:B:11:GLY:CA	3:C:71:HIS:CD2	2.61	0.73
19:B:1205:CLA:H102	19:B:1205:CLA:H142	1.71	0.73
2:B:486:LEU:CD1	2:B:489:GLY:N	2.49	0.73
2:B:545:LYS:HG2	2:B:546:LEU:N	2.01	0.73
7:G:99:HIS:O	7:G:101:GLU:CB	2.36	0.73
12:L:110:LEU:HA	12:L:113:PRO:HG2	1.71	0.73
3:C:52:LYS:O	3:C:52:LYS:CG	2.37	0.73
3:C:73:THR:HG21	3:C:76:SER:HB3	1.70	0.73
12:L:210:PRO:O	12:L:211:TYR:CG	2.42	0.73
8:H:80:GLN:HA	8:H:83:LEU:HD23	1.70	0.73
16:2:269:LYS:CA	16:2:269:LYS:NZ	2.47	0.73
17:3:202:TYR:HB3	17:3:203:PRO:HD2	1.69	0.73
1:A:521:VAL:HG12	1:A:521:VAL:O	1.86	0.73
19:A:9022:CLA:H13	19:B:1206:CLA:HBB2	1.70	0.73
7:G:75:GLY:C	7:G:77:PHE:N	2.35	0.73
7:G:89:LYS:HZ2	7:G:89:LYS:CA	2.02	0.73
7:G:88:ALA:C	7:G:90:GLN:O	2.27	0.73
19:A:1237:CLA:C20	12:L:110:LEU:HD21	2.18	0.73
17:3:92:PHE:CD1	17:3:92:PHE:N	2.57	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:515:GLY:CA	2:B:613:SER:HB2	2.18	0.73
15:1:155:GLU:O	15:1:156:LYS:HB2	1.88	0.73
19:A:1122:CLA:C1D	21:A:6007:BCR:C19	2.67	0.73
2:B:256:THR:O	2:B:272:ASP:CG	2.27	0.73
17:3:238:ILE:HG23	17:3:241:TYR:OH	1.88	0.73
16:2:192:ASP:OD2	16:2:194:GLY:HA2	1.87	0.73
19:K:1146:CLA:CMA	19:K:1146:CLA:O1A	2.37	0.73
8:H:119:ASP:C	8:H:120:ILE:HG22	2.07	0.73
6:F:228:ASP:OD2	6:F:231:PHE:CD1	2.41	0.73
19:H:1145:CLA:HAA1	19:H:1145:CLA:CED	2.19	0.73
21:1:6023:BCR:HC8	21:1:6023:BCR:HC21	1.70	0.73
1:A:635:THR:HG22	1:A:635:THR:O	1.88	0.73
19:A:1124:CLA:HED1	19:A:1125:CLA:CAD	2.12	0.73
1:A:328:LYS:HG3	1:A:332:GLU:CB	2.19	0.73
19:B:1228:CLA:CHD	19:B:1228:CLA:CBC	2.66	0.73
2:B:261:PHE:CE2	2:B:500:ALA:N	2.57	0.73
2:B:493:TRP:O	2:B:495:PRO:HD3	1.88	0.73
2:B:531:THR:O	2:B:535:VAL:HG12	1.89	0.73
3:C:1:MET:N	3:C:3:HIS:C	2.42	0.73
3:C:65:VAL:CG2	3:C:66:ARG:H	1.97	0.73
16:2:153:PHE:CE2	16:2:157:LEU:HD21	2.24	0.73
4:D:141:GLY:N	4:D:144:LEU:H	1.84	0.73
1:A:575:LEU:HD11	1:A:579:PHE:HB3	1.71	0.73
19:3:3008:CLA:CGD	19:3:3008:CLA:CGA	2.66	0.73
5:E:96:ASP:CB	5:E:98:ASN:H	1.94	0.73
15:1:162:LYS:C	15:1:164:PRO:CD	2.56	0.73
12:L:54:TYR:N	12:L:54:TYR:CD1	2.53	0.73
1:A:309:LEU:HD21	19:A:1119:CLA:CMC	2.19	0.73
1:A:349:ILE:HG22	1:A:350:LEU:N	2.01	0.73
2:B:310:PRO:CG	19:B:1220:CLA:HMA1	2.17	0.73
2:B:622:ASP:HB3	2:B:626:LEU:CD1	2.18	0.73
12:L:128:GLN:HG2	12:L:132:LEU:HD22	1.69	0.73
5:E:89:SER:HG	5:E:106:ARG:HD3	1.49	0.73
4:D:100:TYR:HE1	4:D:134:LYS:CE	2.00	0.73
16:2:167:ARG:CA	16:2:167:ARG:NE	2.51	0.73
16:2:177:VAL:CG1	16:2:178:ASN:CG	2.56	0.73
19:J:1311:CLA:H2	19:J:1311:CLA:C16	2.18	0.73
19:H:1145:CLA:HAA2	19:H:1145:CLA:O2D	1.89	0.73
6:F:222:LEU:HD23	6:F:222:LEU:N	2.03	0.73
1:A:150:PHE:O	1:A:151:GLN:CG	2.34	0.72
1:A:93:LEU:HA	1:A:96:MET:H	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:53:GLN:HG2	19:B:1202:CLA:HMB2	1.69	0.72
2:B:190:TRP:HA	19:B:1211:CLA:HBB2	1.69	0.72
2:B:87:ILE:HD12	2:B:87:ILE:N	2.03	0.72
5:E:129:GLU:OE1	5:E:129:GLU:CA	2.35	0.72
10:J:5:LYS:CG	16:2:178:ASN:OD1	2.36	0.72
15:1:170:PRO:CD	15:1:173:TYR:CD2	2.71	0.72
19:4:1304:CLA:C20	19:4:1304:CLA:C15	2.63	0.72
4:D:147:LYS:HA	4:D:148:TYR:CD1	2.23	0.72
1:A:464:ASN:HD22	1:A:464:ASN:N	1.85	0.72
1:A:379:MET:CE	19:A:1125:CLA:HMC2	2.18	0.72
19:B:1205:CLA:H141	19:B:1224:CLA:H91	1.71	0.72
2:B:124:TRP:CD1	2:B:129:LEU:HB3	2.24	0.72
2:B:294:ASN:HB2	7:G:94:GLN:NE2	2.03	0.72
2:B:486:LEU:CD1	2:B:489:GLY:H	2.02	0.72
2:B:553:PHE:O	2:B:555:TYR:N	2.22	0.72
23:B:7101:LMG:HC61	3:C:70:TRP:CH2	2.25	0.72
8:H:109:LEU:CD2	19:H:1207:CLA:C5	2.67	0.72
17:3:150:TYR:C	17:3:151:TRP:HD1	1.90	0.72
2:B:542:ARG:HH11	2:B:542:ARG:HB3	1.52	0.72
17:3:173:PHE:CD1	17:3:174:GLN:N	2.51	0.72
2:B:125:TYR:CE1	2:B:130:ARG:NH1	2.56	0.72
18:4:98:ASN:CB	18:4:212:LEU:HD21	2.20	0.72
1:A:210:LEU:HD13	19:A:1111:CLA:HMB2	1.70	0.72
1:A:588:GLY:N	2:B:668:ARG:HD3	2.03	0.72
2:B:216:LEU:HD21	2:B:221:GLY:HA2	1.71	0.72
2:B:457:PRO:HB3	2:B:517:PHE:CB	2.19	0.72
7:G:129:ALA:O	7:G:131:GLY:N	2.23	0.72
7:G:63:VAL:HG22	7:G:64:ILE:H	1.51	0.72
13:N:157:LYS:N	13:N:157:LYS:CE	2.52	0.72
3:C:5:VAL:HG23	3:C:65:VAL:CG2	2.19	0.72
17:3:94:GLU:CD	17:3:94:GLU:C	2.47	0.72
16:2:188:LEU:HD22	16:2:188:LEU:H	1.53	0.72
1:A:478:SER:HB3	1:A:644:GLN:NE2	1.94	0.72
11:K:127:ILE:O	11:K:130:LEU:HG	1.90	0.72
19:J:1308:CLA:C9	19:2:2014:CLA:CGD	2.67	0.72
1:A:267:THR:HG22	1:A:269:PHE:CD2	2.23	0.72
2:B:131:THR:HB	2:B:134:ASP:HB2	1.71	0.72
19:3:3016:CLA:H2A	19:3:3016:CLA:O2D	1.88	0.72
12:L:51:LYS:N	12:L:52:PRO:HD3	2.04	0.72
8:H:111:TYR:CD1	8:H:112:LEU:CD2	2.72	0.72
15:1:224:PRO:HA	15:1:225:TRP:HB2	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1112:CLA:HBA2	19:3:1147:CLA:HMC3	1.71	0.72
21:A:6011:BCR:C32	21:J:6012:BCR:H391	2.19	0.72
2:B:256:THR:OG1	2:B:258:LEU:N	2.23	0.72
2:B:430:GLY:CA	2:B:525:LEU:HD11	2.17	0.72
1:A:558:LYS:HZ2	2:B:674:LEU:HB2	1.52	0.72
6:F:207:LEU:HD22	6:F:208:PHE:HA	1.70	0.72
7:G:96:GLY:O	7:G:97:LEU:CG	2.37	0.72
8:H:113:SER:OG	19:H:1207:CLA:C5	2.37	0.72
3:C:12:ILE:O	3:C:38:GLN:HG3	1.89	0.72
5:E:79:LYS:CG	5:E:84:TYR:CE1	2.73	0.72
6:F:100:LYS:O	6:F:103:GLN:CB	2.31	0.72
22:F:7036:LMU:H6D	22:F:7036:LMU:O2B	1.89	0.72
15:1:64:PHE:CE1	15:1:66:PRO:HD3	2.24	0.72
1:A:475:ASP:HB3	19:A:1132:CLA:HED3	1.69	0.72
1:A:188:LYS:HE2	1:A:190:ALA:HA	1.72	0.72
2:B:521:HIS:CE1	19:B:1235:CLA:NA	2.56	0.72
3:C:1:MET:H1	3:C:3:HIS:C	1.93	0.72
22:G:7026:LMU:C8	22:G:7026:LMU:H41	2.19	0.72
19:A:1105:CLA:C3B	21:J:6012:BCR:H333	2.19	0.72
4:D:176:LYS:HG3	4:D:177:VAL:N	2.02	0.72
2:B:160:LYS:CD	2:B:161:TRP:CD2	2.72	0.72
1:A:579:PHE:CD1	1:A:579:PHE:N	2.53	0.72
19:4:1304:CLA:O1D	19:4:1304:CLA:H2A	1.90	0.72
17:3:156:THR:CA	17:3:158:PHE:O	2.36	0.72
19:A:1141:CLA:HBC3	19:A:1141:CLA:HHD	1.70	0.72
1:A:345:GLY:C	1:A:347:TYR:N	2.35	0.72
1:A:351:THR:O	19:A:1123:CLA:H201	1.89	0.72
2:B:576:PHE:HE2	19:B:1226:CLA:HAC1	1.53	0.72
2:B:362:ALA:O	2:B:363:GLN:HB3	1.88	0.72
2:B:459:PHE:H	19:B:1235:CLA:CAD	2.02	0.72
4:D:201:LYS:O	4:D:202:PHE:HB3	1.87	0.72
2:B:293:THR:HG23	7:G:94:GLN:HG2	1.69	0.72
13:N:139:LYS:HD2	13:N:142:LYS:NZ	2.01	0.72
15:1:134:LEU:N	15:1:135:PRO:CD	2.52	0.72
3:C:52:LYS:NZ	3:C:64:SER:HB2	2.03	0.72
4:D:162:GLU:C	4:D:163:VAL:HG23	2.10	0.72
16:2:249:ASN:ND2	16:2:254:LEU:HG	2.04	0.72
11:K:97:ASP:CA	11:K:101:PHE:CE2	2.73	0.72
1:A:34:TRP:O	1:A:35:ALA:HB3	1.89	0.72
19:1:1005:CLA:CBC	19:1:1005:CLA:HMC1	2.20	0.72
15:1:70:GLY:C	15:1:73:PRO:HD2	2.08	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:4:1306:CLA:H2A	19:4:1306:CLA:O2A	1.89	0.72
18:4:103:MET:HE2	18:4:207:ASN:C	1.90	0.72
18:4:169:ASP:HB3	19:4:4001:CLA:HMB3	1.70	0.72
1:A:355:HIS:CE1	1:A:416:ILE:HG21	2.24	0.72
1:A:93:LEU:HA	1:A:96:MET:CB	2.19	0.72
19:B:1222:CLA:HBB1	19:B:1236:CLA:CHB	2.19	0.72
19:B:1214:CLA:HBD	19:B:1223:CLA:HBB2	1.70	0.72
2:B:469:LYS:HZ2	2:B:471:THR:C	1.93	0.72
2:B:639:VAL:HG22	2:B:640:CYS:H	1.55	0.72
7:G:89:LYS:HZ2	7:G:89:LYS:H	1.38	0.72
8:H:94:ARG:O	8:H:95:GLY:C	2.28	0.72
17:3:103:VAL:HG13	17:3:107:ARG:CZ	2.19	0.72
16:2:165:GLY:C	16:2:167:ARG:CG	2.58	0.72
2:B:77:TRP:O	2:B:81:PRO:HG3	1.89	0.72
2:B:135:LEU:HD12	2:B:135:LEU:O	1.90	0.72
15:1:161:LYS:HE2	15:1:162:LYS:CB	2.17	0.72
1:A:289:PRO:O	1:A:290:LEU:CB	2.37	0.72
1:A:499:ALA:CB	19:A:1133:CLA:CED	2.64	0.72
19:A:1140:CLA:NC	19:A:1140:CLA:C4	2.53	0.72
1:A:284:ARG:CG	1:A:295:TRP:CG	2.73	0.72
1:A:346:LEU:C	1:A:346:LEU:CD2	2.58	0.72
1:A:355:HIS:ND1	1:A:416:ILE:CG2	2.52	0.72
21:A:6002:BCR:H402	21:A:6002:BCR:C23	2.20	0.72
19:B:1211:CLA:HMB2	21:B:6006:BCR:C8	2.19	0.72
2:B:293:THR:CG2	19:B:1209:CLA:HMA2	2.19	0.72
2:B:430:GLY:HA2	2:B:525:LEU:CD1	2.19	0.72
5:E:93:VAL:HG23	5:E:103:VAL:CB	2.19	0.72
6:F:138:LEU:HD23	6:F:146:PRO:HB3	1.71	0.72
3:C:73:THR:CG2	3:C:76:SER:OG	2.38	0.72
15:1:170:PRO:O	15:1:173:TYR:OH	2.08	0.72
2:B:75:GLU:HB2	2:B:132:ASN:CG	2.09	0.72
1:A:422:TYR:CD1	1:A:422:TYR:N	2.31	0.72
16:2:206:TRP:O	16:2:208:SER:HB2	1.90	0.72
22:4:7009:LMU:H3'	22:4:7009:LMU:O5B	1.89	0.72
15:1:179:LYS:HG2	15:1:180:LEU:O	1.89	0.72
1:A:126:ILE:HD11	19:A:1107:CLA:HMA3	1.70	0.72
19:A:9023:CLA:HBC3	19:A:9023:CLA:HMC1	1.71	0.72
19:B:1203:CLA:H193	19:B:1203:CLA:H91	1.71	0.72
2:B:120:VAL:HA	2:B:123:TRP:NE1	2.05	0.72
2:B:230:TRP:N	7:G:63:VAL:CG2	2.49	0.72
12:L:112:GLY:HA3	19:L:1503:CLA:HHC	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:L:1130:CLA:H52	19:L:1504:CLA:CHB	2.19	0.72
1:A:27:ILE:O	1:A:28:LYS:CG	2.38	0.72
3:C:27:GLU:OE1	3:C:39:ILE:C	2.28	0.72
3:C:62:PHE:CE2	5:E:80:GLU:OE2	2.42	0.72
19:H:1145:CLA:CAA	19:H:1145:CLA:CED	2.68	0.72
18:4:232:LEU:HB2	18:4:236:ILE:CD1	2.18	0.72
15:1:92:LEU:CA	15:1:95:PRO:HD2	2.19	0.72
19:B:1216:CLA:OBD	19:B:1219:CLA:HBC3	1.90	0.72
2:B:639:VAL:HG22	2:B:640:CYS:N	2.05	0.72
3:C:80:ALA:O	3:C:81:TYR:CB	2.35	0.72
7:G:64:ILE:O	7:G:68:THR:HG21	1.88	0.72
5:E:78:ARG:HH12	5:E:125:ILE:CG2	2.00	0.72
3:C:5:VAL:HG23	3:C:65:VAL:HG23	1.71	0.72
3:C:72:GLU:CG	3:C:77:MET:CE	2.66	0.72
16:2:167:ARG:HE	16:2:168:TRP:H	1.37	0.72
22:E:7048:LMU:H22	22:E:7048:LMU:O5'	1.90	0.72
22:N:7049:LMU:H41	22:N:7049:LMU:O1'	1.88	0.72
1:A:316:MET:CG	1:A:317:TYR:HD1	1.97	0.72
22:E:7037:LMU:H12	22:E:7037:LMU:C5	2.20	0.72
7:G:144:THR:HG23	7:G:147:ASN:O	1.90	0.72
18:4:226:LYS:H	18:4:226:LYS:NZ	1.87	0.71
1:A:293:GLY:O	1:A:294:LEU:HB3	1.89	0.71
1:A:57:LEU:C	1:A:57:LEU:CD2	2.57	0.71
2:B:231:ASN:HD21	7:G:61:ALA:HB3	1.53	0.71
2:B:317:ARG:NH2	2:B:410:ARG:HG3	2.05	0.71
2:B:729:THR:O	2:B:729:THR:HG22	1.90	0.71
11:K:63:LEU:H	11:K:63:LEU:CD1	1.99	0.71
6:F:96:LYS:O	6:F:100:LYS:CB	2.37	0.71
11:K:118:VAL:CG2	11:K:121:VAL:CG2	2.68	0.71
19:J:1308:CLA:HMA3	19:2:2014:CLA:CED	2.20	0.71
2:B:74:PHE:O	2:B:76:ALA:N	2.23	0.71
12:L:51:LYS:N	12:L:52:PRO:CD	2.52	0.71
17:3:252:PRO:HB3	17:3:254:GLN:NE2	2.04	0.71
18:4:225:GLY:HA2	18:4:226:LYS:HZ2	1.55	0.71
19:A:1141:CLA:H72	19:A:1141:CLA:C12	2.18	0.71
1:A:246:HIS:CA	1:A:248:PHE:CE2	2.60	0.71
1:A:472:ARG:HH22	12:L:120:LEU:HD11	1.54	0.71
2:B:493:TRP:CZ3	19:B:1232:CLA:HMA2	2.25	0.71
2:B:510:LEU:HD11	2:B:597:LYS:HZ3	1.54	0.71
11:K:56:ILE:HG23	11:K:59:THR:CG2	2.19	0.71
12:L:110:LEU:HB3	12:L:114:PHE:CE1	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:26:LEU:N	3:C:43:PRO:HG3	2.05	0.71
17:3:104:ILE:HG21	19:3:3004:CLA:C4D	2.20	0.71
16:2:184:PRO:HD3	16:2:187:LYS:N	2.05	0.71
11:K:127:ILE:CB	11:K:130:LEU:HG	2.20	0.71
11:K:116:ILE:HG23	11:K:117:GLY:N	2.05	0.71
15:1:150:HIS:CE1	15:1:151:GLN:HE22	2.07	0.71
4:D:188:PHE:CD1	4:D:188:PHE:N	2.52	0.71
15:1:101:GLU:O	15:1:101:GLU:HG2	1.89	0.71
19:A:1117:CLA:H202	19:A:1125:CLA:H3A	1.71	0.71
1:A:472:ARG:NH1	12:L:120:LEU:CD2	2.50	0.71
1:A:92:TRP:O	1:A:93:LEU:CB	2.38	0.71
19:B:1235:CLA:H121	21:F:6016:BCR:H312	1.70	0.71
2:B:693:TRP:CD1	19:B:1238:CLA:C1D	2.74	0.71
2:B:315:LEU:HD11	2:B:317:ARG:HD2	1.73	0.71
2:B:395:ILE:HD12	2:B:396:ARG:HG2	1.73	0.71
5:E:83:TRP:CZ3	5:E:111:ASN:HB2	2.25	0.71
21:L:6019:BCR:C27	21:L:6019:BCR:H403	2.19	0.71
12:L:67:GLY:O	12:L:68:SER:CB	2.38	0.71
16:2:124:GLU:O	16:2:127:THR:CG2	2.37	0.71
16:2:227:LEU:HD21	19:2:2004:CLA:NC	2.05	0.71
3:C:72:GLU:HG2	3:C:77:MET:CE	2.19	0.71
17:3:98:LEU:HD21	19:3:3012:CLA:C3D	2.20	0.71
19:K:1142:CLA:HED2	19:K:1143:CLA:HMB2	1.70	0.71
22:A:7016:LMU:C2	22:A:7016:LMU:H61	2.16	0.71
1:A:387:THR:CG2	1:A:523:VAL:HG11	2.20	0.71
11:K:89:ARG:HG3	11:K:89:ARG:HH11	1.55	0.71
22:B:7038:LMU:O2B	22:B:7038:LMU:H4'	1.88	0.71
15:1:67:LEU:HD12	15:1:68:GLY:H	1.51	0.71
19:A:1102:CLA:HMC3	19:A:1104:CLA:O2D	1.90	0.71
19:A:1124:CLA:H172	21:A:6007:BCR:H332	1.71	0.71
11:K:59:THR:O	11:K:63:LEU:CD2	2.38	0.71
16:2:121:PHE:HD2	16:2:121:PHE:H	1.36	0.71
16:2:226:ARG:HB2	16:2:226:ARG:HH11	1.56	0.71
13:N:139:LYS:CD	13:N:142:LYS:CE	2.68	0.71
16:2:96:PRO:HD3	17:3:85:ASP:OD2	1.87	0.71
6:F:224:GLY:C	6:F:227:VAL:CG1	2.54	0.71
11:K:98:PRO:CD	11:K:99:ALA:H	2.01	0.71
19:A:1102:CLA:H12	19:A:1109:CLA:H92	1.72	0.71
1:A:555:ILE:CD1	19:A:9023:CLA:HMD1	2.19	0.71
19:B:1223:CLA:C8	21:B:6010:BCR:H14C	2.21	0.71
6:F:170:ILE:CG2	21:F:6014:BCR:H372	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:94:SER:O	12:L:96:LEU:CD2	2.38	0.71
16:2:223:LYS:O	16:2:226:ARG:HB3	1.90	0.71
17:3:150:TYR:CD2	17:3:151:TRP:CD2	2.78	0.71
15:1:189:LYS:CB	19:1:1007:CLA:HMC1	2.15	0.71
13:N:99:LYS:CB	13:N:102:ASN:HD21	2.03	0.71
16:2:154:ILE:HG12	16:2:155:VAL:N	2.04	0.71
2:B:331:HIS:CE1	2:B:392:ILE:HG21	2.25	0.71
18:4:226:LYS:N	18:4:226:LYS:HD3	2.04	0.71
1:A:187:HIS:CE1	19:A:1109:CLA:C4D	2.67	0.71
1:A:370:ILE:HG23	1:A:403:GLY:CA	2.16	0.71
1:A:479:ASP:OD1	1:A:536:THR:HG22	1.91	0.71
21:B:6004:BCR:H343	7:G:77:PHE:CD1	2.25	0.71
3:C:63:LEU:HD21	3:C:65:VAL:H	1.53	0.71
1:A:478:SER:HB2	1:A:644:GLN:CD	2.10	0.71
4:D:106:SER:OG	4:D:124:GLU:HG2	1.91	0.71
8:H:77:ASN:OD1	8:H:78:PRO:HD2	1.91	0.71
19:K:1146:CLA:HBC2	19:K:1146:CLA:HMC1	1.73	0.71
17:3:204:GLY:H	17:3:207:PHE:HA	1.56	0.71
4:D:133:ARG:H	4:D:136:GLN:HE22	1.36	0.71
22:L:7029:LMU:C1'	22:L:7029:LMU:H31	2.16	0.71
1:A:258:LEU:HG	1:A:280:PHE:CE1	2.26	0.71
15:1:83:GLU:CA	15:1:86:HIS:CD2	2.74	0.71
18:4:167:ASN:ND2	19:4:4014:CLA:C2	2.53	0.71
18:4:96:LEU:O	18:4:96:LEU:HD12	1.91	0.71
19:A:1102:CLA:O2D	19:A:1102:CLA:H2A	1.90	0.71
1:A:615:HIS:CE1	19:A:1135:CLA:HBC3	2.26	0.71
19:B:1225:CLA:OBD	19:B:1225:CLA:O1D	1.97	0.71
8:H:98:LEU:HD21	12:L:143:LEU:HD22	1.73	0.71
5:E:89:SER:HB3	5:E:106:ARG:NE	2.06	0.71
3:C:44:ARG:HA	4:D:182:GLN:OE1	1.90	0.71
22:3:7003:LMU:O2B	22:3:7005:LMU:O5B	2.09	0.71
17:3:150:TYR:CA	17:3:152:ALA:HB2	2.21	0.71
11:K:70:PHE:HD1	11:K:70:PHE:O	1.74	0.71
2:B:600:THR:O	2:B:604:GLY:HA2	1.89	0.71
18:4:173:LYS:HZ2	18:4:201:LYS:CG	2.01	0.71
1:A:328:LYS:CG	1:A:332:GLU:CB	2.68	0.71
1:A:723:ARG:HH11	1:A:723:ARG:HG2	1.56	0.71
2:B:88:ALA:N	2:B:115:ASN:HA	2.05	0.71
2:B:322:LEU:O	2:B:326:ILE:HG22	1.90	0.71
2:B:622:ASP:HB3	2:B:626:LEU:HG	1.72	0.71
5:E:90:VAL:HG12	5:E:91:VAL:H	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:207:LEU:CG	6:F:208:PHE:N	2.54	0.71
19:H:1241:CLA:HAC1	21:I:6021:BCR:HC31	1.69	0.71
12:L:143:LEU:H	12:L:145:LEU:H	1.35	0.71
3:C:62:PHE:CG	4:D:191:ILE:HG21	2.26	0.71
1:A:252:ARG:NH1	1:A:261:SER:OG	2.23	0.71
18:4:242:ASN:O	18:4:243:THR:CG2	2.35	0.71
18:4:122:ASN:CB	18:4:124:PRO:HD3	2.19	0.71
5:E:94:ASP:HB2	5:E:102:PRO:HB3	1.72	0.71
10:J:2:ARG:NH1	10:J:8:LEU:HD13	2.01	0.71
3:C:52:LYS:NZ	3:C:65:VAL:O	2.24	0.71
12:L:209:LEU:CG	12:L:210:PRO:HD2	2.21	0.71
19:1:1303:CLA:HBA2	19:1:1303:CLA:CMA	2.19	0.71
2:B:125:TYR:CD1	2:B:130:ARG:NH1	2.58	0.71
18:4:174:GLN:O	18:4:194:PHE:CD1	2.44	0.71
19:A:1112:CLA:HMC2	21:A:6002:BCR:C17	2.20	0.71
1:A:62:HIS:N	1:A:62:HIS:ND1	2.39	0.71
19:B:1231:CLA:HMD2	19:B:1232:CLA:C2C	2.21	0.71
5:E:81:SER:OG	5:E:120:TYR:CZ	2.37	0.71
2:B:293:THR:CG2	7:G:94:GLN:CD	2.54	0.71
16:2:171:ILE:HG13	16:2:172:LEU:CA	2.19	0.71
17:3:150:TYR:CA	17:3:151:TRP:HD1	2.04	0.71
19:K:1143:CLA:HBC1	22:K:7001:LMU:C3B	2.21	0.71
18:4:169:ASP:OD1	18:4:174:GLN:HB2	1.90	0.70
18:4:172:PHE:CA	18:4:194:PHE:HE2	1.94	0.70
18:4:211:MET:HG3	19:4:4002:CLA:HBB2	1.73	0.70
1:A:545:HIS:HB3	19:A:1135:CLA:HBB2	1.71	0.70
19:A:1140:CLA:H161	21:A:6011:BCR:HC22	1.72	0.70
1:A:362:LEU:HB3	1:A:410:ALA:HB2	1.73	0.70
1:A:680:LEU:HB3	19:A:9012:CLA:O2A	1.91	0.70
19:A:9022:CLA:C9	19:A:9023:CLA:C9	2.69	0.70
5:E:82:TYR:HB3	5:E:83:TRP:HE3	1.54	0.70
7:G:84:ARG:NE	7:G:89:LYS:CE	2.51	0.70
12:L:82:TYR:O	12:L:83:LEU:HB3	1.91	0.70
16:2:120:ILE:CG1	16:2:121:PHE:N	2.51	0.70
16:2:134:THR:OG1	16:2:135:PRO:HD3	1.89	0.70
3:C:49:VAL:HG22	3:C:50:GLY:H	1.55	0.70
3:C:44:ARG:HB3	4:D:182:GLN:OE1	1.89	0.70
16:2:160:ILE:CG2	19:2:2012:CLA:CAB	2.68	0.70
15:1:151:GLN:HE21	15:1:151:GLN:CA	2.02	0.70
2:B:70:TRP:HB3	2:B:136:TYR:HH	1.55	0.70
1:A:66:SER:O	1:A:67:HIS:HB2	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LEU:HD11	1:A:674:ALA:CB	2.20	0.70
1:A:188:LYS:HD2	1:A:189:ALA:N	2.06	0.70
1:A:379:MET:HE1	19:A:1125:CLA:HHC	1.73	0.70
2:B:663:PHE:O	2:B:664:LEU:CB	2.39	0.70
6:F:139:LEU:HD13	6:F:149:ILE:HD12	1.72	0.70
19:F:1302:CLA:CMA	21:F:6016:BCR:HC32	2.21	0.70
10:J:11:ALA:HB1	10:J:12:PRO:CD	2.12	0.70
16:2:131:ILE:O	16:2:132:LEU:CB	2.39	0.70
3:C:65:VAL:CG2	3:C:66:ARG:N	2.55	0.70
16:2:173:ASN:N	16:2:173:ASN:ND2	2.36	0.70
2:B:400:PRO:HD2	4:D:197:PRO:HD3	1.72	0.70
6:F:225:GLU:O	6:F:227:VAL:HG13	1.92	0.70
17:3:156:THR:HA	17:3:158:PHE:O	1.89	0.70
6:F:213:TRP:CB	6:F:216:ALA:HB2	2.17	0.70
1:A:389:TYR:HE2	1:A:526:LYS:HD3	1.56	0.70
17:3:225:LEU:HD13	17:3:228:VAL:HG21	1.72	0.70
1:A:532:ILE:O	1:A:532:ILE:HG23	1.90	0.70
21:A:6007:BCR:C23	21:A:6007:BCR:H382	2.21	0.70
2:B:127:ILE:CG1	2:B:127:ILE:O	2.38	0.70
21:I:6021:BCR:H322	21:I:6021:BCR:HC42	1.72	0.70
19:A:1237:CLA:C14	12:L:141:LEU:HD23	2.17	0.70
17:3:103:VAL:CG1	17:3:107:ARG:NE	2.42	0.70
14:R:37:UNK:O	14:R:43:UNK:N	2.24	0.70
16:2:176:CYS:O	16:2:177:VAL:CG2	2.36	0.70
22:3:7003:LMU:C2B	22:3:7005:LMU:O5B	2.39	0.70
4:D:123:ARG:O	4:D:124:GLU:HB2	1.91	0.70
11:K:115:ILE:O	11:K:118:VAL:HG22	1.91	0.70
19:2:2014:CLA:CED	19:2:2014:CLA:OBD	2.38	0.70
2:B:110:LEU:CD1	2:B:111:GLY:N	2.53	0.70
6:F:159:GLU:HG2	10:J:38:ILE:HG12	1.72	0.70
3:C:31:TRP:CD1	3:C:32:GLY:N	2.58	0.70
19:K:3009:CLA:H91	19:3:3007:CLA:HAC2	1.74	0.70
2:B:680:TRP:O	2:B:681:ALA:O	2.08	0.70
1:A:284:ARG:CG	1:A:295:TRP:CD1	2.73	0.70
19:B:1223:CLA:HED1	19:B:1231:CLA:CBB	2.19	0.70
6:F:204:SER:O	6:F:207:LEU:CD1	2.38	0.70
10:J:2:ARG:HH12	10:J:8:LEU:CD1	2.00	0.70
2:B:25:ILE:CG2	21:L:6019:BCR:H292	2.15	0.70
5:E:129:GLU:C	5:E:129:GLU:OE1	2.30	0.70
13:N:165:ASN:O	13:N:167:PHE:N	2.24	0.70
3:C:43:PRO:HA	4:D:182:GLN:CB	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:190:LYS:CG	6:F:192:THR:HG23	2.22	0.70
17:3:150:TYR:O	17:3:152:ALA:CA	2.38	0.70
2:B:160:LYS:HZ2	2:B:161:TRP:CB	2.02	0.70
13:N:99:LYS:CB	13:N:102:ASN:ND2	2.55	0.70
17:3:156:THR:O	17:3:156:THR:HG23	1.90	0.70
18:4:111:LEU:HD12	18:4:112:PRO:HG3	1.74	0.70
1:A:86:LEU:CD1	1:A:178:MET:CE	2.69	0.70
19:B:1209:CLA:H61	19:B:1209:CLA:H11	1.73	0.70
19:B:1209:CLA:HMC1	21:B:6005:BCR:H373	1.72	0.70
2:B:244:PHE:O	2:B:244:PHE:HD2	1.75	0.70
2:B:615:TYR:HD1	2:B:615:TYR:N	1.89	0.70
7:G:124:ILE:O	7:G:128:LEU:CB	2.39	0.70
1:A:27:ILE:O	1:A:28:LYS:HG3	1.92	0.70
13:N:131:PHE:C	13:N:132:THR:HG22	2.11	0.70
13:N:152:LEU:C	13:N:153:GLU:CG	2.57	0.70
4:D:100:TYR:HE1	4:D:134:LYS:CD	2.04	0.70
16:2:183:PHE:N	16:2:187:LYS:CG	2.53	0.70
22:4:7053:LMU:C1B	22:4:7053:LMU:H6E	2.20	0.70
1:A:246:HIS:O	1:A:248:PHE:CD2	2.43	0.70
2:B:334:LEU:HB2	19:B:1202:CLA:HMD3	1.71	0.70
2:B:469:LYS:CE	2:B:470:THR:HG23	2.21	0.70
19:B:1235:CLA:H121	21:F:6016:BCR:C31	2.21	0.70
4:D:113:GLU:O	4:D:114:MET:HB3	1.91	0.70
2:B:58:PHE:HB3	2:B:146:SER:HB3	1.73	0.70
22:R:7021:LMU:H1'	22:R:7021:LMU:C3	2.20	0.70
16:2:154:ILE:CG1	16:2:155:VAL:N	2.53	0.70
2:B:314:ARG:HH12	15:1:67:LEU:CD1	2.05	0.70
18:4:211:MET:CG	19:4:4002:CLA:HBB1	2.21	0.70
19:A:1124:CLA:H2	19:A:1125:CLA:HED3	1.73	0.70
1:A:346:LEU:HD23	1:A:346:LEU:C	2.11	0.70
21:A:6008:BCR:C8	21:A:6008:BCR:H331	2.21	0.70
2:B:188:LEU:CD1	19:B:1212:CLA:HBB2	2.20	0.70
2:B:232:LEU:HD11	2:B:235:GLN:HB2	1.72	0.70
2:B:256:THR:O	2:B:257:ILE:HD13	1.92	0.70
2:B:329:SER:OG	2:B:332:PHE:HB2	1.91	0.70
2:B:457:PRO:CB	2:B:517:PHE:HD1	2.04	0.70
7:G:124:ILE:CG2	7:G:125:VAL:N	2.54	0.70
12:L:73:VAL:HG21	19:L:1130:CLA:OBD	1.90	0.70
12:L:91:THR:CA	12:L:98:ARG:HH12	2.05	0.70
5:E:79:LYS:HG3	5:E:84:TYR:OH	1.90	0.70
13:N:139:LYS:HG3	13:N:142:LYS:CE	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3:148:TYR:N	17:3:149:ASN:CG	2.45	0.70
19:K:1142:CLA:HED2	19:K:1143:CLA:CMB	2.21	0.70
15:1:150:HIS:CG	15:1:151:GLN:NE2	2.60	0.70
2:B:131:THR:C	2:B:135:LEU:HD23	2.12	0.70
13:N:120:VAL:CG1	13:N:120:VAL:O	2.40	0.70
19:4:1004:CLA:CHD	19:4:1004:CLA:HBC2	2.16	0.70
18:4:200:ALA:O	18:4:202:GLU:N	2.25	0.70
1:A:207:LEU:HB3	19:A:1119:CLA:CBB	2.22	0.70
1:A:430:ASP:H	1:A:433:ASP:CG	1.95	0.70
19:B:1222:CLA:CBC	19:B:1222:CLA:HHD	2.16	0.70
5:E:83:TRP:CH2	5:E:116:SER:HB2	2.27	0.70
7:G:82:PHE:HB2	7:G:83:GLN:CG	2.21	0.70
11:K:78:ARG:HA	11:K:78:ARG:HE	1.52	0.70
21:B:6020:BCR:C33	19:L:1502:CLA:NB	2.48	0.70
16:2:229:MET:SD	16:2:229:MET:C	2.70	0.70
4:D:95:GLN:HG3	4:D:96:VAL:N	2.06	0.70
10:J:4:LEU:O	10:J:5:LYS:HB2	1.89	0.70
2:B:5:ILE:HG22	2:B:6:PRO:N	2.05	0.70
1:A:581:CYS:HB2	1:A:590:CYS:CA	2.18	0.70
19:R:1144:CLA:H2A	19:R:1144:CLA:O1A	1.92	0.70
1:A:236:GLY:C	1:A:237:VAL:HG22	2.12	0.70
15:1:81:GLU:C	15:1:83:GLU:N	2.40	0.70
18:4:173:LYS:HZ2	18:4:201:LYS:HG2	1.57	0.70
19:A:1112:CLA:HHC	21:A:6002:BCR:C17	2.22	0.70
19:A:1132:CLA:HMC1	19:A:1132:CLA:HBC3	1.73	0.70
19:B:1239:CLA:H192	9:I:21:MET:HB3	1.73	0.70
1:A:244:LEU:HD13	1:A:247:GLU:OE2	1.92	0.70
19:3:2009:CLA:CBA	19:3:2009:CLA:CHA	2.70	0.70
5:E:126:VAL:O	5:E:127:GLU:HB2	1.92	0.70
13:N:157:LYS:HB3	13:N:158:ASP:HA	1.73	0.70
3:C:44:ARG:NH2	4:D:181:ARG:HG2	2.06	0.70
16:2:148:ASP:HB3	16:2:152:LEU:HG	1.71	0.70
12:L:172:GLU:N	12:L:173:PRO:CD	2.40	0.70
15:1:103:LEU:N	15:1:103:LEU:HD23	2.02	0.70
1:A:564:ARG:NH2	1:A:564:ARG:CB	2.54	0.70
18:4:153:GLU:OE2	19:4:4012:CLA:C4B	2.39	0.70
1:A:50:THR:HG22	1:A:52:THR:H	1.57	0.70
2:B:212:PHE:CZ	19:B:1211:CLA:HHD	2.26	0.70
2:B:551:LYS:O	2:B:552:ASP:CG	2.30	0.70
6:F:138:LEU:CD2	6:F:146:PRO:HB3	2.22	0.70
5:E:78:ARG:NH1	5:E:125:ILE:HB	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:182:ILE:HB	16:2:187:LYS:HG3	1.64	0.70
11:K:115:ILE:HD13	11:K:122:LEU:HD12	1.73	0.70
18:4:109:MET:O	18:4:111:LEU:N	2.25	0.70
22:4:7034:LMU:C8	22:4:7052:LMU:H1'	2.14	0.69
18:4:142:PHE:CD1	19:4:4010:CLA:C3C	2.75	0.69
1:A:83:PHE:CE1	19:A:1111:CLA:CED	2.75	0.69
19:A:1115:CLA:H193	11:K:64:MET:HE3	1.71	0.69
19:A:1237:CLA:C6	19:A:1237:CLA:H112	2.20	0.69
1:A:531:PRO:O	1:A:532:ILE:CG2	2.39	0.69
5:E:82:TYR:CE1	5:E:111:ASN:HA	2.27	0.69
19:B:1206:CLA:H41	21:I:6018:BCR:C23	2.21	0.69
12:L:143:LEU:CD2	12:L:146:THR:HG22	2.15	0.69
17:3:187:PHE:CD1	17:3:188:LEU:N	2.60	0.69
13:N:155:GLU:CB	13:N:157:LYS:N	2.17	0.69
4:D:145:ARG:HH12	4:D:173:TYR:HE1	1.38	0.69
19:L:1148:CLA:HED3	19:L:1148:CLA:H2	1.70	0.69
11:K:115:ILE:CG1	11:K:121:VAL:C	2.47	0.69
15:1:112:GLN:HG2	15:1:113:GLU:N	2.03	0.69
12:L:51:LYS:NZ	12:L:51:LYS:HB3	2.06	0.69
22:H:7011:LMU:O6'	22:H:7011:LMU:H4B	1.92	0.69
18:4:120:ILE:HG22	18:4:121:ILE:HG23	1.74	0.69
15:1:98:LEU:HD13	15:1:98:LEU:O	1.92	0.69
19:A:1101:CLA:C4	19:A:1140:CLA:H61	2.07	0.69
1:A:105:ASN:HB2	1:A:119:SER:O	1.93	0.69
1:A:370:ILE:HG22	1:A:400:MET:CA	2.21	0.69
2:B:229:GLN:OE1	2:B:229:GLN:HA	1.92	0.69
16:2:113:ALA:CB	16:2:114:MET:HE3	2.21	0.69
19:1:1014:CLA:CBC	19:1:1014:CLA:HHD	2.12	0.69
3:C:67:VAL:HG22	3:C:67:VAL:O	1.90	0.69
10:J:5:LYS:HD2	16:2:178:ASN:CG	2.12	0.69
17:3:150:TYR:HB3	17:3:151:TRP:HE1	1.56	0.69
19:3:3008:CLA:CBA	19:3:3008:CLA:CBD	2.65	0.69
18:4:188:ILE:HG22	18:4:189:PHE:N	2.05	0.69
19:K:3009:CLA:C9	19:3:3007:CLA:HAC2	2.23	0.69
19:A:1106:CLA:HBB2	19:A:1107:CLA:C4D	2.23	0.69
19:A:1105:CLA:HAA2	19:A:1107:CLA:CED	2.22	0.69
19:A:1119:CLA:HBA1	19:A:1123:CLA:HBB2	1.74	0.69
19:A:1122:CLA:CAB	21:A:6007:BCR:H351	2.22	0.69
2:B:187:SER:O	2:B:189:ALA:N	2.25	0.69
6:F:207:LEU:HD22	6:F:208:PHE:CB	2.22	0.69
7:G:64:ILE:HG13	7:G:68:THR:CG2	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:131:SER:N	12:L:201:TYR:CD2	2.59	0.69
13:N:124:SER:O	13:N:125:CYS:HB2	1.91	0.69
13:N:156:GLY:CA	13:N:157:LYS:HD2	2.22	0.69
19:1:1014:CLA:C5	19:1:1014:CLA:C10	2.58	0.69
4:D:80:SER:HG	4:D:126:PRO:CD	1.94	0.69
16:2:243:GLY:CA	16:2:244:THR:HG23	2.22	0.69
19:1:1303:CLA:HMA3	19:1:1303:CLA:HBA2	1.74	0.69
15:1:201:PHE:CD1	15:1:204:GLN:NE2	2.59	0.69
15:1:157:ASP:CB	15:1:178:LYS:CA	2.50	0.69
15:1:67:LEU:C	15:1:67:LEU:HD12	2.12	0.69
19:A:1237:CLA:HMB2	19:L:1502:CLA:HBC1	1.73	0.69
1:A:472:ARG:HH22	12:L:120:LEU:CD1	2.04	0.69
2:B:118:SER:HB2	19:B:1205:CLA:OBD	1.92	0.69
2:B:373:THR:HA	2:B:376:GLN:HB2	1.73	0.69
2:B:438:VAL:HG22	19:B:1230:CLA:CMC	2.21	0.69
7:G:116:SER:CA	7:G:119:PRO:HG2	2.21	0.69
12:L:137:LEU:O	12:L:137:LEU:HD23	1.91	0.69
17:3:233:LEU:HA	17:3:236:LEU:HB3	1.73	0.69
17:3:98:LEU:HD21	19:3:3012:CLA:C2D	2.22	0.69
17:3:93:ILE:O	17:3:93:ILE:HG23	1.92	0.69
6:F:193:GLN:HA	6:F:195:GLU:OE1	1.92	0.69
22:3:7005:LMU:H3'	22:3:7005:LMU:O2B	1.91	0.69
13:N:89:GLU:OE1	13:N:89:GLU:O	2.11	0.69
15:1:65:ASP:OD2	15:1:66:PRO:CA	2.40	0.69
15:1:97:ILE:HD12	15:1:98:LEU:HB2	1.73	0.69
1:A:351:THR:O	19:A:1123:CLA:C20	2.41	0.69
1:A:690:LEU:HD23	1:A:693:LEU:HD12	1.74	0.69
1:A:74:ILE:O	1:A:77:LYS:N	2.22	0.69
2:B:527:LEU:CD1	19:B:1236:CLA:HMA3	2.22	0.69
2:B:224:PRO:O	2:B:226:LEU:N	2.25	0.69
2:B:508:LEU:HB3	2:B:509:PHE:CD2	2.28	0.69
7:G:76:ARG:NH2	7:G:117:ASN:HA	2.07	0.69
7:G:77:PHE:O	7:G:79:PHE:HB3	1.92	0.69
3:C:14:CYS:C	3:C:17:CYS:SG	2.69	0.69
12:L:205:TYR:CE1	12:L:207:LEU:CD1	2.75	0.69
11:K:114:HIS:O	11:K:115:ILE:C	2.31	0.69
17:3:192:LYS:NZ	17:3:192:LYS:HA	2.06	0.69
15:1:147:PHE:O	15:1:150:HIS:HB3	1.92	0.69
14:R:51:UNK:O	14:R:52:UNK:CB	2.41	0.69
12:L:172:GLU:O	12:L:174:ASP:O	2.10	0.69
12:L:168:GLY:O	12:L:170:LYS:N	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:GLN:OE1	2:B:163:PRO:HB2	1.91	0.69
19:A:1134:CLA:CMA	19:A:1141:CLA:HBB2	2.22	0.69
1:A:281:LEU:HD13	19:A:1115:CLA:O2D	1.89	0.69
1:A:73:GLU:CG	1:A:74:ILE:N	2.55	0.69
19:A:9012:CLA:H12	2:B:616:LEU:HD13	1.73	0.69
6:F:170:ILE:O	6:F:173:TRP:CD1	2.44	0.69
7:G:90:GLN:CB	7:G:91:VAL:O	2.38	0.69
16:2:94:SER:O	16:2:95:ASP:HB2	1.90	0.69
12:L:155:GLU:HA	12:L:178:THR:HG22	1.74	0.69
11:K:125:LYS:HB2	11:K:128:GLY:H	1.57	0.69
19:J:1308:CLA:CBD	19:J:1308:CLA:HBA2	2.14	0.69
15:1:170:PRO:CD	15:1:173:TYR:HE2	2.05	0.69
8:H:114:ALA:O	8:H:115:THR:CG2	2.40	0.69
10:J:42:PHE:HD1	18:4:244:ILE:HG21	1.58	0.69
12:L:54:TYR:HE1	12:L:57:ILE:HG23	1.58	0.69
18:4:145:GLU:CG	18:4:146:PHE:CD1	2.58	0.69
18:4:207:ASN:HD21	19:4:4002:CLA:C1A	2.06	0.69
19:A:1112:CLA:HED2	19:A:1112:CLA:H2A	1.74	0.69
19:A:1123:CLA:OBD	19:A:1123:CLA:H112	1.93	0.69
1:A:173:VAL:HG23	1:A:174:PHE:HD1	1.57	0.69
1:A:217:SER:OG	21:A:6002:BCR:H17C	1.92	0.69
19:A:9023:CLA:CGA	19:A:9023:CLA:H3A	2.22	0.69
19:B:1211:CLA:HMB3	21:B:6006:BCR:H311	1.73	0.69
2:B:21:ILE:HD11	19:B:1238:CLA:HMA1	1.74	0.69
2:B:308:HIS:CG	2:B:309:ILE:N	2.61	0.69
2:B:87:ILE:CD1	2:B:87:ILE:N	2.55	0.69
6:F:138:LEU:O	6:F:140:CYS:SG	2.48	0.69
19:1:1013:CLA:HED2	19:1:1013:CLA:CAD	2.22	0.69
17:3:91:GLY:O	17:3:93:ILE:N	2.25	0.69
12:L:204:LEU:HD13	12:L:205:TYR:N	2.08	0.69
6:F:103:GLN:O	6:F:104:ALA:C	2.30	0.69
13:N:99:LYS:CA	13:N:102:ASN:OD1	2.33	0.69
17:3:243:ILE:HD11	19:3:3005:CLA:C1C	2.20	0.69
22:G:7039:LMU:H6'2	22:G:7039:LMU:H3'	1.74	0.69
1:A:491:TRP:NE1	19:A:1135:CLA:C1	2.50	0.69
21:A:6011:BCR:C8	21:A:6011:BCR:C31	2.70	0.69
1:A:684:PHE:HD2	1:A:684:PHE:C	1.95	0.69
2:B:315:LEU:C	2:B:315:LEU:CD1	2.54	0.69
2:B:53:GLN:HE22	19:B:1201:CLA:HBB1	1.53	0.69
2:B:625:TRP:CE3	2:B:626:LEU:N	2.60	0.69
7:G:136:VAL:O	7:G:137:VAL:C	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:F:1302:CLA:HBC2	19:F:1302:CLA:HHD	1.75	0.69
7:G:87:VAL:O	7:G:88:ALA:HB3	1.92	0.69
1:A:49:ASP:HB2	1:A:720:THR:HA	1.75	0.69
4:D:140:LEU:CD1	4:D:140:LEU:C	2.32	0.69
16:2:95:ASP:HB3	17:3:85:ASP:OD2	1.82	0.69
17:3:191:GLU:O	17:3:192:LYS:HE2	1.91	0.69
4:D:82:ILE:CG2	4:D:121:ILE:O	2.40	0.69
8:H:115:THR:O	8:H:116:ALA:HB3	1.90	0.69
17:3:159:VAL:CG1	17:3:160:LEU:H	2.05	0.69
2:B:141:PHE:HA	2:B:144:PHE:CD1	2.28	0.69
15:1:206:SER:O	15:1:209:PRO:HD3	1.92	0.69
22:H:7011:LMU:C6'	22:H:7011:LMU:H2B	2.22	0.69
16:2:158:VAL:CG2	16:2:159:PHE:N	2.54	0.69
15:1:217:LEU:HD23	15:1:218:ALA:HA	1.74	0.69
19:B:1223:CLA:H41	19:B:1223:CLA:H72	1.74	0.69
2:B:127:ILE:O	2:B:127:ILE:HG13	1.93	0.69
19:A:9022:CLA:H151	21:B:6017:BCR:C19	2.22	0.69
7:G:89:LYS:N	7:G:89:LYS:NZ	2.41	0.69
16:2:215:LYS:O	16:2:215:LYS:HG2	1.92	0.69
3:C:10:THR:CG2	5:E:101:TYR:CD2	2.71	0.69
19:1:1013:CLA:CGD	19:1:1013:CLA:HAA2	2.22	0.69
14:R:34:UNK:C	14:R:38:UNK:CB	2.71	0.69
16:2:172:LEU:C	16:2:173:ASN:HD22	1.95	0.69
22:3:7005:LMU:H32	22:3:7005:LMU:H1'	1.73	0.69
4:D:80:SER:CB	4:D:127:ASN:H	2.06	0.69
1:A:575:LEU:CD1	1:A:576:GLY:CA	2.57	0.69
15:1:170:PRO:O	15:1:173:TYR:HE2	1.73	0.69
15:1:178:LYS:CG	15:1:179:LYS:N	2.55	0.69
15:1:84:LEU:O	15:1:88:ARG:CG	2.38	0.69
15:1:84:LEU:C	15:1:88:ARG:HG3	2.14	0.69
18:4:153:GLU:OE2	19:4:4012:CLA:CHC	2.41	0.69
19:A:1115:CLA:HED3	19:A:1115:CLA:H2A	0.74	0.69
1:A:336:GLY:CA	19:A:1151:CLA:CMC	2.71	0.69
1:A:209:GLY:CA	1:A:213:LEU:HD13	2.23	0.69
1:A:453:LEU:HD13	1:A:547:PHE:HA	1.73	0.69
1:A:443:ILE:HG21	1:A:558:LYS:HB2	1.75	0.69
1:A:740:LEU:HD21	19:A:1140:CLA:HMA3	1.73	0.69
12:L:82:TYR:O	12:L:82:TYR:CG	2.46	0.69
16:2:131:ILE:O	16:2:131:ILE:CG2	2.41	0.69
3:C:44:ARG:HE	4:D:182:GLN:NE2	1.90	0.69
19:3:3011:CLA:HBC1	19:3:3012:CLA:CHA	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2:2014:CLA:H91	19:2:2014:CLA:H152	1.75	0.69
10:J:31:ARG:HA	10:J:34:PRO:HA	1.75	0.69
15:1:66:PRO:CD	15:1:67:LEU:N	2.56	0.68
20:A:5001:PQN:H272	20:A:5001:PQN:H241	1.76	0.68
2:B:530:THR:HG21	19:B:1222:CLA:HAC1	1.74	0.68
2:B:535:VAL:O	2:B:539:LEU:CD2	2.41	0.68
2:B:545:LYS:CD	2:B:546:LEU:N	2.50	0.68
2:B:654:HIS:CE1	19:B:9010:CLA:NB	2.60	0.68
17:3:104:ILE:HG21	19:3:3004:CLA:ND	2.08	0.68
17:3:93:ILE:CD1	17:3:95:PRO:O	2.41	0.68
8:H:119:ASP:CB	8:H:121:LEU:HG	2.22	0.68
12:L:164:LEU:C	12:L:165:THR:CG2	2.61	0.68
2:B:262:HIS:ND1	2:B:265:THR:OG1	2.26	0.68
3:C:55:GLU:C	3:C:57:ALA:H	1.96	0.68
15:1:158:PRO:HA	15:1:175:LYS:CG	2.21	0.68
15:1:95:PRO:C	15:1:98:LEU:CB	2.60	0.68
1:A:103:PHE:CE1	19:A:1105:CLA:O1D	2.43	0.68
1:A:453:LEU:CD2	19:A:1136:CLA:CBB	2.71	0.68
1:A:120:ALA:N	1:A:145:ILE:HD12	1.97	0.68
2:B:90:ALA:N	2:B:113:VAL:CG1	2.55	0.68
12:L:112:GLY:N	12:L:113:PRO:HD2	2.08	0.68
12:L:198:ILE:O	12:L:202:PHE:N	2.21	0.68
13:N:157:LYS:CG	13:N:159:LYS:H	2.07	0.68
16:2:182:ILE:O	16:2:183:PHE:CD1	2.46	0.68
11:K:127:ILE:HA	11:K:130:LEU:CD1	2.23	0.68
6:F:105:SER:O	6:F:106:LEU:C	2.31	0.68
15:1:162:LYS:HG2	15:1:163:TYR:H	1.59	0.68
22:4:7033:LMU:H3'	22:4:7033:LMU:C6B	2.23	0.68
1:A:220:ARG:O	1:A:221:HIS:HB2	1.92	0.68
18:4:121:ILE:HG13	18:4:122:ASN:N	2.07	0.68
18:4:146:PHE:CE1	19:4:4013:CLA:C1C	2.77	0.68
1:A:508:THR:O	1:A:509:ALA:HB2	1.90	0.68
2:B:620:LEU:HD12	2:B:624:LEU:HD21	1.74	0.68
6:F:160:PHE:O	6:F:164:GLY:CA	2.40	0.68
8:H:98:LEU:HD21	12:L:143:LEU:CD2	2.24	0.68
12:L:190:PHE:CZ	12:L:194:ILE:CD1	2.77	0.68
16:2:226:ARG:HD3	16:2:230:LEU:CD2	2.23	0.68
15:1:135:PRO:HD2	15:1:136:THR:H	1.59	0.68
17:3:109:ALA:CA	17:3:111:LEU:HD22	2.23	0.68
22:3:7005:LMU:C1'	22:3:7005:LMU:H32	2.22	0.68
15:1:171:LEU:HA	15:1:173:TYR:CD2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:LEU:O	1:A:259:TYR:CB	2.42	0.68
19:A:1133:CLA:C3D	19:A:1134:CLA:HAC1	2.22	0.68
1:A:217:SER:OG	21:A:6002:BCR:C16	2.40	0.68
21:A:6011:BCR:H313	19:A:9013:CLA:H143	1.74	0.68
2:B:314:ARG:HH12	15:1:67:LEU:HD11	1.59	0.68
1:A:668:TYR:CB	2:B:445:ALA:HB2	2.23	0.68
2:B:469:LYS:NZ	2:B:471:THR:O	2.27	0.68
5:E:103:VAL:CG1	5:E:120:TYR:O	2.42	0.68
7:G:64:ILE:HG13	7:G:68:THR:HG23	1.74	0.68
11:K:55:LEU:O	11:K:58:VAL:HG12	1.94	0.68
13:N:139:LYS:CA	13:N:142:LYS:NZ	2.51	0.68
13:N:147:SER:CA	13:N:149:ASP:HB2	2.23	0.68
1:A:249:ILE:N	17:3:137:PHE:HZ	1.91	0.68
17:3:206:PRO:HG2	17:3:208:PHE:CZ	2.28	0.68
18:4:154:ILE:O	18:4:158:GLN:HG2	1.93	0.68
1:A:57:LEU:HD23	1:A:58:HIS:N	2.08	0.68
19:B:1215:CLA:H3A	19:B:1215:CLA:CGA	2.23	0.68
19:B:1209:CLA:CMC	21:B:6005:BCR:H373	2.24	0.68
9:I:11:LEU:HG	21:I:6021:BCR:C7	2.23	0.68
11:K:47:ASP:OD2	11:K:48:PHE:N	2.27	0.68
16:2:131:ILE:O	16:2:132:LEU:CD1	2.41	0.68
13:N:139:LYS:CG	13:N:142:LYS:CE	2.71	0.68
16:2:171:ILE:HD11	16:2:173:ASN:HD21	1.59	0.68
16:2:184:PRO:HD2	16:2:185:ASN:O	1.93	0.68
4:D:124:GLU:OE1	4:D:125:GLY:CA	2.41	0.68
16:2:240:ILE:HG22	16:2:263:PHE:HB3	1.72	0.68
15:1:170:PRO:C	15:1:171:LEU:HD23	2.14	0.68
8:H:114:ALA:O	8:H:115:THR:HG23	1.93	0.68
2:B:475:ASP:CA	2:B:480:SER:HA	2.23	0.68
12:L:161:ALA:N	12:L:162:PRO:HD2	2.07	0.68
18:4:145:GLU:CG	18:4:146:PHE:HD1	2.03	0.68
1:A:193:LEU:CA	1:A:196:PHE:HE2	2.03	0.68
2:B:22:TRP:NE1	19:B:1238:CLA:CBB	2.47	0.68
2:B:454:LEU:C	2:B:454:LEU:HD12	2.13	0.68
3:C:17:CYS:CB	3:C:58:CYS:SG	2.74	0.68
3:C:66:ARG:NH2	3:C:66:ARG:CG	2.49	0.68
16:2:167:ARG:HE	16:2:168:TRP:N	1.90	0.68
16:2:182:ILE:O	16:2:183:PHE:CG	2.47	0.68
2:B:633:ASN:O	2:B:633:ASN:OD1	2.11	0.68
2:B:247:THR:C	2:B:250:ALA:H	1.96	0.68
17:3:154:ASN:O	17:3:155:TYR:CG	2.46	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:3017:CLA:HMC1	19:3:3017:CLA:HBC3	1.74	0.68
18:4:202:GLU:O	18:4:205:ILE:CG1	2.40	0.68
1:A:110:LEU:O	1:A:113:PRO:HD3	1.94	0.68
2:B:266:GLN:O	2:B:267:SER:CB	2.41	0.68
2:B:666:SER:HB3	2:B:671:TRP:NE1	2.05	0.68
19:B:1226:CLA:H62	23:B:7101:LMG:H182	1.75	0.68
6:F:200:VAL:CG1	10:J:7:TYR:CA	2.71	0.68
11:K:79:LYS:O	11:K:80:ALA:HB3	1.91	0.68
3:C:52:LYS:NZ	3:C:64:SER:HB3	2.08	0.68
22:A:7016:LMU:H51	22:A:7016:LMU:O6'	1.94	0.68
22:H:7011:LMU:H1B	22:H:7011:LMU:O6'	1.93	0.68
18:4:194:PHE:O	18:4:195:ALA:HB3	1.91	0.68
19:A:1125:CLA:H143	19:A:1125:CLA:H101	1.74	0.68
1:A:281:LEU:CD1	1:A:282:THR:H	2.07	0.68
2:B:444:LEU:CD2	2:B:452:GLN:NE2	2.56	0.68
2:B:98:GLN:O	2:B:100:ALA:CA	2.42	0.68
7:G:86:ASN:O	7:G:89:LYS:NZ	2.26	0.68
12:L:68:SER:O	12:L:69:LEU:C	2.30	0.68
12:L:69:LEU:O	12:L:71:THR:HG23	1.94	0.68
3:C:12:ILE:HG22	3:C:38:GLN:O	1.93	0.68
3:C:44:ARG:NH2	4:D:181:ARG:CB	2.56	0.68
8:H:89:ALA:O	8:H:92:THR:N	2.27	0.68
6:F:92:ALA:O	6:F:95:GLU:HB2	1.94	0.68
22:A:7023:LMU:H91	22:A:7023:LMU:C2	2.24	0.68
1:A:464:ASN:HD22	1:A:464:ASN:H	1.41	0.68
2:B:82:PHE:O	2:B:84:VAL:N	2.22	0.68
15:1:177:PRO:HG2	15:1:180:LEU:N	2.09	0.68
19:A:1129:CLA:HMB2	19:L:1130:CLA:C1D	2.23	0.68
1:A:63:ASP:HA	19:A:1128:CLA:HED2	1.76	0.68
1:A:728:VAL:HG22	1:A:731:ARG:NH1	2.09	0.68
2:B:190:TRP:HE3	19:B:1211:CLA:CBB	2.06	0.68
2:B:57:ILE:HD13	21:B:6005:BCR:H321	1.76	0.68
5:E:111:ASN:C	5:E:111:ASN:ND2	2.46	0.68
12:L:150:ILE:HD12	12:L:151:SER:N	2.08	0.68
15:1:142:PHE:HA	15:1:145:ILE:HD12	1.74	0.68
3:C:43:PRO:O	3:C:43:PRO:HD2	1.94	0.68
16:2:183:PHE:C	16:2:185:ASN:HA	2.14	0.68
16:2:184:PRO:N	16:2:187:LYS:HG2	2.09	0.68
16:2:263:PHE:O	16:2:263:PHE:CG	2.47	0.68
19:2:2014:CLA:C9	19:2:2014:CLA:H152	2.24	0.68
17:3:215:LYS:HB2	17:3:216:ASP:HA	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:GLN:HG3	1:A:490:GLN:O	1.93	0.68
15:1:73:PRO:CD	15:1:74:ALA:H	2.07	0.68
1:A:545:HIS:CG	19:A:1135:CLA:CBB	2.69	0.68
19:A:1126:CLA:H102	21:A:6011:BCR:H372	1.76	0.68
7:G:76:ARG:NH1	7:G:120:VAL:HB	2.08	0.68
5:E:78:ARG:HH12	5:E:125:ILE:CB	2.07	0.68
15:1:140:ILE:HD13	15:1:140:ILE:N	2.09	0.68
18:4:141:LEU:N	18:4:141:LEU:HD22	2.01	0.68
2:B:476:ILE:O	2:B:476:ILE:HG23	1.93	0.68
1:A:628:ILE:HD12	1:A:629:ASN:N	2.09	0.68
18:4:100:ARG:O	18:4:104:LEU:CD1	2.42	0.67
18:4:172:PHE:O	18:4:173:LYS:HB2	1.94	0.67
18:4:214:PHE:O	18:4:215:LEU:C	2.29	0.67
1:A:445:HIS:O	1:A:446:LEU:CB	2.42	0.67
1:A:555:ILE:CD1	19:A:9023:CLA:CMD	2.71	0.67
1:A:553:VAL:H	1:A:556:LEU:HD12	1.59	0.67
1:A:75:SER:HB3	1:A:354:TRP:CZ2	2.29	0.67
2:B:104:PHE:O	2:B:105:THR:OG1	2.09	0.67
19:B:1203:CLA:H71	23:B:7101:LMG:H381	1.76	0.67
16:2:122:ILE:O	16:2:126:LEU:CG	2.40	0.67
15:1:137:ILE:CG2	19:1:1013:CLA:HBB2	2.22	0.67
16:2:166:ARG:CA	16:2:167:ARG:CB	2.70	0.67
16:2:167:ARG:HE	16:2:167:ARG:HA	1.55	0.67
16:2:184:PRO:HD3	16:2:187:LYS:HD2	1.75	0.67
16:2:174:PRO:HD2	16:2:189:THR:OG1	1.94	0.67
22:D:7050:LMU:H5B	22:D:7050:LMU:O2B	1.92	0.67
18:4:198:LEU:HG	18:4:199:GLU:H	1.58	0.67
18:4:124:PRO:HB2	18:4:126:TRP:N	2.07	0.67
18:4:173:LYS:CA	18:4:194:PHE:HD2	2.08	0.67
1:A:304:LEU:HG	19:A:1115:CLA:CAB	2.24	0.67
1:A:684:PHE:HD2	1:A:685:VAL:N	1.93	0.67
19:B:1202:CLA:OBD	19:B:1202:CLA:H151	1.94	0.67
2:B:310:PRO:HG2	2:B:311:PRO:HD3	1.75	0.67
1:A:21:LEU:N	1:A:22:VAL:CB	2.57	0.67
5:E:101:TYR:HA	5:E:121:ALA:HB2	1.76	0.67
15:1:145:ILE:HA	15:1:148:VAL:HG12	1.76	0.67
1:A:249:ILE:CG1	1:A:250:LEU:N	2.52	0.67
16:2:164:GLU:OE2	19:2:2012:CLA:NB	2.26	0.67
13:N:99:LYS:HB3	13:N:102:ASN:ND2	2.09	0.67
14:R:26:UNK:O	14:R:27:UNK:C	2.42	0.67
2:B:69:ALA:CB	2:B:135:LEU:CD1	2.71	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:225:TRP:HB3	15:1:226:HIS:HA	1.73	0.67
2:B:424:TRP:CZ2	19:B:1228:CLA:HAC1	2.29	0.67
2:B:176:ASN:ND2	2:B:291:TYR:O	2.27	0.67
2:B:294:ASN:HD21	7:G:94:GLN:HA	1.57	0.67
2:B:501:ILE:HG13	2:B:502:ASN:N	2.09	0.67
21:B:6020:BCR:H383	21:B:6020:BCR:H23C	1.75	0.67
9:I:12:VAL:O	9:I:17:PRO:CD	2.41	0.67
19:A:1126:CLA:H111	21:J:6012:BCR:H353	1.74	0.67
12:L:92:ALA:H	12:L:98:ARG:HH12	1.22	0.67
5:E:122:LEU:O	5:E:125:ILE:N	2.28	0.67
13:N:139:LYS:CE	13:N:142:LYS:NZ	2.57	0.67
17:3:238:ILE:HA	17:3:241:TYR:CE1	2.30	0.67
1:A:720:THR:HG22	1:A:720:THR:O	1.95	0.67
4:D:114:MET:HG3	4:D:115:PRO:CA	2.23	0.67
11:K:127:ILE:O	11:K:129:ALA:HA	1.94	0.67
19:J:1308:CLA:H92	19:2:2014:CLA:O2D	1.93	0.67
22:N:7049:LMU:C6	22:N:7049:LMU:C1	2.71	0.67
15:1:129:VAL:CB	15:1:130:PRO:HD3	2.24	0.67
22:H:7011:LMU:H111	22:H:7011:LMU:C7	2.23	0.67
18:4:121:ILE:CG1	18:4:122:ASN:N	2.57	0.67
15:1:68:GLY:O	15:1:72:VAL:CB	2.40	0.67
19:A:1115:CLA:H193	11:K:64:MET:HE1	1.76	0.67
1:A:536:THR:HA	1:A:539:PHE:HB2	1.76	0.67
2:B:459:PHE:CZ	19:B:1235:CLA:HMD2	2.29	0.67
2:B:233:TYR:O	2:B:253:ALA:HB1	1.94	0.67
16:2:100:ARG:O	16:2:102:ASN:N	2.26	0.67
16:2:226:ARG:HH11	16:2:226:ARG:CG	2.08	0.67
5:E:107:PHE:CD2	5:E:109:LYS:HE3	2.28	0.67
4:D:95:GLN:C	4:D:95:GLN:CD	2.52	0.67
4:D:102:ILE:O	4:D:102:ILE:HG23	1.93	0.67
15:1:151:GLN:NE2	15:1:151:GLN:CA	2.57	0.67
2:B:85:ARG:HH11	2:B:85:ARG:CG	2.05	0.67
15:1:201:PHE:O	15:1:204:GLN:HB2	1.95	0.67
22:4:7053:LMU:H1B	22:4:7053:LMU:C6'	2.17	0.67
1:A:408:VAL:HG21	1:A:602:LEU:HG	1.76	0.67
15:1:73:PRO:CG	15:1:74:ALA:H	2.07	0.67
1:A:207:LEU:HA	1:A:211:LEU:CG	2.25	0.67
1:A:304:LEU:CG	19:A:1115:CLA:CBB	2.72	0.67
1:A:373:ALA:O	1:A:396:PHE:CD1	2.48	0.67
2:B:411:MET:CE	19:B:1220:CLA:CMC	2.72	0.67
6:F:170:ILE:HG22	21:F:6014:BCR:H372	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:62:LEU:O	7:G:65:SER:HB3	1.94	0.67
11:K:56:ILE:HA	11:K:59:THR:HG23	1.76	0.67
19:3:2009:CLA:CBA	19:3:2009:CLA:HBD	2.22	0.67
15:1:93:ALA:CB	19:1:1006:CLA:HHC	2.09	0.67
1:A:251:ASN:OD1	17:3:137:PHE:HD1	1.55	0.67
6:F:103:GLN:OE1	6:F:103:GLN:CA	2.42	0.67
6:F:103:GLN:CD	6:F:104:ALA:N	2.47	0.67
14:R:26:UNK:O	14:R:28:UNK:N	2.27	0.67
16:2:211:PRO:O	16:2:212:GLN:CB	2.41	0.67
21:1:6023:BCR:C8	21:1:6023:BCR:HC21	2.23	0.67
22:2:7027:LMU:O2'	22:2:7027:LMU:H12	1.95	0.67
15:1:85:ILE:CG1	15:1:88:ARG:CZ	2.69	0.67
18:4:175:TYR:HB2	18:4:195:ALA:N	2.09	0.67
2:B:292:ARG:NH2	2:B:297:ILE:HG13	2.10	0.67
2:B:414:HIS:CD2	19:B:1227:CLA:HMA3	2.30	0.67
19:B:1223:CLA:H71	21:B:6010:BCR:H14C	1.76	0.67
8:H:113:SER:OG	19:H:1207:CLA:H52	1.92	0.67
16:2:103:VAL:HG12	16:2:104:GLN:OE1	1.94	0.67
19:2:2001:CLA:HBC2	19:2:2001:CLA:HMC1	1.74	0.67
2:B:542:ARG:HH21	4:D:197:PRO:HG3	1.59	0.67
19:4:4015:CLA:HBA1	19:4:4015:CLA:CBD	2.25	0.67
2:B:324:ASP:O	2:B:328:ASN:HB2	1.94	0.67
7:G:114:LEU:HD12	7:G:115:LYS:N	2.09	0.67
18:4:205:ILE:HD12	19:4:4004:CLA:CHA	2.25	0.67
1:A:193:LEU:O	1:A:196:PHE:CD2	2.48	0.67
1:A:207:LEU:HB3	19:A:1119:CLA:HBB2	1.76	0.67
1:A:87:SER:O	1:A:88:ILE:HB	1.94	0.67
2:B:299:HIS:HE1	19:B:1219:CLA:HMD1	1.58	0.67
2:B:29:HIS:CD2	19:B:1202:CLA:CBB	2.77	0.67
2:B:594:TRP:C	2:B:594:TRP:CD1	2.68	0.67
2:B:73:ASN:ND2	2:B:73:ASN:H	1.90	0.67
5:E:83:TRP:HH2	5:E:116:SER:CB	2.07	0.67
7:G:68:THR:HB	7:G:128:LEU:HG	1.77	0.67
17:3:96:ARG:N	17:3:99:ALA:H	1.93	0.67
4:D:103:THR:CG2	4:D:128:LEU:HD12	2.23	0.67
22:A:7016:LMU:C2	22:A:7016:LMU:C6	2.72	0.67
15:1:199:VAL:CG1	15:1:200:GLY:N	2.56	0.67
18:4:83:GLU:HB3	18:4:84:ASP:OD1	1.94	0.67
18:4:159:ASP:CG	18:4:171:ILE:CD1	2.55	0.67
1:A:102:ARG:C	1:A:103:PHE:CD2	2.62	0.67
1:A:224:HIS:O	1:A:225:VAL:HG22	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:HIS:C	1:A:248:PHE:CD2	2.68	0.67
1:A:283:PHE:C	1:A:284:ARG:HH11	1.98	0.67
1:A:334:HIS:ND1	1:A:334:HIS:N	2.41	0.67
1:A:503:THR:HB	19:A:1134:CLA:HBA1	1.75	0.67
2:B:438:VAL:CG2	19:B:1230:CLA:HMC1	2.24	0.67
2:B:292:ARG:NH1	2:B:296:GLY:N	2.41	0.67
2:B:318:GLY:O	2:B:407:VAL:HG13	1.95	0.67
2:B:606:VAL:O	2:B:607:SER:C	2.33	0.67
11:K:49:ILE:C	11:K:52:PRO:HD3	2.15	0.67
19:1:1008:CLA:HAA2	19:1:1008:CLA:CGD	2.25	0.67
15:1:182:GLU:O	15:1:183:LEU:HB2	1.93	0.67
18:4:167:ASN:HD21	19:4:4014:CLA:C2	2.08	0.67
1:A:127:VAL:CG2	1:A:128:GLY:H	2.03	0.67
19:B:1231:CLA:HMD2	19:B:1232:CLA:C1C	2.24	0.67
2:B:273:VAL:O	2:B:277:HIS:HD2	1.78	0.67
19:B:1235:CLA:CBC	6:F:160:PHE:CZ	2.77	0.67
12:L:110:LEU:HA	12:L:113:PRO:CG	2.25	0.67
16:2:126:LEU:O	16:2:128:LYS:N	2.27	0.67
5:E:125:ILE:O	5:E:125:ILE:CG1	2.30	0.67
5:E:127:GLU:C	5:E:128:VAL:HG23	2.15	0.67
13:N:139:LYS:CD	13:N:142:LYS:NZ	2.55	0.67
19:1:1007:CLA:H122	19:1:1007:CLA:H61	1.77	0.67
17:3:191:GLU:O	17:3:192:LYS:HD2	1.95	0.67
1:A:40:PHE:N	1:A:44:ILE:HG23	2.10	0.67
18:4:122:ASN:C	18:4:124:PRO:HD3	2.15	0.67
18:4:220:GLN:CD	19:4:1306:CLA:HAC2	2.14	0.67
1:A:79:PHE:CE1	19:A:1111:CLA:CED	2.78	0.67
19:B:1226:CLA:HBC3	19:B:1226:CLA:HMC1	1.74	0.67
19:B:1222:CLA:CBB	19:B:1236:CLA:CMB	2.73	0.67
2:B:270:LEU:HD12	2:B:270:LEU:C	2.15	0.67
2:B:353:TYR:HB2	2:B:594:TRP:HH2	1.60	0.67
8:H:108:THR:O	8:H:109:LEU:C	2.29	0.67
19:H:1207:CLA:CHD	21:I:6018:BCR:H342	2.25	0.67
16:2:107:LEU:HD12	16:2:107:LEU:C	2.15	0.67
16:2:226:ARG:CD	16:2:230:LEU:HD22	2.25	0.67
13:N:139:LYS:O	13:N:142:LYS:CD	2.43	0.67
13:N:143:VAL:HG12	13:N:144:PRO:HD3	1.77	0.67
3:C:52:LYS:CE	3:C:64:SER:HB3	2.24	0.67
4:D:102:ILE:CG2	4:D:102:ILE:O	2.43	0.67
19:H:1145:CLA:CMA	19:H:1145:CLA:C2	2.71	0.67
17:3:154:ASN:HA	17:3:155:TYR:CE2	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:212:GLN:HG2	16:2:213:LYS:N	2.07	0.67
4:D:146:SER:C	4:D:147:LYS:HG3	2.12	0.67
2:B:92:TRP:CD1	2:B:92:TRP:O	2.48	0.67
7:G:139:TYR:CG	7:G:139:TYR:O	2.45	0.67
18:4:98:ASN:HB3	18:4:212:LEU:HD21	1.77	0.66
1:A:214:GLY:O	1:A:215:SER:HB3	1.94	0.66
1:A:64:PHE:CD2	1:A:74:ILE:HD13	2.30	0.66
1:A:711:HIS:NE2	19:A:1139:CLA:HAC1	2.10	0.66
1:A:458:PHE:CD2	19:A:9022:CLA:HMB2	2.29	0.66
2:B:638:LEU:O	2:B:639:VAL:CG1	2.40	0.66
8:H:61:THR:CA	8:H:62:THR:CG2	2.24	0.66
8:H:58:LEU:CB	8:H:61:THR:HG21	2.08	0.66
17:3:108:PHE:CB	19:3:3013:CLA:H42	2.24	0.66
16:2:148:ASP:CB	16:2:152:LEU:CB	2.51	0.66
16:2:182:ILE:CG2	16:2:187:LYS:CG	2.65	0.66
17:3:197:SER:HB3	17:3:206:PRO:CD	2.21	0.66
11:K:112:VAL:O	11:K:113:GLY:C	2.34	0.66
15:1:170:PRO:HG2	15:1:171:LEU:N	2.09	0.66
2:B:75:GLU:HB2	2:B:132:ASN:HB3	1.76	0.66
18:4:109:MET:C	18:4:111:LEU:H	1.97	0.66
18:4:232:LEU:CB	18:4:236:ILE:CD1	2.72	0.66
15:1:128:PRO:CG	15:1:131:TRP:CH2	2.75	0.66
1:A:577:PHE:O	1:A:593:SER:OG	2.13	0.66
19:A:1102:CLA:H2A	19:A:1102:CLA:CED	2.25	0.66
1:A:451:ILE:HD11	19:A:1131:CLA:HED1	1.78	0.66
1:A:149:PHE:HB3	1:A:153:TRP:CE3	2.31	0.66
21:A:6003:BCR:C23	21:A:6003:BCR:C40	2.73	0.66
2:B:310:PRO:HB2	2:B:311:PRO:CD	2.12	0.66
2:B:315:LEU:HD11	2:B:317:ARG:HG2	1.72	0.66
2:B:576:PHE:CE2	19:B:1226:CLA:HAC1	2.29	0.66
19:B:1239:CLA:HED1	23:B:7101:LMG:C21	2.25	0.66
7:G:84:ARG:CG	7:G:85:GLU:HB3	2.26	0.66
8:H:109:LEU:HD23	19:H:1207:CLA:H72	1.77	0.66
11:K:56:ILE:O	11:K:59:THR:HG23	1.95	0.66
3:C:61:ASP:OD2	5:E:118:ASN:ND2	2.26	0.66
5:E:122:LEU:HD12	5:E:122:LEU:O	1.95	0.66
16:2:182:ILE:CA	16:2:187:LYS:HG3	2.25	0.66
16:2:237:PHE:HD1	16:2:237:PHE:O	1.77	0.66
19:2:2014:CLA:H41	19:2:2014:CLA:H93	1.75	0.66
11:K:99:ALA:O	11:K:103:LEU:HD12	1.95	0.66
6:F:188:GLU:OE2	16:2:180:ASP:OD1	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:755:ILE:O	1:A:756:ALA:HB3	1.95	0.66
15:1:58:ALA:HB3	15:1:59:PRO:CD	2.25	0.66
19:4:4006:CLA:H41	19:4:4006:CLA:C10	2.25	0.66
19:3:1147:CLA:CMC	19:3:1147:CLA:HBC2	2.20	0.66
18:4:158:GLN:CA	19:4:1004:CLA:CMA	2.67	0.66
1:A:295:TRP:C	1:A:297:THR:H	1.96	0.66
2:B:455:ILE:HD13	6:F:148:LEU:HD21	1.77	0.66
4:D:86:SER:HA	12:L:69:LEU:HD21	1.78	0.66
11:K:47:ASP:HA	11:K:51:SER:CB	2.25	0.66
8:H:121:LEU:CB	8:H:122:PRO:HD2	2.05	0.66
19:1:1008:CLA:HMC1	19:1:1008:CLA:HBC3	1.77	0.66
13:N:168:TRP:HE3	13:N:168:TRP:O	1.78	0.66
15:1:219:THR:O	15:1:220:HIS:HB3	1.95	0.66
2:B:691:ILE:CG2	2:B:691:ILE:O	2.43	0.66
1:A:308:ILE:HG23	19:A:1115:CLA:H111	1.77	0.66
19:A:1138:CLA:H191	6:F:181:TYR:CB	2.19	0.66
19:A:1140:CLA:H43	19:A:1140:CLA:NC	2.11	0.66
2:B:231:ASN:O	2:B:233:TYR:N	2.28	0.66
2:B:459:PHE:HB2	19:B:1235:CLA:CBD	2.26	0.66
5:E:82:TYR:CZ	5:E:111:ASN:HA	2.30	0.66
5:E:82:TYR:CB	5:E:83:TRP:CE3	2.74	0.66
5:E:90:VAL:O	5:E:91:VAL:HG23	1.94	0.66
11:K:52:PRO:CD	11:K:53:THR:N	2.51	0.66
12:L:70:GLU:CG	12:L:74:THR:HG21	2.24	0.66
3:C:73:THR:CG2	3:C:76:SER:CB	2.74	0.66
4:D:167:HIS:NE2	4:D:172:VAL:CB	2.57	0.66
17:3:96:ARG:NH1	17:3:100:TYR:CE2	2.63	0.66
16:2:166:ARG:NH2	19:2:4009:CLA:O1D	2.29	0.66
17:3:130:GLN:CA	17:3:132:THR:H	2.08	0.66
8:H:78:PRO:HG3	19:L:1501:CLA:HMD1	1.76	0.66
6:F:130:PHE:HB3	6:F:132:ASN:ND2	2.09	0.66
2:B:80:ASP:O	2:B:80:ASP:OD1	2.14	0.66
2:B:479:SER:O	2:B:480:SER:HB3	1.96	0.66
13:N:120:VAL:O	13:N:121:GLU:C	2.34	0.66
11:K:87:GLU:CD	11:K:87:GLU:O	2.34	0.66
16:2:97:GLU:HG2	16:2:97:GLU:O	1.96	0.66
19:B:1217:CLA:H2	19:B:1217:CLA:NB	2.09	0.66
2:B:411:MET:CE	19:B:1220:CLA:HMC2	2.25	0.66
2:B:120:VAL:O	2:B:123:TRP:N	2.28	0.66
2:B:317:ARG:NE	2:B:317:ARG:CA	2.55	0.66
2:B:469:LYS:CB	2:B:470:THR:OG1	2.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:HIS:O	2:B:88:ALA:O	2.14	0.66
11:K:47:ASP:CA	11:K:51:SER:CB	2.73	0.66
13:N:151:ASP:O	13:N:152:LEU:HG	1.96	0.66
16:2:148:ASP:CG	16:2:152:LEU:CB	2.63	0.66
22:A:7010:LMU:C6'	22:K:7047:LMU:H111	2.25	0.66
18:4:169:ASP:OD1	18:4:174:GLN:CB	2.43	0.66
19:A:1115:CLA:CMC	19:A:1115:CLA:HBC3	2.14	0.66
19:A:1124:CLA:C5	19:A:1125:CLA:HED1	2.25	0.66
19:A:1138:CLA:CBC	21:F:6014:BCR:H332	2.25	0.66
1:A:207:LEU:HD11	1:A:314:GLY:HA2	1.78	0.66
2:B:123:TRP:CA	2:B:126:THR:HG21	2.18	0.66
2:B:175:LEU:O	2:B:179:LEU:HG	1.96	0.66
5:E:111:ASN:HD22	5:E:111:ASN:C	1.99	0.66
6:F:202:LEU:O	6:F:203:ALA:HB3	1.94	0.66
11:K:63:LEU:HB3	11:K:102:THR:OG1	1.95	0.66
12:L:73:VAL:CG1	19:L:1504:CLA:HMA3	2.23	0.66
5:E:79:LYS:CE	5:E:84:TYR:OH	2.43	0.66
8:H:66:ASP:O	8:H:67:SER:C	2.34	0.66
17:3:110:MET:O	17:3:114:VAL:N	2.29	0.66
17:3:100:TYR:CB	17:3:229:LYS:HE2	2.24	0.66
19:J:1311:CLA:CED	19:J:1311:CLA:CHA	2.74	0.66
12:L:174:ASP:CG	12:L:175:GLN:N	2.48	0.66
7:G:145:THR:CG2	7:G:146:SER:N	2.57	0.66
18:4:126:TRP:CG	18:4:127:TYR:N	2.63	0.66
15:1:77:GLU:CA	15:1:80:LYS:HD2	2.25	0.66
18:4:143:VAL:HG12	18:4:144:ILE:N	2.11	0.66
18:4:209:ARG:HB2	19:4:4004:CLA:C3A	2.26	0.66
19:A:1124:CLA:HBB2	19:A:1137:CLA:HMA1	1.76	0.66
1:A:109:TRP:HA	1:A:116:ILE:HG13	1.77	0.66
1:A:377:TYR:CD1	1:A:616:PHE:HE1	2.14	0.66
2:B:310:PRO:O	19:B:1301:CLA:C1D	2.44	0.66
2:B:117:TYR:HE2	2:B:366:THR:HG21	1.60	0.66
2:B:508:LEU:CB	2:B:509:PHE:HD2	2.08	0.66
12:L:142:SER:O	12:L:143:LEU:CD2	2.43	0.66
4:D:140:LEU:HD22	4:D:144:LEU:CD1	2.26	0.66
17:3:207:PHE:CD1	17:3:207:PHE:O	2.39	0.66
11:K:111:VAL:HA	11:K:114:HIS:CG	2.30	0.66
2:B:131:THR:HG22	2:B:134:ASP:CA	2.26	0.66
2:B:211:ASN:HB2	2:B:214:ASP:HB3	1.75	0.66
18:4:103:MET:HE2	18:4:207:ASN:O	1.96	0.66
18:4:175:TYR:HB3	18:4:194:PHE:HD1	1.54	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:223:VAL:O	18:4:223:VAL:CG1	2.38	0.66
1:A:150:PHE:N	1:A:153:TRP:CE3	2.62	0.66
1:A:203:LEU:HD21	19:A:1123:CLA:C3D	2.26	0.66
1:A:488:PHE:CD2	1:A:533:PRO:HB2	2.31	0.66
1:A:710:ALA:CB	19:A:1138:CLA:HED2	2.26	0.66
7:G:102:ALA:CA	7:G:104:ASP:CG	2.60	0.66
7:G:131:GLY:O	7:G:136:VAL:CB	2.42	0.66
9:I:9:VAL:HG12	9:I:10:PRO:HD3	1.78	0.66
12:L:153:PHE:CB	12:L:155:GLU:OE1	2.38	0.66
16:2:269:LYS:CE	16:2:269:LYS:CA	2.73	0.66
15:1:162:LYS:CA	15:1:164:PRO:HG3	2.26	0.66
4:D:148:TYR:O	4:D:149:LYS:CG	2.44	0.66
6:F:110:ALA:HA	6:F:113:SER:HB2	1.78	0.66
13:N:91:TYR:O	13:N:93:GLU:N	2.27	0.66
19:A:1105:CLA:HMB3	19:A:1106:CLA:HMB	1.78	0.66
19:A:1125:CLA:CBB	19:A:1133:CLA:C3A	2.70	0.66
19:A:1139:CLA:H42	19:A:1139:CLA:CGA	2.25	0.66
19:A:1140:CLA:C14	21:A:6011:BCR:HC21	2.25	0.66
1:A:358:LEU:HD11	1:A:413:HIS:CB	2.26	0.66
1:A:396:PHE:CE2	1:A:616:PHE:CG	2.84	0.66
1:A:678:PHE:O	1:A:680:LEU:N	2.28	0.66
2:B:123:TRP:HA	2:B:126:THR:HB	1.58	0.66
6:F:149:ILE:O	6:F:150:VAL:HG12	1.96	0.66
5:E:128:VAL:O	5:E:129:GLU:C	2.30	0.66
11:K:127:ILE:O	11:K:130:LEU:CG	2.44	0.66
1:A:715:LYS:CE	6:F:230:ASN:OD1	2.44	0.66
11:K:69:ARG:HG3	11:K:73:ALA:HB2	1.77	0.66
1:A:483:GLN:CB	1:A:485:GLN:NE2	2.56	0.66
4:D:185:GLY:O	4:D:186:GLN:CB	2.43	0.66
3:C:31:TRP:O	3:C:33:GLY:N	2.29	0.66
1:A:606:TYR:O	1:A:610:SER:CB	2.44	0.66
22:A:7023:LMU:H2B	22:A:7023:LMU:C6B	2.24	0.66
1:A:112:ASP:O	1:A:115:HIS:CD2	2.49	0.66
1:A:733:VAL:CG1	1:A:733:VAL:O	2.44	0.66
2:B:527:LEU:HD12	19:B:1236:CLA:HMA3	1.78	0.66
2:B:305:LEU:CD2	19:B:1220:CLA:O1D	2.45	0.66
7:G:102:ALA:CA	7:G:104:ASP:OD1	2.39	0.66
12:L:92:ALA:N	12:L:98:ARG:NH2	2.41	0.66
3:C:12:ILE:HG21	3:C:27:GLU:OE1	1.96	0.66
19:2:4009:CLA:H8	19:2:4009:CLA:H151	1.75	0.66
16:2:237:PHE:CE1	16:2:241:TYR:CE1	2.79	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:H:7017:LMU:O3'	22:H:7017:LMU:H1B	1.96	0.66
15:1:66:PRO:O	15:1:69:LEU:O	2.14	0.65
19:A:1106:CLA:HBB2	19:A:1107:CLA:C3D	2.26	0.65
1:A:402:ILE:CG1	19:A:1127:CLA:HBB2	2.26	0.65
1:A:328:LYS:HZ2	1:A:345:GLY:HA3	1.60	0.65
19:B:1205:CLA:CBB	19:B:1205:CLA:C9	2.73	0.65
6:F:181:TYR:HB2	6:F:203:ALA:HB2	1.78	0.65
7:G:125:VAL:O	7:G:129:ALA:N	2.29	0.65
13:N:148:ASP:H	13:N:149:ASP:CB	2.08	0.65
19:1:1006:CLA:CAC	19:1:1010:CLA:CMB	2.73	0.65
12:L:205:TYR:HD2	12:L:205:TYR:H	1.40	0.65
4:D:140:LEU:CD1	4:D:141:GLY:H	1.82	0.65
1:A:578:ARG:O	1:A:579:PHE:C	2.33	0.65
22:F:7036:LMU:O2B	22:F:7036:LMU:C6'	2.45	0.65
2:B:79:GLN:O	2:B:80:ASP:CB	2.43	0.65
19:4:1304:CLA:H202	19:4:1304:CLA:H151	1.77	0.65
15:1:86:HIS:CD2	15:1:86:HIS:H	2.01	0.65
18:4:103:MET:HE1	18:4:207:ASN:HB3	1.79	0.65
19:A:1131:CLA:O1A	19:A:1237:CLA:H11	1.96	0.65
19:A:9011:CLA:HMC3	2:B:624:LEU:HG	1.77	0.65
19:A:9022:CLA:H13	19:B:1206:CLA:CBB	2.26	0.65
2:B:120:VAL:O	2:B:123:TRP:HD1	1.79	0.65
16:2:115:LEU:HD21	19:2:2011:CLA:NB	2.12	0.65
8:H:64:GLN:CB	8:H:67:SER:H	2.09	0.65
3:C:73:THR:CB	3:C:76:SER:OG	2.43	0.65
4:D:99:PHE:HB3	4:D:157:VAL:CB	2.25	0.65
8:H:85:GLU:CG	8:H:86:THR:H	1.98	0.65
2:B:58:PHE:HB2	2:B:146:SER:HB2	1.78	0.65
2:B:476:ILE:HG23	2:B:479:SER:OG	1.94	0.65
15:1:201:PHE:CD1	15:1:204:GLN:CD	2.70	0.65
22:4:7034:LMU:C11	22:4:7052:LMU:C2'	2.72	0.65
18:4:211:MET:SD	19:4:4002:CLA:HBB1	2.36	0.65
2:B:596:TRP:CH2	2:B:612:SER:C	2.67	0.65
19:A:1115:CLA:H191	11:K:64:MET:HE3	1.79	0.65
12:L:141:LEU:HD12	12:L:145:LEU:CD1	2.24	0.65
8:H:58:LEU:CD1	8:H:61:THR:HA	2.26	0.65
11:K:89:ARG:NH1	11:K:89:ARG:CG	2.58	0.65
15:1:79:TYR:CB	19:1:1012:CLA:OBD	2.44	0.65
6:F:172:GLY:O	6:F:176:TRP:HB2	1.96	0.65
19:A:1126:CLA:CBA	19:A:1126:CLA:H43	2.25	0.65
1:A:385:LEU:O	1:A:386:ALA:CB	2.43	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:HIS:CE1	19:A:1139:CLA:HAC1	2.31	0.65
2:B:292:ARG:NH2	2:B:297:ILE:CG1	2.60	0.65
2:B:320:LYS:O	2:B:406:ASN:ND2	2.18	0.65
19:A:9012:CLA:C1	2:B:616:LEU:HD12	2.14	0.65
7:G:89:LYS:O	7:G:90:GLN:HG2	1.95	0.65
8:H:119:ASP:HB3	8:H:121:LEU:HG	1.78	0.65
18:4:245:VAL:HG22	18:4:246:GLN:N	2.10	0.65
15:1:91:MET:O	15:1:91:MET:SD	2.55	0.65
19:A:1112:CLA:HMC2	21:A:6002:BCR:C15	2.26	0.65
1:A:660:GLN:O	1:A:661:ALA:CB	2.43	0.65
1:A:90:PHE:CD1	19:A:1103:CLA:H91	2.31	0.65
19:B:1219:CLA:CBB	19:B:1219:CLA:H72	2.24	0.65
19:B:1224:CLA:HBC3	19:B:1224:CLA:HMC1	1.79	0.65
2:B:615:TYR:CD1	2:B:615:TYR:N	2.62	0.65
2:B:645:VAL:HG22	19:B:1206:CLA:HHD	1.77	0.65
8:H:67:SER:C	8:H:68:TYR:CG	2.69	0.65
1:A:250:LEU:HD12	17:3:136:TRP:HZ2	1.61	0.65
4:D:95:GLN:NE2	4:D:96:VAL:CA	2.52	0.65
13:N:110:THR:CG2	13:N:111:GLY:H	2.10	0.65
2:B:69:ALA:HB2	2:B:135:LEU:CD1	2.27	0.65
17:3:254:GLN:CG	17:3:255:ASN:H	2.06	0.65
3:C:55:GLU:O	3:C:57:ALA:N	2.20	0.65
18:4:158:GLN:CG	19:4:1004:CLA:HMA3	2.23	0.65
18:4:169:ASP:O	18:4:173:LYS:CA	2.45	0.65
1:A:101:ALA:HB2	1:A:164:LEU:HB2	1.77	0.65
19:A:1119:CLA:HMD1	19:A:1120:CLA:HHD	1.79	0.65
1:A:747:TRP:CE3	21:A:6011:BCR:H401	2.31	0.65
2:B:444:LEU:HD21	2:B:452:GLN:HE22	1.61	0.65
2:B:98:GLN:N	2:B:99:PRO:HD2	2.11	0.65
13:N:152:LEU:CB	13:N:153:GLU:HG3	2.27	0.65
3:C:73:THR:CG2	3:C:76:SER:HB3	2.26	0.65
17:3:91:GLY:C	17:3:92:PHE:CD1	2.69	0.65
2:B:5:ILE:CG2	2:B:6:PRO:CD	2.62	0.65
15:1:150:HIS:CE1	15:1:151:GLN:NE2	2.65	0.65
1:A:525:ASN:ND2	1:A:526:LYS:HE3	2.12	0.65
13:N:169:LYS:CB	13:N:170:TRP:CD1	2.74	0.65
1:A:40:PHE:N	1:A:44:ILE:CG2	2.59	0.65
11:K:87:GLU:O	11:K:87:GLU:OE1	2.15	0.65
18:4:158:GLN:HA	19:4:1004:CLA:H2A	1.78	0.65
1:A:356:ALA:HB2	1:A:417:PHE:HD2	1.61	0.65
1:A:740:LEU:CD2	19:A:1140:CLA:CMA	2.75	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:LEU:HD22	2:B:124:TRP:CE3	2.31	0.65
2:B:171:ALA:O	2:B:172:GLU:HB2	1.97	0.65
1:A:588:GLY:H	2:B:668:ARG:NH1	1.95	0.65
6:F:205:SER:C	6:F:207:LEU:HD12	2.17	0.65
7:G:69:GLY:CA	7:G:72:LEU:HG	2.26	0.65
7:G:89:LYS:H	7:G:89:LYS:NZ	1.95	0.65
11:K:75:SER:O	11:K:76:ALA:HB3	1.97	0.65
3:C:26:LEU:H	3:C:43:PRO:CG	2.08	0.65
1:A:586:ARG:CG	3:C:49:VAL:HG21	2.24	0.65
17:3:96:ARG:CA	17:3:99:ALA:N	2.51	0.65
14:R:36:UNK:O	14:R:38:UNK:N	2.30	0.65
16:2:156:GLU:O	16:2:160:ILE:HD13	1.96	0.65
4:D:140:LEU:CD1	4:D:144:LEU:H	2.10	0.65
1:A:425:THR:OG1	1:A:428:TYR:CE1	2.49	0.65
15:1:208:TYR:N	15:1:209:PRO:CD	2.59	0.65
15:1:176:ASP:HB3	15:1:180:LEU:CG	2.24	0.65
18:4:149:SER:HB2	18:4:153:GLU:OE1	1.95	0.65
1:A:105:ASN:OD1	1:A:119:SER:N	2.28	0.65
19:A:1115:CLA:H191	11:K:64:MET:CE	2.26	0.65
1:A:692:PHE:CZ	19:A:1140:CLA:HBC3	2.32	0.65
21:A:6011:BCR:H313	19:A:9013:CLA:H142	1.79	0.65
2:B:280:ILE:HD13	19:B:1215:CLA:HBB2	1.79	0.65
19:B:1220:CLA:C4	19:B:1220:CLA:C1A	2.65	0.65
2:B:127:ILE:O	2:B:127:ILE:HD12	1.97	0.65
6:F:139:LEU:CD1	6:F:149:ILE:CD1	2.71	0.65
8:H:98:LEU:CD2	12:L:146:THR:CG2	2.71	0.65
19:L:1502:CLA:HAC1	21:L:6019:BCR:H322	1.78	0.65
17:3:112:GLY:HA2	17:3:115:GLY:O	1.97	0.65
17:3:136:TRP:O	17:3:139:THR:N	2.29	0.65
22:3:7005:LMU:H51	22:3:7005:LMU:O1'	1.97	0.65
6:F:101:LYS:C	6:F:103:GLN:N	2.46	0.65
2:B:394:PHE:O	2:B:542:ARG:CD	2.45	0.65
22:F:7036:LMU:H72	22:F:7036:LMU:C11	2.27	0.65
15:1:65:ASP:OD2	15:1:66:PRO:N	2.29	0.65
19:A:1131:CLA:C16	21:L:6019:BCR:C36	2.75	0.65
1:A:246:HIS:O	1:A:248:PHE:N	2.25	0.65
1:A:331:LEU:HD21	1:A:343:HIS:C	2.16	0.65
2:B:196:HIS:CE1	19:B:1212:CLA:HED2	2.32	0.65
2:B:312:GLY:CA	2:B:315:LEU:HB2	2.24	0.65
5:E:111:ASN:ND2	5:E:112:TYR:N	2.45	0.65
19:A:1139:CLA:H43	6:F:198:ILE:HD13	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:6020:BCR:H333	19:L:1502:CLA:C1C	2.26	0.65
3:C:17:CYS:C	3:C:58:CYS:HB2	2.17	0.65
19:3:3011:CLA:HBC2	19:3:3012:CLA:CHA	2.26	0.65
16:2:152:LEU:CD1	16:2:153:PHE:N	2.55	0.65
11:K:128:GLY:N	11:K:129:ALA:CA	2.55	0.65
22:N:7049:LMU:C6	22:N:7049:LMU:H12	2.12	0.65
17:3:210:PRO:HD2	17:3:211:LEU:H	1.62	0.65
22:4:7009:LMU:H3'	22:4:7009:LMU:C5B	2.27	0.65
16:2:258:GLY:O	16:2:259:HIS:ND1	2.29	0.65
18:4:193:ASN:C	18:4:194:PHE:CD1	2.69	0.65
19:B:1235:CLA:H152	21:F:6016:BCR:H313	1.76	0.65
19:B:1222:CLA:HBB1	19:B:1236:CLA:HMB3	1.78	0.65
2:B:123:TRP:HB2	2:B:126:THR:CG2	2.26	0.65
2:B:361:ILE:CG2	2:B:368:GLN:OE1	2.44	0.65
2:B:456:GLU:HA	2:B:514:PRO:CD	2.27	0.65
7:G:62:LEU:O	7:G:65:SER:CB	2.44	0.65
19:L:1502:CLA:HMC1	19:L:1502:CLA:HBC3	1.78	0.65
12:L:72:PRO:C	12:L:73:VAL:HG22	2.15	0.65
5:E:121:ALA:O	5:E:125:ILE:HG21	1.97	0.65
13:N:146:LEU:HD11	17:3:142:ILE:C	2.03	0.65
16:2:152:LEU:HD22	16:2:153:PHE:N	2.12	0.65
6:F:97:GLN:O	6:F:98:ALA:C	2.32	0.65
18:4:112:PRO:HA	18:4:117:SER:OG	1.96	0.65
17:3:177:ALA:O	17:3:178:LYS:CB	2.45	0.65
19:A:1102:CLA:HBA2	19:A:1109:CLA:H62	1.79	0.64
19:A:1120:CLA:H2A	19:A:1120:CLA:O1D	1.97	0.64
19:A:1124:CLA:HMA1	21:A:6008:BCR:H16C	1.79	0.64
19:A:1133:CLA:O1A	19:A:1134:CLA:HBC3	1.97	0.64
1:A:740:LEU:HD21	19:A:1140:CLA:HMA1	1.77	0.64
1:A:328:LYS:HD2	1:A:332:GLU:CB	2.19	0.64
1:A:467:MET:HA	1:A:470:LEU:HB2	1.79	0.64
2:B:292:ARG:HH21	2:B:297:ILE:C	1.99	0.64
2:B:292:ARG:NH2	2:B:297:ILE:O	2.30	0.64
2:B:444:LEU:O	2:B:445:ALA:HB3	1.97	0.64
10:J:18:TRP:CH2	10:J:22:LEU:HD22	2.32	0.64
12:L:71:THR:HB	12:L:72:PRO:HD2	1.78	0.64
16:2:133:ASN:HD22	16:2:134:THR:HB	0.92	0.64
19:1:1014:CLA:CHD	19:1:1014:CLA:CBC	2.72	0.64
15:1:170:PRO:HG2	15:1:173:TYR:CE2	2.32	0.64
12:L:174:ASP:OD2	12:L:175:GLN:N	2.29	0.64
15:1:58:ALA:HB1	19:1:1015:CLA:C3B	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:78:ARG:HH21	15:1:179:LYS:HD3	1.55	0.64
19:A:1133:CLA:CAD	19:A:1134:CLA:HAC1	2.27	0.64
1:A:223:VAL:HG23	1:A:227:LEU:HD12	0.79	0.64
1:A:207:LEU:CD1	1:A:314:GLY:CA	2.75	0.64
1:A:370:ILE:CD1	19:A:1124:CLA:CAD	2.74	0.64
1:A:388:ASP:CG	1:A:391:THR:HG1	1.97	0.64
21:A:6011:BCR:H323	21:J:6012:BCR:H391	1.77	0.64
19:B:1227:CLA:HED2	19:B:1227:CLA:HAA1	1.80	0.64
2:B:188:LEU:O	2:B:191:ALA:N	2.30	0.64
2:B:607:SER:O	2:B:610:ASN:HB2	1.96	0.64
2:B:558:PRO:CG	2:B:703:VAL:CG2	2.62	0.64
16:2:125:PHE:O	16:2:126:LEU:C	2.36	0.64
3:C:73:THR:CB	3:C:76:SER:HG	2.05	0.64
4:D:102:ILE:HG13	4:D:153:GLN:O	1.97	0.64
12:L:154:ASN:C	12:L:178:THR:CG2	2.62	0.64
19:2:2014:CLA:H41	19:2:2014:CLA:C8	2.26	0.64
6:F:117:LEU:HA	6:F:119:ILE:HG12	1.78	0.64
19:R:1150:CLA:H92	22:R:7007:LMU:O4'	1.97	0.64
1:A:274:TRP:CG	1:A:277:TYR:O	2.49	0.64
1:A:43:THR:HG22	1:A:46:LYS:NZ	2.11	0.64
1:A:382:TYR:CE2	19:A:1127:CLA:HED3	2.33	0.64
19:A:1132:CLA:C4	12:L:110:LEU:HD23	2.27	0.64
1:A:204:ASN:O	1:A:205:HIS:CB	2.45	0.64
1:A:281:LEU:HD12	1:A:282:THR:H	1.62	0.64
1:A:374:GLN:O	1:A:377:TYR:HD2	1.81	0.64
1:A:618:TRP:O	1:A:622:SER:HB3	1.98	0.64
1:A:705:GLU:HA	1:A:708:VAL:HB	1.80	0.64
1:A:555:ILE:CG1	19:A:9023:CLA:OBD	2.45	0.64
2:B:152:ALA:O	2:B:153:GLY:C	2.35	0.64
2:B:362:ALA:O	2:B:363:GLN:CB	2.46	0.64
19:B:1235:CLA:CBC	6:F:160:PHE:HZ	2.10	0.64
8:H:58:LEU:CD1	8:H:61:THR:CB	2.52	0.64
2:B:561:GLY:HA3	3:C:52:LYS:CG	2.25	0.64
14:R:38:UNK:C	14:R:39:UNK:O	2.45	0.64
16:2:184:PRO:HD3	16:2:187:LYS:HB2	1.71	0.64
22:3:7003:LMU:H3B	22:3:7005:LMU:C6B	2.19	0.64
13:N:114:PHE:CE2	13:N:116:ARG:HD2	2.33	0.64
11:K:115:ILE:HG12	11:K:122:LEU:CD1	2.27	0.64
19:3:3017:CLA:CMC	19:3:3017:CLA:HBC3	2.24	0.64
1:A:113:PRO:O	1:A:114:THR:CG2	2.35	0.64
1:A:296:LEU:CD1	1:A:297:THR:HG22	2.22	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:LEU:HG	1:A:394:SER:H	1.62	0.64
1:A:52:THR:OG1	1:A:53:TRP:CE3	2.50	0.64
2:B:174:ARG:NH1	19:B:1221:CLA:HMD1	2.13	0.64
7:G:61:ALA:O	7:G:63:VAL:HG13	1.97	0.64
19:2:2001:CLA:CGA	19:2:2001:CLA:C4	2.74	0.64
13:N:139:LYS:CD	13:N:142:LYS:HE2	2.28	0.64
13:N:150:LEU:HD22	13:N:150:LEU:H	1.63	0.64
3:C:63:LEU:CD2	3:C:65:VAL:N	2.59	0.64
17:3:150:TYR:CB	17:3:151:TRP:NE1	2.48	0.64
6:F:97:GLN:NE2	6:F:98:ALA:N	2.45	0.64
12:L:104:LEU:HD21	12:L:199:TRP:CZ2	2.29	0.64
1:A:392:GLN:HA	1:A:395:LEU:HD23	1.78	0.64
15:1:223:ASP:OD1	18:4:140:THR:CG2	2.46	0.64
1:A:174:PHE:CE2	19:A:1103:CLA:H152	2.31	0.64
1:A:302:HIS:HB2	19:A:1116:CLA:CHB	2.27	0.64
19:B:1212:CLA:OBD	19:B:1212:CLA:O2D	2.11	0.64
2:B:622:ASP:HB3	2:B:626:LEU:CG	2.27	0.64
13:N:135:GLN:HA	13:N:136:ASP:C	2.12	0.64
15:1:93:ALA:HA	19:1:1006:CLA:C4B	2.28	0.64
17:3:111:LEU:O	17:3:114:VAL:CB	2.45	0.64
16:2:177:VAL:HG13	16:2:178:ASN:CG	2.17	0.64
12:L:209:LEU:CD1	12:L:210:PRO:CD	2.59	0.64
18:4:111:LEU:CD1	18:4:112:PRO:HG3	2.26	0.64
1:A:40:PHE:H	1:A:44:ILE:HG23	1.62	0.64
4:D:77:ASN:HB3	4:D:79:PRO:CD	2.27	0.64
1:A:554:LEU:CD2	19:A:9023:CLA:O2D	2.46	0.64
2:B:310:PRO:HG2	2:B:311:PRO:CD	2.27	0.64
21:B:6020:BCR:C38	21:B:6020:BCR:H23C	2.28	0.64
19:F:1302:CLA:HHB	21:F:6016:BCR:H333	1.79	0.64
11:K:62:SER:OG	11:K:63:LEU:CD1	2.42	0.64
11:K:63:LEU:N	11:K:63:LEU:CD1	2.45	0.64
16:2:126:LEU:C	16:2:128:LYS:H	1.97	0.64
19:2:2007:CLA:HMC1	19:2:2007:CLA:HBC3	1.79	0.64
3:C:67:VAL:HG13	3:C:68:TYR:N	2.09	0.64
3:C:26:LEU:CD2	4:D:181:ARG:NH1	2.61	0.64
13:N:110:THR:HG22	13:N:111:GLY:N	2.12	0.64
1:A:44:ILE:O	1:A:45:ALA:C	2.36	0.64
18:4:158:GLN:NE2	19:4:1004:CLA:CHA	2.44	0.64
18:4:169:ASP:C	18:4:173:LYS:CA	2.57	0.64
1:A:76:ARG:HH12	1:A:193:LEU:HD22	1.62	0.64
1:A:645:SER:OG	1:A:655:ASP:OD1	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:469:LYS:NZ	2:B:471:THR:N	2.46	0.64
11:K:59:THR:O	11:K:63:LEU:CD1	2.46	0.64
12:L:83:LEU:CD1	12:L:83:LEU:O	2.46	0.64
3:C:63:LEU:HD23	3:C:65:VAL:N	2.13	0.64
17:3:135:ALA:HB3	17:3:139:THR:HB	1.77	0.64
4:D:98:GLU:CB	4:D:100:TYR:HE2	2.11	0.64
4:D:93:LYS:NZ	4:D:97:GLU:OE2	2.30	0.64
16:2:184:PRO:HG2	16:2:185:ASN:N	2.12	0.64
12:L:210:PRO:HB2	12:L:211:TYR:CD2	2.33	0.64
16:2:256:ASP:OD1	16:2:256:ASP:N	2.29	0.64
6:F:214:PRO:O	6:F:215:VAL:CB	2.45	0.64
16:2:211:PRO:HD2	16:2:212:GLN:N	2.12	0.64
18:4:202:GLU:O	18:4:205:ILE:CD1	2.45	0.64
1:A:338:PHE:CD1	19:A:1151:CLA:HBB2	2.33	0.64
1:A:336:GLY:C	1:A:339:THR:HG1	2.01	0.64
1:A:378:SER:O	1:A:379:MET:HG3	1.97	0.64
1:A:57:LEU:HD23	1:A:57:LEU:O	1.98	0.64
1:A:62:HIS:ND1	19:A:1128:CLA:HBA1	2.12	0.64
19:A:9023:CLA:C4	19:A:9023:CLA:HHB	2.27	0.64
1:A:92:TRP:O	1:A:93:LEU:HB3	1.97	0.64
2:B:73:ASN:O	2:B:121:TYR:HE1	1.79	0.64
2:B:202:SER:O	2:B:245:GLY:HA2	1.98	0.64
2:B:280:ILE:HA	2:B:283:LEU:HD12	1.79	0.64
2:B:293:THR:CG2	7:G:94:GLN:CG	2.72	0.64
2:B:295:PHE:N	2:B:295:PHE:CD2	2.59	0.64
2:B:3:LEU:CD1	9:I:29:GLU:OE1	2.44	0.64
19:A:9013:CLA:H93	2:B:431:PHE:CD1	2.33	0.64
2:B:683:GLU:OE2	2:B:693:TRP:HH2	1.80	0.64
2:B:692:ARG:HH22	2:B:694:ARG:HH22	1.44	0.64
5:E:127:GLU:HB3	5:E:128:VAL:C	2.18	0.64
13:N:157:LYS:HB3	13:N:158:ASP:C	2.17	0.64
15:1:143:LEU:N	15:1:143:LEU:HD12	2.13	0.64
4:D:103:THR:CG2	4:D:128:LEU:CG	2.75	0.64
1:A:497:ALA:CB	1:A:510:SER:OG	2.45	0.64
22:A:7045:LMU:H5'	22:A:7045:LMU:O5B	1.97	0.64
15:1:224:PRO:HA	15:1:225:TRP:CB	2.26	0.64
1:A:401:TRP:CD1	19:A:1126:CLA:CHC	2.80	0.64
1:A:130:GLU:CA	1:A:130:GLU:OE1	2.45	0.64
1:A:345:GLY:O	1:A:347:TYR:N	2.23	0.64
2:B:232:LEU:HD11	2:B:235:GLN:CB	2.27	0.64
2:B:418:ILE:O	2:B:422:LEU:HD12	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:510:LEU:HD22	2:B:597:LYS:HD2	1.79	0.64
8:H:97:LEU:HD13	8:H:100:PHE:CB	2.28	0.64
19:2:2007:CLA:CAC	19:3:2009:CLA:HED1	2.09	0.64
1:A:261:SER:O	1:A:262:PHE:CG	2.51	0.64
22:A:7016:LMU:C7	22:A:7016:LMU:H112	2.28	0.64
14:R:27:UNK:O	14:R:29:UNK:N	2.31	0.64
19:4:1304:CLA:C2A	19:4:1304:CLA:CGD	2.75	0.64
18:4:112:PRO:HB3	18:4:116:THR:O	1.98	0.64
4:D:186:GLN:C	4:D:187:ASN:ND2	2.50	0.64
17:3:176:TRP:O	17:3:178:LYS:CG	2.45	0.64
7:G:114:LEU:HD12	7:G:114:LEU:C	2.18	0.64
19:A:1117:CLA:H203	19:A:1125:CLA:HAA1	1.80	0.64
1:A:455:PHE:HD1	19:A:1131:CLA:HMA2	1.63	0.64
1:A:430:ASP:OD1	1:A:433:ASP:OD2	2.15	0.64
1:A:59:ALA:O	1:A:60:ASP:C	2.36	0.64
12:L:146:THR:O	12:L:148:TYR:N	2.30	0.64
12:L:71:THR:HB	12:L:72:PRO:CD	2.27	0.64
13:N:139:LYS:CA	13:N:142:LYS:HD3	2.27	0.64
18:4:87:ASN:O	18:4:90:TRP:HB2	1.98	0.64
8:H:120:ILE:CG1	8:H:120:ILE:O	2.40	0.64
19:4:1304:CLA:H203	19:4:1304:CLA:C15	2.23	0.64
2:B:476:ILE:HG22	2:B:479:SER:OG	1.98	0.64
2:B:453:ILE:CG2	2:B:453:ILE:O	2.41	0.64
16:2:206:TRP:O	16:2:208:SER:N	2.31	0.64
15:1:95:PRO:C	15:1:98:LEU:HB2	2.17	0.63
18:4:207:ASN:O	18:4:211:MET:HE2	1.97	0.63
19:A:1111:CLA:C2	19:A:1111:CLA:HMA2	2.28	0.63
1:A:451:ILE:HD11	19:A:1131:CLA:CED	2.29	0.63
1:A:188:LYS:CE	1:A:190:ALA:HA	2.27	0.63
1:A:245:PRO:O	1:A:248:PHE:CE2	2.51	0.63
1:A:555:ILE:HD13	19:A:9023:CLA:HMD2	1.78	0.63
1:A:58:HIS:HE1	19:A:1101:CLA:ND	1.97	0.63
2:B:212:PHE:CZ	19:B:1211:CLA:HAC1	2.33	0.63
2:B:622:ASP:CB	2:B:626:LEU:HD11	2.28	0.63
2:B:711:VAL:HG22	23:B:7101:LMG:H391	1.80	0.63
21:F:6016:BCR:HC8	21:F:6016:BCR:H311	1.79	0.63
16:2:131:ILE:O	16:2:132:LEU:HD12	1.98	0.63
17:3:141:VAL:CG2	17:3:142:ILE:HG12	2.16	0.63
13:N:142:LYS:HE3	13:N:142:LYS:CA	2.11	0.63
4:D:100:TYR:CZ	4:D:134:LYS:HE3	2.32	0.63
4:D:163:VAL:C	4:D:164:GLN:HG3	2.18	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:103:THR:CG2	4:D:128:LEU:CD1	2.76	0.63
8:H:78:PRO:CG	19:L:1501:CLA:CMD	2.69	0.63
16:2:211:PRO:CD	16:2:212:GLN:H	2.09	0.63
4:D:129:LEU:HD13	12:L:65:PHE:CE1	2.33	0.63
16:2:145:TYR:O	16:2:146:PHE:CG	2.51	0.63
15:1:158:PRO:CG	15:1:159:GLU:N	2.61	0.63
15:1:176:ASP:HB2	15:1:180:LEU:HD12	1.72	0.63
18:4:158:GLN:HE22	19:4:1004:CLA:C4D	2.12	0.63
18:4:158:GLN:NE2	19:4:1004:CLA:C2A	2.61	0.63
1:A:218:TRP:N	19:A:1112:CLA:HBB2	2.13	0.63
2:B:120:VAL:C	2:B:123:TRP:HD1	2.00	0.63
2:B:256:THR:HG1	2:B:258:LEU:H	1.44	0.63
2:B:292:ARG:NH2	2:B:297:ILE:H	1.95	0.63
2:B:454:LEU:HB2	2:B:514:PRO:HB3	1.79	0.63
19:F:1305:CLA:C4	19:4:1306:CLA:HAA1	2.23	0.63
3:C:73:THR:O	3:C:77:MET:HG2	1.97	0.63
13:N:169:LYS:HB3	13:N:170:TRP:HD1	1.48	0.63
22:4:7053:LMU:H6E	22:4:7053:LMU:H2B	1.79	0.63
2:B:117:TYR:CE2	2:B:366:THR:HG21	2.33	0.63
5:E:74:VAL:CG2	5:E:90:VAL:HG22	2.27	0.63
19:A:1129:CLA:HMB2	19:L:1130:CLA:C2D	2.27	0.63
15:1:133:THR:C	15:1:135:PRO:CD	2.66	0.63
3:C:73:THR:OG1	3:C:76:SER:CB	2.46	0.63
16:2:163:ALA:O	16:2:167:ARG:HD2	1.98	0.63
16:2:182:ILE:HD13	16:2:187:LYS:O	1.98	0.63
16:2:189:THR:HG23	16:2:193:VAL:O	1.97	0.63
22:3:7005:LMU:H1B	22:3:7005:LMU:O3'	1.99	0.63
4:D:83:PHE:CZ	4:D:114:MET:HE2	2.33	0.63
4:D:140:LEU:HD13	4:D:144:LEU:N	2.13	0.63
12:L:153:PHE:HD2	12:L:153:PHE:N	1.92	0.63
11:K:115:ILE:HG12	11:K:122:LEU:HD13	1.78	0.63
22:R:7020:LMU:C5B	22:R:7020:LMU:C6'	2.64	0.63
22:H:7032:LMU:C2B	22:H:7032:LMU:H31	2.28	0.63
22:K:7042:LMU:H6D	22:K:7042:LMU:H32	1.80	0.63
15:1:77:GLU:N	15:1:77:GLU:OE1	2.31	0.63
19:A:1237:CLA:H92	21:L:6019:BCR:H321	1.81	0.63
1:A:434:ARG:O	1:A:437:ARG:HB2	1.98	0.63
1:A:432:LEU:HA	1:A:435:VAL:HG13	1.81	0.63
1:A:536:THR:O	1:A:537:ALA:HB3	1.98	0.63
1:A:699:TYR:OH	2:B:533:ILE:CG2	2.43	0.63
2:B:616:LEU:O	2:B:619:TRP:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:91:VAL:O	5:E:93:VAL:N	2.31	0.63
7:G:72:LEU:HD22	7:G:124:ILE:CD1	2.02	0.63
7:G:82:PHE:HB2	7:G:83:GLN:HG3	1.79	0.63
1:A:569:ILE:HB	1:A:572:LYS:HB2	1.80	0.63
1:A:585:GLY:O	1:A:589:THR:OG1	2.17	0.63
18:4:87:ASN:ND2	18:4:90:TRP:CE2	2.67	0.63
16:2:165:GLY:C	16:2:167:ARG:HG2	2.19	0.63
4:D:83:PHE:CZ	4:D:114:MET:CE	2.81	0.63
16:2:252:ALA:HB1	16:2:254:LEU:HB2	1.80	0.63
11:K:81:THR:OG1	11:K:82:ALA:N	2.32	0.63
17:3:243:ILE:HD13	19:3:3005:CLA:C1C	2.29	0.63
22:K:7042:LMU:O3'	22:K:7042:LMU:H1B	1.96	0.63
1:A:54:ILE:O	1:A:58:HIS:HD2	1.80	0.63
21:A:6003:BCR:H403	21:A:6003:BCR:H23C	1.80	0.63
1:A:711:HIS:NE2	19:A:1139:CLA:CAC	2.62	0.63
2:B:551:LYS:HZ1	4:D:194:ASN:C	2.01	0.63
6:F:139:LEU:HD12	6:F:147:HIS:O	1.99	0.63
21:F:6016:BCR:H403	21:F:6016:BCR:H271	1.80	0.63
16:2:160:ILE:O	16:2:161:GLY:C	2.34	0.63
15:1:201:PHE:HA	15:1:204:GLN:HB2	1.80	0.63
1:A:42:ARG:O	1:A:42:ARG:NH1	2.32	0.63
14:R:7:UNK:O	14:R:10:UNK:CB	2.47	0.63
4:D:112:PHE:O	4:D:119:ALA:HB1	1.98	0.63
18:4:175:TYR:HB2	18:4:195:ALA:H	1.63	0.63
1:A:368:LEU:HD22	19:A:1117:CLA:H92	1.77	0.63
1:A:197:GLN:NE2	1:A:351:THR:O	2.32	0.63
1:A:281:LEU:HD12	1:A:282:THR:N	2.14	0.63
1:A:58:HIS:HB3	19:A:1102:CLA:HBC1	1.81	0.63
2:B:568:CYS:O	2:B:570:ILE:N	2.31	0.63
7:G:84:ARG:HE	7:G:85:GLU:HB3	1.60	0.63
8:H:94:ARG:O	8:H:95:GLY:O	2.16	0.63
9:I:10:PRO:HA	9:I:14:LEU:HB2	1.80	0.63
11:K:59:THR:O	11:K:63:LEU:HD11	1.98	0.63
19:2:2002:CLA:HBC2	19:2:2002:CLA:CHD	2.23	0.63
1:A:582:ASP:HB3	1:A:589:THR:HG22	1.80	0.63
17:3:96:ARG:CB	17:3:99:ALA:HB3	2.27	0.63
6:F:191:PRO:HG2	6:F:191:PRO:O	1.99	0.63
8:H:86:THR:O	8:H:88:ALA:C	2.37	0.63
1:A:71:LEU:HD12	1:A:71:LEU:C	2.18	0.63
18:4:145:GLU:CG	18:4:146:PHE:CE1	2.78	0.63
19:A:1110:CLA:C3D	19:A:1111:CLA:HMC3	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1140:CLA:H62	19:A:9013:CLA:H193	1.79	0.63
1:A:401:TRP:O	1:A:405:PHE:HB2	1.98	0.63
1:A:691:MET:HB2	19:A:9013:CLA:C1C	2.28	0.63
2:B:225:LEU:C	2:B:227:THR:O	2.37	0.63
2:B:544:SER:O	2:B:547:MET:N	2.32	0.63
6:F:206:LEU:O	6:F:209:ARG:HB2	1.99	0.63
6:F:204:SER:C	6:F:207:LEU:HD12	2.19	0.63
17:3:131:GLU:O	17:3:134:LEU:N	2.17	0.63
19:R:1144:CLA:C4D	19:R:1144:CLA:HED3	2.28	0.63
1:A:568:LEU:HG	2:B:676:GLU:OE2	1.98	0.63
18:4:86:GLU:H	18:4:86:GLU:CD	1.98	0.63
15:1:225:TRP:CD1	15:1:226:HIS:CE1	2.86	0.63
1:A:448:TRP:CD1	19:A:1131:CLA:HED2	2.32	0.63
1:A:98:PHE:HD1	1:A:99:HIS:H	1.43	0.63
2:B:348:VAL:HA	19:B:1215:CLA:H42	1.79	0.63
2:B:21:ILE:O	2:B:24:GLY:N	2.31	0.63
2:B:292:ARG:NE	2:B:297:ILE:O	2.31	0.63
2:B:353:TYR:C	2:B:355:LEU:H	2.02	0.63
3:C:12:ILE:HD13	3:C:39:ILE:HG13	1.81	0.63
4:D:100:TYR:N	4:D:100:TYR:CD2	2.65	0.63
12:L:210:PRO:O	12:L:211:TYR:CB	2.46	0.63
16:2:233:MET:HA	16:2:236:TRP:HB2	1.80	0.63
11:K:98:PRO:HD2	11:K:99:ALA:N	2.06	0.63
22:K:7041:LMU:H6'2	22:K:7042:LMU:H21	1.79	0.63
18:4:172:PHE:CA	18:4:194:PHE:CE2	2.77	0.63
18:4:157:TRP:HB2	19:4:4012:CLA:CMA	2.29	0.63
1:A:210:LEU:HD12	19:A:1111:CLA:HMB2	1.81	0.63
19:A:1113:CLA:HAA1	19:A:1113:CLA:CED	2.29	0.63
19:A:1119:CLA:H92	21:A:6007:BCR:H373	0.74	0.63
1:A:370:ILE:HD11	19:A:1124:CLA:C3D	2.29	0.63
19:A:1124:CLA:HED2	19:A:1124:CLA:CAA	2.29	0.63
2:B:103:ALA:CA	2:B:105:THR:N	2.61	0.63
2:B:174:ARG:HH11	19:B:1221:CLA:HMD1	1.64	0.63
2:B:422:LEU:CD1	2:B:535:VAL:HG11	2.26	0.63
7:G:93:GLU:OE2	7:G:98:THR:N	2.31	0.63
12:L:131:SER:N	12:L:201:TYR:CZ	2.58	0.63
21:L:6019:BCR:H271	21:L:6019:BCR:H403	1.79	0.63
5:E:78:ARG:H	5:E:78:ARG:CD	2.11	0.63
8:H:58:LEU:HD11	8:H:62:THR:CG2	1.92	0.63
3:C:44:ARG:CB	4:D:182:GLN:NE2	2.51	0.63
14:R:31:UNK:C	14:R:32:UNK:O	2.47	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3:202:TYR:HB3	17:3:203:PRO:HD3	1.79	0.63
11:K:70:PHE:CD1	11:K:70:PHE:O	2.51	0.63
18:4:133:GLU:O	18:4:134:TYR:CD1	2.51	0.63
4:D:112:PHE:O	4:D:119:ALA:CB	2.47	0.63
15:1:75:ASN:O	15:1:76:LEU:C	2.34	0.62
19:A:1111:CLA:HBA1	19:A:1123:CLA:C4	2.27	0.62
19:A:1134:CLA:H3A	19:A:1141:CLA:CBB	2.19	0.62
1:A:336:GLY:C	1:A:339:THR:OG1	2.36	0.62
1:A:364:MET:O	1:A:368:LEU:HB2	1.99	0.62
19:B:1222:CLA:HBB1	19:B:1236:CLA:CMB	2.29	0.62
19:B:1227:CLA:HMB2	19:B:1228:CLA:CHB	2.28	0.62
19:B:1235:CLA:HHB	19:B:1236:CLA:OBD	1.98	0.62
2:B:356:PRO:HD2	2:B:356:PRO:O	1.99	0.62
2:B:470:THR:H	2:B:502:ASN:H	1.45	0.62
2:B:598:HIS:HB3	2:B:602:TRP:CZ3	2.34	0.62
2:B:663:PHE:O	2:B:664:LEU:HG	1.99	0.62
19:G:1242:CLA:H11	22:G:7026:LMU:H61	1.81	0.62
7:G:72:LEU:HD12	7:G:73:PHE:CZ	2.33	0.62
8:H:94:ARG:HH11	8:H:94:ARG:HB2	1.64	0.62
16:2:128:LYS:CB	16:2:131:ILE:HG23	2.29	0.62
19:1:1010:CLA:CBC	19:1:1010:CLA:HHD	2.09	0.62
3:C:7:ILE:O	3:C:8:TYR:C	2.36	0.62
4:D:158:PHE:CB	4:D:159:PRO:HD2	2.17	0.62
18:4:90:TRP:O	18:4:91:PHE:CD1	2.52	0.62
16:2:171:ILE:CG1	16:2:173:ASN:HD21	2.12	0.62
19:J:1311:CLA:H152	19:2:2014:CLA:HMB1	1.79	0.62
16:2:247:ILE:O	16:2:248:ASP:HB2	1.98	0.62
19:1:1008:CLA:HBA2	19:1:1008:CLA:HMA3	1.80	0.62
7:G:111:VAL:O	7:G:111:VAL:HG23	1.97	0.62
15:1:78:ARG:O	15:1:81:GLU:HG2	1.98	0.62
19:4:4002:CLA:CGA	19:4:4002:CLA:HMA2	2.29	0.62
1:A:105:ASN:OD1	1:A:118:PRO:CA	2.44	0.62
1:A:381:PRO:CB	19:A:1117:CLA:HAA2	2.29	0.62
1:A:681:GLY:HA2	1:A:684:PHE:HB3	1.79	0.62
1:A:723:ARG:NH1	1:A:723:ARG:HG2	2.13	0.62
19:B:1220:CLA:O2D	19:B:1220:CLA:C2A	2.47	0.62
2:B:230:TRP:HH2	7:G:67:SER:HB2	1.64	0.62
2:B:32:GLU:HG2	2:B:42:LEU:HD21	1.81	0.62
2:B:459:PHE:HB2	19:B:1235:CLA:HBD	1.80	0.62
2:B:552:ASP:OD1	2:B:553:PHE:CE2	2.52	0.62
2:B:625:TRP:C	2:B:625:TRP:CD2	2.71	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:173:TRP:HE3	6:F:210:GLY:C	2.01	0.62
11:K:56:ILE:CA	11:K:59:THR:HG23	2.29	0.62
12:L:86:LEU:H	12:L:86:LEU:HD12	1.64	0.62
5:E:85:LYS:O	5:E:86:GLY:C	2.37	0.62
15:1:138:LEU:HA	15:1:141:GLU:CG	2.29	0.62
3:C:25:VAL:HA	3:C:43:PRO:HG3	1.80	0.62
11:K:127:ILE:O	11:K:130:LEU:CD2	2.47	0.62
6:F:89:LYS:O	6:F:92:ALA:N	2.32	0.62
22:A:7016:LMU:C1'	22:A:7016:LMU:H31	2.29	0.62
16:2:201:PHE:CE1	16:2:202:ASP:HB3	2.34	0.62
22:H:7011:LMU:H1B	22:H:7011:LMU:C6'	2.28	0.62
18:4:146:PHE:HD1	18:4:146:PHE:N	1.97	0.62
18:4:223:VAL:O	18:4:224:THR:HG23	1.99	0.62
19:A:1124:CLA:C6	19:A:1125:CLA:CED	2.77	0.62
1:A:364:MET:O	1:A:368:LEU:N	2.32	0.62
2:B:269:TRP:HA	2:B:269:TRP:CE3	2.34	0.62
2:B:353:TYR:HB2	2:B:594:TRP:CH2	2.33	0.62
2:B:538:ALA:O	2:B:539:LEU:C	2.38	0.62
2:B:664:LEU:O	2:B:667:TRP:CZ3	2.52	0.62
5:E:103:VAL:CG2	5:E:104:VAL:O	2.47	0.62
11:K:47:ASP:O	11:K:48:PHE:HB2	1.99	0.62
3:C:11:CYS:SG	3:C:12:ILE:N	2.72	0.62
5:E:79:LYS:CB	5:E:84:TYR:CE1	2.82	0.62
13:N:142:LYS:O	13:N:145:PHE:O	2.16	0.62
17:3:135:ALA:C	17:3:139:THR:OG1	2.38	0.62
6:F:101:LYS:O	6:F:103:GLN:N	2.32	0.62
1:A:426:THR:CG2	1:A:428:TYR:HE2	2.04	0.62
19:J:1311:CLA:CHD	19:J:1311:CLA:HBC3	2.28	0.62
1:A:389:TYR:CD1	1:A:625:TRP:CG	2.87	0.62
22:H:7011:LMU:H72	22:H:7011:LMU:H111	1.81	0.62
2:B:691:ILE:O	2:B:691:ILE:HG22	1.98	0.62
15:1:85:ILE:CG1	15:1:88:ARG:NH2	2.62	0.62
1:A:443:ILE:HG22	2:B:674:LEU:HD11	1.80	0.62
7:G:84:ARG:CD	7:G:85:GLU:HB3	2.30	0.62
9:I:9:VAL:CG1	9:I:10:PRO:HD3	2.29	0.62
6:F:200:VAL:HG11	10:J:7:TYR:CG	2.34	0.62
16:2:118:ALA:CB	16:2:121:PHE:HE2	2.11	0.62
13:N:142:LYS:CA	13:N:145:PHE:O	2.47	0.62
17:3:113:ALA:HB2	17:3:239:LEU:HD12	1.70	0.62
16:2:174:PRO:HB2	16:2:194:GLY:CA	2.22	0.62
17:3:148:TYR:CG	17:3:148:TYR:O	2.51	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:4:1304:CLA:CAA	19:4:1304:CLA:CED	2.66	0.62
16:2:137:TRP:O	16:2:139:THR:CG2	2.47	0.62
7:G:139:TYR:O	7:G:139:TYR:CD1	2.52	0.62
2:B:488:ALA:HB1	19:B:1233:CLA:C1C	2.29	0.62
1:A:284:ARG:HB2	1:A:295:TRP:HB2	1.80	0.62
1:A:747:TRP:CD2	21:A:6011:BCR:H401	2.34	0.62
19:B:1222:CLA:HED2	19:B:1223:CLA:HMD1	1.81	0.62
19:B:1222:CLA:CBB	19:B:1236:CLA:HHB	2.24	0.62
7:G:89:LYS:O	7:G:90:GLN:CB	2.48	0.62
10:J:26:LEU:C	10:J:26:LEU:HD23	2.20	0.62
16:2:98:SER:O	16:2:100:ARG:CB	2.47	0.62
5:E:107:PHE:CE2	5:E:109:LYS:CD	2.82	0.62
8:H:86:THR:HG22	8:H:87:PHE:C	2.19	0.62
2:B:550:LYS:CG	2:B:550:LYS:O	2.46	0.62
2:B:144:PHE:CD2	2:B:144:PHE:O	2.52	0.62
15:1:112:GLN:CG	15:1:113:GLU:N	2.62	0.62
6:F:94:ARG:HA	6:F:94:ARG:HE	1.62	0.62
2:B:207:VAL:O	2:B:207:VAL:HG13	1.99	0.62
18:4:120:ILE:CG1	18:4:226:LYS:HG3	2.17	0.62
15:1:225:TRP:CB	15:1:226:HIS:HA	2.29	0.62
19:A:1125:CLA:HBA2	21:A:6008:BCR:H12C	1.81	0.62
19:A:1151:CLA:HBA2	19:A:1151:CLA:O2D	2.00	0.62
1:A:57:LEU:O	1:A:61:ALA:HB2	1.99	0.62
21:A:6011:BCR:HC31	21:F:6014:BCR:H17C	1.81	0.62
2:B:337:ALA:HA	19:B:1221:CLA:HAA1	1.82	0.62
2:B:255:LEU:H	2:B:271:THR:CG2	2.13	0.62
2:B:379:ALA:O	2:B:383:MET:HG2	1.98	0.62
2:B:98:GLN:NE2	2:B:98:GLN:HA	2.14	0.62
7:G:100:PHE:CD2	7:G:100:PHE:O	2.53	0.62
7:G:84:ARG:HG3	7:G:85:GLU:HB2	1.76	0.62
8:H:113:SER:CB	19:H:1207:CLA:H2	2.29	0.62
5:E:107:PHE:CD2	5:E:109:LYS:HD2	2.34	0.62
17:3:130:GLN:CA	17:3:132:THR:N	2.63	0.62
2:B:247:THR:N	2:B:250:ALA:HB2	2.15	0.62
1:A:104:SER:C	1:A:106:TYR:H	2.02	0.62
1:A:123:VAL:O	1:A:124:TRP:HB2	1.99	0.62
1:A:150:PHE:C	1:A:151:GLN:HG3	2.19	0.62
1:A:159:THR:HG22	1:A:160:SER:H	1.64	0.62
1:A:63:ASP:HB2	19:A:1128:CLA:CED	2.28	0.62
1:A:733:VAL:CG2	19:A:1140:CLA:C3D	2.78	0.62
2:B:295:PHE:HE2	7:G:94:GLN:NE2	1.97	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:74:THR:HG23	3:C:75:ARG:N	2.13	0.62
8:H:98:LEU:O	8:H:98:LEU:HG	1.99	0.62
3:C:52:LYS:C	3:C:54:CYS:H	2.03	0.62
10:J:5:LYS:HD2	16:2:178:ASN:CB	2.30	0.62
16:2:186:ASN:O	16:2:187:LYS:HB2	1.99	0.62
4:D:140:LEU:CD2	4:D:144:LEU:HD11	2.30	0.62
6:F:103:GLN:OE1	6:F:103:GLN:HA	2.00	0.62
11:K:115:ILE:CD1	11:K:122:LEU:HD12	2.29	0.62
17:3:155:TYR:O	17:3:157:LEU:N	2.32	0.62
19:1:1001:CLA:HBA1	19:1:1001:CLA:HMA2	1.82	0.62
15:1:65:ASP:HA	15:1:69:LEU:HD13	1.80	0.62
19:A:1101:CLA:HBB2	19:A:1102:CLA:NC	2.15	0.62
1:A:452:PHE:CE1	19:A:1136:CLA:HBB2	2.34	0.62
1:A:207:LEU:CD1	1:A:314:GLY:N	2.62	0.62
1:A:360:ILE:O	1:A:361:ASN:CB	2.47	0.62
1:A:532:ILE:O	1:A:533:PRO:C	2.34	0.62
2:B:686:PRO:HG2	19:L:1130:CLA:H12	1.82	0.62
19:2:2004:CLA:O1A	19:3:2009:CLA:CBC	2.48	0.62
1:A:21:LEU:HD12	1:A:21:LEU:C	2.20	0.62
3:C:14:CYS:O	3:C:14:CYS:SG	2.58	0.62
3:C:58:CYS:HB3	24:C:8003:SF4:S2	2.40	0.62
4:D:167:HIS:NE2	4:D:172:VAL:HG13	2.02	0.62
4:D:172:VAL:O	4:D:173:TYR:CB	2.48	0.62
1:A:250:LEU:CG	17:3:136:TRP:CZ2	2.83	0.62
17:3:204:GLY:CA	17:3:206:PRO:O	2.48	0.62
1:A:485:GLN:OE1	1:A:485:GLN:N	2.32	0.62
3:C:20:ALA:O	3:C:21:CYS:CB	2.47	0.62
13:N:91:TYR:C	13:N:93:GLU:N	2.50	0.62
18:4:201:LYS:CD	18:4:201:LYS:H	2.12	0.62
1:A:224:HIS:CE1	19:A:1113:CLA:C4C	2.83	0.62
1:A:211:LEU:O	1:A:214:GLY:O	2.18	0.62
1:A:229:ILE:CG2	1:A:229:ILE:O	2.46	0.62
1:A:298:ASP:OD2	1:A:298:ASP:N	2.32	0.62
1:A:351:THR:O	19:A:1123:CLA:H18	1.98	0.62
1:A:682:ALA:H	1:A:685:VAL:HG23	1.65	0.62
1:A:603:PHE:HZ	1:A:693:LEU:CD2	2.13	0.62
19:B:1203:CLA:H191	19:B:1224:CLA:H141	1.82	0.62
19:B:1221:CLA:H61	19:B:1221:CLA:HMA2	1.82	0.62
2:B:233:TYR:N	2:B:233:TYR:CD2	2.68	0.62
2:B:438:VAL:HG23	19:B:1230:CLA:HAC1	1.82	0.62
3:C:1:MET:CG	3:C:4:SER:OG	2.42	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:24:LEU:C	9:I:26:LEU:N	2.51	0.62
16:2:128:LYS:O	16:2:129:LEU:C	2.37	0.62
3:C:39:ILE:HG12	3:C:40:ALA:H	1.65	0.62
3:C:25:VAL:HA	3:C:43:PRO:HG2	1.79	0.62
17:3:110:MET:O	17:3:113:ALA:CB	2.41	0.62
18:4:90:TRP:CD1	18:4:91:PHE:N	2.67	0.62
16:2:156:GLU:HG3	16:2:157:LEU:HD13	1.74	0.62
13:N:110:THR:H	13:N:113:ASN:ND2	1.98	0.62
2:B:400:PRO:HD2	4:D:197:PRO:CD	2.29	0.62
15:1:190:ASN:ND2	19:1:1002:CLA:ND	2.48	0.62
2:B:141:PHE:O	2:B:143:LEU:N	2.33	0.62
16:2:266:PHE:CZ	16:2:267:THR:O	2.53	0.62
1:A:497:ALA:HB1	1:A:510:SER:OG	1.99	0.62
16:2:144:GLU:HA	16:2:144:GLU:OE2	1.97	0.62
1:A:98:PHE:O	1:A:101:ALA:N	2.33	0.62
19:A:1115:CLA:C2A	19:A:1115:CLA:CED	2.44	0.62
19:A:1117:CLA:C20	19:A:1125:CLA:H3A	2.30	0.62
19:A:1104:CLA:H51	19:A:1128:CLA:C4C	2.30	0.62
1:A:373:ALA:HB1	1:A:396:PHE:CD1	2.35	0.62
1:A:399:HIS:O	1:A:400:MET:HB2	2.00	0.62
19:A:9023:CLA:H92	19:B:1239:CLA:HBB2	1.82	0.62
1:A:93:LEU:N	1:A:96:MET:H	1.98	0.62
2:B:178:HIS:HE1	19:B:1210:CLA:NC	1.97	0.62
19:L:1503:CLA:CBC	19:L:1503:CLA:CHD	2.65	0.62
4:D:93:LYS:CG	4:D:96:VAL:CG1	2.74	0.62
17:3:134:LEU:H	17:3:134:LEU:HD12	1.64	0.62
16:2:95:ASP:OD2	17:3:85:ASP:O	2.13	0.62
17:3:201:ALA:O	17:3:202:TYR:HB2	2.00	0.62
22:H:7043:LMU:C10	22:H:7043:LMU:H62	2.28	0.62
2:B:262:HIS:O	2:B:265:THR:O	2.18	0.62
1:A:96:MET:CE	19:A:1106:CLA:HED2	2.29	0.61
1:A:126:ILE:O	1:A:127:VAL:CG2	2.41	0.61
1:A:227:LEU:HD22	1:A:296:LEU:O	1.99	0.61
1:A:54:ILE:O	1:A:58:HIS:CD2	2.53	0.61
19:B:1235:CLA:H202	21:F:6016:BCR:HC41	1.82	0.61
2:B:449:PRO:O	2:B:452:GLN:HB2	2.00	0.61
2:B:557:PHE:CD1	2:B:571:SER:HB3	2.34	0.61
2:B:663:PHE:O	2:B:664:LEU:HB2	1.99	0.61
2:B:685:THR:OG1	19:L:1130:CLA:C3A	2.47	0.61
6:F:203:ALA:HB1	6:F:206:LEU:HD12	1.80	0.61
19:L:1503:CLA:HAA1	19:L:1503:CLA:O1D	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:150:ILE:CD1	12:L:150:ILE:C	2.63	0.61
13:N:148:ASP:N	13:N:149:ASP:C	2.53	0.61
3:C:44:ARG:NE	4:D:182:GLN:HE21	1.97	0.61
17:3:151:TRP:HD1	17:3:151:TRP:N	1.93	0.61
4:D:142:THR:O	4:D:143:ARG:C	2.38	0.61
1:A:578:ARG:NH1	1:A:578:ARG:CB	2.63	0.61
15:1:170:PRO:HD2	15:1:173:TYR:HD2	1.56	0.61
2:B:139:ALA:O	2:B:140:ILE:C	2.36	0.61
22:4:7033:LMU:H6'2	22:4:7033:LMU:H3'	1.82	0.61
22:4:7052:LMU:C1	22:4:7052:LMU:H61	2.29	0.61
18:4:96:LEU:HD13	18:4:100:ARG:CZ	2.30	0.61
19:A:1117:CLA:OBD	19:A:1127:CLA:H43	2.01	0.61
1:A:188:LYS:O	1:A:190:ALA:CB	2.43	0.61
1:A:193:LEU:O	1:A:196:PHE:CE2	2.52	0.61
1:A:459:GLY:O	1:A:462:ILE:HG22	2.00	0.61
1:A:701:GLN:O	1:A:704:ILE:N	2.33	0.61
2:B:278:LEU:HG	19:B:1213:CLA:HMA2	1.82	0.61
19:A:1131:CLA:C16	21:L:6019:BCR:H361	2.29	0.61
16:2:104:GLN:H	16:2:104:GLN:CD	2.02	0.61
5:E:107:PHE:HD2	5:E:109:LYS:HD2	1.65	0.61
13:N:147:SER:O	13:N:148:ASP:CB	2.48	0.61
15:1:93:ALA:CB	19:1:1006:CLA:C4B	2.78	0.61
16:2:168:TRP:HA	16:2:171:ILE:CG2	2.19	0.61
4:D:141:GLY:H	4:D:144:LEU:N	1.86	0.61
11:K:110:GLY:O	11:K:114:HIS:CD2	2.53	0.61
17:3:192:LYS:CA	17:3:192:LYS:HZ3	2.12	0.61
17:3:202:TYR:CD2	17:3:202:TYR:N	2.67	0.61
17:3:243:ILE:CG1	19:3:3005:CLA:C3C	2.78	0.61
1:A:389:TYR:CE1	1:A:625:TRP:CG	2.87	0.61
6:F:171:ALA:HA	6:F:174:ILE:HG12	1.80	0.61
15:1:184:LYS:HE3	19:1:1001:CLA:OBD	2.00	0.61
1:A:302:HIS:HB2	19:A:1116:CLA:C1B	2.30	0.61
19:A:1119:CLA:CBC	19:A:1119:CLA:HMC1	2.29	0.61
1:A:309:LEU:O	1:A:310:PHE:HB2	2.00	0.61
19:A:1124:CLA:CHC	21:A:6008:BCR:H373	2.30	0.61
2:B:438:VAL:HG22	19:B:1230:CLA:HMC3	1.81	0.61
2:B:175:LEU:HD21	19:B:1216:CLA:CMA	2.30	0.61
2:B:298:GLY:HA2	19:B:1218:CLA:CMD	2.28	0.61
2:B:493:TRP:O	2:B:495:PRO:CD	2.47	0.61
2:B:525:LEU:HD23	2:B:525:LEU:O	1.99	0.61
3:C:74:THR:OG1	3:C:80:ALA:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:74:THR:OG1	3:C:80:ALA:CB	2.48	0.61
6:F:157:TRP:HE3	19:F:1305:CLA:HMC2	1.65	0.61
16:2:104:GLN:N	16:2:104:GLN:OE1	2.33	0.61
19:2:2007:CLA:O1D	19:2:2007:CLA:H2A	2.01	0.61
3:C:42:ALA:HB1	3:C:43:PRO:CD	2.30	0.61
1:A:263:ALA:O	1:A:264:GLU:CG	2.47	0.61
18:4:87:ASN:ND2	18:4:90:TRP:CZ2	2.68	0.61
16:2:160:ILE:O	16:2:163:ALA:N	2.34	0.61
16:2:172:LEU:CA	16:2:173:ASN:ND2	2.62	0.61
19:2:4009:CLA:ND	19:2:4009:CLA:H18	2.14	0.61
12:L:204:LEU:HD13	12:L:205:TYR:C	2.19	0.61
1:A:575:LEU:CD1	1:A:579:PHE:HB3	2.30	0.61
15:1:112:GLN:O	15:1:113:GLU:HB2	2.00	0.61
22:H:7032:LMU:C5B	22:H:7032:LMU:H3'	2.29	0.61
1:A:236:GLY:O	1:A:237:VAL:CG1	2.48	0.61
22:4:7034:LMU:C10	22:4:7052:LMU:O3'	2.48	0.61
15:1:184:LYS:CE	19:1:1001:CLA:OBD	2.47	0.61
19:A:1112:CLA:C3B	21:A:6002:BCR:C19	2.72	0.61
19:A:1124:CLA:H52	19:A:1125:CLA:HED1	1.81	0.61
19:A:1237:CLA:H152	21:B:6020:BCR:H352	1.80	0.61
1:A:93:LEU:HA	1:A:96:MET:N	2.15	0.61
2:B:120:VAL:HG13	2:B:123:TRP:CD1	2.35	0.61
19:B:1215:CLA:C3A	19:B:1215:CLA:CGA	2.77	0.61
19:B:1227:CLA:CAA	19:B:1227:CLA:HED2	2.30	0.61
2:B:202:SER:C	2:B:204:GLY:H	2.03	0.61
2:B:266:GLN:O	2:B:267:SER:HB3	1.98	0.61
2:B:544:SER:N	2:B:547:MET:O	2.34	0.61
2:B:714:SER:O	2:B:718:ILE:HG22	2.01	0.61
21:F:6016:BCR:H403	21:F:6016:BCR:C27	2.30	0.61
9:I:14:LEU:C	9:I:17:PRO:HD2	2.20	0.61
11:K:60:SER:CA	11:K:63:LEU:HD21	2.28	0.61
12:L:201:TYR:O	12:L:202:PHE:C	2.37	0.61
13:N:147:SER:C	13:N:149:ASP:HB2	2.21	0.61
3:C:72:GLU:OE2	3:C:77:MET:HE1	2.00	0.61
17:3:238:ILE:CG1	19:3:3003:CLA:HMC2	2.31	0.61
4:D:83:PHE:CE1	4:D:114:MET:HE2	2.35	0.61
13:N:112:ALA:N	13:N:118:TYR:CD1	2.69	0.61
4:D:80:SER:N	4:D:81:PRO:HD3	2.16	0.61
17:3:204:GLY:HA3	17:3:207:PHE:C	2.20	0.61
18:4:243:THR:HG23	18:4:244:ILE:C	2.20	0.61
1:A:483:GLN:HB3	1:A:485:GLN:HE22	1.61	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:177:LEU:N	18:4:178:PRO:HD2	2.16	0.61
18:4:201:LYS:CD	18:4:201:LYS:N	2.63	0.61
19:A:1116:CLA:HMC1	19:A:1116:CLA:HBC3	1.81	0.61
1:A:379:MET:HE2	19:A:1125:CLA:HMC2	1.80	0.61
1:A:304:LEU:HG	19:A:1115:CLA:HBB2	1.82	0.61
1:A:438:HIS:CE1	1:A:442:ILE:HD11	2.35	0.61
1:A:554:LEU:HD21	19:A:9023:CLA:O2D	1.99	0.61
1:A:604:TRP:HE1	19:A:9023:CLA:C1D	2.14	0.61
2:B:293:THR:O	2:B:295:PHE:HD2	1.82	0.61
2:B:421:HIS:NE2	19:B:1228:CLA:C4D	2.63	0.61
7:G:76:ARG:NH2	7:G:117:ASN:C	2.54	0.61
6:F:101:LYS:O	6:F:102:LEU:C	2.38	0.61
6:F:228:ASP:O	6:F:231:PHE:CB	2.49	0.61
21:3:6022:BCR:C8	21:3:6022:BCR:H311	2.29	0.61
1:A:258:LEU:O	1:A:259:TYR:CD2	2.54	0.61
19:1:1005:CLA:HMC3	19:1:1012:CLA:CAC	2.29	0.61
18:4:142:PHE:HA	18:4:145:GLU:CD	2.20	0.61
1:A:296:LEU:CD1	1:A:296:LEU:C	2.69	0.61
1:A:296:LEU:HD12	1:A:297:THR:N	2.16	0.61
19:A:1103:CLA:H42	21:A:6003:BCR:H313	1.82	0.61
1:A:618:TRP:CZ2	1:A:655:ASP:HB2	2.35	0.61
1:A:700:TRP:CZ3	19:A:9013:CLA:O1D	2.53	0.61
2:B:552:ASP:OD1	2:B:553:PHE:HD2	1.82	0.61
19:A:1131:CLA:HAA1	21:B:6020:BCR:C13	2.30	0.61
6:F:204:SER:O	6:F:206:LEU:N	2.33	0.61
16:2:133:ASN:HD21	16:2:134:THR:CB	2.10	0.61
3:C:62:PHE:CG	4:D:191:ILE:CG2	2.84	0.61
8:H:67:SER:C	8:H:68:TYR:CD2	2.74	0.61
4:D:173:TYR:CD2	4:D:173:TYR:O	2.52	0.61
16:2:160:ILE:CG2	19:2:2012:CLA:HBB2	2.11	0.61
17:3:130:GLN:C	17:3:132:THR:N	2.49	0.61
18:4:115:PHE:O	18:4:116:THR:C	2.38	0.61
16:2:154:ILE:O	16:2:158:VAL:HG12	2.01	0.61
22:A:7010:LMU:O6'	22:K:7047:LMU:H111	2.00	0.61
15:1:158:PRO:CA	15:1:175:LYS:HG3	2.26	0.61
19:A:1106:CLA:H142	21:J:6012:BCR:C14	2.31	0.61
19:A:1119:CLA:CMD	19:A:1121:CLA:CBB	2.64	0.61
1:A:375:HIS:CE1	19:A:1125:CLA:NC	2.69	0.61
1:A:648:THR:CG2	1:A:651:GLY:H	2.09	0.61
1:A:707:ILE:O	1:A:711:HIS:CD2	2.53	0.61
2:B:98:GLN:O	2:B:100:ALA:HB3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1220:CLA:HBD	19:B:1220:CLA:HAA2	1.81	0.61
2:B:315:LEU:HD12	2:B:317:ARG:N	2.15	0.61
2:B:378:ILE:HA	2:B:381:PHE:HB2	1.82	0.61
2:B:607:SER:O	2:B:610:ASN:CB	2.49	0.61
2:B:623:TYR:H	2:B:626:LEU:HB2	1.66	0.61
2:B:638:LEU:C	2:B:639:VAL:HG12	2.21	0.61
19:F:1302:CLA:C3B	19:F:1305:CLA:CAC	2.68	0.61
17:3:98:LEU:O	17:3:99:ALA:C	2.39	0.61
19:K:1142:CLA:HMD1	19:K:1143:CLA:C1A	2.30	0.61
2:B:480:SER:O	2:B:481:THR:CG2	2.45	0.61
12:L:51:LYS:CA	12:L:51:LYS:CE	2.75	0.61
2:B:8:PHE:O	2:B:35:ASP:OD2	2.18	0.61
15:1:177:PRO:CG	15:1:180:LEU:HD23	2.31	0.61
1:A:690:LEU:HD21	1:A:738:TYR:HE1	1.66	0.61
2:B:123:TRP:CB	2:B:126:THR:HG22	2.26	0.61
2:B:390:GLY:N	2:B:391:PRO:CD	2.64	0.61
2:B:558:PRO:HG2	2:B:703:VAL:CG1	2.31	0.61
2:B:692:ARG:HH22	2:B:694:ARG:NH2	1.98	0.61
2:B:696:LYS:HG2	3:C:80:ALA:CA	2.24	0.61
3:C:78:GLY:O	3:C:81:TYR:HE1	1.84	0.61
13:N:130:ASN:HB2	13:N:139:LYS:HD3	1.80	0.61
3:C:51:CYS:N	24:C:8002:SF4:S4	2.63	0.61
4:D:156:ARG:HB2	4:D:166:LEU:HD12	1.81	0.61
2:B:633:ASN:CG	2:B:636:THR:HB	2.19	0.61
4:D:82:ILE:O	4:D:82:ILE:CG1	2.46	0.61
22:R:7020:LMU:O6'	22:R:7020:LMU:H5B	1.99	0.61
17:3:156:THR:O	17:3:158:PHE:O	2.18	0.61
15:1:67:LEU:CD1	15:1:68:GLY:H	2.10	0.61
19:A:1120:CLA:CAD	19:A:1121:CLA:HMA1	2.31	0.61
19:A:1122:CLA:HBC1	21:A:6007:BCR:H393	1.83	0.61
19:A:1134:CLA:O1A	19:A:1141:CLA:CBB	2.49	0.61
1:A:284:ARG:CB	1:A:295:TRP:CD1	2.84	0.61
1:A:393:LEU:CD1	1:A:750:PHE:CE1	2.83	0.61
2:B:426:SER:O	2:B:430:GLY:N	2.33	0.61
2:B:668:ARG:HG3	2:B:699:ALA:O	2.01	0.61
12:L:106:HIS:HD2	19:L:1502:CLA:HED1	1.64	0.61
12:L:209:LEU:O	12:L:210:PRO:C	2.38	0.61
19:K:1146:CLA:C2A	19:K:1146:CLA:O1A	2.48	0.61
15:1:77:GLU:O	15:1:80:LYS:CG	2.41	0.61
19:4:4002:CLA:O1D	19:4:4002:CLA:HAA2	2.01	0.61
1:A:342:GLY:O	1:A:343:HIS:C	2.39	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:716:VAL:O	19:A:1139:CLA:HMD3	2.01	0.61
2:B:122:GLN:O	2:B:126:THR:CA	2.49	0.61
2:B:178:HIS:O	2:B:180:SER:N	2.34	0.61
2:B:463:ILE:O	2:B:464:GLN:CB	2.49	0.61
2:B:469:LYS:CD	2:B:470:THR:HG23	2.30	0.61
11:K:76:ALA:HA	11:K:78:ARG:HH11	1.65	0.61
12:L:82:TYR:CE1	19:L:1130:CLA:H93	2.35	0.61
16:2:101:TRP:N	16:2:103:VAL:N	2.49	0.61
13:N:143:VAL:HG12	13:N:144:PRO:CD	2.31	0.61
19:1:1014:CLA:H101	19:1:1014:CLA:C5	2.29	0.61
2:B:75:GLU:HB3	2:B:132:ASN:HD22	1.64	0.61
22:R:7007:LMU:H1'	22:R:7007:LMU:O6'	2.00	0.61
18:4:158:GLN:CD	19:4:1004:CLA:O1D	2.37	0.60
18:4:174:GLN:C	18:4:176:SER:N	2.49	0.60
1:A:101:ALA:HB1	1:A:161:GLU:O	2.01	0.60
1:A:545:HIS:HB3	19:A:1135:CLA:CBB	2.30	0.60
1:A:76:ARG:O	1:A:186:TYR:HD2	1.84	0.60
19:B:1222:CLA:HMB2	19:B:1236:CLA:O1A	1.99	0.60
6:F:152:GLY:O	19:F:1302:CLA:HAC2	2.00	0.60
3:C:12:ILE:CG2	3:C:38:GLN:O	2.49	0.60
3:C:24:ASP:O	3:C:43:PRO:HG2	2.01	0.60
14:R:41:UNK:CA	14:R:42:UNK:CB	2.77	0.60
16:2:172:LEU:CB	16:2:173:ASN:HD22	2.13	0.60
10:J:5:LYS:CD	16:2:178:ASN:HA	2.28	0.60
19:J:1308:CLA:HBC3	19:J:1308:CLA:CHD	2.25	0.60
16:2:155:VAL:O	16:2:158:VAL:HG13	2.01	0.60
2:B:681:ALA:O	2:B:684:ARG:N	2.33	0.60
1:A:107:GLU:CD	1:A:161:GLU:HG3	2.21	0.60
1:A:207:LEU:O	1:A:310:PHE:CB	2.49	0.60
1:A:346:LEU:O	1:A:346:LEU:HD22	2.01	0.60
1:A:534:LEU:HD12	1:A:535:GLY:CA	2.26	0.60
1:A:723:ARG:HH11	1:A:723:ARG:HG3	1.65	0.60
2:B:230:TRP:O	2:B:231:ASN:C	2.39	0.60
2:B:440:ASN:OD1	2:B:614:THR:HG23	1.96	0.60
2:B:553:PHE:CD1	2:B:557:PHE:HB3	2.36	0.60
2:B:664:LEU:O	2:B:667:TRP:HZ3	1.84	0.60
7:G:100:PHE:H	7:G:101:GLU:HB2	1.62	0.60
3:C:9:ASP:OD1	3:C:61:ASP:OD2	2.19	0.60
14:R:35:UNK:C	14:R:38:UNK:CB	2.79	0.60
18:4:89:ARG:NH1	18:4:90:TRP:HA	2.16	0.60
16:2:167:ARG:CA	16:2:167:ARG:HE	2.13	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3:131:GLU:O	17:3:134:LEU:HD12	2.02	0.60
8:H:81:SER:O	8:H:82:LYS:C	2.37	0.60
15:1:189:LYS:N	15:1:189:LYS:HE2	2.16	0.60
4:D:208:TYR:CG	4:D:208:TYR:O	2.53	0.60
1:A:425:THR:O	1:A:427:ARG:NE	2.33	0.60
15:1:169:ASP:OD2	15:1:170:PRO:HD2	2.00	0.60
2:B:27:THR:O	2:B:28:ALA:C	2.39	0.60
22:4:7034:LMU:C10	22:4:7052:LMU:C2'	2.78	0.60
1:A:362:LEU:HD11	19:A:1128:CLA:HBB2	1.84	0.60
19:A:1141:CLA:HBC3	19:A:1141:CLA:CHD	2.32	0.60
1:A:174:PHE:O	1:A:175:ALA:HB2	2.01	0.60
1:A:246:HIS:ND1	1:A:246:HIS:N	2.50	0.60
1:A:679:PHE:HE1	1:A:749:PHE:HB2	1.66	0.60
19:A:9012:CLA:HMB3	19:B:9010:CLA:C18	2.30	0.60
19:B:1216:CLA:HBB2	19:B:1221:CLA:H41	1.83	0.60
2:B:25:ILE:CG2	21:L:6019:BCR:C29	2.77	0.60
2:B:302:LYS:O	2:B:303:TYR:CB	2.37	0.60
2:B:553:PHE:O	2:B:554:GLY:O	2.19	0.60
2:B:704:GLN:O	2:B:708:VAL:HG23	2.02	0.60
7:G:128:LEU:CD2	7:G:128:LEU:C	2.70	0.60
7:G:76:ARG:NH2	7:G:117:ASN:CA	2.64	0.60
11:K:56:ILE:CG2	11:K:59:THR:HG23	2.28	0.60
19:A:1132:CLA:H41	12:L:110:LEU:HD23	1.82	0.60
12:L:142:SER:O	12:L:143:LEU:HD23	2.01	0.60
16:2:101:TRP:HA	16:2:103:VAL:H	1.64	0.60
13:N:145:PHE:CA	13:N:146:LEU:O	2.49	0.60
1:A:68:THR:HG22	1:A:70:ASP:N	2.14	0.60
2:B:715:VAL:HG13	2:B:719:PHE:HD2	1.64	0.60
15:1:85:ILE:HA	15:1:88:ARG:NE	2.14	0.60
18:4:149:SER:CB	18:4:153:GLU:OE1	2.50	0.60
18:4:174:GLN:C	18:4:176:SER:H	2.03	0.60
19:A:1115:CLA:C17	19:A:1115:CLA:H141	2.13	0.60
1:A:442:ILE:CG2	19:A:1129:CLA:HMC3	2.31	0.60
1:A:50:THR:CG2	1:A:51:THR:H	2.15	0.60
21:A:6008:BCR:C8	21:A:6008:BCR:C33	2.75	0.60
19:B:1212:CLA:H2A	19:B:1212:CLA:O1D	2.02	0.60
2:B:469:LYS:NZ	2:B:471:THR:C	2.55	0.60
19:A:9012:CLA:H11	2:B:616:LEU:CB	2.30	0.60
5:E:82:TYR:CB	5:E:83:TRP:CZ3	2.72	0.60
6:F:207:LEU:N	6:F:207:LEU:CD1	2.64	0.60
11:K:47:ASP:N	11:K:51:SER:HB2	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:122:ILE:N	16:2:123:PRO:CD	2.64	0.60
5:E:78:ARG:CZ	5:E:125:ILE:HG22	2.32	0.60
1:A:250:LEU:CG	17:3:136:TRP:HZ2	2.15	0.60
4:D:156:ARG:CZ	4:D:164:GLN:HB2	2.32	0.60
16:2:152:LEU:HD22	16:2:152:LEU:C	2.21	0.60
15:1:150:HIS:NE2	15:1:151:GLN:NE2	2.47	0.60
1:A:23:ASP:CB	1:A:33:GLN:OE1	2.50	0.60
2:B:478:LEU:CD2	2:B:478:LEU:O	2.44	0.60
7:G:144:THR:OG1	7:G:148:GLY:N	2.34	0.60
18:4:127:TYR:CD1	18:4:127:TYR:O	2.54	0.60
18:4:205:ILE:HG13	18:4:206:ALA:N	2.14	0.60
1:A:206:HIS:O	1:A:211:LEU:HD23	2.00	0.60
1:A:287:LEU:HD22	1:A:292:GLY:O	2.00	0.60
1:A:327:ILE:O	1:A:328:LYS:C	2.37	0.60
1:A:331:LEU:C	1:A:331:LEU:CD2	2.69	0.60
1:A:704:ILE:HA	1:A:707:ILE:HG13	1.83	0.60
1:A:725:LEU:HD21	19:A:1140:CLA:HMD3	1.83	0.60
1:A:735:VAL:O	1:A:739:LEU:HG	2.00	0.60
19:B:1212:CLA:HMA1	21:B:6006:BCR:H372	1.83	0.60
21:B:6010:BCR:H23C	21:B:6010:BCR:C38	2.27	0.60
2:B:652:PHE:O	2:B:656:VAL:HG23	2.00	0.60
7:G:83:GLN:O	7:G:84:ARG:HB3	2.01	0.60
2:B:294:ASN:CG	7:G:94:GLN:CG	2.57	0.60
9:I:8:PHE:CE1	19:I:1204:CLA:H43	2.36	0.60
16:2:130:GLY:CA	16:2:131:ILE:HG12	1.99	0.60
5:E:107:PHE:CD2	5:E:109:LYS:CE	2.84	0.60
15:1:143:LEU:CD1	15:1:143:LEU:N	2.63	0.60
16:2:184:PRO:CB	16:2:187:LYS:CD	2.68	0.60
16:2:184:PRO:N	16:2:185:ASN:HA	2.16	0.60
17:3:150:TYR:C	17:3:152:ALA:H	2.01	0.60
15:1:170:PRO:HG2	15:1:171:LEU:C	2.22	0.60
19:H:1145:CLA:C19	19:H:1145:CLA:H143	2.29	0.60
16:2:266:PHE:CG	16:2:267:THR:N	2.70	0.60
1:A:34:TRP:O	1:A:35:ALA:CB	2.49	0.60
4:D:112:PHE:CD2	4:D:112:PHE:C	2.75	0.60
22:2:7031:LMU:O2B	22:2:7031:LMU:H4'	2.01	0.60
19:4:4006:CLA:CMA	22:4:7034:LMU:H62	2.23	0.60
15:1:97:ILE:HD11	15:1:98:LEU:CD2	2.27	0.60
1:A:109:TRP:O	1:A:113:PRO:N	2.35	0.60
1:A:242:ILE:HG13	1:A:243:PRO:HD3	0.74	0.60
2:B:493:TRP:HH2	19:B:1232:CLA:HMA2	1.61	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1239:CLA:H151	12:L:144:CYS:SG	2.42	0.60
5:E:107:PHE:HD2	5:E:109:LYS:CD	2.12	0.60
5:E:127:GLU:CD	5:E:129:GLU:O	2.40	0.60
17:3:104:ILE:HG21	19:3:3004:CLA:C2D	2.30	0.60
22:2:7006:LMU:O2'	22:2:7006:LMU:H22	2.01	0.60
17:3:150:TYR:CG	17:3:151:TRP:NE1	2.47	0.60
2:B:159:PRO:O	2:B:160:LYS:C	2.38	0.60
2:B:131:THR:O	2:B:134:ASP:N	2.34	0.60
2:B:131:THR:CG2	2:B:134:ASP:CB	2.74	0.60
4:D:148:TYR:C	4:D:149:LYS:HG2	2.22	0.60
16:2:154:ILE:O	16:2:158:VAL:CG1	2.49	0.60
7:G:144:THR:HG23	7:G:144:THR:O	2.01	0.60
17:3:245:GLY:C	17:3:246:LEU:HD22	2.22	0.60
13:N:127:PHE:CD2	13:N:127:PHE:N	2.68	0.60
15:1:64:PHE:C	15:1:69:LEU:CD1	2.70	0.60
19:A:1141:CLA:H121	19:A:1141:CLA:H72	1.79	0.60
1:A:479:ASP:CG	1:A:536:THR:CG2	2.70	0.60
19:A:9012:CLA:H92	19:A:9012:CLA:H122	1.83	0.60
2:B:493:TRP:CZ2	19:B:1214:CLA:H122	2.36	0.60
2:B:315:LEU:HD11	2:B:317:ARG:CD	2.30	0.60
2:B:31:PHE:HB2	2:B:42:LEU:CD1	2.32	0.60
2:B:686:PRO:HD2	19:L:1130:CLA:O1A	2.01	0.60
5:E:110:VAL:O	5:E:111:ASN:HB3	2.00	0.60
7:G:131:GLY:CA	7:G:136:VAL:CG2	2.75	0.60
7:G:94:GLN:O	7:G:97:LEU:CD2	2.46	0.60
4:D:87:THR:H	12:L:69:LEU:HD11	1.67	0.60
14:R:35:UNK:N	14:R:38:UNK:CB	2.65	0.60
19:3:3008:CLA:O1A	19:3:3008:CLA:HED3	2.01	0.60
2:B:141:PHE:HD2	2:B:144:PHE:CE1	2.20	0.60
7:G:145:THR:CG2	7:G:146:SER:H	2.13	0.60
15:1:179:LYS:CG	15:1:180:LEU:O	2.49	0.60
1:A:281:LEU:CG	19:A:1115:CLA:HED2	2.23	0.60
1:A:281:LEU:O	1:A:282:THR:C	2.38	0.60
1:A:707:ILE:C	1:A:711:HIS:HD2	2.05	0.60
1:A:92:TRP:CD1	19:A:1105:CLA:CBB	2.83	0.60
19:B:1206:CLA:H143	19:B:1224:CLA:H18	1.83	0.60
2:B:349:ALA:CB	2:B:375:HIS:HB3	2.31	0.60
2:B:443:MET:O	2:B:446:PHE:CB	2.48	0.60
5:E:129:GLU:HA	5:E:129:GLU:OE1	2.00	0.60
4:D:95:GLN:CG	4:D:96:VAL:N	2.63	0.60
12:L:153:PHE:O	12:L:178:THR:HG22	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:129:ARG:HB3	6:F:133:TYR:CE1	2.37	0.60
15:1:150:HIS:C	15:1:150:HIS:ND1	2.53	0.60
22:L:7029:LMU:C6'	22:L:7029:LMU:O2B	2.50	0.60
1:A:343:HIS:HA	1:A:431:LEU:HD22	1.83	0.60
21:A:6008:BCR:HC8	21:A:6008:BCR:H331	1.82	0.60
19:A:9022:CLA:C13	19:B:1206:CLA:HBB2	2.32	0.60
2:B:275:HIS:HD1	19:B:1214:CLA:HMB1	1.65	0.60
19:F:1305:CLA:H42	19:4:1306:CLA:CAA	2.25	0.60
11:K:62:SER:HG	11:K:63:LEU:HD13	1.62	0.60
5:E:72:ALA:O	5:E:73:LYS:HB3	2.02	0.60
13:N:132:THR:CG2	13:N:139:LYS:CD	2.46	0.60
13:N:165:ASN:OD1	13:N:167:PHE:CA	2.49	0.60
3:C:43:PRO:CA	4:D:182:GLN:HG3	2.32	0.60
16:2:112:TRP:HZ3	16:2:164:GLU:HG3	1.66	0.60
4:D:114:MET:HG3	4:D:115:PRO:N	2.17	0.60
2:B:4:ARG:NE	2:B:4:ARG:C	2.55	0.60
17:3:191:GLU:O	17:3:191:GLU:CG	2.49	0.60
12:L:169:ARG:HG2	12:L:172:GLU:HA	1.84	0.60
22:R:7014:LMU:C6	22:R:7014:LMU:H11	2.22	0.60
1:A:29:THR:OG1	1:A:31:PHE:HB2	2.02	0.60
18:4:161:LYS:HD2	18:4:161:LYS:C	2.22	0.60
2:B:508:LEU:CB	2:B:509:PHE:CD2	2.85	0.60
2:B:732:LYS:CG	2:B:733:PHE:CA	2.78	0.60
6:F:207:LEU:CD2	6:F:208:PHE:CB	2.80	0.60
7:G:105:THR:OG1	7:G:106:ARG:N	2.34	0.60
16:2:223:LYS:O	16:2:226:ARG:CB	2.50	0.60
3:C:62:PHE:HZ	5:E:80:GLU:OE2	1.74	0.60
8:H:60:ASN:O	8:H:62:THR:HA	2.01	0.60
8:H:62:THR:H	8:H:63:GLY:HA2	1.67	0.60
4:D:96:VAL:O	4:D:96:VAL:HG22	2.00	0.60
8:H:89:ALA:O	8:H:93:LYS:N	2.32	0.60
12:L:155:GLU:CA	12:L:178:THR:CG2	2.75	0.60
6:F:228:ASP:HA	6:F:231:PHE:HB3	1.84	0.60
15:1:114:TRP:HH2	15:1:121:GLN:HA	1.65	0.60
14:R:4:UNK:O	14:R:5:UNK:CB	2.50	0.60
15:1:157:ASP:CB	15:1:178:LYS:HB2	2.23	0.59
15:1:95:PRO:HA	15:1:98:LEU:CB	2.31	0.59
18:4:103:MET:CE	18:4:207:ASN:O	2.48	0.59
18:4:221:HIS:O	18:4:224:THR:N	2.33	0.59
1:A:107:GLU:HA	1:A:110:LEU:HD21	1.83	0.59
1:A:158:ILE:HG13	1:A:163:GLN:HE22	1.65	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:ASP:CA	1:A:536:THR:HG21	2.21	0.59
1:A:84:GLY:O	1:A:87:SER:O	2.19	0.59
2:B:438:VAL:O	2:B:441:ASP:N	2.35	0.59
2:B:607:SER:O	2:B:610:ASN:N	2.35	0.59
6:F:167:PHE:HA	21:F:6014:BCR:H392	1.84	0.59
19:L:1148:CLA:C2	19:L:1148:CLA:O1A	2.50	0.59
16:2:183:PHE:CA	16:2:187:LYS:HG2	2.31	0.59
1:A:165:TYR:CD2	1:A:165:TYR:O	2.55	0.59
15:1:170:PRO:O	15:1:171:LEU:HD23	2.02	0.59
1:A:266:ALA:O	1:A:267:THR:C	2.37	0.59
1:A:253:ASP:HB3	1:A:254:LEU:HD22	1.83	0.59
6:F:159:GLU:CG	10:J:38:ILE:HG12	2.31	0.59
22:B:7040:LMU:O3'	22:B:7040:LMU:C1B	2.50	0.59
22:B:7038:LMU:C6	22:B:7038:LMU:H101	2.31	0.59
3:C:55:GLU:C	3:C:57:ALA:N	2.50	0.59
2:B:246:THR:O	2:B:246:THR:HG23	2.00	0.59
18:4:165:SER:O	18:4:168:GLN:N	2.34	0.59
1:A:195:TRP:CH2	19:A:1108:CLA:HMA1	2.38	0.59
1:A:361:ASN:O	1:A:365:LEU:N	2.34	0.59
21:A:6002:BCR:H402	21:A:6002:BCR:H23C	1.83	0.59
1:A:580:PRO:HB3	1:A:727:ILE:HG21	1.84	0.59
2:B:222:LEU:HD13	2:B:225:LEU:HD23	1.84	0.59
19:F:1302:CLA:O1D	19:F:1302:CLA:H2A	2.02	0.59
7:G:88:ALA:O	7:G:90:GLN:O	2.20	0.59
8:H:94:ARG:NH2	8:H:97:LEU:O	2.35	0.59
19:2:2001:CLA:O2A	19:2:2001:CLA:C4	2.50	0.59
5:E:121:ALA:O	5:E:125:ILE:CG2	2.50	0.59
5:E:78:ARG:H	5:E:78:ARG:HD2	1.66	0.59
3:C:52:LYS:C	3:C:54:CYS:N	2.54	0.59
18:4:90:TRP:O	18:4:91:PHE:HD1	1.84	0.59
22:D:7050:LMU:C4'	22:D:7050:LMU:O2B	2.46	0.59
20:A:5001:PQN:H142	21:F:6014:BCR:HC22	1.83	0.59
1:A:90:PHE:CE1	19:A:1103:CLA:C9	2.82	0.59
2:B:180:SER:OG	2:B:181:GLY:N	2.35	0.59
2:B:189:ALA:HB2	19:B:1225:CLA:C20	2.26	0.59
2:B:126:THR:OG1	2:B:358:TYR:CD1	2.49	0.59
2:B:378:ILE:HG22	2:B:379:ALA:H	1.66	0.59
21:B:6020:BCR:C33	21:B:6020:BCR:C8	2.77	0.59
1:A:447:ASN:ND2	2:B:678:LEU:HD21	2.17	0.59
7:G:82:PHE:HB2	7:G:83:GLN:HG2	1.84	0.59
19:A:1126:CLA:H171	21:J:6012:BCR:H15C	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:74:THR:HG22	12:L:75:SER:CB	2.31	0.59
19:2:2002:CLA:H2A	19:2:2002:CLA:O1D	2.02	0.59
5:E:78:ARG:HB2	5:E:80:GLU:OE2	2.02	0.59
16:2:164:GLU:HG2	19:2:2012:CLA:HMA3	1.84	0.59
6:F:105:SER:HB2	6:F:108:LEU:HD13	1.83	0.59
16:2:240:ILE:HG23	16:2:263:PHE:CB	2.27	0.59
13:N:169:LYS:HA	13:N:170:TRP:CD1	2.37	0.59
22:4:7052:LMU:O1'	22:4:7052:LMU:C6	2.45	0.59
15:1:81:GLU:C	15:1:83:GLU:H	2.05	0.59
19:A:1106:CLA:HBB1	19:A:1126:CLA:H151	1.84	0.59
1:A:112:ASP:HB3	1:A:116:ILE:HD11	1.84	0.59
19:A:1237:CLA:HAA2	19:L:1130:CLA:HMB1	1.84	0.59
1:A:130:GLU:HA	1:A:130:GLU:OE1	2.02	0.59
1:A:308:ILE:CD1	19:A:1115:CLA:CBB	2.77	0.59
1:A:472:ARG:HH12	12:L:120:LEU:CD2	2.10	0.59
1:A:679:PHE:O	1:A:683:HIS:HB2	2.03	0.59
2:B:89:HIS:CA	2:B:113:VAL:HG11	2.22	0.59
2:B:32:GLU:HG2	2:B:42:LEU:HD22	1.85	0.59
2:B:463:ILE:O	2:B:464:GLN:HG2	2.01	0.59
2:B:46:ILE:HD11	19:B:1202:CLA:H192	1.83	0.59
2:B:618:GLY:HA2	2:B:621:ARG:H	1.67	0.59
6:F:180:SER:C	6:F:182:LEU:N	2.56	0.59
18:4:87:ASN:OD1	18:4:88:LEU:N	2.35	0.59
8:H:79:LEU:O	8:H:80:GLN:C	2.40	0.59
15:1:189:LYS:HB3	19:1:1007:CLA:HMC2	1.77	0.59
11:K:118:VAL:O	11:K:121:VAL:HG22	1.99	0.59
6:F:225:GLU:N	6:F:227:VAL:CG1	2.64	0.59
17:3:154:ASN:C	17:3:155:TYR:CG	2.75	0.59
15:1:193:LEU:C	15:1:193:LEU:CD2	2.68	0.59
15:1:76:LEU:CB	15:1:77:GLU:OE1	2.48	0.59
19:A:1151:CLA:HBA2	19:A:1151:CLA:CED	2.32	0.59
1:A:368:LEU:HD21	19:A:1117:CLA:H91	1.75	0.59
1:A:451:ILE:HD12	19:A:1131:CLA:CED	2.03	0.59
1:A:472:ARG:O	1:A:474:GLN:N	2.36	0.59
1:A:60:ASP:O	1:A:60:ASP:CG	2.40	0.59
1:A:73:GLU:HB2	1:A:186:TYR:HE2	1.67	0.59
20:B:5002:PQN:H291	23:B:7101:LMG:H201	1.83	0.59
4:D:201:LYS:CD	4:D:201:LYS:N	2.47	0.59
7:G:136:VAL:HG22	7:G:137:VAL:HG13	1.83	0.59
11:K:58:VAL:O	11:K:62:SER:HB3	2.02	0.59
2:B:549:ASP:CG	3:C:63:LEU:HB2	2.22	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3:98:LEU:CD2	19:3:3012:CLA:C3D	2.81	0.59
4:D:162:GLU:O	4:D:163:VAL:CG2	2.30	0.59
22:D:7050:LMU:C6'	22:D:7050:LMU:O2B	2.51	0.59
15:1:189:LYS:HB3	19:1:1007:CLA:CMC	2.27	0.59
16:2:240:ILE:HG21	16:2:263:PHE:HB3	1.79	0.59
1:A:23:ASP:OD1	1:A:33:GLN:CG	2.51	0.59
7:G:144:THR:OG1	7:G:148:GLY:CA	2.50	0.59
22:4:7034:LMU:H81	22:4:7052:LMU:O2'	1.97	0.59
18:4:158:GLN:NE2	19:4:1004:CLA:C4A	2.65	0.59
18:4:155:ARG:O	18:4:158:GLN:HB2	2.02	0.59
18:4:142:PHE:CG	19:4:4010:CLA:C3C	2.85	0.59
1:A:349:ILE:O	1:A:350:LEU:C	2.39	0.59
1:A:454:GLY:H	1:A:457:SER:CB	2.05	0.59
1:A:747:TRP:CD2	21:A:6011:BCR:C40	2.85	0.59
19:B:1201:CLA:C4C	21:I:6021:BCR:H401	2.33	0.59
2:B:195:VAL:HA	2:B:199:ILE:HG13	1.84	0.59
2:B:293:THR:HG22	7:G:94:GLN:NE2	2.18	0.59
2:B:388:ALA:C	2:B:391:PRO:CD	2.69	0.59
2:B:455:ILE:HG23	6:F:148:LEU:CD1	2.32	0.59
7:G:125:VAL:O	7:G:129:ALA:HB3	2.03	0.59
15:1:145:ILE:O	15:1:148:VAL:CG1	2.51	0.59
4:D:173:TYR:O	4:D:175:GLU:CG	2.51	0.59
4:D:96:VAL:O	4:D:96:VAL:CG2	2.49	0.59
4:D:141:GLY:O	4:D:142:THR:C	2.39	0.59
16:2:263:PHE:CD2	16:2:263:PHE:O	2.56	0.59
1:A:575:LEU:CD1	1:A:576:GLY:N	2.48	0.59
6:F:185:ILE:C	6:F:186:ARG:CG	2.71	0.59
14:R:26:UNK:C	14:R:28:UNK:N	2.66	0.59
15:1:102:ALA:CA	15:1:103:LEU:HD23	2.33	0.59
1:A:274:TRP:CD2	1:A:277:TYR:O	2.55	0.59
13:N:126:LYS:CB	13:N:126:LYS:NZ	2.65	0.59
1:A:455:PHE:HD1	19:A:1131:CLA:CMA	2.15	0.59
19:A:1139:CLA:O1A	19:A:1139:CLA:H42	2.02	0.59
1:A:330:ILE:O	1:A:334:HIS:HE1	1.86	0.59
1:A:393:LEU:HG	1:A:394:SER:N	2.17	0.59
2:B:90:ALA:N	2:B:113:VAL:HG13	2.18	0.59
19:B:1213:CLA:HED2	19:B:1213:CLA:HBA2	1.85	0.59
9:I:22:ALA:O	9:I:23:SER:C	2.40	0.59
11:K:78:ARG:CA	11:K:78:ARG:CZ	2.80	0.59
16:2:217:LEU:HD12	16:2:218:ARG:HG3	1.85	0.59
17:3:184:LYS:O	17:3:185:GLN:HB3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:147:SER:HA	13:N:149:ASP:CB	2.32	0.59
3:C:44:ARG:NH2	4:D:181:ARG:HB3	2.16	0.59
14:R:39:UNK:CB	14:R:40:UNK:HA	2.33	0.59
1:A:426:THR:HA	1:A:428:TYR:CE1	2.36	0.59
15:1:171:LEU:CD2	15:1:173:TYR:OH	2.51	0.59
1:A:636:HIS:O	1:A:637:ILE:C	2.41	0.59
18:4:225:GLY:CA	18:4:226:LYS:NZ	2.66	0.59
1:A:129:GLN:HE21	19:A:1107:CLA:MG	1.09	0.59
1:A:492:ILE:HA	1:A:495:THR:HG22	1.83	0.59
2:B:90:ALA:CA	2:B:113:VAL:CG1	2.63	0.59
2:B:289:LEU:HD21	19:B:1217:CLA:NA	2.17	0.59
2:B:290:MET:HA	19:B:1218:CLA:CAC	2.32	0.59
19:B:1223:CLA:C7	21:B:6010:BCR:H14C	2.33	0.59
2:B:255:LEU:CA	2:B:271:THR:CB	2.70	0.59
2:B:489:GLY:HA3	19:B:1232:CLA:OBD	2.01	0.59
7:G:69:GLY:C	7:G:72:LEU:HG	2.23	0.59
7:G:99:HIS:CB	7:G:100:PHE:HB3	2.33	0.59
11:K:55:LEU:O	11:K:58:VAL:CG1	2.51	0.59
16:2:226:ARG:CD	16:2:230:LEU:HD23	2.30	0.59
13:N:133:GLY:HA3	13:N:134:CYS:C	2.21	0.59
13:N:147:SER:HA	13:N:149:ASP:HB2	1.83	0.59
4:D:181:ARG:HB3	4:D:182:GLN:HG2	1.83	0.59
19:L:1148:CLA:CGA	19:L:1148:CLA:CED	2.80	0.59
16:2:184:PRO:HG2	16:2:186:ASN:N	2.17	0.59
19:1:1007:CLA:O1D	22:4:7008:LMU:O2'	2.19	0.59
1:A:426:THR:HG23	1:A:428:TYR:CZ	2.38	0.59
16:2:246:PRO:HB2	16:2:247:ILE:CG1	2.32	0.59
19:H:1145:CLA:HAA2	19:H:1145:CLA:CED	2.33	0.59
1:A:71:LEU:HD12	1:A:72:GLU:O	2.03	0.59
12:L:164:LEU:CD1	12:L:165:THR:N	2.61	0.59
18:4:133:GLU:O	18:4:134:TYR:HB2	2.01	0.59
1:A:46:LYS:HB2	1:A:48:PRO:O	2.03	0.59
12:L:158:PRO:O	12:L:159:SER:CB	2.51	0.59
18:4:146:PHE:N	18:4:146:PHE:CD1	2.70	0.59
18:4:177:LEU:HD22	18:4:177:LEU:C	2.22	0.59
1:A:136:VAL:CG2	1:A:140:PHE:O	2.51	0.59
1:A:360:ILE:O	1:A:361:ASN:HB2	2.02	0.59
1:A:555:ILE:HD13	19:A:9023:CLA:HMD1	1.83	0.59
2:B:178:HIS:C	2:B:180:SER:H	2.04	0.59
2:B:102:GLU:OE1	2:B:640:CYS:O	2.20	0.59
19:A:9011:CLA:HAA1	19:B:9010:CLA:HBB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:76:ARG:HH12	7:G:120:VAL:CA	2.16	0.59
7:G:88:ALA:CB	7:G:90:GLN:O	2.49	0.59
16:2:129:LEU:O	16:2:130:GLY:O	2.20	0.59
3:C:39:ILE:O	3:C:40:ALA:HB3	2.03	0.59
5:E:76:ILE:HG23	5:E:78:ARG:HD3	1.85	0.59
6:F:129:ARG:C	6:F:133:TYR:CE1	2.76	0.59
11:K:115:ILE:HD12	11:K:118:VAL:HG23	1.85	0.59
1:A:267:THR:CG2	1:A:267:THR:O	2.50	0.59
18:4:232:LEU:HD12	18:4:234:GLN:CA	2.32	0.59
1:A:40:PHE:C	1:A:41:SER:O	2.41	0.59
1:A:43:THR:HG22	1:A:46:LYS:HZ3	1.67	0.59
2:B:207:VAL:O	2:B:207:VAL:CG1	2.50	0.59
1:A:461:TYR:CE1	1:A:540:LEU:CD1	2.85	0.59
15:1:64:PHE:CE1	15:1:65:ASP:HB3	2.38	0.59
1:A:63:ASP:OD2	1:A:65:ASP:N	2.30	0.59
1:A:700:TRP:CZ2	20:A:5001:PQN:H2M3	2.38	0.59
19:A:9012:CLA:CAD	19:A:9012:CLA:CED	2.81	0.59
19:B:1222:CLA:CED	19:B:1223:CLA:OBD	2.50	0.59
2:B:224:PRO:C	2:B:227:THR:HB	2.23	0.59
2:B:315:LEU:HD11	2:B:317:ARG:CG	2.30	0.59
2:B:623:TYR:O	2:B:624:LEU:HB3	2.03	0.59
19:B:1226:CLA:HMD2	23:B:7101:LMG:H341	1.85	0.59
12:L:73:VAL:CA	19:L:1504:CLA:HMA3	2.31	0.59
12:L:76:SER:O	12:L:77:PRO:C	2.41	0.59
16:2:103:VAL:C	16:2:105:ALA:N	2.53	0.59
16:2:217:LEU:O	16:2:218:ARG:C	2.42	0.59
19:1:1013:CLA:CED	19:1:1013:CLA:CAD	2.79	0.59
13:N:104:LYS:O	13:N:107:LEU:CB	2.49	0.59
17:3:96:ARG:HA	17:3:99:ALA:HB2	1.78	0.59
19:J:1308:CLA:O1D	19:J:1308:CLA:CGA	2.51	0.59
1:A:628:ILE:CD1	1:A:629:ASN:H	2.13	0.59
16:2:145:TYR:O	16:2:146:PHE:CB	2.51	0.59
15:1:179:LYS:HE3	15:1:181:GLU:HA	1.85	0.58
1:A:105:ASN:CB	1:A:119:SER:O	2.51	0.58
1:A:197:GLN:NE2	1:A:351:THR:C	2.57	0.58
1:A:154:ARG:CD	1:A:384:TYR:HE1	2.11	0.58
1:A:604:TRP:O	1:A:607:ASN:N	2.31	0.58
1:A:699:TYR:HD1	1:A:700:TRP:CD1	2.21	0.58
2:B:277:HIS:HE1	19:B:1215:CLA:NC	2.01	0.58
19:B:1222:CLA:H72	19:B:1236:CLA:C2D	2.33	0.58
2:B:127:ILE:O	2:B:127:ILE:CD1	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:503:GLU:CG	2:B:503:GLU:O	2.49	0.58
2:B:535:VAL:HG13	2:B:536:LYS:N	2.17	0.58
2:B:551:LYS:O	2:B:553:PHE:CE2	2.56	0.58
12:L:102:VAL:HG13	19:L:1502:CLA:CED	2.33	0.58
16:2:130:GLY:HA3	16:2:131:ILE:CG1	1.92	0.58
5:E:79:LYS:N	5:E:84:TYR:HE1	2.00	0.58
3:C:73:THR:OG1	3:C:76:SER:CA	2.51	0.58
17:3:238:ILE:HG13	19:3:3003:CLA:CMC	2.33	0.58
16:2:160:ILE:HB	19:2:2012:CLA:CBB	2.33	0.58
1:A:253:ASP:O	1:A:256:ALA:HB3	2.02	0.58
2:B:8:PHE:HE2	2:B:27:THR:HG1	1.50	0.58
2:B:433:THR:O	2:B:436:LEU:O	2.20	0.58
22:4:7034:LMU:H81	22:4:7052:LMU:C3'	2.23	0.58
19:A:1101:CLA:HBB2	19:A:1102:CLA:C1C	2.32	0.58
19:A:1115:CLA:C19	11:K:64:MET:HE1	2.32	0.58
19:A:1117:CLA:H121	19:A:1117:CLA:CBB	2.34	0.58
1:A:93:LEU:O	1:A:97:TYR:HD2	1.85	0.58
19:B:1214:CLA:HBD	19:B:1223:CLA:CBB	2.31	0.58
2:B:455:ILE:O	2:B:514:PRO:HG3	2.02	0.58
20:B:5002:PQN:C19	21:B:6017:BCR:C10	2.80	0.58
19:B:1239:CLA:C19	9:I:21:MET:HB3	2.32	0.58
12:L:146:THR:C	12:L:148:TYR:H	2.05	0.58
18:4:87:ASN:OD1	18:4:90:TRP:CG	2.55	0.58
16:2:167:ARG:HD3	19:2:2012:CLA:HMA3	1.85	0.58
16:2:183:PHE:C	16:2:183:PHE:CD1	2.77	0.58
6:F:128:LYS:O	6:F:129:ARG:HD3	2.03	0.58
22:R:7022:LMU:C2'	22:R:7022:LMU:C2	2.76	0.58
3:C:34:CYS:H	3:C:37:LYS:CB	2.09	0.58
16:2:203:PRO:O	16:2:204:LEU:HB2	2.03	0.58
1:A:278:ALA:O	1:A:281:LEU:HD11	2.03	0.58
2:B:175:LEU:HD12	19:B:1221:CLA:HED1	1.84	0.58
19:B:1229:CLA:H51	21:F:6016:BCR:C40	2.33	0.58
2:B:298:GLY:N	19:B:1218:CLA:HMD3	2.17	0.58
2:B:555:TYR:O	2:B:571:SER:HB2	2.03	0.58
19:B:1223:CLA:H122	21:B:6010:BCR:C13	2.32	0.58
5:E:90:VAL:O	5:E:91:VAL:HG22	2.03	0.58
6:F:173:TRP:CZ3	6:F:211:PHE:CB	2.68	0.58
7:G:99:HIS:O	7:G:101:GLU:N	2.37	0.58
8:H:109:LEU:HD22	19:H:1207:CLA:H52	1.85	0.58
19:A:1136:CLA:C19	19:L:1130:CLA:HBB1	2.29	0.58
5:E:84:TYR:CD2	5:E:85:LYS:HG3	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:132:THR:CB	13:N:139:LYS:HD3	2.29	0.58
19:1:1014:CLA:H71	19:1:1014:CLA:C4	2.19	0.58
18:4:88:LEU:O	18:4:90:TRP:CD1	2.55	0.58
16:2:148:ASP:C	16:2:149:THR:HG1	2.00	0.58
11:K:112:VAL:C	11:K:114:HIS:H	2.06	0.58
18:4:228:PRO:CB	18:4:229:PHE:CD1	2.72	0.58
2:B:631:LEU:HD23	2:B:631:LEU:H	1.68	0.58
22:R:7020:LMU:O6'	22:R:7020:LMU:H3B	2.03	0.58
17:3:162:MET:CE	19:3:3010:CLA:C3D	2.81	0.58
1:A:581:CYS:CB	1:A:590:CYS:O	2.50	0.58
18:4:232:LEU:CD1	18:4:234:GLN:HA	2.33	0.58
16:2:266:PHE:CE1	16:2:267:THR:O	2.55	0.58
15:1:223:ASP:OD1	18:4:140:THR:HG21	2.03	0.58
18:4:161:LYS:CD	18:4:161:LYS:C	2.72	0.58
18:4:220:GLN:NE2	19:4:1306:CLA:HAC2	2.18	0.58
1:A:50:THR:HG23	1:A:51:THR:H	1.69	0.58
1:A:746:THR:HG1	19:A:9011:CLA:CGD	2.13	0.58
1:A:90:PHE:HA	1:A:93:LEU:CD2	2.34	0.58
19:B:1222:CLA:CBC	19:B:1222:CLA:CHD	2.79	0.58
2:B:378:ILE:CA	2:B:381:PHE:HB2	2.34	0.58
2:B:409:ALA:O	2:B:410:ARG:CB	2.34	0.58
2:B:654:HIS:HE1	19:B:9010:CLA:NB	2.01	0.58
23:B:7101:LMG:HO3	3:C:70:TRP:HE1	1.46	0.58
9:I:23:SER:O	9:I:26:LEU:HG	2.04	0.58
16:2:226:ARG:HH11	16:2:226:ARG:CA	2.16	0.58
5:E:78:ARG:HH12	5:E:125:ILE:HB	1.65	0.58
13:N:130:ASN:OD1	13:N:130:ASN:O	2.20	0.58
14:R:35:UNK:C	14:R:36:UNK:O	2.51	0.58
19:L:1501:CLA:HED2	19:L:1501:CLA:HAA2	1.85	0.58
19:K:1142:CLA:CMD	19:K:1143:CLA:C1A	2.82	0.58
1:A:255:LEU:CD1	1:A:280:PHE:CZ	2.82	0.58
19:1:1005:CLA:HBC3	19:1:1005:CLA:HMC1	1.85	0.58
1:A:368:LEU:CD2	19:A:1117:CLA:H93	2.24	0.58
1:A:338:PHE:CZ	19:A:1151:CLA:CBB	2.81	0.58
1:A:216:LEU:HD12	21:A:6002:BCR:H353	1.85	0.58
1:A:230:ASN:HA	1:A:233:LEU:HB2	1.85	0.58
1:A:332:GLU:HA	1:A:344:LYS:HG2	1.85	0.58
2:B:29:HIS:CG	19:B:1202:CLA:HBB2	2.38	0.58
19:B:1213:CLA:CHD	19:B:1213:CLA:CBC	2.81	0.58
19:B:1223:CLA:H8	21:B:6010:BCR:H14C	1.84	0.58
2:B:194:LEU:O	2:B:199:ILE:HG13	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:460:ALA:O	2:B:461:GLN:C	2.42	0.58
5:E:103:VAL:HG22	5:E:104:VAL:O	2.03	0.58
12:L:143:LEU:N	12:L:145:LEU:H	2.01	0.58
13:N:139:LYS:CA	13:N:142:LYS:CD	2.81	0.58
4:D:156:ARG:HE	4:D:164:GLN:HB2	1.64	0.58
8:H:77:ASN:ND2	8:H:78:PRO:CG	2.66	0.58
6:F:99:LEU:HB3	6:F:127:LYS:HE2	1.85	0.58
16:2:195:TYR:CE2	16:2:198:GLY:CA	2.87	0.58
5:E:96:ASP:OD2	5:E:98:ASN:ND2	2.36	0.58
2:B:213:LEU:CD1	2:B:214:ASP:N	2.60	0.58
3:C:34:CYS:O	3:C:35:LYS:HB2	2.04	0.58
4:D:150:ILE:O	4:D:151:LYS:CG	2.47	0.58
22:K:7042:LMU:H3'	22:K:7042:LMU:H2B	1.85	0.58
15:1:116:ALA:O	15:1:117:LEU:HD22	2.02	0.58
13:N:127:PHE:O	13:N:128:PRO:C	2.42	0.58
18:4:121:ILE:C	18:4:123:VAL:H	2.07	0.58
19:A:1107:CLA:HMC1	19:A:1107:CLA:HBC3	1.85	0.58
2:B:290:MET:HA	19:B:1218:CLA:HAC2	1.85	0.58
19:A:1237:CLA:HBB2	19:B:1238:CLA:HMD1	1.85	0.58
2:B:182:LEU:HA	19:B:1210:CLA:HMB2	1.86	0.58
2:B:469:LYS:CG	2:B:470:THR:HA	2.31	0.58
2:B:558:PRO:HB3	2:B:706:ARG:HH21	1.68	0.58
2:B:732:LYS:C	2:B:733:PHE:O	2.41	0.58
12:L:70:GLU:HG2	12:L:74:THR:CG2	2.31	0.58
16:2:122:ILE:HG13	16:2:126:LEU:HD21	1.84	0.58
19:1:1013:CLA:HED2	19:1:1013:CLA:OBD	2.03	0.58
3:C:66:ARG:NH2	3:C:66:ARG:HB3	2.18	0.58
6:F:129:ARG:C	6:F:133:TYR:HE1	2.07	0.58
17:3:192:LYS:CA	17:3:192:LYS:CE	2.59	0.58
14:R:52:UNK:CB	14:R:53:UNK:CB	2.82	0.58
6:F:227:VAL:O	6:F:230:ASN:N	2.37	0.58
17:3:161:GLU:C	17:3:161:GLU:CD	2.61	0.58
2:B:70:TRP:CD1	2:B:70:TRP:N	2.71	0.58
18:4:172:PHE:O	18:4:173:LYS:CB	2.51	0.58
1:A:210:LEU:HD13	19:A:1111:CLA:HBB	1.85	0.58
19:A:1117:CLA:O1A	19:A:1127:CLA:H71	2.04	0.58
19:A:1124:CLA:O2A	19:A:1137:CLA:O2D	2.21	0.58
1:A:453:LEU:HD23	19:A:1136:CLA:HBB1	1.86	0.58
1:A:603:PHE:CZ	1:A:735:VAL:CG2	2.86	0.58
19:A:9022:CLA:C14	19:B:1206:CLA:HBB2	2.34	0.58
19:B:1205:CLA:HMC2	21:B:6017:BCR:C28	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1218:CLA:HMD2	21:B:6004:BCR:C32	2.34	0.58
2:B:438:VAL:CG2	19:B:1230:CLA:CMC	2.80	0.58
2:B:190:TRP:CA	19:B:1211:CLA:HBB2	2.34	0.58
2:B:294:ASN:HB2	7:G:94:GLN:OE1	1.89	0.58
2:B:697:PRO:O	3:C:79:LEU:CD1	2.49	0.58
2:B:696:LYS:CG	3:C:80:ALA:HA	2.24	0.58
5:E:90:VAL:CG1	5:E:91:VAL:N	2.65	0.58
12:L:91:THR:O	12:L:92:ALA:C	2.41	0.58
15:1:133:THR:C	15:1:135:PRO:HD2	2.24	0.58
2:B:560:ASP:OD1	3:C:52:LYS:NZ	2.35	0.58
19:1:1007:CLA:CHD	19:1:1007:CLA:CBC	2.82	0.58
2:B:394:PHE:O	2:B:542:ARG:HD3	2.04	0.58
2:B:145:LEU:HA	2:B:148:ILE:HD12	1.85	0.58
15:1:162:LYS:CB	15:1:164:PRO:HG3	2.34	0.58
4:D:77:ASN:HB3	4:D:79:PRO:HD2	1.85	0.58
2:B:341:LEU:O	2:B:345:THR:OG1	2.14	0.58
18:4:173:LYS:NZ	18:4:201:LYS:HG2	2.14	0.58
18:4:210:LEU:HD23	19:4:4002:CLA:CBB	2.34	0.58
1:A:281:LEU:HB2	19:A:1115:CLA:HED2	1.85	0.58
1:A:159:THR:C	1:A:163:GLN:NE2	2.57	0.58
1:A:284:ARG:HG2	1:A:295:TRP:CG	2.37	0.58
1:A:443:ILE:CG1	1:A:557:LEU:HD22	2.32	0.58
1:A:397:THR:HG21	1:A:613:ILE:HG13	1.82	0.58
1:A:396:PHE:HE2	1:A:616:PHE:CB	2.17	0.58
19:A:9013:CLA:HMA1	19:A:9013:CLA:H2	1.85	0.58
2:B:115:ASN:OD1	2:B:115:ASN:C	2.41	0.58
2:B:388:ALA:O	2:B:391:PRO:HD2	2.02	0.58
2:B:692:ARG:NH2	2:B:694:ARG:NH2	2.52	0.58
14:R:37:UNK:C	14:R:42:UNK:O	2.52	0.58
10:J:5:LYS:HD2	16:2:178:ASN:OD1	2.02	0.58
22:3:7005:LMU:C1'	22:3:7005:LMU:C3	2.80	0.58
2:B:154:TRP:O	2:B:157:LEU:N	2.36	0.58
2:B:475:ASP:O	2:B:480:SER:N	2.26	0.58
17:3:171:ARG:CG	17:3:175:ASP:OD1	2.50	0.58
3:C:34:CYS:N	3:C:37:LYS:HB3	2.10	0.58
1:A:29:THR:OG1	1:A:31:PHE:CB	2.51	0.58
19:4:4006:CLA:H43	22:4:7034:LMU:H91	1.86	0.58
15:1:157:ASP:OD2	15:1:175:LYS:HD2	2.04	0.58
15:1:65:ASP:O	15:1:68:GLY:N	2.37	0.58
1:A:104:SER:O	1:A:106:TYR:N	2.28	0.58
1:A:711:HIS:HB3	1:A:717:ALA:CB	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:HIS:CD2	19:B:1202:CLA:HBB1	2.39	0.58
2:B:212:PHE:CE1	19:B:1211:CLA:HHD	2.38	0.58
2:B:25:ILE:O	2:B:26:ALA:CB	2.51	0.58
2:B:34:HIS:O	2:B:36:ASP:N	2.37	0.58
2:B:375:HIS:HE1	19:B:1225:CLA:NC	2.01	0.58
19:A:9013:CLA:H11	2:B:431:PHE:CE1	2.39	0.58
10:J:11:ALA:CB	10:J:12:PRO:HD2	2.10	0.58
11:K:60:SER:HA	11:K:63:LEU:CD2	2.28	0.58
12:L:108:TYR:HB2	12:L:200:ALA:HB2	1.85	0.58
12:L:73:VAL:CA	19:L:1504:CLA:CMA	2.78	0.58
13:N:156:GLY:C	13:N:157:LYS:HD2	2.24	0.58
17:3:103:VAL:HG11	17:3:229:LYS:HG2	1.84	0.58
19:K:1142:CLA:HMD3	19:K:1143:CLA:ND	2.19	0.58
16:2:201:PHE:HD1	16:2:202:ASP:CA	2.16	0.58
13:N:120:VAL:O	13:N:122:PHE:CD2	2.57	0.58
15:1:155:GLU:N	15:1:155:GLU:OE2	2.30	0.58
1:A:284:ARG:NH1	1:A:284:ARG:C	2.57	0.58
1:A:329:ASP:O	1:A:332:GLU:O	2.22	0.58
19:B:1220:CLA:H93	19:B:1227:CLA:HBC1	1.86	0.58
2:B:187:SER:O	2:B:188:LEU:C	2.40	0.58
19:B:1229:CLA:CBB	21:F:6014:BCR:H23C	2.34	0.58
8:H:97:LEU:HD12	8:H:100:PHE:HB2	1.83	0.58
12:L:128:GLN:HG2	12:L:132:LEU:CD2	2.02	0.58
5:E:107:PHE:HD2	5:E:109:LYS:CG	2.17	0.58
16:2:171:ILE:HG13	16:2:172:LEU:HB2	1.84	0.58
8:H:77:ASN:ND2	8:H:78:PRO:CD	2.67	0.58
16:2:249:ASN:C	16:2:249:ASN:OD1	2.42	0.58
15:1:171:LEU:HB3	15:1:173:TYR:CZ	2.39	0.58
1:A:253:ASP:O	1:A:256:ALA:CB	2.52	0.58
1:A:111:ASN:O	1:A:113:PRO:HD2	2.03	0.57
1:A:270:PHE:CZ	19:A:1141:CLA:H2	2.39	0.57
1:A:217:SER:CA	21:A:6002:BCR:H351	2.34	0.57
19:B:1214:CLA:H52	19:B:1223:CLA:CMB	2.30	0.57
2:B:37:ILE:HD12	2:B:37:ILE:O	2.04	0.57
11:K:79:LYS:HG3	11:K:79:LYS:O	2.04	0.57
16:2:113:ALA:HB1	16:2:114:MET:HE3	1.84	0.57
16:2:121:PHE:N	16:2:121:PHE:CD2	2.72	0.57
13:N:131:PHE:N	13:N:132:THR:HG22	2.19	0.57
13:N:143:VAL:CG1	13:N:144:PRO:CD	2.82	0.57
19:1:1006:CLA:CAB	19:1:1013:CLA:CHD	2.82	0.57
19:2:2014:CLA:H41	19:2:2014:CLA:C9	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:PHE:O	2:B:77:TRP:N	2.36	0.57
15:1:73:PRO:HG2	15:1:74:ALA:H	1.65	0.57
18:4:172:PHE:C	18:4:194:PHE:CE2	2.77	0.57
1:A:187:HIS:HE1	19:A:1109:CLA:CHA	2.17	0.57
1:A:346:LEU:O	1:A:347:TYR:HB2	2.04	0.57
1:A:51:THR:HG22	1:A:723:ARG:HB2	1.84	0.57
21:A:6002:BCR:C8	21:A:6002:BCR:C31	2.69	0.57
1:A:705:GLU:HB3	2:B:545:LYS:NZ	2.19	0.57
2:B:317:ARG:HE	2:B:317:ARG:HA	1.68	0.57
5:E:91:VAL:HG12	5:E:92:ALA:N	2.18	0.57
6:F:152:GLY:O	6:F:157:TRP:CH2	2.57	0.57
7:G:103:GLY:N	7:G:104:ASP:HA	2.19	0.57
12:L:79:ILE:HD12	19:L:1504:CLA:CMA	2.34	0.57
3:C:12:ILE:O	3:C:12:ILE:HG22	2.03	0.57
3:C:12:ILE:HB	3:C:39:ILE:HA	1.86	0.57
2:B:560:ASP:CB	3:C:66:ARG:NE	2.65	0.57
14:R:38:UNK:C	14:R:42:UNK:O	2.52	0.57
22:2:7006:LMU:H22	22:2:7006:LMU:H2'	1.86	0.57
16:2:251:PHE:CG	16:2:251:PHE:O	2.57	0.57
1:A:423:ASP:N	1:A:424:PRO:CD	2.65	0.57
19:J:1308:CLA:H2A	19:J:1308:CLA:H2	1.86	0.57
15:1:170:PRO:HG2	15:1:171:LEU:HA	1.85	0.57
1:A:40:PHE:H	1:A:44:ILE:HG22	1.68	0.57
13:N:127:PHE:HD2	13:N:127:PHE:H	1.50	0.57
18:4:93:GLN:OE1	18:4:170:PRO:HB2	2.04	0.57
1:A:707:ILE:C	1:A:711:HIS:CD2	2.77	0.57
19:B:1203:CLA:C4	23:B:7101:LMG:H321	2.34	0.57
19:B:1235:CLA:C1A	19:B:1235:CLA:CGA	2.82	0.57
2:B:282:PHE:O	2:B:286:ILE:HG13	2.03	0.57
2:B:414:HIS:O	2:B:414:HIS:CG	2.57	0.57
19:A:9023:CLA:HMC1	2:B:661:PHE:CB	2.34	0.57
15:1:134:LEU:CA	15:1:137:ILE:CD1	2.71	0.57
17:3:226:LYS:HG3	17:3:229:LYS:HE3	1.86	0.57
13:N:114:PHE:HE2	13:N:116:ARG:HD2	1.69	0.57
2:B:154:TRP:O	2:B:157:LEU:CB	2.52	0.57
2:B:393:PHE:CD2	2:B:397:ASP:OD1	2.49	0.57
3:C:33:GLY:HA2	3:C:37:LYS:CE	2.33	0.57
18:4:120:ILE:O	18:4:121:ILE:C	2.43	0.57
19:4:1004:CLA:CHD	19:4:1004:CLA:CBC	2.75	0.57
18:4:209:ARG:O	18:4:212:LEU:C	2.42	0.57
18:4:222:ASN:O	18:4:223:VAL:CB	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1102:CLA:HBB2	19:A:1104:CLA:C4D	2.34	0.57
19:A:1109:CLA:HBC3	19:A:1109:CLA:HMC1	1.86	0.57
1:A:111:ASN:OD1	1:A:238:ASP:HA	2.04	0.57
1:A:282:THR:O	1:A:283:PHE:O	2.22	0.57
19:A:9023:CLA:CMC	2:B:661:PHE:CB	2.81	0.57
2:B:51:PHE:CD1	19:B:1210:CLA:HED1	2.40	0.57
2:B:486:LEU:HD13	2:B:489:GLY:N	2.19	0.57
1:A:558:LYS:HZ1	2:B:674:LEU:HB2	1.67	0.57
2:B:710:LEU:C	2:B:712:HIS:N	2.56	0.57
2:B:711:VAL:O	2:B:711:VAL:CG1	2.52	0.57
12:L:82:TYR:O	12:L:82:TYR:CD1	2.57	0.57
13:N:147:SER:CB	13:N:151:ASP:OD1	2.52	0.57
4:D:98:GLU:HB2	4:D:100:TYR:HE2	1.68	0.57
16:2:182:ILE:CB	16:2:187:LYS:CB	2.61	0.57
19:K:1142:CLA:HED1	19:K:1143:CLA:CMB	2.30	0.57
2:B:155:LEU:O	2:B:161:TRP:NE1	2.38	0.57
11:K:116:ILE:CG2	11:K:117:GLY:N	2.68	0.57
12:L:55:GLN:C	12:L:57:ILE:N	2.57	0.57
12:L:55:GLN:O	12:L:57:ILE:N	2.38	0.57
15:1:129:VAL:HB	15:1:130:PRO:HD3	1.85	0.57
16:2:154:ILE:HG12	16:2:155:VAL:H	1.70	0.57
18:4:225:GLY:CA	18:4:226:LYS:HZ2	2.17	0.57
15:1:78:ARG:HH22	15:1:179:LYS:CB	2.16	0.57
18:4:194:PHE:O	18:4:195:ALA:CB	2.51	0.57
19:A:1133:CLA:H2A	19:A:1133:CLA:O1D	2.04	0.57
1:A:174:PHE:O	1:A:175:ALA:CB	2.51	0.57
1:A:225:VAL:O	1:A:229:ILE:HB	2.04	0.57
1:A:246:HIS:C	1:A:248:PHE:HD2	2.05	0.57
1:A:338:PHE:CD1	1:A:338:PHE:N	2.72	0.57
1:A:344:LYS:C	1:A:346:LEU:H	2.08	0.57
1:A:412:ALA:HA	1:A:598:VAL:HG21	1.86	0.57
21:A:6011:BCR:H19C	19:A:9012:CLA:H172	1.86	0.57
2:B:486:LEU:HD12	2:B:489:GLY:H	1.68	0.57
20:B:5002:PQN:H161	21:B:6017:BCR:H331	1.87	0.57
21:B:6020:BCR:H331	19:L:1502:CLA:C4B	2.06	0.57
8:H:91:PHE:HB3	12:L:187:GLY:HA3	1.86	0.57
16:2:115:LEU:O	16:2:118:ALA:CB	2.52	0.57
13:N:146:LEU:HD13	17:3:142:ILE:O	1.75	0.57
17:3:103:VAL:O	17:3:107:ARG:CB	2.49	0.57
19:3:3013:CLA:O1D	19:3:3013:CLA:C2A	2.52	0.57
2:B:155:LEU:O	2:B:161:TRP:CD1	2.57	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:118:VAL:O	11:K:120:VAL:HA	2.03	0.57
15:1:171:LEU:HD22	15:1:173:TYR:OH	2.05	0.57
3:C:31:TRP:C	3:C:31:TRP:CD1	2.78	0.57
15:1:115:ALA:O	15:1:116:ALA:HB3	2.05	0.57
9:I:2:ILE:HG12	9:I:3:ASN:ND2	2.20	0.57
19:1:1001:CLA:CMC	19:1:1001:CLA:CBC	2.80	0.57
15:1:182:GLU:O	15:1:183:LEU:CB	2.53	0.57
15:1:77:GLU:C	15:1:80:LYS:HG3	2.23	0.57
1:A:723:ARG:N	19:A:1139:CLA:HBB1	2.16	0.57
1:A:278:ALA:O	1:A:279:ASP:O	2.22	0.57
1:A:340:GLY:O	1:A:343:HIS:CB	2.45	0.57
19:A:1122:CLA:NC	21:A:6007:BCR:H19C	2.20	0.57
1:A:665:ILE:O	2:B:621:ARG:HD3	2.04	0.57
2:B:347:LEU:HD13	2:B:351:HIS:HD1	1.70	0.57
20:B:5002:PQN:H191	21:B:6017:BCR:C10	2.34	0.57
3:C:1:MET:N	3:C:4:SER:CB	2.67	0.57
5:E:83:TRP:CH2	5:E:116:SER:CB	2.86	0.57
12:L:95:PRO:O	12:L:97:LEU:N	2.38	0.57
16:2:171:ILE:CD1	16:2:173:ASN:HD21	2.17	0.57
11:K:125:LYS:HE3	11:K:125:LYS:O	2.04	0.57
17:3:155:TYR:CD2	17:3:155:TYR:N	2.72	0.57
17:3:210:PRO:CD	17:3:211:LEU:N	2.67	0.57
2:B:70:TRP:H	2:B:70:TRP:HD1	1.50	0.57
18:4:133:GLU:O	18:4:134:TYR:CB	2.51	0.57
12:L:100:ILE:CG2	12:L:191:PHE:O	2.50	0.57
2:B:93:ASP:OD1	2:B:96:PHE:HD1	1.87	0.57
15:1:69:LEU:O	15:1:70:GLY:C	2.39	0.57
15:1:97:ILE:HG12	15:1:98:LEU:N	2.18	0.57
18:4:159:ASP:O	18:4:163:PRO:HA	2.04	0.57
19:A:1119:CLA:C2C	19:A:1125:CLA:C17	2.82	0.57
1:A:51:THR:CG2	19:A:1139:CLA:CBB	2.61	0.57
19:A:1134:CLA:O2A	19:A:1141:CLA:HBB1	2.04	0.57
1:A:240:LYS:CA	1:A:243:PRO:HD2	2.33	0.57
19:A:9013:CLA:H93	2:B:431:PHE:HD1	1.69	0.57
2:B:120:VAL:O	2:B:121:TYR:C	2.41	0.57
2:B:438:VAL:HG21	19:B:1230:CLA:HMC1	1.86	0.57
2:B:457:PRO:HG3	2:B:517:PHE:HB2	1.87	0.57
11:K:76:ALA:HA	11:K:78:ARG:NH1	2.18	0.57
13:N:146:LEU:O	13:N:147:SER:HB2	2.04	0.57
15:1:93:ALA:HB1	19:1:1006:CLA:C4B	2.24	0.57
17:3:104:ILE:CG2	19:3:3004:CLA:C1D	2.83	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:100:TYR:N	4:D:100:TYR:HD2	2.01	0.57
18:4:90:TRP:C	18:4:91:PHE:CD1	2.74	0.57
22:D:7050:LMU:H82	22:D:7050:LMU:H42	1.85	0.57
11:K:114:HIS:O	11:K:116:ILE:N	2.38	0.57
15:1:92:LEU:CA	15:1:95:PRO:HD3	2.35	0.57
1:A:213:LEU:O	1:A:217:SER:HB2	2.04	0.57
1:A:331:LEU:C	1:A:331:LEU:HD23	2.17	0.57
1:A:86:LEU:HD13	1:A:178:MET:HE2	1.85	0.57
19:B:1222:CLA:HMB3	21:B:6010:BCR:C35	2.35	0.57
2:B:254:ILE:HB	2:B:255:LEU:CD2	2.32	0.57
2:B:649:MET:O	2:B:653:GLY:N	2.37	0.57
2:B:91:ILE:HG12	2:B:112:PRO:O	2.04	0.57
3:C:1:MET:H2	3:C:3:HIS:N	2.02	0.57
6:F:200:VAL:HG13	10:J:7:TYR:N	2.02	0.57
13:N:139:LYS:HA	13:N:142:LYS:CE	2.34	0.57
13:N:144:PRO:HG2	13:N:158:ASP:O	2.05	0.57
4:D:181:ARG:CB	4:D:182:GLN:HG2	2.35	0.57
17:3:204:GLY:N	17:3:207:PHE:HA	2.18	0.57
19:3:3016:CLA:HMA2	19:3:3016:CLA:O1A	2.04	0.57
1:A:259:TYR:CE2	1:A:280:PHE:HA	2.40	0.57
7:G:144:THR:OG1	7:G:148:GLY:HA3	2.05	0.57
15:1:71:GLU:HG2	15:1:72:VAL:HG23	1.85	0.57
15:1:78:ARG:HH21	15:1:179:LYS:CB	2.07	0.57
15:1:77:GLU:CD	15:1:80:LYS:HZ1	2.08	0.57
15:1:97:ILE:HD11	15:1:98:LEU:HD23	1.85	0.57
19:4:4014:CLA:CBC	19:4:4014:CLA:CHD	2.83	0.57
19:A:1106:CLA:HMC3	19:A:1107:CLA:HHD	1.86	0.57
1:A:110:LEU:HD11	1:A:239:PRO:HG2	1.86	0.57
1:A:308:ILE:CG2	19:A:1115:CLA:H111	2.35	0.57
1:A:603:PHE:CE2	1:A:735:VAL:HG22	2.40	0.57
19:B:1205:CLA:H42	19:B:1205:CLA:C4C	2.35	0.57
2:B:276:HIS:HB2	19:B:1214:CLA:C1B	2.35	0.57
2:B:303:TYR:N	2:B:306:GLU:HB2	2.19	0.57
2:B:469:LYS:HG3	2:B:470:THR:CB	2.35	0.57
2:B:471:THR:CG2	2:B:502:ASN:HD22	2.18	0.57
2:B:486:LEU:HD13	2:B:489:GLY:H	1.70	0.57
2:B:454:LEU:HD13	2:B:514:PRO:HG2	1.86	0.57
2:B:53:GLN:C	2:B:55:ALA:N	2.58	0.57
3:C:2:SER:O	3:C:69:LEU:HB3	2.05	0.57
6:F:150:VAL:HG21	6:F:160:PHE:CB	2.31	0.57
6:F:157:TRP:HB3	19:F:1305:CLA:HHC	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:302:LYS:NZ	7:G:103:GLY:HA3	2.19	0.57
7:G:63:VAL:HG23	7:G:64:ILE:H	1.59	0.57
7:G:69:GLY:O	7:G:72:LEU:CB	2.53	0.57
16:2:128:LYS:CG	16:2:131:ILE:HG23	2.35	0.57
5:E:89:SER:OG	5:E:106:ARG:HG3	2.05	0.57
4:D:172:VAL:O	4:D:173:TYR:HB3	2.05	0.57
1:A:250:LEU:CB	17:3:136:TRP:HH2	2.02	0.57
16:2:168:TRP:O	16:2:169:ALA:C	2.43	0.57
17:3:130:GLN:CB	17:3:132:THR:N	2.37	0.57
22:E:7048:LMU:C5B	22:E:7048:LMU:H3'	2.34	0.57
1:A:389:TYR:CD1	1:A:625:TRP:CD1	2.92	0.57
12:L:54:TYR:O	12:L:55:GLN:HB3	2.05	0.57
19:A:1132:CLA:O1D	12:L:119:PRO:HA	2.05	0.57
19:A:1136:CLA:C1A	19:A:1136:CLA:CGA	2.83	0.57
1:A:284:ARG:CA	1:A:298:ASP:OD1	2.53	0.57
1:A:502:THR:C	1:A:504:ALA:N	2.51	0.57
1:A:697:ARG:HD3	2:B:566:GLY:O	2.05	0.57
2:B:232:LEU:CD1	2:B:235:GLN:HB2	2.35	0.57
2:B:233:TYR:HB3	2:B:254:ILE:O	2.04	0.57
2:B:643:LEU:HD22	2:B:646:TRP:CD1	2.40	0.57
2:B:668:ARG:NE	2:B:699:ALA:O	2.38	0.57
5:E:111:ASN:CG	5:E:116:SER:HB3	2.25	0.57
19:2:2002:CLA:HHD	19:2:2002:CLA:CBC	2.28	0.57
13:N:139:LYS:C	13:N:142:LYS:HZ2	2.09	0.57
13:N:146:LEU:CG	13:N:148:ASP:O	2.52	0.57
6:F:195:GLU:H	6:F:195:GLU:CD	2.07	0.57
18:4:87:ASN:OD1	18:4:90:TRP:CD1	2.58	0.57
8:H:78:PRO:O	8:H:79:LEU:C	2.39	0.57
16:2:195:TYR:CD1	16:2:196:PRO:CD	2.60	0.57
16:2:201:PHE:HD1	16:2:202:ASP:N	2.00	0.57
1:A:567:ARG:HH11	4:D:89:GLY:CA	2.16	0.57
1:A:484:LEU:H	1:A:484:LEU:HD23	1.66	0.57
15:1:95:PRO:CA	15:1:98:LEU:CB	2.83	0.56
18:4:146:PHE:HE2	19:4:4013:CLA:C3C	2.17	0.56
19:A:1131:CLA:C14	19:A:1131:CLA:H101	2.35	0.56
19:A:1135:CLA:HBD	19:A:1135:CLA:HBA2	1.85	0.56
1:A:206:HIS:C	1:A:211:LEU:HD23	2.26	0.56
1:A:390:ALA:HB1	1:A:754:ILE:HD13	1.86	0.56
1:A:73:GLU:O	1:A:74:ILE:C	2.43	0.56
2:B:457:PRO:CG	2:B:517:PHE:HB2	2.34	0.56
1:A:705:GLU:HB3	2:B:545:LYS:HZ1	1.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:570:ILE:O	2:B:570:ILE:HG13	2.04	0.56
21:B:6020:BCR:C38	21:B:6020:BCR:C23	2.82	0.56
2:B:725:LEU:HD12	2:B:726:ILE:N	2.20	0.56
2:B:88:ALA:H	2:B:115:ASN:CA	2.17	0.56
7:G:96:GLY:O	7:G:97:LEU:CD2	2.53	0.56
7:G:99:HIS:HA	7:G:100:PHE:HB2	1.85	0.56
11:K:58:VAL:HG12	11:K:59:THR:N	2.19	0.56
11:K:76:ALA:N	11:K:78:ARG:NH1	2.46	0.56
19:2:2004:CLA:O1A	19:3:2009:CLA:HBC2	2.05	0.56
13:N:132:THR:OG1	13:N:137:LEU:C	2.43	0.56
13:N:148:ASP:CA	13:N:149:ASP:O	2.53	0.56
4:D:177:VAL:HG13	4:D:177:VAL:O	2.05	0.56
4:D:177:VAL:HG22	4:D:178:ASN:HA	1.87	0.56
4:D:100:TYR:HE1	4:D:134:LYS:HG3	1.58	0.56
4:D:102:ILE:CG1	4:D:154:PHE:HB3	2.35	0.56
6:F:102:LEU:C	6:F:103:GLN:O	2.42	0.56
11:K:115:ILE:HD12	11:K:118:VAL:CG2	2.34	0.56
16:2:195:TYR:CE1	16:2:196:PRO:HD2	2.37	0.56
19:H:1145:CLA:C14	19:H:1145:CLA:H101	2.22	0.56
17:3:159:VAL:O	17:3:161:GLU:CA	2.53	0.56
12:L:164:LEU:HD12	12:L:165:THR:CA	2.34	0.56
12:L:164:LEU:C	12:L:165:THR:HG23	2.24	0.56
6:F:114:ALA:N	6:F:115:PRO:HD3	2.20	0.56
1:A:638:THR:O	1:A:639:ALA:C	2.44	0.56
15:1:78:ARG:CD	19:1:1011:CLA:HMC2	2.16	0.56
19:A:1105:CLA:HHB	19:A:1106:CLA:HMB3	1.86	0.56
19:A:1124:CLA:CBC	19:A:1124:CLA:CHD	2.77	0.56
19:A:1124:CLA:O1A	19:A:1124:CLA:C2	2.51	0.56
1:A:146:THR:O	19:A:1126:CLA:HMA2	2.04	0.56
1:A:370:ILE:CD1	19:A:1124:CLA:O1D	2.53	0.56
1:A:438:HIS:HB2	1:A:441:ALA:HB3	1.85	0.56
1:A:97:TYR:O	1:A:98:PHE:O	2.23	0.56
19:B:1213:CLA:HED2	19:B:1213:CLA:CBA	2.36	0.56
2:B:371:LEU:HD21	19:B:1225:CLA:HED3	1.87	0.56
1:A:558:LYS:NZ	2:B:674:LEU:HD22	2.20	0.56
6:F:207:LEU:CD2	6:F:208:PHE:CG	2.88	0.56
6:F:82:LEU:CG	6:F:83:THR:N	2.58	0.56
16:2:117:ALA:HB3	16:2:230:LEU:CG	2.20	0.56
5:E:106:ARG:HE	5:E:106:ARG:C	2.09	0.56
4:D:167:HIS:CD2	4:D:167:HIS:O	2.59	0.56
3:C:26:LEU:HD21	4:D:181:ARG:NH1	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:138:LEU:HD23	4:D:138:LEU:O	2.05	0.56
16:2:195:TYR:HB3	16:2:201:PHE:CE2	2.39	0.56
2:B:143:LEU:C	2:B:145:LEU:H	2.08	0.56
4:D:187:ASN:N	4:D:187:ASN:ND2	2.37	0.56
19:4:4015:CLA:CHD	19:4:4015:CLA:HBC3	2.34	0.56
1:A:236:GLY:O	1:A:237:VAL:CG2	2.53	0.56
17:3:214:GLY:HA3	17:3:215:LYS:HE2	1.85	0.56
1:A:497:ALA:HB1	1:A:510:SER:HG	1.71	0.56
7:G:133:ILE:O	7:G:133:ILE:HG23	2.03	0.56
22:H:7002:LMU:O6B	22:H:7002:LMU:H1B	2.05	0.56
18:4:226:LYS:N	18:4:226:LYS:HZ3	2.04	0.56
15:1:64:PHE:CD1	15:1:65:ASP:HB3	2.40	0.56
15:1:91:MET:SD	15:1:94:VAL:HB	2.45	0.56
18:4:154:ILE:CD1	19:4:1009:CLA:HMD1	2.35	0.56
18:4:156:ARG:HD2	19:4:4011:CLA:C2D	2.35	0.56
1:A:224:HIS:HE1	19:A:1113:CLA:C4C	2.18	0.56
1:A:203:LEU:CD2	19:A:1123:CLA:CED	2.83	0.56
1:A:462:ILE:HD11	19:A:9022:CLA:C5	2.32	0.56
19:A:1112:CLA:CAB	21:A:6002:BCR:H19C	2.36	0.56
19:A:9023:CLA:H142	21:I:6018:BCR:C4	2.36	0.56
19:B:1206:CLA:H122	21:I:6018:BCR:H373	1.87	0.56
19:B:1206:CLA:H203	21:I:6018:BCR:H372	1.85	0.56
7:G:90:GLN:N	7:G:90:GLN:OE1	2.39	0.56
12:L:141:LEU:CD1	21:L:6019:BCR:H312	2.17	0.56
19:4:1306:CLA:H2	19:4:1306:CLA:CED	2.31	0.56
18:4:177:LEU:N	18:4:178:PRO:CD	2.68	0.56
19:A:1119:CLA:C4C	19:A:1125:CLA:H172	2.35	0.56
1:A:111:ASN:HB3	1:A:112:ASP:OD1	2.04	0.56
1:A:733:VAL:HG22	19:A:1140:CLA:C3D	2.35	0.56
19:A:9022:CLA:CBB	19:A:9023:CLA:CHB	2.79	0.56
2:B:293:THR:H	19:B:1217:CLA:CED	2.18	0.56
2:B:457:PRO:O	2:B:458:ILE:C	2.44	0.56
2:B:495:PRO:O	2:B:499:ASN:ND2	2.39	0.56
21:B:6010:BCR:H321	21:B:6010:BCR:HC8	1.88	0.56
10:J:10:VAL:CG1	10:J:11:ALA:N	2.68	0.56
11:K:57:MET:O	11:K:61:THR:OG1	2.22	0.56
17:3:184:LYS:O	17:3:185:GLN:CB	2.53	0.56
19:2:2001:CLA:C1A	19:2:2001:CLA:O1A	2.53	0.56
1:A:263:ALA:O	1:A:264:GLU:HG2	2.06	0.56
16:2:150:THR:O	16:2:152:LEU:HD13	2.05	0.56
16:2:172:LEU:O	16:2:174:PRO:CD	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:104:TRP:CD1	4:D:104:TRP:N	2.73	0.56
19:H:1145:CLA:CBC	19:H:1145:CLA:CMC	2.77	0.56
11:K:70:PHE:CB	11:K:98:PRO:HB3	2.32	0.56
6:F:215:VAL:O	6:F:218:TYR:N	2.38	0.56
18:4:111:LEU:HD12	18:4:112:PRO:HD3	1.78	0.56
1:A:631:GLN:O	1:A:632:GLY:C	2.41	0.56
18:4:246:GLN:CG	18:4:246:GLN:O	2.52	0.56
18:4:121:ILE:CG1	18:4:122:ASN:H	2.18	0.56
18:4:95:GLU:HA	18:4:98:ASN:OD1	2.05	0.56
1:A:187:HIS:CE1	19:A:1109:CLA:C1A	2.74	0.56
19:A:1138:CLA:H101	19:A:1138:CLA:CBB	2.35	0.56
1:A:430:ASP:C	1:A:432:LEU:H	2.08	0.56
19:B:1220:CLA:H43	19:B:1220:CLA:CAA	2.31	0.56
2:B:175:LEU:CD1	19:B:1221:CLA:HED1	2.35	0.56
2:B:312:GLY:C	2:B:314:ARG:N	2.59	0.56
2:B:315:LEU:HD22	2:B:315:LEU:O	2.06	0.56
2:B:558:PRO:HG3	2:B:574:ASP:OD1	2.06	0.56
11:K:50:GLY:N	11:K:52:PRO:CD	2.68	0.56
2:B:25:ILE:CG2	21:L:6019:BCR:C28	2.83	0.56
3:C:7:ILE:HD13	3:C:54:CYS:SG	2.45	0.56
3:C:23:THR:HG21	3:C:47:ASP:OD2	2.06	0.56
16:2:165:GLY:HA2	16:2:167:ARG:HG2	1.86	0.56
16:2:192:ASP:OD1	16:2:194:GLY:C	2.43	0.56
16:2:112:TRP:CG	19:2:2012:CLA:O1D	2.58	0.56
15:1:189:LYS:CA	15:1:189:LYS:CE	2.74	0.56
15:1:170:PRO:O	15:1:173:TYR:CZ	2.58	0.56
17:3:162:MET:HE1	19:3:3010:CLA:C3D	2.36	0.56
1:A:68:THR:HG23	1:A:69:SER:N	2.20	0.56
15:1:85:ILE:C	15:1:88:ARG:HB2	2.26	0.56
18:4:145:GLU:OE2	18:4:146:PHE:HE1	1.88	0.56
18:4:207:ASN:OD1	19:4:4002:CLA:NB	2.39	0.56
19:A:1102:CLA:CBA	19:A:1109:CLA:H62	2.35	0.56
1:A:242:ILE:CB	1:A:243:PRO:HD3	2.34	0.56
1:A:281:LEU:HD22	19:A:1115:CLA:HED2	1.83	0.56
19:A:9023:CLA:HED3	19:A:9023:CLA:HBA2	1.87	0.56
3:C:1:MET:H3	3:C:4:SER:CB	2.16	0.56
1:A:438:HIS:HA	4:D:87:THR:OG1	2.05	0.56
2:B:230:TRP:H	7:G:63:VAL:HG21	1.63	0.56
20:B:5002:PQN:H302	21:L:6019:BCR:H24C	1.86	0.56
5:E:78:ARG:NH1	5:E:125:ILE:CB	2.65	0.56
13:N:133:GLY:O	13:N:134:CYS:SG	2.60	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:146:LEU:HG	13:N:148:ASP:O	2.06	0.56
1:A:570:PRO:C	1:A:572:LYS:H	2.07	0.56
2:B:560:ASP:CG	3:C:66:ARG:NH1	2.59	0.56
3:C:67:VAL:CG1	3:C:68:TYR:N	2.68	0.56
17:3:124:LYS:HZ1	17:3:148:TYR:N	2.04	0.56
11:K:127:ILE:HG12	11:K:130:LEU:CD1	2.28	0.56
11:K:127:ILE:HG23	11:K:130:LEU:HG	1.64	0.56
17:3:204:GLY:O	17:3:205:GLY:C	2.42	0.56
1:A:578:ARG:NH1	1:A:578:ARG:HB2	2.19	0.56
1:A:267:THR:CG2	1:A:269:PHE:CE2	2.59	0.56
17:3:164:LEU:CD1	17:3:165:MET:SD	2.93	0.56
2:B:131:THR:O	2:B:131:THR:HG22	2.04	0.56
6:F:221:LEU:CD2	6:F:222:LEU:HD21	2.31	0.56
15:1:221:LEU:CD1	19:1:1003:CLA:HAC1	2.29	0.56
1:A:564:ARG:CZ	1:A:564:ARG:CB	2.83	0.56
4:D:147:LYS:O	4:D:148:TYR:CG	2.58	0.56
15:1:123:THR:O	15:1:124:TYR:CB	2.53	0.56
18:4:158:GLN:CD	19:4:1004:CLA:C1A	2.70	0.56
18:4:212:LEU:O	18:4:213:ALA:HB3	2.04	0.56
1:A:685:VAL:HG22	19:A:1140:CLA:HBB2	1.86	0.56
1:A:331:LEU:O	1:A:331:LEU:CD2	2.52	0.56
1:A:700:TRP:HZ3	19:A:9013:CLA:O1D	1.89	0.56
2:B:117:TYR:H	19:B:1205:CLA:HMD1	1.71	0.56
19:B:1205:CLA:C10	19:B:1205:CLA:H142	2.34	0.56
2:B:193:HIS:HB2	19:B:1211:CLA:CHC	2.36	0.56
2:B:351:HIS:O	2:B:355:LEU:HB2	2.05	0.56
2:B:355:LEU:HD21	2:B:508:LEU:HD21	1.87	0.56
5:E:90:VAL:CG1	5:E:91:VAL:H	2.19	0.56
6:F:199:ASP:HA	10:J:9:SER:HA	1.87	0.56
16:2:157:LEU:N	16:2:157:LEU:HD13	2.19	0.56
13:N:113:ASN:OD1	13:N:113:ASN:O	2.24	0.56
4:D:140:LEU:CD1	4:D:144:LEU:N	2.69	0.56
8:H:82:LYS:HG2	8:H:85:GLU:CB	2.36	0.56
8:H:82:LYS:HG2	8:H:85:GLU:HB3	1.87	0.56
15:1:151:GLN:NE2	15:1:151:GLN:HA	2.19	0.56
15:1:170:PRO:CG	15:1:173:TYR:CE2	2.88	0.56
22:R:7021:LMU:H41	22:R:7021:LMU:H6D	1.87	0.56
15:1:81:GLU:CG	15:1:82:SER:N	2.68	0.56
19:A:1112:CLA:CHC	21:A:6002:BCR:C17	2.82	0.56
19:A:1127:CLA:H51	21:A:6003:BCR:H331	1.87	0.56
1:A:349:ILE:CG2	1:A:350:LEU:N	2.66	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:ILE:HD13	19:A:1131:CLA:HED1	1.84	0.56
1:A:462:ILE:CG2	19:A:1132:CLA:HMC3	2.35	0.56
1:A:57:LEU:CD2	1:A:58:HIS:N	2.68	0.56
2:B:614:THR:O	2:B:614:THR:CG2	2.50	0.56
6:F:148:LEU:CD1	6:F:148:LEU:O	2.48	0.56
5:E:75:LYS:HA	5:E:87:THR:CG2	2.31	0.56
16:2:185:ASN:OD1	16:2:185:ASN:C	2.43	0.56
8:H:121:LEU:C	8:H:122:PRO:O	2.44	0.56
7:G:151:PRO:O	7:G:151:PRO:HD2	2.05	0.56
6:F:88:SER:O	6:F:91:PHE:N	2.39	0.56
1:A:426:THR:CG2	1:A:428:TYR:CZ	2.88	0.56
10:J:31:ARG:NH2	19:J:1311:CLA:C3B	2.69	0.56
15:1:170:PRO:CG	15:1:171:LEU:N	2.58	0.56
17:3:125:VAL:HG21	19:3:3010:CLA:C1C	2.35	0.56
22:R:7021:LMU:H22	22:R:7021:LMU:C6	2.33	0.56
15:1:117:LEU:CD1	15:1:117:LEU:N	2.67	0.56
2:B:436:LEU:O	2:B:437:TYR:HB2	2.06	0.56
2:B:730:SER:C	2:B:731:GLY:O	2.42	0.56
19:1:1001:CLA:CBC	19:1:1001:CLA:HMC1	2.17	0.56
15:1:78:ARG:HH21	15:1:179:LYS:CG	2.15	0.56
18:4:103:MET:HE1	18:4:207:ASN:CA	2.35	0.56
1:A:58:HIS:CE1	19:A:1101:CLA:ND	2.74	0.56
19:A:1116:CLA:H52	19:A:1133:CLA:HBA1	1.87	0.56
1:A:190:ALA:HB1	1:A:191:PRO:HD2	1.85	0.56
19:A:1127:CLA:CHD	21:A:6003:BCR:H333	2.36	0.56
19:A:1119:CLA:H18	21:A:6007:BCR:H383	1.87	0.56
1:A:544:ILE:HD11	19:A:9011:CLA:H193	1.88	0.56
2:B:317:ARG:CZ	2:B:410:ARG:CG	2.68	0.56
23:B:7101:LMG:O3	3:C:70:TRP:HZ2	1.84	0.56
10:J:2:ARG:HB3	10:J:7:TYR:CZ	2.41	0.56
12:L:67:GLY:C	12:L:68:SER:OG	2.45	0.56
12:L:93:VAL:O	12:L:94:SER:C	2.41	0.56
16:2:226:ARG:HA	16:2:229:MET:HB3	1.87	0.56
5:E:73:LYS:HG3	5:E:73:LYS:O	2.06	0.56
3:C:43:PRO:O	3:C:43:PRO:CD	2.54	0.56
3:C:66:ARG:NH2	3:C:66:ARG:HG2	1.95	0.56
22:3:7003:LMU:C2B	22:3:7005:LMU:H6'1	2.36	0.56
15:1:147:PHE:CD1	15:1:147:PHE:O	2.59	0.56
16:2:269:LYS:C	16:2:269:LYS:HE3	2.26	0.56
1:A:567:ARG:HH11	4:D:88:GLY:C	2.09	0.56
17:3:210:PRO:CG	17:3:211:LEU:N	2.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:215:VAL:O	6:F:218:TYR:HB2	2.06	0.56
15:1:161:LYS:O	15:1:161:LYS:HD2	2.06	0.56
16:2:146:PHE:N	16:2:146:PHE:CD1	2.73	0.56
18:4:172:PHE:C	18:4:194:PHE:CD2	2.79	0.56
19:4:4002:CLA:CBA	19:4:4002:CLA:CMA	2.67	0.56
19:A:1124:CLA:CHB	21:A:6008:BCR:H363	2.35	0.56
1:A:580:PRO:HA	1:A:728:VAL:CG2	2.36	0.56
2:B:197:VAL:O	2:B:198:ALA:HB2	2.06	0.56
2:B:419:ILE:HG12	2:B:536:LYS:HB2	1.88	0.56
2:B:457:PRO:HB3	2:B:517:PHE:CG	2.40	0.56
7:G:102:ALA:C	7:G:104:ASP:OD1	2.44	0.56
7:G:89:LYS:HZ1	7:G:89:LYS:HA	1.63	0.56
8:H:109:LEU:HD23	19:H:1207:CLA:H52	1.86	0.56
19:A:9023:CLA:H142	21:I:6018:BCR:HC42	1.87	0.56
5:E:79:LYS:N	5:E:84:TYR:CE1	2.74	0.56
13:N:131:PHE:CA	13:N:132:THR:HG22	2.35	0.56
1:A:586:ARG:HG3	3:C:49:VAL:CG2	2.31	0.56
14:R:36:UNK:C	14:R:38:UNK:N	2.66	0.56
1:A:252:ARG:NH2	1:A:261:SER:OG	2.39	0.56
19:3:3013:CLA:H91	19:3:3013:CLA:H121	1.87	0.56
2:B:154:TRP:CD1	2:B:154:TRP:C	2.78	0.56
6:F:228:ASP:C	6:F:231:PHE:HB3	2.25	0.56
1:A:426:THR:CA	1:A:428:TYR:CE2	2.84	0.56
11:K:97:ASP:O	11:K:98:PRO:C	2.44	0.56
1:A:484:LEU:C	1:A:485:GLN:NE2	2.59	0.56
1:A:639:ALA:O	1:A:641:ASN:N	2.39	0.56
2:B:505:SER:OG	2:B:506:ASN:OD1	2.23	0.56
1:A:177:LEU:C	1:A:179:LEU:H	2.09	0.56
2:B:12:ILE:HG22	2:B:13:ALA:N	2.20	0.56
1:A:159:THR:HG22	1:A:160:SER:N	2.20	0.56
1:A:193:LEU:O	1:A:194:ALA:C	2.44	0.56
1:A:358:LEU:HD21	1:A:413:HIS:ND1	2.21	0.56
1:A:545:HIS:CE1	1:A:612:VAL:HG22	2.41	0.56
19:B:1203:CLA:C19	19:B:1224:CLA:H141	2.36	0.56
2:B:655:LEU:CD2	19:B:1239:CLA:CBB	2.84	0.56
2:B:471:THR:HG22	2:B:502:ASN:HD22	1.71	0.56
2:B:493:TRP:O	2:B:495:PRO:HG3	2.06	0.56
2:B:707:LEU:O	2:B:710:LEU:HB3	2.06	0.56
2:B:732:LYS:HG2	2:B:733:PHE:HA	1.88	0.56
2:B:86:PRO:C	2:B:87:ILE:HD12	2.26	0.56
5:E:103:VAL:HG13	5:E:120:TYR:C	2.26	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:10:PRO:O	9:I:15:LEU:N	2.32	0.56
11:K:56:ILE:HG22	11:K:56:ILE:O	2.05	0.56
16:2:122:ILE:N	16:2:123:PRO:HD3	2.20	0.56
16:2:122:ILE:HD12	19:2:2002:CLA:HMB1	1.87	0.56
19:K:1146:CLA:H2A	19:K:1146:CLA:O1A	2.05	0.56
17:3:204:GLY:C	17:3:206:PRO:C	2.65	0.56
15:1:170:PRO:HG2	15:1:173:TYR:CD2	2.41	0.56
12:L:164:LEU:O	12:L:165:THR:HG22	2.05	0.56
4:D:184:VAL:HG12	4:D:185:GLY:N	2.21	0.56
12:L:51:LYS:N	12:L:51:LYS:CD	2.66	0.56
6:F:168:LEU:O	6:F:171:ALA:O	2.23	0.56
10:J:32:PHE:HE2	10:J:33:PHE:CZ	2.23	0.56
19:A:9012:CLA:C3B	2:B:589:TRP:CH2	2.85	0.55
19:B:1220:CLA:H93	19:B:1227:CLA:CBC	2.37	0.55
2:B:382:ILE:CG2	2:B:383:MET:N	2.48	0.55
2:B:438:VAL:CG2	19:B:1230:CLA:HAC1	2.35	0.55
2:B:596:TRP:O	2:B:597:LYS:HB3	2.06	0.55
2:B:440:ASN:CG	2:B:614:THR:CG2	2.71	0.55
6:F:149:ILE:HG22	6:F:151:SER:N	2.21	0.55
6:F:200:VAL:CG2	6:F:204:SER:N	2.70	0.55
9:I:14:LEU:O	9:I:17:PRO:HD2	2.06	0.55
11:K:50:GLY:C	11:K:52:PRO:CD	2.71	0.55
12:L:82:TYR:O	12:L:83:LEU:CB	2.54	0.55
19:L:1148:CLA:C1	19:L:1148:CLA:CED	2.77	0.55
16:2:150:THR:O	16:2:153:PHE:N	2.39	0.55
19:K:1146:CLA:HMD2	22:K:7001:LMU:H32	1.87	0.55
11:K:124:LEU:O	11:K:126:ASN:CB	2.54	0.55
16:2:254:LEU:HD22	16:2:256:ASP:H	1.69	0.55
1:A:630:ASP:O	1:A:631:GLN:C	2.45	0.55
1:A:42:ARG:C	1:A:44:ILE:N	2.60	0.55
12:L:104:LEU:HD11	12:L:199:TRP:CZ2	2.41	0.55
15:1:125:LEU:HD23	15:1:125:LEU:O	2.06	0.55
19:A:1124:CLA:HED2	19:A:1124:CLA:HAA1	1.87	0.55
19:A:1131:CLA:H52	21:B:6017:BCR:C34	2.34	0.55
19:A:1141:CLA:H71	19:A:1141:CLA:C12	2.09	0.55
1:A:362:LEU:CB	1:A:410:ALA:HB2	2.36	0.55
2:B:463:ILE:HD11	19:B:1231:CLA:HMC3	1.88	0.55
2:B:290:MET:HG2	2:B:290:MET:O	2.06	0.55
2:B:347:LEU:HD22	2:B:351:HIS:CE1	2.42	0.55
2:B:356:PRO:CD	2:B:356:PRO:O	2.55	0.55
9:I:28:VAL:O	9:I:29:GLU:CD	2.45	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:155:GLU:CB	13:N:157:LYS:CA	2.79	0.55
16:2:183:PHE:C	16:2:183:PHE:HD1	2.09	0.55
4:D:123:ARG:NH2	22:D:7050:LMU:H6'1	1.59	0.55
6:F:90:GLN:HG2	6:F:143:ASP:H	1.70	0.55
22:N:7049:LMU:C6	22:N:7049:LMU:O1'	2.55	0.55
12:L:169:ARG:HG2	12:L:172:GLU:CA	2.37	0.55
12:L:172:GLU:C	12:L:173:PRO:O	2.41	0.55
8:H:111:TYR:CD1	8:H:112:LEU:HD21	2.41	0.55
18:4:191:PRO:O	18:4:192:LEU:HB2	2.06	0.55
19:A:1124:CLA:H2	19:A:1125:CLA:CED	2.35	0.55
1:A:245:PRO:C	1:A:248:PHE:HE2	2.09	0.55
1:A:393:LEU:HD11	1:A:750:PHE:CE1	2.41	0.55
2:B:98:GLN:O	2:B:100:ALA:CB	2.55	0.55
2:B:293:THR:HG21	19:B:1209:CLA:HMA3	1.88	0.55
2:B:292:ARG:HH21	2:B:297:ILE:HG13	1.70	0.55
2:B:459:PHE:CD2	19:B:1235:CLA:C1D	2.66	0.55
2:B:556:SER:C	2:B:558:PRO:CD	2.71	0.55
7:G:106:ARG:HB2	7:G:107:ALA:HA	1.88	0.55
19:A:1126:CLA:C20	21:J:6012:BCR:C17	2.79	0.55
11:K:78:ARG:CZ	11:K:78:ARG:H	2.20	0.55
12:L:141:LEU:O	12:L:145:LEU:HD12	2.07	0.55
3:C:11:CYS:C	3:C:13:GLY:H	2.10	0.55
8:H:61:THR:HA	8:H:62:THR:HG23	0.63	0.55
13:N:139:LYS:HG3	13:N:142:LYS:CG	2.37	0.55
13:N:99:LYS:HA	13:N:102:ASN:CG	2.23	0.55
11:K:81:THR:HG23	11:K:82:ALA:N	2.22	0.55
1:A:316:MET:CA	1:A:317:TYR:HB2	2.31	0.55
11:K:97:ASP:HA	11:K:101:PHE:CE2	2.41	0.55
15:1:112:GLN:C	15:1:113:GLU:OE2	2.44	0.55
22:4:7053:LMU:H6E	22:4:7053:LMU:C2B	2.36	0.55
18:4:95:GLU:CG	18:4:96:LEU:N	2.69	0.55
1:A:541:VAL:HG12	1:A:545:HIS:NE2	2.22	0.55
1:A:74:ILE:O	1:A:75:SER:C	2.44	0.55
19:A:9011:CLA:HMB3	19:A:9012:CLA:CAD	2.37	0.55
19:A:9023:CLA:HBC1	2:B:665:ILE:HD12	1.89	0.55
2:B:352:MET:HE2	19:B:1225:CLA:OBD	2.04	0.55
2:B:459:PHE:CG	19:B:1235:CLA:CAD	2.89	0.55
2:B:617:MET:HG3	2:B:618:GLY:N	2.21	0.55
2:B:622:ASP:CB	2:B:626:LEU:CG	2.85	0.55
5:E:102:PRO:O	5:E:120:TYR:O	2.24	0.55
7:G:68:THR:OG1	7:G:69:GLY:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:92:ALA:CB	12:L:98:ARG:CZ	2.84	0.55
3:C:12:ILE:HB	3:C:38:GLN:O	2.07	0.55
15:1:141:GLU:O	15:1:145:ILE:CG1	2.53	0.55
17:3:94:GLU:HB3	17:3:95:PRO:HD3	1.88	0.55
19:L:1148:CLA:HAA1	19:L:1148:CLA:O1D	2.03	0.55
22:3:7003:LMU:O2B	22:3:7005:LMU:C6B	2.55	0.55
5:E:96:ASP:CB	5:E:98:ASN:OD1	2.54	0.55
1:A:629:ASN:O	1:A:632:GLY:N	2.39	0.55
1:A:29:THR:CG2	1:A:29:THR:O	2.54	0.55
6:F:94:ARG:HA	6:F:94:ARG:NE	2.21	0.55
15:1:60:GLY:O	15:1:61:ASP:C	2.45	0.55
15:1:68:GLY:C	15:1:72:VAL:HB	2.25	0.55
19:4:4002:CLA:CAA	19:4:4002:CLA:CGD	2.75	0.55
1:A:107:GLU:OE2	1:A:161:GLU:CG	2.45	0.55
1:A:158:ILE:HD13	19:A:1112:CLA:CED	2.36	0.55
1:A:201:SER:O	1:A:204:ASN:N	2.40	0.55
1:A:338:PHE:HB3	19:A:1129:CLA:HBD	1.89	0.55
1:A:430:ASP:C	1:A:432:LEU:N	2.60	0.55
2:B:670:TYR:C	2:B:670:TYR:CD1	2.80	0.55
12:L:102:VAL:CA	19:L:1502:CLA:HED2	2.33	0.55
15:1:137:ILE:C	15:1:141:GLU:OE2	2.45	0.55
22:3:7003:LMU:H3B	22:3:7005:LMU:C3B	2.31	0.55
4:D:80:SER:H	4:D:81:PRO:HD3	1.70	0.55
6:F:100:LYS:O	6:F:100:LYS:CD	2.53	0.55
2:B:542:ARG:HB3	2:B:542:ARG:NH1	2.18	0.55
17:3:161:GLU:HA	17:3:164:LEU:CG	2.32	0.55
18:4:174:GLN:CA	18:4:176:SER:H	2.19	0.55
18:4:173:LYS:CA	18:4:194:PHE:CD2	2.89	0.55
19:A:1106:CLA:H111	21:J:6012:BCR:C11	2.36	0.55
1:A:507:ALA:O	1:A:508:THR:C	2.44	0.55
1:A:64:PHE:CD1	1:A:64:PHE:N	2.73	0.55
1:A:470:LEU:HG	19:B:1206:CLA:HMC3	1.89	0.55
19:B:1229:CLA:HMB3	19:B:1230:CLA:HBB2	1.87	0.55
2:B:175:LEU:HA	2:B:178:HIS:HB2	1.88	0.55
2:B:275:HIS:ND1	19:B:1214:CLA:HMB1	2.22	0.55
21:B:6010:BCR:H382	21:B:6010:BCR:C23	2.34	0.55
21:B:6017:BCR:C38	21:B:6017:BCR:H23C	2.26	0.55
5:E:82:TYR:CB	5:E:83:TRP:HZ3	2.14	0.55
7:G:74:LEU:C	7:G:77:PHE:H	2.10	0.55
13:N:139:LYS:HG3	13:N:142:LYS:HE2	1.87	0.55
15:1:137:ILE:HB	15:1:141:GLU:OE2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:173:TYR:O	4:D:175:GLU:HG3	2.07	0.55
13:N:104:LYS:O	13:N:107:LEU:CA	2.55	0.55
16:2:165:GLY:O	16:2:167:ARG:CG	2.54	0.55
8:H:89:ALA:N	8:H:90:PRO:HD2	2.22	0.55
6:F:123:MET:O	6:F:126:THR:N	2.39	0.55
11:K:112:VAL:C	11:K:114:HIS:N	2.53	0.55
2:B:49:SER:O	2:B:52:GLY:N	2.40	0.55
1:A:710:ALA:HB1	19:A:1138:CLA:HED2	1.88	0.55
1:A:230:ASN:OD1	1:A:296:LEU:HD22	2.07	0.55
1:A:373:ALA:O	1:A:396:PHE:HD1	1.88	0.55
19:A:9012:CLA:CED	19:B:9010:CLA:H2	2.36	0.55
19:B:1205:CLA:CGA	19:B:1205:CLA:C1A	2.85	0.55
19:B:1225:CLA:H101	21:B:6006:BCR:H343	1.89	0.55
2:B:18:THR:O	2:B:21:ILE:N	2.40	0.55
2:B:312:GLY:C	2:B:314:ARG:H	2.07	0.55
2:B:707:LEU:CD1	2:B:711:VAL:HG21	2.37	0.55
2:B:732:LYS:CG	2:B:733:PHE:HA	2.37	0.55
19:G:1242:CLA:O1A	22:G:7026:LMU:H101	2.07	0.55
5:E:106:ARG:NE	5:E:106:ARG:C	2.60	0.55
13:N:146:LEU:HD13	17:3:142:ILE:HB	1.89	0.55
13:N:155:GLU:CB	13:N:157:LYS:CE	2.78	0.55
13:N:105:LYS:O	13:N:106:ARG:C	2.44	0.55
17:3:110:MET:CE	17:3:238:ILE:H	2.20	0.55
22:3:7005:LMU:C2B	22:3:7005:LMU:C3'	2.85	0.55
17:3:154:ASN:HA	17:3:155:TYR:CD2	2.41	0.55
13:N:169:LYS:CA	13:N:170:TRP:HD1	2.20	0.55
4:D:129:LEU:HD12	4:D:130:LYS:H	1.71	0.55
15:1:122:ALA:HB3	15:1:124:TYR:H	1.72	0.55
1:A:420:ARG:CZ	1:A:420:ARG:HB3	2.32	0.55
5:E:69:LYS:H	5:E:69:LYS:HE3	1.71	0.55
18:4:124:PRO:O	18:4:125:LYS:CB	2.55	0.55
18:4:158:GLN:HE21	19:4:1004:CLA:C4A	2.18	0.55
18:4:169:ASP:O	18:4:173:LYS:CB	2.54	0.55
19:4:4002:CLA:O1A	19:4:4002:CLA:C2	2.52	0.55
1:A:109:TRP:CH2	1:A:154:ARG:HD3	2.42	0.55
19:A:1113:CLA:H42	19:A:1113:CLA:HBA2	1.88	0.55
19:A:1237:CLA:H112	19:A:1237:CLA:H61	1.87	0.55
21:A:6011:BCR:C19	19:A:9012:CLA:H172	2.37	0.55
2:B:334:LEU:O	2:B:334:LEU:CG	2.51	0.55
2:B:376:GLN:OE1	2:B:376:GLN:HA	2.06	0.55
2:B:502:ASN:ND2	2:B:511:THR:HG21	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:507:SER:O	2:B:508:LEU:HB2	2.05	0.55
19:A:1131:CLA:HAA1	21:B:6020:BCR:C14	2.37	0.55
2:B:607:SER:OG	2:B:608:GLN:N	2.39	0.55
5:E:93:VAL:O	5:E:93:VAL:CG1	2.54	0.55
19:F:1305:CLA:HED2	19:F:1305:CLA:CAD	2.36	0.55
16:2:101:TRP:CA	16:2:103:VAL:N	2.62	0.55
17:3:96:ARG:CA	17:3:99:ALA:HB2	2.34	0.55
6:F:194:LYS:O	6:F:197:ILE:O	2.25	0.55
4:D:98:GLU:HB2	4:D:100:TYR:CE2	2.42	0.55
2:B:160:LYS:CE	2:B:161:TRP:CD2	2.90	0.55
22:H:7032:LMU:O5B	22:H:7032:LMU:H31	2.07	0.55
4:D:146:SER:O	4:D:147:LYS:CG	2.51	0.55
7:G:134:GLY:O	7:G:135:HIS:ND1	2.40	0.55
22:A:7010:LMU:H22	22:K:7047:LMU:H101	1.89	0.55
22:4:7033:LMU:H3'	22:4:7033:LMU:O5B	2.05	0.55
2:B:473:GLY:O	2:B:474:PHE:HB2	2.06	0.55
18:4:172:PHE:HB2	18:4:173:LYS:O	2.06	0.55
1:A:229:ILE:O	1:A:229:ILE:HG22	2.06	0.55
1:A:281:LEU:HD22	19:A:1115:CLA:H2A	1.87	0.55
1:A:472:ARG:N	1:A:473:PRO:CD	2.68	0.55
19:B:1210:CLA:H41	19:B:1215:CLA:CBC	2.36	0.55
2:B:224:PRO:HB2	2:B:227:THR:CG2	2.36	0.55
2:B:348:VAL:HG12	2:B:349:ALA:N	2.22	0.55
1:A:466:THR:HG22	2:B:648:TRP:NE1	2.21	0.55
19:G:1242:CLA:O2A	19:G:1242:CLA:H3A	2.06	0.55
3:C:62:PHE:CE1	5:E:80:GLU:CB	2.87	0.55
13:N:145:PHE:C	13:N:146:LEU:O	2.45	0.55
4:D:167:HIS:O	4:D:167:HIS:HD2	1.90	0.55
12:L:205:TYR:CD1	12:L:207:LEU:HD13	2.33	0.55
17:3:206:PRO:HD2	17:3:206:PRO:O	2.07	0.55
22:E:7048:LMU:C11	22:E:7048:LMU:C7	2.83	0.55
19:2:2014:CLA:C4A	19:2:2014:CLA:HBA2	2.35	0.55
15:1:171:LEU:HD23	15:1:171:LEU:N	2.22	0.55
15:1:170:PRO:HB2	15:1:171:LEU:O	2.06	0.55
19:H:1145:CLA:O2D	19:H:1145:CLA:CAA	2.55	0.55
22:1:7004:LMU:C1	22:1:7004:LMU:H3'	2.25	0.55
8:H:107:SER:O	8:H:111:TYR:HB2	2.07	0.55
7:G:134:GLY:O	7:G:135:HIS:CD2	2.60	0.55
18:4:202:GLU:HA	18:4:205:ILE:HG23	1.89	0.55
19:A:1140:CLA:H192	10:J:19:PHE:CD2	2.42	0.55
1:A:86:LEU:CD1	1:A:178:MET:HE2	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:9013:CLA:H3A	19:A:9013:CLA:CGA	2.37	0.55
1:A:607:ASN:HD21	19:A:9022:CLA:C2C	2.19	0.55
2:B:104:PHE:O	2:B:105:THR:CB	2.54	0.55
19:B:1213:CLA:HBC2	19:B:1213:CLA:CHD	2.29	0.55
19:B:1235:CLA:C15	21:F:6016:BCR:H313	2.25	0.55
2:B:256:THR:C	2:B:257:ILE:HD13	2.27	0.55
19:G:1242:CLA:HAA2	19:G:1242:CLA:HBD	1.88	0.55
12:L:125:ILE:HG12	12:L:127:GLY:H	1.72	0.55
17:3:185:GLN:CG	17:3:186:TYR:N	2.33	0.55
2:B:560:ASP:OD1	3:C:65:VAL:O	2.25	0.55
3:C:26:LEU:HD22	4:D:181:ARG:HH11	1.71	0.55
17:3:98:LEU:HD21	17:3:102:GLU:HG3	1.88	0.55
1:A:250:LEU:CD1	17:3:136:TRP:HZ2	2.20	0.55
16:2:149:THR:O	16:2:152:LEU:HD11	2.07	0.55
16:2:184:PRO:N	16:2:187:LYS:CD	2.70	0.55
13:N:118:TYR:O	13:N:119:THR:CG2	2.53	0.55
6:F:225:GLU:O	6:F:227:VAL:CG1	2.54	0.55
15:1:170:PRO:CD	15:1:173:TYR:HD2	2.16	0.55
1:A:70:ASP:O	1:A:71:LEU:C	2.44	0.55
6:F:158:GLY:O	10:J:38:ILE:HG23	2.06	0.55
13:N:169:LYS:HA	13:N:170:TRP:HD1	1.71	0.55
4:D:203:THR:HG22	4:D:205:LYS:N	2.16	0.55
22:4:7053:LMU:H72	22:4:7053:LMU:C11	2.37	0.55
15:1:193:LEU:HD23	15:1:193:LEU:O	2.07	0.55
22:K:7042:LMU:H32	22:K:7042:LMU:O5'	2.06	0.55
4:D:101:VAL:HA	4:D:130:LYS:HA	1.87	0.55
1:A:461:TYR:CE1	1:A:540:LEU:HD11	2.42	0.55
2:B:314:ARG:NH1	15:1:67:LEU:HD11	2.23	0.54
1:A:448:TRP:CD1	19:A:1131:CLA:CED	2.90	0.54
1:A:75:SER:HB3	1:A:354:TRP:HZ2	1.71	0.54
1:A:622:SER:OG	1:A:642:PHE:HB2	2.07	0.54
1:A:728:VAL:HG22	1:A:731:ARG:HH12	1.72	0.54
2:B:330:ILE:HD11	19:B:1202:CLA:H193	1.87	0.54
2:B:167:TRP:CZ2	19:B:1208:CLA:HMA1	2.42	0.54
19:B:1201:CLA:HBC3	19:B:1226:CLA:H51	1.88	0.54
2:B:261:PHE:HE2	2:B:500:ALA:N	1.98	0.54
2:B:594:TRP:C	2:B:594:TRP:HD1	2.10	0.54
21:I:6021:BCR:C39	21:L:6019:BCR:C40	2.81	0.54
10:J:10:VAL:HG13	10:J:11:ALA:N	2.21	0.54
11:K:56:ILE:CG2	11:K:56:ILE:O	2.55	0.54
15:1:145:ILE:O	15:1:148:VAL:HG12	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:3011:CLA:H3A	19:3:3011:CLA:CGA	2.37	0.54
19:J:1311:CLA:H141	19:2:2014:CLA:HMB3	1.88	0.54
16:2:269:LYS:HA	16:2:269:LYS:HZ1	1.65	0.54
15:1:130:PRO:O	15:1:131:TRP:CE3	2.42	0.54
8:H:111:TYR:C	8:H:112:LEU:CD2	2.70	0.54
22:A:7023:LMU:C2B	22:A:7023:LMU:C6B	2.82	0.54
19:A:1101:CLA:HBA2	19:A:1101:CLA:O1D	2.07	0.54
1:A:146:THR:H	19:A:1106:CLA:HMD1	1.72	0.54
19:A:1120:CLA:HBC3	19:A:1122:CLA:HED1	1.90	0.54
1:A:51:THR:OG1	19:A:1139:CLA:CAB	2.54	0.54
1:A:286:GLY:O	1:A:295:TRP:CD1	2.59	0.54
1:A:295:TRP:N	1:A:295:TRP:CD1	2.75	0.54
1:A:396:PHE:HE2	1:A:616:PHE:CG	2.26	0.54
21:A:6007:BCR:H23C	21:A:6007:BCR:C38	2.21	0.54
19:B:1221:CLA:C8	19:B:1223:CLA:H43	2.38	0.54
2:B:124:TRP:NE1	2:B:129:LEU:O	2.36	0.54
2:B:20:ARG:CG	2:B:20:ARG:NH1	2.49	0.54
2:B:229:GLN:CA	2:B:229:GLN:OE1	2.53	0.54
2:B:462:TRP:CZ3	19:B:1231:CLA:HBC1	2.42	0.54
3:C:79:LEU:CD2	3:C:81:TYR:C	2.76	0.54
12:L:76:SER:OG	12:L:78:LEU:CD1	2.55	0.54
4:D:125:GLY:HA2	4:D:127:ASN:N	2.22	0.54
1:A:426:THR:HA	1:A:428:TYR:CD2	2.43	0.54
11:K:69:ARG:O	11:K:70:PHE:C	2.42	0.54
17:3:174:GLN:O	17:3:175:ASP:C	2.46	0.54
4:D:112:PHE:HD2	4:D:112:PHE:C	2.09	0.54
18:4:127:TYR:O	18:4:128:ALA:CB	2.55	0.54
1:A:203:LEU:HD21	19:A:1123:CLA:C4D	2.37	0.54
19:A:1126:CLA:C10	21:A:6011:BCR:H372	2.38	0.54
19:A:1135:CLA:HBD	19:A:1135:CLA:CBA	2.37	0.54
1:A:285:GLY:O	1:A:294:LEU:CD1	2.56	0.54
2:B:174:ARG:NH1	19:B:1221:CLA:CMD	2.70	0.54
2:B:303:TYR:HA	2:B:306:GLU:CG	2.36	0.54
2:B:326:ILE:O	2:B:326:ILE:HG12	2.07	0.54
7:G:84:ARG:HG2	7:G:85:GLU:H	1.72	0.54
7:G:88:ALA:O	7:G:89:LYS:C	2.41	0.54
16:2:133:ASN:ND2	16:2:134:THR:CA	2.52	0.54
19:2:2006:CLA:H161	19:2:2006:CLA:H102	1.89	0.54
17:3:239:LEU:HA	17:3:242:PHE:HB2	1.89	0.54
16:2:150:THR:C	16:2:152:LEU:CD1	2.76	0.54
4:D:115:PRO:C	4:D:116:THR:HG1	1.96	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:160:LYS:NZ	2:B:161:TRP:CB	2.69	0.54
2:B:70:TRP:NE1	2:B:71:GLN:OE1	2.40	0.54
19:A:1105:CLA:HAA2	19:A:1107:CLA:HED1	1.90	0.54
1:A:76:ARG:HD3	1:A:191:PRO:O	2.07	0.54
1:A:302:HIS:HD2	19:A:1116:CLA:NB	2.03	0.54
1:A:471:GLY:O	1:A:472:ARG:HG2	2.07	0.54
1:A:672:LEU:HD23	1:A:672:LEU:H	1.72	0.54
1:A:693:LEU:HD11	1:A:738:TYR:CD1	2.43	0.54
1:A:73:GLU:HB2	1:A:186:TYR:CE2	2.42	0.54
2:B:22:TRP:CE2	19:B:1238:CLA:HMB1	2.41	0.54
2:B:124:TRP:C	2:B:124:TRP:CD1	2.80	0.54
2:B:233:TYR:H	2:B:233:TYR:HD2	1.55	0.54
2:B:292:ARG:HH22	2:B:297:ILE:HG12	1.73	0.54
2:B:297:ILE:HG21	7:G:77:PHE:CZ	2.43	0.54
2:B:450:GLU:O	2:B:451:LYS:CB	2.52	0.54
2:B:454:LEU:HD11	6:F:147:HIS:CA	2.29	0.54
10:J:22:LEU:O	10:J:25:LEU:N	2.41	0.54
12:L:91:THR:C	12:L:98:ARG:HH12	2.11	0.54
3:C:44:ARG:NE	4:D:182:GLN:NE2	2.55	0.54
13:N:104:LYS:H	13:N:107:LEU:HD13	1.73	0.54
17:3:107:ARG:NH1	17:3:233:LEU:H	2.06	0.54
1:A:261:SER:C	1:A:262:PHE:CD1	2.79	0.54
4:D:100:TYR:HE1	4:D:134:LYS:HE3	1.61	0.54
16:2:184:PRO:CG	16:2:186:ASN:N	2.71	0.54
22:3:7005:LMU:O2B	22:3:7005:LMU:C3'	2.55	0.54
16:2:249:ASN:HD22	16:2:254:LEU:HG	1.71	0.54
17:3:156:THR:C	17:3:158:PHE:C	2.65	0.54
22:K:7041:LMU:H1B	22:K:7041:LMU:O6'	2.08	0.54
15:1:70:GLY:O	15:1:71:GLU:C	2.42	0.54
18:4:168:GLN:O	18:4:173:LYS:C	2.46	0.54
18:4:178:PRO:O	18:4:194:PHE:HZ	1.89	0.54
18:4:201:LYS:O	18:4:201:LYS:CG	2.52	0.54
19:A:1237:CLA:C14	12:L:141:LEU:HD22	2.36	0.54
1:A:129:GLN:HE22	19:A:1107:CLA:C1A	2.13	0.54
1:A:370:ILE:HD12	19:A:1124:CLA:O1D	2.07	0.54
1:A:656:PHE:HD2	1:A:657:LEU:HD12	1.72	0.54
1:A:73:GLU:O	1:A:76:ARG:CA	2.55	0.54
2:B:33:SER:H	2:B:37:ILE:HD13	1.73	0.54
2:B:668:ARG:NH2	2:B:672:GLN:OE1	2.41	0.54
2:B:720:THR:O	2:B:724:PHE:N	2.41	0.54
2:B:646:TRP:CH2	2:B:726:ILE:HG21	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:84:ARG:CG	7:G:85:GLU:CB	2.71	0.54
13:N:139:LYS:O	13:N:142:LYS:NZ	2.40	0.54
17:3:139:THR:CG2	17:3:140:GLY:N	2.38	0.54
1:A:261:SER:C	1:A:263:ALA:H	2.08	0.54
4:D:163:VAL:O	4:D:164:GLN:CB	2.56	0.54
4:D:83:PHE:CE1	4:D:114:MET:CE	2.91	0.54
2:B:160:LYS:HE3	2:B:161:TRP:CE3	2.41	0.54
16:2:243:GLY:C	16:2:244:THR:CG2	2.76	0.54
15:1:201:PHE:CE1	15:1:204:GLN:NE2	2.75	0.54
13:N:169:LYS:CA	13:N:170:TRP:CD1	2.91	0.54
2:B:241:ASN:CG	2:B:241:ASN:O	2.45	0.54
15:1:69:LEU:O	15:1:73:PRO:HD3	2.07	0.54
19:A:1133:CLA:C1B	21:A:6008:BCR:H333	2.37	0.54
1:A:491:TRP:CE2	19:A:1135:CLA:H12	2.42	0.54
1:A:706:SER:HB3	2:B:419:ILE:O	2.07	0.54
19:A:9023:CLA:HBC3	2:B:661:PHE:HB3	1.89	0.54
19:B:1218:CLA:CBC	19:B:1218:CLA:CHD	2.76	0.54
19:B:1220:CLA:CBD	19:B:1220:CLA:HAA2	2.37	0.54
19:B:1232:CLA:HBB2	21:B:6010:BCR:H281	1.89	0.54
2:B:228:GLY:O	2:B:229:GLN:OE1	2.26	0.54
2:B:361:ILE:O	2:B:362:ALA:HB3	2.08	0.54
2:B:557:PHE:N	2:B:558:PRO:HD2	2.16	0.54
19:A:9022:CLA:H152	21:B:6017:BCR:H20C	1.85	0.54
2:B:663:PHE:O	2:B:664:LEU:CG	2.55	0.54
5:E:90:VAL:C	5:E:91:VAL:HG23	2.28	0.54
19:A:1138:CLA:C6	21:F:6014:BCR:H12C	2.33	0.54
7:G:98:THR:OG1	7:G:101:GLU:CG	2.54	0.54
19:H:1241:CLA:O1D	19:H:1241:CLA:H2A	2.07	0.54
11:K:47:ASP:O	11:K:48:PHE:CB	2.55	0.54
12:L:60:ILE:HG12	12:L:68:SER:OG	2.08	0.54
16:2:128:LYS:HB3	16:2:131:ILE:CG2	2.33	0.54
13:N:123:GLY:CA	13:N:131:PHE:CD1	2.90	0.54
4:D:170:ASP:HB2	4:D:181:ARG:HH21	1.71	0.54
17:3:103:VAL:CG1	17:3:107:ARG:CZ	2.85	0.54
17:3:96:ARG:O	17:3:100:TYR:CD2	2.61	0.54
10:J:5:LYS:CD	16:2:178:ASN:CG	2.76	0.54
13:N:110:THR:HG23	13:N:111:GLY:N	2.22	0.54
6:F:92:ALA:O	6:F:96:LYS:HG3	2.06	0.54
2:B:631:LEU:HB3	2:B:727:ALA:HB1	1.90	0.54
1:A:436:LEU:O	1:A:439:ARG:HB3	2.07	0.54
17:3:176:TRP:CZ2	17:3:199:ASN:OD1	2.61	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:G:7051:LMU:H5'	22:G:7051:LMU:O2'	2.04	0.54
19:4:4006:CLA:HBA2	19:4:4006:CLA:HBD	1.89	0.54
15:1:225:TRP:HB3	15:1:226:HIS:ND1	2.22	0.54
19:A:1140:CLA:C19	10:J:19:PHE:CD2	2.90	0.54
1:A:207:LEU:HA	1:A:211:LEU:HB2	1.89	0.54
1:A:284:ARG:CB	1:A:295:TRP:HB2	2.37	0.54
1:A:432:LEU:C	1:A:434:ARG:N	2.60	0.54
19:B:1222:CLA:HED2	19:B:1223:CLA:OBD	2.07	0.54
2:B:233:TYR:N	2:B:233:TYR:HD2	2.04	0.54
2:B:236:ASN:N	2:B:237:PRO:HD3	2.23	0.54
2:B:544:SER:O	2:B:545:LYS:C	2.45	0.54
6:F:204:SER:O	6:F:207:LEU:CB	2.55	0.54
7:G:72:LEU:HD21	7:G:124:ILE:HD11	1.84	0.54
8:H:109:LEU:HD23	19:H:1207:CLA:C5	2.36	0.54
11:K:76:ALA:CA	11:K:78:ARG:NH1	2.71	0.54
13:N:156:GLY:CA	13:N:157:LYS:HE2	2.36	0.54
17:3:150:TYR:CE2	17:3:151:TRP:CD2	2.96	0.54
8:H:81:SER:O	8:H:83:LEU:N	2.41	0.54
16:2:249:ASN:O	16:2:250:LEU:HB3	2.06	0.54
19:J:1308:CLA:O1D	19:J:1308:CLA:C1	2.56	0.54
15:1:170:PRO:CG	15:1:173:TYR:CD2	2.91	0.54
2:B:137:THR:OG1	2:B:140:ILE:HG12	2.08	0.54
22:H:7011:LMU:C6'	22:H:7011:LMU:C1B	2.86	0.54
16:2:211:PRO:CD	16:2:212:GLN:N	2.70	0.54
15:1:177:PRO:O	15:1:179:LYS:N	2.41	0.54
15:1:183:LEU:O	15:1:184:LYS:CG	2.55	0.54
15:1:67:LEU:O	15:1:69:LEU:O	2.26	0.54
15:1:68:GLY:O	15:1:73:PRO:HD3	2.07	0.54
18:4:103:MET:HE1	18:4:207:ASN:CB	2.38	0.54
18:4:148:LEU:O	18:4:149:SER:C	2.45	0.54
1:A:618:TRP:CZ2	1:A:655:ASP:CB	2.91	0.54
2:B:225:LEU:O	2:B:230:TRP:NE1	2.40	0.54
2:B:334:LEU:CA	19:B:1202:CLA:HMD3	2.38	0.54
2:B:486:LEU:HD12	2:B:489:GLY:N	2.21	0.54
2:B:625:TRP:CE3	2:B:625:TRP:O	2.59	0.54
22:G:7026:LMU:H51	22:G:7026:LMU:H12	1.89	0.54
8:H:108:THR:OG1	8:H:109:LEU:N	2.38	0.54
12:L:81:TRP:O	12:L:83:LEU:N	2.37	0.54
1:A:25:ASP:OD1	1:A:26:PRO:CG	2.56	0.54
13:N:144:PRO:CG	13:N:158:ASP:O	2.56	0.54
19:K:1142:CLA:OBD	19:K:1143:CLA:CHB	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:K:1146:CLA:C3A	19:K:1146:CLA:O1A	2.56	0.54
2:B:393:PHE:CZ	2:B:398:TYR:HD2	2.24	0.54
1:A:425:THR:OG1	1:A:428:TYR:HE1	1.82	0.54
12:L:172:GLU:O	12:L:173:PRO:O	2.25	0.54
15:1:104:GLY:O	15:1:105:TYR:HB2	2.08	0.54
15:1:71:GLU:CG	15:1:72:VAL:N	2.71	0.54
18:4:193:ASN:O	18:4:194:PHE:CB	2.52	0.54
19:A:1125:CLA:CGD	19:A:1125:CLA:HBA1	2.37	0.54
1:A:394:SER:HB2	19:A:1126:CLA:CMA	2.30	0.54
1:A:398:HIS:CD2	19:A:1126:CLA:ND	2.76	0.54
1:A:402:ILE:HG13	19:A:1127:CLA:CBB	2.33	0.54
1:A:453:LEU:HD21	19:A:1136:CLA:CBB	2.38	0.54
2:B:440:ASN:O	2:B:444:LEU:HD23	2.07	0.54
3:C:79:LEU:CD2	3:C:81:TYR:O	2.56	0.54
6:F:149:ILE:HG22	6:F:150:VAL:N	2.21	0.54
7:G:80:PHE:O	7:G:81:ASN:C	2.44	0.54
7:G:89:LYS:CA	7:G:89:LYS:HE3	2.22	0.54
8:H:97:LEU:HD11	8:H:100:PHE:HB2	1.66	0.54
5:E:118:ASN:OD1	5:E:119:ASN:N	2.41	0.54
13:N:150:LEU:O	13:N:151:ASP:HB2	2.07	0.54
4:D:100:TYR:HD1	4:D:134:LYS:CG	2.18	0.54
4:D:99:PHE:HB3	4:D:157:VAL:CG1	2.38	0.54
4:D:157:VAL:HG13	4:D:158:PHE:O	2.06	0.54
4:D:99:PHE:CB	4:D:157:VAL:CG1	2.84	0.54
6:F:228:ASP:CA	6:F:231:PHE:HB3	2.38	0.54
15:1:171:LEU:N	15:1:173:TYR:CE2	2.76	0.54
2:B:324:ASP:O	2:B:328:ASN:CB	2.54	0.54
18:4:197:THR:OG1	19:4:4001:CLA:HBA2	2.07	0.54
18:4:98:ASN:HB2	18:4:212:LEU:HD21	1.90	0.54
19:A:1104:CLA:H51	19:A:1128:CLA:NC	2.23	0.54
1:A:79:PHE:CE1	19:A:1111:CLA:HED3	2.39	0.54
1:A:119:SER:HA	1:A:145:ILE:HD12	1.90	0.54
1:A:158:ILE:HG12	1:A:159:THR:H	1.68	0.54
1:A:479:ASP:OD1	1:A:536:THR:CG2	2.55	0.54
2:B:343:VAL:CG1	19:B:1223:CLA:H2	2.38	0.54
2:B:55:ALA:HB1	2:B:150:LEU:CD1	2.38	0.54
2:B:255:LEU:H	2:B:271:THR:HG21	1.73	0.54
2:B:269:TRP:HE3	2:B:270:LEU:H	1.55	0.54
2:B:442:VAL:HG21	19:B:1230:CLA:CAC	2.33	0.54
2:B:545:LYS:O	2:B:548:PRO:HD3	2.09	0.54
19:B:1205:CLA:CMC	21:B:6017:BCR:H281	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:89:SER:C	5:E:106:ARG:H	2.07	0.54
15:1:188:ILE:O	15:1:189:LYS:C	2.44	0.54
16:2:254:LEU:HD22	16:2:256:ASP:N	2.23	0.54
16:2:244:THR:O	16:2:246:PRO:C	2.46	0.54
6:F:215:VAL:O	6:F:216:ALA:C	2.45	0.54
22:R:7007:LMU:H71	22:R:7007:LMU:H11	1.90	0.54
1:A:628:ILE:CG1	1:A:629:ASN:N	2.70	0.54
15:1:114:TRP:CH2	15:1:121:GLN:CA	2.89	0.54
1:A:29:THR:OG1	1:A:31:PHE:N	2.40	0.54
13:N:93:GLU:HG2	13:N:94:LYS:N	2.23	0.54
1:A:155:ALA:O	1:A:156:SER:C	2.40	0.54
18:4:124:PRO:O	18:4:125:LYS:HG3	2.08	0.53
18:4:226:LYS:H	18:4:226:LYS:HD3	1.57	0.53
18:4:217:PHE:CD1	18:4:221:HIS:ND1	2.76	0.53
2:B:212:PHE:HZ	19:B:1211:CLA:HHD	1.73	0.53
19:B:1216:CLA:C3	19:B:1221:CLA:H92	2.38	0.53
2:B:462:TRP:CH2	19:B:1231:CLA:HBC1	2.43	0.53
2:B:509:PHE:CD2	2:B:509:PHE:N	2.76	0.53
16:2:215:LYS:HA	16:2:217:LEU:HD23	1.89	0.53
16:2:218:ARG:CB	16:2:219:THR:HG22	2.28	0.53
5:E:79:LYS:CB	5:E:84:TYR:HE1	2.19	0.53
8:H:64:GLN:C	8:H:66:ASP:HA	2.29	0.53
13:N:132:THR:CA	13:N:137:LEU:O	2.56	0.53
13:N:150:LEU:CB	13:N:152:LEU:HD23	2.38	0.53
17:3:232:ARG:HA	17:3:235:MET:HB2	1.90	0.53
1:A:249:ILE:CG2	17:3:137:PHE:CE2	2.92	0.53
1:A:252:ARG:N	1:A:252:ARG:CD	2.52	0.53
16:2:172:LEU:C	16:2:174:PRO:HD3	2.26	0.53
16:2:254:LEU:CD2	16:2:256:ASP:H	2.20	0.53
2:B:135:LEU:O	2:B:135:LEU:HG	2.07	0.53
12:L:51:LYS:HD2	12:L:51:LYS:N	2.23	0.53
1:A:274:TRP:HB3	1:A:277:TYR:H	1.73	0.53
15:1:123:THR:O	15:1:124:TYR:HB2	2.08	0.53
15:1:66:PRO:O	15:1:69:LEU:C	2.46	0.53
15:1:77:GLU:CD	15:1:80:LYS:HE3	2.28	0.53
18:4:209:ARG:HG2	18:4:210:LEU:N	2.15	0.53
18:4:209:ARG:O	18:4:212:LEU:N	2.41	0.53
19:A:1137:CLA:CMC	19:A:1137:CLA:HBC3	2.34	0.53
1:A:453:LEU:HD23	19:A:1136:CLA:CBB	2.37	0.53
1:A:62:HIS:CE1	19:A:1128:CLA:CGA	2.92	0.53
1:A:64:PHE:HE2	1:A:74:ILE:CG2	2.12	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:278:LEU:HG	19:B:1213:CLA:CMA	2.38	0.53
2:B:304:ILE:O	2:B:308:HIS:CB	2.52	0.53
2:B:391:PRO:HB3	2:B:538:ALA:CA	2.30	0.53
2:B:469:LYS:HE3	2:B:470:THR:CG2	2.34	0.53
4:D:87:THR:N	12:L:69:LEU:HD11	2.22	0.53
8:H:98:LEU:O	8:H:102:ILE:HG13	2.08	0.53
19:3:2009:CLA:CBA	19:3:2009:CLA:CBD	2.85	0.53
5:E:84:TYR:HD2	5:E:85:LYS:HG3	1.72	0.53
4:D:158:PHE:CB	4:D:159:PRO:O	2.46	0.53
16:2:164:GLU:HA	16:2:167:ARG:NH1	2.22	0.53
2:B:247:THR:HG22	2:B:248:GLN:N	2.15	0.53
1:A:23:ASP:OD2	1:A:24:ARG:CZ	2.56	0.53
18:4:198:LEU:O	18:4:199:GLU:C	2.46	0.53
18:4:131:LYS:HG2	18:4:131:LYS:O	2.08	0.53
18:4:142:PHE:HA	18:4:145:GLU:CG	2.38	0.53
18:4:165:SER:O	18:4:166:VAL:C	2.45	0.53
1:A:534:LEU:HD12	1:A:534:LEU:C	2.17	0.53
1:A:462:ILE:CD1	19:A:9022:CLA:H72	2.38	0.53
19:B:1220:CLA:HMD2	19:B:1221:CLA:HBB1	1.88	0.53
2:B:196:HIS:CE1	19:B:1212:CLA:ND	2.75	0.53
2:B:223:GLY:O	2:B:224:PRO:C	2.45	0.53
2:B:353:TYR:C	2:B:355:LEU:N	2.61	0.53
2:B:625:TRP:CD2	2:B:625:TRP:O	2.61	0.53
2:B:551:LYS:NZ	4:D:194:ASN:O	2.34	0.53
3:C:62:PHE:CD1	5:E:80:GLU:HB3	2.43	0.53
22:3:7005:LMU:O2B	22:3:7005:LMU:H5'	2.09	0.53
11:K:113:GLY:O	11:K:116:ILE:CG2	2.34	0.53
6:F:227:VAL:HG23	6:F:228:ASP:N	2.23	0.53
19:1:1303:CLA:HBC2	19:4:1304:CLA:HMB3	1.88	0.53
16:2:266:PHE:CE2	16:2:267:THR:O	2.62	0.53
13:N:90:GLU:OE1	13:N:91:TYR:CZ	2.61	0.53
15:1:183:LEU:C	15:1:184:LYS:CG	2.69	0.53
15:1:81:GLU:HG2	15:1:82:SER:N	2.22	0.53
18:4:215:LEU:O	18:4:217:PHE:N	2.41	0.53
19:A:1107:CLA:HBB2	19:B:1230:CLA:HMD1	1.86	0.53
1:A:328:LYS:O	1:A:329:ASP:C	2.46	0.53
1:A:431:LEU:H	1:A:434:ARG:NE	2.06	0.53
1:A:534:LEU:HB2	1:A:538:ASP:CB	2.39	0.53
2:B:65:LEU:HD22	2:B:124:TRP:HE3	1.72	0.53
1:A:696:GLY:HA3	2:B:569:ASP:HB2	1.89	0.53
16:2:125:PHE:O	16:2:127:THR:CG2	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:228:ALA:O	16:2:229:MET:C	2.44	0.53
3:C:65:VAL:H	3:C:66:ARG:HH22	1.57	0.53
3:C:65:VAL:N	3:C:66:ARG:HH22	2.06	0.53
4:D:156:ARG:HB2	4:D:166:LEU:HD11	1.89	0.53
22:2:7006:LMU:H3'	22:2:7006:LMU:O6B	2.08	0.53
4:D:80:SER:HB2	4:D:127:ASN:HA	1.90	0.53
13:N:99:LYS:HB2	13:N:102:ASN:ND2	2.24	0.53
17:3:156:THR:O	17:3:157:LEU:C	2.46	0.53
22:R:7021:LMU:H41	22:R:7021:LMU:C6'	2.38	0.53
2:B:482:ASN:O	2:B:484:PRO:HD2	2.08	0.53
11:K:108:ALA:O	11:K:109:CYS:C	2.45	0.53
2:B:367:THR:O	2:B:367:THR:CG2	2.56	0.53
2:B:66:PHE:CG	2:B:66:PHE:O	2.60	0.53
1:A:79:PHE:CE2	1:A:185:HIS:NE2	2.76	0.53
1:A:466:THR:O	1:A:470:LEU:HG	2.08	0.53
1:A:703:LEU:O	1:A:707:ILE:HG12	2.08	0.53
2:B:459:PHE:N	19:B:1235:CLA:CAD	2.71	0.53
2:B:316:GLY:O	2:B:317:ARG:NE	2.41	0.53
2:B:508:LEU:HB3	2:B:509:PHE:CE2	2.42	0.53
2:B:509:PHE:N	2:B:509:PHE:HD2	2.06	0.53
3:C:2:SER:O	3:C:3:HIS:ND1	2.42	0.53
6:F:203:ALA:O	6:F:205:SER:N	2.42	0.53
12:L:190:PHE:CE2	12:L:194:ILE:HD12	2.44	0.53
8:H:58:LEU:CB	8:H:61:THR:CB	2.60	0.53
13:N:148:ASP:CA	13:N:149:ASP:C	2.77	0.53
13:N:143:VAL:O	13:N:151:ASP:OD1	2.26	0.53
16:2:168:TRP:CD1	16:2:171:ILE:HD13	2.43	0.53
17:3:132:THR:HG23	17:3:133:ALA:N	2.23	0.53
17:3:156:THR:O	17:3:156:THR:HG22	2.06	0.53
1:A:624:VAL:HG12	1:A:625:TRP:N	2.22	0.53
15:1:199:VAL:HG13	15:1:200:GLY:N	2.23	0.53
1:A:628:ILE:CD1	1:A:629:ASN:N	2.71	0.53
6:F:176:TRP:CZ3	6:F:217:ALA:HB2	2.43	0.53
13:N:126:LYS:HD2	13:N:127:PHE:HD2	1.74	0.53
1:A:482:ILE:O	1:A:482:ILE:CG2	2.55	0.53
15:1:176:ASP:C	15:1:180:LEU:HG	2.29	0.53
18:4:217:PHE:CE1	18:4:221:HIS:ND1	2.77	0.53
19:A:1106:CLA:CMB	19:A:1107:CLA:H11	2.36	0.53
19:A:1119:CLA:C2C	19:A:1125:CLA:H172	2.38	0.53
1:A:281:LEU:HD12	1:A:282:THR:HG23	1.91	0.53
1:A:362:LEU:HB3	1:A:406:LEU:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:ILE:HG22	1:A:711:HIS:CD2	2.41	0.53
19:A:9012:CLA:NB	19:A:9013:CLA:HBB2	2.24	0.53
19:B:1216:CLA:HBD	19:B:1216:CLA:HBA1	1.90	0.53
19:B:1222:CLA:CMB	21:B:6010:BCR:H352	2.39	0.53
2:B:464:GLN:HG3	2:B:464:GLN:O	2.01	0.53
2:B:574:ASP:O	2:B:578:LEU:HG	2.08	0.53
1:A:466:THR:HG22	2:B:648:TRP:HE1	1.72	0.53
7:G:123:ASN:O	7:G:126:ASP:OD2	2.27	0.53
19:A:1126:CLA:C17	21:J:6012:BCR:H17C	2.36	0.53
12:L:109:LEU:O	12:L:110:LEU:C	2.47	0.53
12:L:141:LEU:HD11	12:L:145:LEU:HD11	1.90	0.53
6:F:192:THR:O	6:F:193:GLN:CG	2.56	0.53
12:L:205:TYR:CD2	12:L:205:TYR:O	2.62	0.53
8:H:77:ASN:ND2	8:H:78:PRO:O	2.42	0.53
8:H:119:ASP:OD2	8:H:121:LEU:CG	2.50	0.53
6:F:228:ASP:O	6:F:231:PHE:HD1	1.90	0.53
15:1:199:VAL:O	15:1:200:GLY:C	2.47	0.53
15:1:199:VAL:O	15:1:201:PHE:N	2.41	0.53
17:3:88:GLY:O	17:3:89:THR:C	2.47	0.53
22:H:7028:LMU:O6'	22:H:7028:LMU:H1'	2.09	0.53
15:1:177:PRO:HD3	15:1:180:LEU:HD21	1.85	0.53
19:A:1106:CLA:H93	21:J:6012:BCR:H311	1.89	0.53
1:A:307:ALA:O	1:A:308:ILE:C	2.48	0.53
1:A:449:VAL:HG22	19:A:1137:CLA:HMC3	1.90	0.53
1:A:472:ARG:N	1:A:473:PRO:HD2	2.22	0.53
21:A:6002:BCR:C40	21:A:6002:BCR:C23	2.87	0.53
2:B:411:MET:HE2	19:B:1220:CLA:CMC	2.39	0.53
19:B:1235:CLA:H61	21:F:6016:BCR:H323	1.91	0.53
19:B:1239:CLA:H51	20:B:5002:PQN:H251	1.90	0.53
2:B:278:LEU:O	2:B:281:ALA:N	2.42	0.53
2:B:292:ARG:NH2	2:B:297:ILE:CA	2.71	0.53
19:A:1131:CLA:H152	21:L:6019:BCR:C36	2.39	0.53
16:2:118:ALA:C	16:2:121:PHE:CD2	2.75	0.53
3:C:12:ILE:CB	3:C:38:GLN:O	2.56	0.53
4:D:100:TYR:CD1	4:D:134:LYS:HG2	2.42	0.53
16:2:156:GLU:HG3	16:2:157:LEU:CD1	2.36	0.53
17:3:150:TYR:N	17:3:152:ALA:CB	2.32	0.53
14:R:26:UNK:O	14:R:28:UNK:CA	2.57	0.53
22:B:7038:LMU:H61	22:B:7038:LMU:H101	1.91	0.53
12:L:63:ASP:OD1	12:L:63:ASP:O	2.26	0.53
15:1:176:ASP:CB	15:1:180:LEU:CD1	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:HIS:CE1	19:A:1113:CLA:NC	2.77	0.53
19:A:1122:CLA:CBB	21:A:6007:BCR:H353	2.36	0.53
1:A:492:ILE:CD1	19:A:1133:CLA:C2C	2.85	0.53
1:A:209:GLY:HA2	1:A:213:LEU:CD1	2.38	0.53
19:A:1125:CLA:HMA2	21:A:6008:BCR:H10C	1.90	0.53
1:A:750:PHE:O	1:A:752:ALA:N	2.41	0.53
19:B:1220:CLA:C9	19:B:1227:CLA:HBC2	2.39	0.53
6:F:160:PHE:O	6:F:164:GLY:N	2.42	0.53
7:G:98:THR:HB	7:G:101:GLU:OE2	1.81	0.53
12:L:98:ARG:O	12:L:102:VAL:HG23	2.07	0.53
16:2:126:LEU:O	16:2:129:LEU:N	2.41	0.53
5:E:100:ARG:O	5:E:121:ALA:CB	2.57	0.53
13:N:130:ASN:HB2	13:N:132:THR:HG21	1.91	0.53
19:1:1014:CLA:H101	19:1:1014:CLA:H52	1.79	0.53
4:D:140:LEU:HD12	4:D:144:LEU:H	1.74	0.53
16:2:240:ILE:CG2	16:2:263:PHE:CB	2.65	0.53
17:3:155:TYR:C	17:3:157:LEU:H	2.12	0.53
16:2:137:TRP:O	16:2:137:TRP:CD1	2.62	0.53
22:4:7053:LMU:O2B	22:4:7053:LMU:H5B	2.08	0.53
15:1:101:GLU:O	15:1:101:GLU:CG	2.54	0.53
2:B:364:ASP:OD2	2:B:367:THR:HB	2.08	0.53
2:B:367:THR:O	2:B:367:THR:HG22	2.08	0.53
15:1:81:GLU:O	15:1:82:SER:C	2.46	0.53
19:4:1004:CLA:H2A	19:4:1004:CLA:O1D	2.08	0.53
18:4:150:HIS:CE1	18:4:154:ILE:HD11	2.43	0.53
19:A:1131:CLA:H11	19:A:1237:CLA:H43	1.90	0.53
1:A:284:ARG:NE	1:A:284:ARG:O	2.42	0.53
1:A:612:VAL:O	1:A:615:HIS:HB3	2.09	0.53
2:B:282:PHE:HE2	19:B:1213:CLA:H3A	1.74	0.53
2:B:232:LEU:CD1	2:B:235:GLN:CB	2.86	0.53
2:B:298:GLY:H	19:B:1218:CLA:HMD3	1.73	0.53
2:B:311:PRO:HG3	19:B:1301:CLA:NC	2.24	0.53
2:B:312:GLY:HA3	2:B:315:LEU:HB3	1.87	0.53
2:B:440:ASN:CG	2:B:614:THR:HG23	2.29	0.53
2:B:469:LYS:C	2:B:470:THR:OG1	2.47	0.53
2:B:595:HIS:CE1	2:B:599:ILE:HD11	2.43	0.53
2:B:622:ASP:HB3	2:B:626:LEU:HD11	1.91	0.53
6:F:181:TYR:CD2	6:F:181:TYR:O	2.61	0.53
19:A:1126:CLA:C17	21:J:6012:BCR:H15C	2.39	0.53
16:2:128:LYS:O	16:2:131:ILE:HA	2.08	0.53
19:2:2007:CLA:C1B	19:2:2007:CLA:H2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:78:ARG:HB2	5:E:80:GLU:CD	2.29	0.53
17:3:104:ILE:HG21	19:3:3004:CLA:C3D	2.39	0.53
19:L:1148:CLA:O2D	19:L:1148:CLA:CAA	2.52	0.53
16:2:237:PHE:O	16:2:237:PHE:CD1	2.57	0.53
1:A:32:GLU:OE1	1:A:33:GLN:N	2.38	0.53
16:2:246:PRO:HB2	16:2:247:ILE:CD1	2.36	0.53
15:1:77:GLU:C	15:1:80:LYS:CG	2.77	0.53
18:4:220:GLN:NE2	19:4:1306:CLA:CAC	2.72	0.53
1:A:302:HIS:HE1	19:A:1117:CLA:CHB	2.22	0.53
1:A:157:GLY:C	1:A:229:ILE:HG21	2.28	0.53
1:A:346:LEU:O	1:A:346:LEU:CD2	2.56	0.53
1:A:415:ALA:HB2	1:A:560:VAL:HG12	1.91	0.53
1:A:435:VAL:HA	1:A:438:HIS:CE1	2.44	0.53
1:A:443:ILE:HG22	2:B:674:LEU:CD1	2.39	0.53
2:B:486:LEU:HD13	19:B:1232:CLA:HMD1	1.89	0.53
2:B:120:VAL:CB	2:B:123:TRP:HE1	2.21	0.53
2:B:310:PRO:CD	2:B:311:PRO:CD	2.87	0.53
2:B:330:ILE:CD1	19:B:1202:CLA:C19	2.86	0.53
2:B:325:THR:HG21	2:B:403:ASN:HD21	1.74	0.53
2:B:577:TYR:CE2	2:B:578:LEU:HD23	2.45	0.53
19:A:9023:CLA:H111	21:B:6017:BCR:C35	2.39	0.53
2:B:580:VAL:CG1	2:B:710:LEU:HD21	2.39	0.53
9:I:20:ALA:O	9:I:24:LEU:HB3	2.08	0.53
5:E:75:LYS:CA	5:E:87:THR:HG22	2.31	0.53
5:E:89:SER:O	5:E:105:VAL:CB	2.56	0.53
15:1:134:LEU:O	15:1:137:ILE:HG12	2.09	0.53
16:2:184:PRO:HD2	16:2:186:ASN:N	2.22	0.53
17:3:150:TYR:CG	17:3:151:TRP:N	2.77	0.53
6:F:228:ASP:O	6:F:231:PHE:CD1	2.62	0.53
22:E:7048:LMU:O5'	22:E:7048:LMU:C2	2.57	0.53
2:B:609:PHE:O	2:B:613:SER:N	2.36	0.53
4:D:129:LEU:CD1	12:L:65:PHE:CD1	2.92	0.53
1:A:464:ASN:ND2	1:A:464:ASN:H	2.07	0.53
2:B:66:PHE:O	2:B:66:PHE:CD2	2.61	0.53
18:4:193:ASN:C	18:4:201:LYS:NZ	2.62	0.52
1:A:106:TYR:O	1:A:107:GLU:C	2.43	0.52
19:A:1124:CLA:HED3	19:A:1125:CLA:CMD	2.30	0.52
1:A:479:ASP:CG	1:A:536:THR:HG22	2.29	0.52
19:B:1203:CLA:H161	19:B:1203:CLA:H91	1.91	0.52
19:B:1216:CLA:OBD	19:B:1219:CLA:CBC	2.57	0.52
2:B:127:ILE:HD13	2:B:193:HIS:HE1	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:244:PHE:CD2	2:B:245:GLY:N	2.77	0.52
2:B:294:ASN:ND2	7:G:94:GLN:CB	2.46	0.52
2:B:347:LEU:CD2	2:B:351:HIS:CE1	2.92	0.52
2:B:353:TYR:O	2:B:355:LEU:N	2.41	0.52
2:B:687:LEU:HD12	21:B:6020:BCR:HC31	1.91	0.52
2:B:708:VAL:O	2:B:710:LEU:O	2.27	0.52
12:L:143:LEU:H	12:L:145:LEU:N	2.05	0.52
16:2:101:TRP:H	16:2:103:VAL:CG1	2.21	0.52
1:A:582:ASP:HB3	1:A:589:THR:CG2	2.38	0.52
4:D:167:HIS:H	4:D:168:PRO:CD	2.21	0.52
14:R:32:UNK:CB	14:R:33:UNK:CA	2.76	0.52
6:F:228:ASP:OD2	6:F:231:PHE:CG	2.63	0.52
4:D:133:ARG:H	4:D:136:GLN:HE21	1.53	0.52
22:1:7004:LMU:O2'	22:1:7004:LMU:C1	2.50	0.52
22:1:7004:LMU:C1B	22:1:7004:LMU:O6B	2.55	0.52
4:D:205:LYS:N	4:D:205:LYS:HE2	2.24	0.52
15:1:65:ASP:OD2	15:1:66:PRO:HA	2.08	0.52
18:4:93:GLN:CD	18:4:170:PRO:HB2	2.30	0.52
18:4:174:GLN:HB3	18:4:195:ALA:HA	1.92	0.52
18:4:195:ALA:CB	18:4:197:THR:O	2.55	0.52
1:A:746:THR:O	1:A:750:PHE:N	2.36	0.52
19:A:9012:CLA:HED1	19:B:9010:CLA:H61	1.90	0.52
2:B:414:HIS:HD2	19:B:1227:CLA:HMA3	1.71	0.52
19:B:1231:CLA:ND	19:B:1232:CLA:HBB1	2.24	0.52
2:B:429:LEU:HD11	19:B:1235:CLA:CMB	2.39	0.52
2:B:486:LEU:HB2	19:B:1232:CLA:CMD	2.28	0.52
2:B:569:ASP:OD1	2:B:706:ARG:NE	2.42	0.52
2:B:608:GLN:O	2:B:612:SER:HB2	2.08	0.52
7:G:136:VAL:O	7:G:137:VAL:HG22	2.09	0.52
7:G:84:ARG:CG	7:G:85:GLU:H	2.13	0.52
11:K:62:SER:O	11:K:63:LEU:C	2.46	0.52
11:K:62:SER:HG	11:K:63:LEU:CD1	2.21	0.52
12:L:73:VAL:HA	19:L:1504:CLA:HMA1	1.85	0.52
13:N:133:GLY:CA	13:N:134:CYS:O	2.54	0.52
13:N:143:VAL:CG1	13:N:144:PRO:HD2	2.39	0.52
13:N:150:LEU:HD13	13:N:150:LEU:N	2.25	0.52
13:N:152:LEU:CA	13:N:153:GLU:HG3	2.39	0.52
16:2:176:CYS:H	16:2:188:LEU:HB2	1.73	0.52
22:3:7005:LMU:C1B	22:3:7005:LMU:O3'	2.57	0.52
12:L:205:TYR:HD1	12:L:207:LEU:CD1	1.90	0.52
19:J:1308:CLA:H2A	19:J:1308:CLA:C2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:214:PRO:C	6:F:215:VAL:HG23	2.30	0.52
12:L:55:GLN:O	12:L:57:ILE:HG13	2.08	0.52
4:D:129:LEU:HD13	12:L:65:PHE:CZ	2.44	0.52
17:3:225:LEU:HD13	17:3:228:VAL:CG2	2.38	0.52
15:1:69:LEU:C	15:1:73:PRO:CD	2.72	0.52
19:A:1105:CLA:C4B	21:J:6012:BCR:C33	2.86	0.52
19:A:1117:CLA:H93	19:A:1117:CLA:H193	1.91	0.52
19:A:1126:CLA:CGA	19:A:1126:CLA:H43	2.39	0.52
1:A:309:LEU:O	1:A:310:PHE:CB	2.56	0.52
1:A:690:LEU:CD2	2:B:661:PHE:HE1	2.21	0.52
19:A:9023:CLA:HMB3	19:B:1239:CLA:HMC3	1.92	0.52
19:B:1226:CLA:HBC2	19:B:1226:CLA:CMC	2.36	0.52
19:B:1227:CLA:HMB2	19:B:1228:CLA:C4A	2.39	0.52
2:B:376:GLN:HB3	2:B:587:ILE:HD12	1.92	0.52
7:G:125:VAL:HG13	7:G:129:ALA:HB2	1.88	0.52
7:G:60:SER:OG	7:G:61:ALA:N	2.42	0.52
7:G:72:LEU:CD1	7:G:73:PHE:CZ	2.93	0.52
2:B:297:ILE:HG21	7:G:77:PHE:HZ	1.73	0.52
12:L:102:VAL:HA	19:L:1502:CLA:HED1	1.89	0.52
16:2:113:ALA:HB1	16:2:114:MET:CE	2.38	0.52
16:2:133:ASN:HD21	16:2:134:THR:HB	1.57	0.52
13:N:136:ASP:OD1	13:N:137:LEU:O	2.28	0.52
3:C:26:LEU:HD22	4:D:181:ARG:NH1	2.23	0.52
17:3:233:LEU:O	17:3:236:LEU:N	2.43	0.52
13:N:114:PHE:O	13:N:118:TYR:N	2.42	0.52
19:K:1143:CLA:CGA	19:K:1143:CLA:C3A	2.85	0.52
6:F:132:ASN:C	6:F:133:TYR:CD1	2.74	0.52
19:J:1308:CLA:CBA	19:J:1308:CLA:CBF	2.83	0.52
19:4:1304:CLA:CAA	19:4:1304:CLA:CGD	2.87	0.52
10:J:37:LEU:C	10:J:38:ILE:HG13	2.25	0.52
4:D:148:TYR:O	4:D:149:LYS:CB	2.56	0.52
1:A:205:HIS:CE1	19:A:1111:CLA:HMC2	2.44	0.52
19:A:1135:CLA:HBA2	19:A:1135:CLA:O1D	2.09	0.52
1:A:458:PHE:CD2	19:A:9022:CLA:CMB	2.92	0.52
19:B:1222:CLA:HBB2	19:B:1236:CLA:HMB3	1.91	0.52
2:B:221:GLY:O	2:B:222:LEU:C	2.46	0.52
2:B:42:LEU:O	2:B:43:TYR:C	2.47	0.52
2:B:444:LEU:C	2:B:446:PHE:H	2.11	0.52
2:B:624:LEU:CD2	19:B:9010:CLA:H93	2.40	0.52
2:B:668:ARG:HH12	2:B:672:GLN:HG2	1.73	0.52
2:B:574:ASP:OD2	2:B:706:ARG:NE	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:85:GLU:HG3	7:G:86:ASN:N	2.24	0.52
16:2:114:MET:N	16:2:114:MET:HE3	2.25	0.52
6:F:190:LYS:CG	6:F:192:THR:CG2	2.88	0.52
1:A:252:ARG:NH2	1:A:252:ARG:O	2.42	0.52
8:H:116:ALA:CB	8:H:117:SER:CA	2.85	0.52
2:B:673:GLU:O	2:B:676:GLU:HB2	2.09	0.52
2:B:715:VAL:O	2:B:716:GLY:C	2.48	0.52
17:3:213:PHE:HB2	17:3:215:LYS:N	2.24	0.52
1:A:592:VAL:HG23	1:A:593:SER:N	2.25	0.52
19:H:1505:CLA:H42	19:H:1505:CLA:HAA1	1.92	0.52
18:4:174:GLN:HA	18:4:176:SER:H	1.74	0.52
18:4:177:LEU:HD22	18:4:178:PRO:CA	2.40	0.52
1:A:365:LEU:HD22	19:A:1103:CLA:HED3	1.87	0.52
1:A:240:LYS:HD2	1:A:240:LYS:O	2.10	0.52
1:A:245:PRO:C	1:A:248:PHE:CE2	2.82	0.52
1:A:607:ASN:ND2	19:A:9022:CLA:C2C	2.73	0.52
1:A:599:PHE:CE2	1:A:735:VAL:HG21	2.45	0.52
19:A:9012:CLA:HBB2	19:A:9013:CLA:C1B	2.39	0.52
2:B:183:PHE:HB3	2:B:284:PHE:HD2	1.74	0.52
2:B:350:GLN:O	2:B:353:TYR:CD1	2.62	0.52
2:B:353:TYR:O	2:B:354:SER:CB	2.47	0.52
2:B:662:MET:HE2	20:B:5002:PQN:H2M3	1.92	0.52
5:E:91:VAL:HB	5:E:104:VAL:CG1	2.40	0.52
7:G:69:GLY:HA2	7:G:72:LEU:CG	2.38	0.52
19:I:1204:CLA:C14	21:I:6018:BCR:H392	2.37	0.52
12:L:194:ILE:O	12:L:195:SER:CB	2.58	0.52
16:2:103:VAL:C	16:2:105:ALA:H	2.13	0.52
16:2:113:ALA:CB	16:2:114:MET:CE	2.87	0.52
8:H:67:SER:O	8:H:68:TYR:CD1	2.62	0.52
13:N:123:GLY:CA	13:N:131:PHE:HD1	2.22	0.52
13:N:147:SER:O	13:N:148:ASP:HB2	2.10	0.52
19:L:1148:CLA:CGA	19:L:1148:CLA:O2D	2.57	0.52
4:D:100:TYR:HD1	4:D:134:LYS:HG3	1.64	0.52
12:L:205:TYR:CG	12:L:207:LEU:HD12	2.36	0.52
19:3:3008:CLA:O2A	19:3:3008:CLA:H2A	2.09	0.52
19:1:1303:CLA:CMC	19:1:1303:CLA:HBC2	2.18	0.52
2:B:135:LEU:O	2:B:135:LEU:CD1	2.57	0.52
18:4:241:HIS:CE1	18:4:242:ASN:OD1	2.62	0.52
15:1:163:TYR:N	15:1:164:PRO:HD3	2.23	0.52
12:L:51:LYS:HZ3	12:L:51:LYS:HB3	1.73	0.52
3:C:36:ALA:O	3:C:37:LYS:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1149:CLA:HBC2	19:A:1149:CLA:CMC	2.33	0.52
2:B:465:SER:O	2:B:466:ALA:C	2.44	0.52
18:4:174:GLN:O	18:4:175:TYR:CB	2.58	0.52
1:A:553:VAL:HG23	19:A:1124:CLA:HMC2	1.91	0.52
2:B:272:ASP:C	2:B:274:ALA:H	2.13	0.52
2:B:443:MET:HG2	2:B:451:LYS:O	2.10	0.52
2:B:510:LEU:C	2:B:510:LEU:HD12	2.29	0.52
19:A:9012:CLA:H12	2:B:616:LEU:CD1	2.32	0.52
2:B:694:ARG:CD	9:I:28:VAL:CG1	2.87	0.52
19:H:1241:CLA:HAC1	21:I:6021:BCR:HC32	1.90	0.52
12:L:76:SER:O	12:L:79:ILE:N	2.42	0.52
19:2:2004:CLA:O1A	19:3:2009:CLA:HBC3	2.10	0.52
19:3:2009:CLA:C5	19:3:2009:CLA:C9	2.26	0.52
3:C:12:ILE:CB	3:C:39:ILE:HA	2.39	0.52
5:E:127:GLU:CG	5:E:129:GLU:O	2.57	0.52
17:3:103:VAL:HG11	17:3:229:LYS:CG	2.39	0.52
17:3:109:ALA:HA	17:3:111:LEU:CD1	2.39	0.52
1:A:49:ASP:OD2	1:A:49:ASP:N	2.41	0.52
19:3:3008:CLA:HBC2	19:3:3008:CLA:CMC	2.19	0.52
22:F:7036:LMU:C4'	22:F:7036:LMU:O2B	2.58	0.52
1:A:629:ASN:OD1	1:A:630:ASP:N	2.43	0.52
1:A:39:HIS:ND1	1:A:39:HIS:O	2.43	0.52
16:2:155:VAL:HA	16:2:158:VAL:CG1	2.40	0.52
1:A:396:PHE:O	1:A:396:PHE:CG	2.62	0.52
1:A:63:ASP:CG	1:A:65:ASP:H	2.13	0.52
2:B:224:PRO:HG3	7:G:153:PHE:CB	2.40	0.52
2:B:323:TYR:CE1	19:B:1221:CLA:HBC1	2.45	0.52
19:A:9022:CLA:H151	21:B:6017:BCR:H19C	1.92	0.52
1:A:587:GLY:HA3	2:B:668:ARG:CZ	2.40	0.52
10:J:26:LEU:H	10:J:28:GLU:H	1.56	0.52
12:L:93:VAL:HG12	12:L:94:SER:O	2.10	0.52
13:N:157:LYS:HG2	13:N:159:LYS:HG3	1.92	0.52
14:R:39:UNK:CA	14:R:41:UNK:CB	2.88	0.52
15:1:149:GLU:HG2	15:1:152:ARG:HH11	1.61	0.52
19:3:3008:CLA:CED	19:3:3008:CLA:O1A	2.58	0.52
15:1:171:LEU:CB	15:1:173:TYR:CZ	2.93	0.52
17:3:155:TYR:C	17:3:157:LEU:N	2.62	0.52
18:4:112:PRO:CB	18:4:116:THR:O	2.57	0.52
18:4:131:LYS:CG	18:4:131:LYS:O	2.57	0.52
1:A:100:GLY:HA3	1:A:153:TRP:HH2	1.75	0.52
1:A:218:TRP:CZ3	19:A:1112:CLA:HMB3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:VAL:HA	1:A:438:HIS:HE1	1.75	0.52
1:A:692:PHE:CD2	1:A:733:VAL:HG12	2.45	0.52
1:A:711:HIS:CD2	19:A:1139:CLA:CBC	2.84	0.52
1:A:73:GLU:HG3	1:A:74:ILE:CA	2.40	0.52
19:A:9012:CLA:H11	2:B:616:LEU:HB2	1.92	0.52
19:A:9011:CLA:H192	19:A:9022:CLA:C2B	2.39	0.52
2:B:334:LEU:CB	19:B:1202:CLA:HMD3	2.38	0.52
19:B:1221:CLA:CMA	19:B:1221:CLA:H61	2.40	0.52
2:B:186:SER:C	2:B:187:SER:O	2.48	0.52
2:B:25:ILE:O	2:B:26:ALA:HB3	2.08	0.52
2:B:278:LEU:HD21	19:B:1213:CLA:CGA	2.40	0.52
2:B:463:ILE:O	2:B:464:GLN:HB3	2.08	0.52
10:J:9:SER:O	10:J:10:VAL:CB	2.57	0.52
13:N:165:ASN:OD1	13:N:167:PHE:N	2.42	0.52
3:C:43:PRO:HA	4:D:182:GLN:HG3	1.92	0.52
3:C:44:ARG:NH2	4:D:181:ARG:NE	2.49	0.52
3:C:5:VAL:HG23	3:C:65:VAL:HG21	1.91	0.52
6:F:193:GLN:CA	6:F:195:GLU:OE1	2.57	0.52
16:2:182:ILE:CA	16:2:187:LYS:CG	2.87	0.52
17:3:148:TYR:CD2	17:3:148:TYR:C	2.78	0.52
2:B:393:PHE:CE2	2:B:398:TYR:HD2	2.27	0.52
2:B:135:LEU:O	2:B:135:LEU:CG	2.58	0.52
12:L:104:LEU:HD12	12:L:196:GLY:CA	2.38	0.52
2:B:609:PHE:O	2:B:613:SER:OG	2.27	0.52
15:1:78:ARG:CG	19:1:1011:CLA:HMC1	2.40	0.52
18:4:93:GLN:HE22	18:4:171:ILE:HG12	1.75	0.52
1:A:379:MET:HE1	19:A:1125:CLA:HMC2	1.90	0.52
19:A:1137:CLA:CHA	19:A:1137:CLA:HBA2	2.39	0.52
1:A:181:ALA:HB2	19:A:1108:CLA:HBC2	1.92	0.52
1:A:246:HIS:C	1:A:248:PHE:CE2	2.83	0.52
1:A:373:ALA:HB1	1:A:396:PHE:HD1	1.75	0.52
1:A:553:VAL:HG22	21:A:6008:BCR:H401	1.91	0.52
1:A:595:TRP:HE3	1:A:596:ASP:OD2	1.92	0.52
2:B:123:TRP:HB2	2:B:126:THR:HG21	1.82	0.52
2:B:363:GLN:HG3	2:B:363:GLN:O	2.09	0.52
2:B:387:PHE:HE2	19:B:1222:CLA:HHC	1.75	0.52
19:A:1237:CLA:H152	21:B:6020:BCR:C35	2.40	0.52
2:B:694:ARG:CG	2:B:694:ARG:NH2	2.47	0.52
19:F:1305:CLA:HED2	19:F:1305:CLA:OBD	2.09	0.52
13:N:136:ASP:N	13:N:136:ASP:OD1	2.43	0.52
1:A:574:ASN:OD1	1:A:574:ASN:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:636:THR:HG23	2:B:636:THR:O	2.08	0.52
22:3:7003:LMU:O4'	22:3:7005:LMU:C4B	2.56	0.52
11:K:122:LEU:HD22	11:K:122:LEU:C	2.30	0.52
18:4:139:SER:O	18:4:141:LEU:HD22	2.09	0.52
2:B:110:LEU:HD12	2:B:111:GLY:HA2	1.88	0.52
2:B:211:ASN:CB	2:B:214:ASP:HB3	2.39	0.52
19:1:1008:CLA:HAA2	19:1:1008:CLA:CB	2.40	0.52
19:R:1144:CLA:CED	19:R:1144:CLA:C1A	2.83	0.52
2:B:44:GLN:OE1	2:B:163:PRO:CB	2.57	0.52
22:K:7042:LMU:H71	22:K:7042:LMU:H22	1.92	0.52
12:L:161:ALA:H	12:L:162:PRO:HD2	1.72	0.52
1:A:176:GLY:O	1:A:180:PHE:HB2	2.10	0.52
15:1:77:GLU:CD	15:1:80:LYS:CE	2.78	0.52
1:A:130:GLU:O	1:A:130:GLU:CD	2.48	0.52
1:A:157:GLY:CA	1:A:229:ILE:HG22	2.25	0.52
1:A:51:THR:HG23	1:A:52:THR:N	2.25	0.52
1:A:664:VAL:CG2	1:A:665:ILE:HG23	2.40	0.52
1:A:733:VAL:HG21	19:A:1140:CLA:C3D	2.40	0.52
19:A:9022:CLA:O2A	2:B:651:LEU:HB3	2.10	0.52
2:B:200:PRO:O	2:B:204:GLY:HA2	2.10	0.52
2:B:455:ILE:HA	6:F:148:LEU:HG	1.91	0.52
2:B:693:TRP:CD1	19:B:1238:CLA:HMD3	2.45	0.52
6:F:207:LEU:CD1	6:F:208:PHE:N	2.51	0.52
11:K:60:SER:O	11:K:61:THR:C	2.44	0.52
16:2:103:VAL:O	16:2:104:GLN:C	2.48	0.52
16:2:118:ALA:HA	16:2:121:PHE:CD2	2.34	0.52
5:E:78:ARG:NH2	5:E:125:ILE:HG22	2.19	0.52
13:N:132:THR:CA	13:N:136:ASP:OD1	2.54	0.52
4:D:155:TYR:CE1	4:D:168:PRO:HG3	2.45	0.52
4:D:173:TYR:O	4:D:175:GLU:HG2	2.10	0.52
16:2:152:LEU:N	16:2:152:LEU:CD1	2.73	0.52
1:A:478:SER:HB2	1:A:644:GLN:OE1	2.08	0.52
2:B:628:SER:O	2:B:630:GLN:N	2.43	0.52
16:2:247:ILE:O	16:2:248:ASP:CB	2.58	0.52
12:L:169:ARG:NE	12:L:169:ARG:O	2.43	0.52
1:A:483:GLN:CB	1:A:485:GLN:HE22	2.21	0.52
19:A:1149:CLA:CBA	19:A:1149:CLA:O1D	2.58	0.52
1:A:44:ILE:O	1:A:45:ALA:O	2.28	0.52
8:H:104:GLY:O	8:H:105:GLY:C	2.47	0.52
18:4:121:ILE:O	18:4:123:VAL:N	2.41	0.51
15:1:157:ASP:O	15:1:158:PRO:C	2.48	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:90:ALA:O	15:1:91:MET:C	2.45	0.51
18:4:144:ILE:O	18:4:145:GLU:C	2.46	0.51
1:A:545:HIS:ND1	19:A:1135:CLA:HBB2	2.22	0.51
1:A:291:THR:O	1:A:293:GLY:N	2.36	0.51
1:A:154:ARG:HG3	1:A:383:PRO:HB2	1.92	0.51
1:A:402:ILE:C	1:A:404:GLY:H	2.13	0.51
1:A:555:ILE:HG23	2:B:670:TYR:HE2	1.75	0.51
1:A:691:MET:HE2	20:A:5001:PQN:H2M2	1.92	0.51
19:A:9022:CLA:H71	19:A:9022:CLA:H122	1.92	0.51
19:A:9023:CLA:CAD	2:B:670:TYR:OH	2.58	0.51
2:B:527:LEU:CD2	19:B:1222:CLA:C1D	2.87	0.51
19:B:1238:CLA:HBC2	19:B:1238:CLA:HMC1	1.92	0.51
2:B:597:LYS:O	2:B:598:HIS:HB2	2.10	0.51
2:B:693:TRP:NE1	19:B:1238:CLA:HMD3	2.24	0.51
19:A:1132:CLA:HBC2	19:H:1207:CLA:HBC1	1.92	0.51
11:K:56:ILE:HG12	11:K:59:THR:HG21	1.92	0.51
21:I:6021:BCR:H392	21:L:6019:BCR:C40	2.39	0.51
3:C:28:MET:HG3	4:D:175:GLU:HA	1.92	0.51
13:N:109:THR:O	13:N:111:GLY:N	2.42	0.51
12:L:178:THR:HG22	12:L:179:ALA:H	1.74	0.51
4:D:129:LEU:HD11	12:L:65:PHE:CD1	2.44	0.51
13:N:90:GLU:OE1	13:N:91:TYR:CE1	2.62	0.51
15:1:157:ASP:OD2	15:1:178:LYS:HA	2.08	0.51
18:4:173:LYS:HD2	18:4:201:LYS:CE	2.33	0.51
19:A:1103:CLA:H201	21:A:6003:BCR:C18	2.40	0.51
1:A:374:GLN:O	1:A:377:TYR:CD2	2.63	0.51
19:A:1112:CLA:CMB	21:A:6002:BCR:H382	2.36	0.51
1:A:603:PHE:CZ	1:A:693:LEU:CD2	2.93	0.51
1:A:694:PHE:HZ	2:B:661:PHE:CD1	2.28	0.51
19:A:9011:CLA:HMB3	19:A:9012:CLA:HMD1	1.92	0.51
19:A:9023:CLA:HED3	19:A:9023:CLA:CBA	2.40	0.51
19:B:1203:CLA:CBB	19:B:1225:CLA:HHC	2.39	0.51
19:B:1239:CLA:C19	9:I:21:MET:CB	2.88	0.51
19:A:9022:CLA:H62	2:B:648:TRP:CZ2	2.45	0.51
7:G:89:LYS:O	7:G:90:GLN:CG	2.57	0.51
12:L:110:LEU:CA	12:L:113:PRO:HG2	2.40	0.51
3:C:67:VAL:CG2	3:C:67:VAL:O	2.57	0.51
4:D:171:GLY:O	4:D:172:VAL:CG2	2.53	0.51
14:R:39:UNK:CA	14:R:42:UNK:CB	2.85	0.51
8:H:121:LEU:O	8:H:122:PRO:C	2.47	0.51
15:1:150:HIS:O	15:1:150:HIS:ND1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3:159:VAL:HG12	17:3:160:LEU:H	1.75	0.51
17:3:210:PRO:CG	17:3:211:LEU:H	2.23	0.51
17:3:176:TRP:O	17:3:178:LYS:CA	2.57	0.51
1:A:421:ASP:N	1:A:421:ASP:OD1	2.43	0.51
19:1:1005:CLA:HBC2	19:1:1005:CLA:HMC1	1.93	0.51
22:B:7038:LMU:C10	22:B:7038:LMU:C6	2.88	0.51
15:1:77:GLU:HG3	15:1:80:LYS:NZ	2.25	0.51
19:A:1126:CLA:CGA	19:A:1126:CLA:C1A	2.89	0.51
1:A:411:ALA:CB	21:A:6008:BCR:H392	2.34	0.51
2:B:620:LEU:CD1	19:B:9010:CLA:H93	2.39	0.51
2:B:102:GLU:OE2	2:B:641:ASN:HA	2.09	0.51
6:F:150:VAL:CG1	6:F:150:VAL:O	2.49	0.51
6:F:83:THR:HB	6:F:84:PRO:CD	2.36	0.51
15:1:93:ALA:HA	19:1:1006:CLA:C3B	2.41	0.51
14:R:38:UNK:O	14:R:42:UNK:C	2.59	0.51
16:2:177:VAL:CG1	16:2:178:ASN:N	2.73	0.51
12:L:205:TYR:CE1	12:L:207:LEU:HD13	2.45	0.51
12:L:211:TYR:HD2	12:L:211:TYR:N	2.07	0.51
8:H:80:GLN:CA	8:H:83:LEU:HD23	2.40	0.51
16:2:249:ASN:O	16:2:249:ASN:OD1	2.28	0.51
17:3:192:LYS:NZ	17:3:192:LYS:CA	2.71	0.51
6:F:184:ALA:C	6:F:185:ILE:HG23	2.29	0.51
1:A:23:ASP:CB	1:A:33:GLN:CD	2.74	0.51
13:N:120:VAL:HG12	13:N:122:PHE:CE2	2.45	0.51
22:H:7011:LMU:C2B	22:H:7011:LMU:H6E	2.32	0.51
22:B:7038:LMU:H1B	22:B:7038:LMU:O6'	2.10	0.51
1:A:461:TYR:CZ	1:A:540:LEU:CD1	2.93	0.51
15:1:182:GLU:OE1	19:1:1001:CLA:C2D	2.58	0.51
18:4:96:LEU:O	18:4:96:LEU:CD1	2.57	0.51
18:4:95:GLU:O	18:4:98:ASN:N	2.43	0.51
19:A:1126:CLA:H18	19:A:9012:CLA:H18	1.92	0.51
19:A:1135:CLA:CGD	19:A:1135:CLA:HBA2	2.39	0.51
1:A:207:LEU:CD2	19:A:1119:CLA:CBB	2.83	0.51
1:A:368:LEU:CD1	19:A:1125:CLA:C6	2.88	0.51
2:B:315:LEU:CD1	2:B:317:ARG:HD2	2.40	0.51
2:B:317:ARG:CZ	2:B:317:ARG:HB3	2.39	0.51
2:B:494:LEU:O	2:B:494:LEU:HD12	2.11	0.51
19:A:1132:CLA:H111	21:B:6020:BCR:H10C	1.91	0.51
2:B:662:MET:HG2	20:B:5002:PQN:O1	2.11	0.51
2:B:98:GLN:CA	2:B:98:GLN:NE2	2.71	0.51
6:F:202:LEU:O	6:F:203:ALA:CB	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:64:MET:O	11:K:67:ALA:HB3	2.11	0.51
16:2:122:ILE:HD11	19:2:2002:CLA:CBB	2.26	0.51
5:E:73:LYS:HG3	5:E:128:VAL:HG11	1.93	0.51
13:N:157:LYS:N	13:N:157:LYS:CD	2.74	0.51
2:B:561:GLY:HA3	3:C:52:LYS:CB	2.41	0.51
2:B:561:GLY:CA	3:C:52:LYS:HG2	2.36	0.51
17:3:113:ALA:CB	17:3:239:LEU:HD12	2.28	0.51
4:D:95:GLN:C	4:D:95:GLN:NE2	2.64	0.51
17:3:134:LEU:CD1	17:3:134:LEU:N	2.65	0.51
19:K:1142:CLA:HMD1	19:K:1143:CLA:C4A	2.39	0.51
19:J:1308:CLA:C2	19:J:1308:CLA:O1D	2.58	0.51
6:F:221:LEU:C	6:F:222:LEU:HD23	2.31	0.51
15:1:67:LEU:CG	15:1:68:GLY:N	2.73	0.51
15:1:84:LEU:N	15:1:86:HIS:HD2	2.07	0.51
1:A:295:TRP:HB3	1:A:297:THR:HG23	1.92	0.51
1:A:374:GLN:O	1:A:376:MET:N	2.43	0.51
19:A:1125:CLA:HBA2	21:A:6008:BCR:C12	2.41	0.51
1:A:665:ILE:C	1:A:665:ILE:HD12	2.30	0.51
1:A:678:PHE:O	1:A:681:GLY:O	2.29	0.51
2:B:340:SER:O	2:B:344:ILE:HG13	2.11	0.51
2:B:404:ALA:O	2:B:405:ASP:CG	2.48	0.51
2:B:639:VAL:CG2	2:B:640:CYS:N	2.74	0.51
2:B:558:PRO:HG2	2:B:703:VAL:HG13	1.92	0.51
19:F:1302:CLA:CHD	19:F:1302:CLA:HBC2	2.38	0.51
1:A:571:ASP:HB3	3:C:53:ARG:HH12	1.74	0.51
16:2:184:PRO:CA	16:2:187:LYS:HD2	2.40	0.51
19:2:4009:CLA:C19	19:2:4009:CLA:H152	2.33	0.51
16:2:200:TRP:CD1	16:2:200:TRP:N	2.79	0.51
15:1:168:PHE:O	15:1:169:ASP:CB	2.39	0.51
1:A:628:ILE:HG13	1:A:629:ASN:N	2.25	0.51
18:4:201:LYS:H	18:4:201:LYS:HD3	1.71	0.51
19:A:1105:CLA:HBA2	19:A:1107:CLA:C1	2.40	0.51
19:A:1107:CLA:HBA2	19:A:1107:CLA:CHA	2.40	0.51
19:A:1101:CLA:HBB1	19:A:1109:CLA:H151	1.91	0.51
19:A:1124:CLA:HAA2	19:A:1125:CLA:CAD	2.41	0.51
1:A:214:GLY:O	1:A:215:SER:CB	2.58	0.51
1:A:488:PHE:HB3	1:A:535:GLY:H	1.76	0.51
19:A:1124:CLA:CHC	21:A:6008:BCR:C37	2.89	0.51
19:A:9012:CLA:C4B	19:A:9013:CLA:HBB2	2.41	0.51
2:B:98:GLN:HE21	2:B:101:VAL:HG23	1.76	0.51
19:B:1220:CLA:HAA1	19:B:1220:CLA:H12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:225:LEU:N	2:B:227:THR:O	2.44	0.51
2:B:257:ILE:N	2:B:257:ILE:HD13	2.25	0.51
2:B:365:PHE:HD1	2:B:602:TRP:CE2	2.29	0.51
2:B:555:TYR:CD2	2:B:573:TRP:HB2	2.44	0.51
2:B:558:PRO:CB	2:B:703:VAL:CG2	2.64	0.51
6:F:161:ILE:O	6:F:164:GLY:N	2.36	0.51
11:K:60:SER:O	11:K:63:LEU:HD22	2.11	0.51
13:N:152:LEU:O	13:N:153:GLU:HG3	2.08	0.51
2:B:564:ARG:NH2	3:C:66:ARG:HH12	2.09	0.51
14:R:37:UNK:O	14:R:42:UNK:O	2.29	0.51
1:A:575:LEU:HD11	1:A:579:PHE:CG	2.45	0.51
16:2:201:PHE:CD1	16:2:202:ASP:CA	2.93	0.51
1:A:483:GLN:CA	1:A:485:GLN:HE22	2.23	0.51
13:N:168:TRP:CE3	13:N:168:TRP:O	2.63	0.51
1:A:274:TRP:NE1	1:A:277:TYR:CD2	2.78	0.51
2:B:324:ASP:O	2:B:328:ASN:CG	2.48	0.51
4:D:74:LEU:HD11	12:L:58:GLN:OE1	2.10	0.51
15:1:178:LYS:C	15:1:178:LYS:CD	2.71	0.51
18:4:94:ALA:HA	19:4:4012:CLA:OBD	2.11	0.51
19:A:1115:CLA:HED3	19:A:1115:CLA:C1A	2.36	0.51
19:A:1131:CLA:C16	21:L:6019:BCR:H362	2.40	0.51
19:A:1126:CLA:H71	21:A:6011:BCR:H372	1.93	0.51
1:A:660:GLN:HE21	1:A:660:GLN:H	1.58	0.51
1:A:79:PHE:CD1	19:A:1111:CLA:CED	2.90	0.51
19:B:1205:CLA:C14	19:B:1205:CLA:H102	2.40	0.51
19:B:1228:CLA:CHD	19:B:1228:CLA:HBC2	2.35	0.51
2:B:493:TRP:CB	19:B:1232:CLA:HED2	2.41	0.51
2:B:230:TRP:O	2:B:232:LEU:N	2.43	0.51
2:B:292:ARG:HH22	2:B:297:ILE:CG1	2.24	0.51
2:B:378:ILE:H	2:B:381:PHE:HD1	1.59	0.51
2:B:621:ARG:O	2:B:625:TRP:CB	2.52	0.51
3:C:1:MET:N	3:C:3:HIS:N	2.59	0.51
3:C:5:VAL:O	3:C:5:VAL:HG23	2.11	0.51
4:D:172:VAL:HG12	4:D:173:TYR:N	2.26	0.51
17:3:96:ARG:CG	17:3:96:ARG:NH1	2.39	0.51
6:F:131:ASP:OD2	6:F:131:ASP:N	2.43	0.51
19:J:1311:CLA:CED	19:J:1311:CLA:C1A	2.83	0.51
5:E:96:ASP:CG	5:E:98:ASN:OD1	2.49	0.51
1:A:468:SER:HB2	1:A:476:MET:SD	2.51	0.51
1:A:240:LYS:O	1:A:240:LYS:CG	2.58	0.51
1:A:332:GLU:HA	1:A:344:LYS:CG	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:VAL:O	1:A:438:HIS:ND1	2.43	0.51
19:B:1222:CLA:CHB	19:B:1236:CLA:HAA2	2.41	0.51
2:B:288:GLY:O	2:B:289:LEU:HB2	2.10	0.51
2:B:596:TRP:O	2:B:597:LYS:CB	2.58	0.51
5:E:103:VAL:HG23	5:E:104:VAL:O	2.11	0.51
8:H:94:ARG:NH1	8:H:94:ARG:HB2	2.25	0.51
12:L:107:GLY:O	12:L:109:LEU:N	2.44	0.51
19:2:2004:CLA:H43	19:3:2009:CLA:HBC3	1.93	0.51
8:H:58:LEU:N	8:H:61:THR:HG21	2.23	0.51
13:N:146:LEU:C	13:N:147:SER:O	2.48	0.51
17:3:96:ARG:H	17:3:99:ALA:H	1.58	0.51
14:R:30:UNK:O	14:R:32:UNK:N	2.43	0.51
22:2:7006:LMU:H122	22:3:7005:LMU:O3'	2.10	0.51
4:D:123:ARG:HG2	4:D:124:GLU:N	2.24	0.51
2:B:160:LYS:NZ	2:B:161:TRP:CG	2.65	0.51
14:R:27:UNK:C	14:R:29:UNK:N	2.74	0.51
19:4:1304:CLA:CGD	19:4:1304:CLA:H2A	2.41	0.51
17:3:125:VAL:CB	17:3:126:GLY:HA2	2.31	0.51
17:3:159:VAL:C	17:3:161:GLU:N	2.56	0.51
15:1:162:LYS:N	15:1:164:PRO:CG	2.49	0.51
18:4:108:GLY:C	18:4:109:MET:O	2.49	0.51
1:A:755:ILE:O	1:A:756:ALA:CB	2.59	0.51
18:4:226:LYS:N	18:4:226:LYS:NZ	2.56	0.51
19:A:1117:CLA:ND	19:A:1127:CLA:H72	2.26	0.51
19:A:1126:CLA:C7	21:A:6011:BCR:C37	2.88	0.51
19:A:1106:CLA:H112	19:A:1126:CLA:H91	1.93	0.51
1:A:431:LEU:CA	1:A:434:ARG:HB2	2.41	0.51
2:B:304:ILE:HD13	19:B:1216:CLA:CED	2.38	0.51
2:B:189:ALA:HB1	19:B:1225:CLA:H203	1.91	0.51
2:B:194:LEU:O	2:B:198:ALA:HB3	2.11	0.51
2:B:256:THR:O	2:B:272:ASP:OD2	2.29	0.51
2:B:290:MET:SD	2:B:291:TYR:CE1	3.04	0.51
2:B:297:ILE:HD11	19:B:1217:CLA:O2D	2.10	0.51
2:B:458:ILE:O	2:B:461:GLN:N	2.43	0.51
2:B:89:HIS:C	2:B:113:VAL:HG13	1.98	0.51
6:F:82:LEU:O	6:F:140:CYS:O	2.29	0.51
13:N:123:GLY:HA3	13:N:131:PHE:CD1	2.45	0.51
3:C:63:LEU:HD21	3:C:65:VAL:N	2.24	0.51
16:2:157:LEU:N	16:2:157:LEU:CD1	2.73	0.51
16:2:183:PHE:O	16:2:185:ASN:HA	2.11	0.51
19:K:1143:CLA:HMC1	19:K:1143:CLA:HBC2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3:191:GLU:O	17:3:192:LYS:CE	2.57	0.51
17:3:162:MET:O	17:3:163:ALA:C	2.46	0.51
17:3:201:ALA:O	17:3:202:TYR:CB	2.58	0.51
10:J:42:PHE:CD1	18:4:244:ILE:HG21	2.43	0.51
18:4:133:GLU:O	18:4:134:TYR:HD1	1.93	0.51
15:1:177:PRO:HG3	15:1:180:LEU:HD23	1.93	0.51
15:1:69:LEU:HA	15:1:73:PRO:HD3	1.91	0.51
19:A:1113:CLA:HAA1	19:A:1113:CLA:HED2	1.91	0.51
19:A:1122:CLA:CAB	21:A:6007:BCR:C35	2.86	0.51
1:A:270:PHE:N	1:A:270:PHE:CD2	2.79	0.51
2:B:544:SER:O	2:B:547:MET:C	2.49	0.51
19:1:1010:CLA:O1D	19:1:1010:CLA:C4D	2.50	0.51
1:A:583:GLY:O	1:A:585:GLY:N	2.44	0.51
2:B:560:ASP:OD2	3:C:66:ARG:NH1	2.44	0.51
3:C:42:ALA:CB	3:C:43:PRO:CD	2.88	0.51
17:3:226:LYS:O	17:3:229:LYS:HB3	2.11	0.51
17:3:233:LEU:C	17:3:235:MET:N	2.65	0.51
16:2:153:PHE:CD2	16:2:157:LEU:HD22	2.45	0.51
11:K:115:ILE:CG1	11:K:122:LEU:CD1	2.89	0.51
16:2:201:PHE:CD1	16:2:202:ASP:HB3	2.46	0.51
18:4:127:TYR:O	18:4:128:ALA:HB3	2.10	0.50
1:A:233:LEU:C	1:A:235:ALA:H	2.14	0.50
1:A:333:ALA:HB3	1:A:334:HIS:ND1	2.27	0.50
19:A:1106:CLA:H43	21:A:6011:BCR:H383	1.92	0.50
2:B:229:GLN:O	7:G:63:VAL:HG11	2.12	0.50
2:B:122:GLN:HG2	2:B:361:ILE:HG13	1.94	0.50
2:B:710:LEU:C	2:B:712:HIS:H	2.13	0.50
4:D:91:LEU:C	4:D:91:LEU:HD12	2.32	0.50
7:G:75:GLY:O	7:G:78:VAL:N	2.45	0.50
9:I:29:GLU:HA	9:I:29:GLU:OE2	2.11	0.50
12:L:106:HIS:HD2	19:L:1502:CLA:CED	2.23	0.50
12:L:96:LEU:HG	12:L:97:LEU:CD2	2.41	0.50
8:H:60:ASN:C	8:H:60:ASN:OD1	2.47	0.50
13:N:123:GLY:HA3	13:N:131:PHE:HD1	1.76	0.50
13:N:142:LYS:O	13:N:145:PHE:CD1	2.64	0.50
17:3:100:TYR:HB3	17:3:229:LYS:HE2	1.92	0.50
14:R:38:UNK:C	14:R:42:UNK:C	2.89	0.50
16:2:161:GLY:N	19:2:2012:CLA:HBB2	2.26	0.50
6:F:88:SER:O	6:F:89:LYS:C	2.48	0.50
1:A:484:LEU:C	1:A:485:GLN:CD	2.70	0.50
1:A:39:HIS:HA	1:A:44:ILE:HG21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:147:ILE:O	18:4:150:HIS:HB3	2.10	0.50
1:A:285:GLY:O	1:A:294:LEU:HD11	2.11	0.50
1:A:340:GLY:O	1:A:343:HIS:N	2.33	0.50
1:A:377:TYR:HD1	1:A:616:PHE:HE1	1.56	0.50
1:A:492:ILE:O	1:A:493:GLN:C	2.47	0.50
19:A:9012:CLA:HED2	19:A:9012:CLA:C3D	2.41	0.50
19:A:9012:CLA:H152	19:A:9012:CLA:H91	1.92	0.50
19:B:1220:CLA:CMC	19:B:1220:CLA:CBC	2.74	0.50
2:B:583:MET:HA	19:B:1222:CLA:HBC1	1.93	0.50
2:B:120:VAL:HG13	2:B:123:TRP:NE1	2.27	0.50
2:B:303:TYR:H	2:B:306:GLU:HB2	1.76	0.50
2:B:598:HIS:HB3	2:B:602:TRP:CH2	2.46	0.50
2:B:556:SER:O	23:B:7101:LMG:HC2	2.11	0.50
7:G:99:HIS:C	7:G:101:GLU:CB	2.68	0.50
19:B:1238:CLA:H91	21:I:6018:BCR:H333	1.93	0.50
16:2:120:ILE:C	16:2:123:PRO:HD2	2.31	0.50
16:2:126:LEU:HB3	19:2:2006:CLA:C19	2.29	0.50
16:2:126:LEU:HD13	19:2:2006:CLA:H172	1.93	0.50
5:E:128:VAL:O	5:E:129:GLU:O	2.28	0.50
13:N:144:PRO:HA	13:N:151:ASP:CG	2.31	0.50
3:C:44:ARG:CA	4:D:182:GLN:CD	2.69	0.50
17:3:233:LEU:C	17:3:235:MET:H	2.14	0.50
17:3:95:PRO:O	17:3:96:ARG:CD	2.58	0.50
17:3:97:TRP:O	17:3:98:LEU:C	2.48	0.50
14:R:35:UNK:O	14:R:42:UNK:O	2.30	0.50
4:D:126:PRO:HB2	4:D:128:LEU:HB2	1.93	0.50
16:2:236:TRP:CZ2	19:2:2003:CLA:CHB	2.94	0.50
10:J:14:VAL:O	10:J:14:VAL:HG13	2.11	0.50
1:A:135:ASP:OD2	1:A:141:ARG:N	2.44	0.50
18:4:161:LYS:NZ	18:4:162:ASN:ND2	2.60	0.50
19:A:1102:CLA:HHD	19:A:1102:CLA:HBC3	1.92	0.50
19:A:1128:CLA:C10	19:A:1128:CLA:H152	2.41	0.50
19:A:1135:CLA:CBD	19:A:1135:CLA:HBA2	2.41	0.50
1:A:472:ARG:O	1:A:474:GLN:HG3	2.12	0.50
19:A:1103:CLA:C4	21:A:6003:BCR:H313	2.41	0.50
2:B:429:LEU:HD21	19:B:1235:CLA:C3B	2.42	0.50
2:B:573:TRP:O	2:B:577:TYR:N	2.37	0.50
6:F:209:ARG:O	6:F:212:SER:C	2.50	0.50
16:2:114:MET:HG3	16:2:230:LEU:HB2	1.92	0.50
13:N:142:LYS:CE	13:N:142:LYS:CA	2.80	0.50
13:N:148:ASP:H	13:N:150:LEU:N	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:180:GLY:O	4:D:182:GLN:N	2.44	0.50
16:2:241:TYR:HD2	16:2:242:THR:N	2.10	0.50
11:K:115:ILE:O	11:K:118:VAL:N	2.44	0.50
17:3:154:ASN:O	17:3:155:TYR:CD2	2.62	0.50
17:3:176:TRP:O	17:3:177:ALA:C	2.49	0.50
1:A:626:GLY:O	1:A:627:THR:HG22	2.11	0.50
14:R:44:UNK:O	14:R:45:UNK:O	2.30	0.50
15:1:225:TRP:HB3	15:1:226:HIS:CA	2.41	0.50
1:A:109:TRP:O	1:A:112:ASP:N	2.44	0.50
1:A:284:ARG:HG3	1:A:295:TRP:NE1	2.26	0.50
1:A:502:THR:O	1:A:504:ALA:O	2.30	0.50
1:A:536:THR:HG23	1:A:536:THR:O	2.11	0.50
1:A:550:HIS:O	1:A:552:THR:O	2.29	0.50
1:A:734:GLY:O	1:A:736:THR:N	2.44	0.50
19:B:1203:CLA:H43	23:B:7101:LMG:H321	1.92	0.50
19:B:1218:CLA:HMA3	19:B:1219:CLA:C4D	2.41	0.50
2:B:351:HIS:NE2	19:B:1223:CLA:NC	2.59	0.50
2:B:594:TRP:HD1	2:B:595:HIS:HB2	1.76	0.50
2:B:622:ASP:HB2	2:B:626:LEU:HD11	1.84	0.50
2:B:682:HIS:O	2:B:683:GLU:C	2.50	0.50
19:L:1130:CLA:H92	19:L:1504:CLA:H2	1.92	0.50
16:2:227:LEU:CD2	19:2:2004:CLA:NC	2.72	0.50
3:C:10:THR:HG23	5:E:101:TYR:CG	2.41	0.50
13:N:104:LYS:O	13:N:107:LEU:N	2.44	0.50
16:2:187:LYS:C	16:2:187:LYS:HE3	2.31	0.50
19:K:1143:CLA:CAC	22:K:7001:LMU:C3B	2.86	0.50
6:F:88:SER:HG	6:F:91:PHE:HB3	1.73	0.50
17:3:201:ALA:CB	17:3:202:TYR:CE2	2.74	0.50
18:4:232:LEU:HD12	18:4:233:LEU:C	2.31	0.50
13:N:120:VAL:CG1	13:N:122:PHE:CE2	2.94	0.50
16:2:261:THR:CG2	16:2:262:ILE:N	2.59	0.50
22:R:7025:LMU:O2'	22:R:7025:LMU:H21	2.11	0.50
1:A:455:PHE:CD1	19:A:1131:CLA:HMA2	2.45	0.50
1:A:245:PRO:O	1:A:248:PHE:CZ	2.64	0.50
1:A:747:TRP:CE3	21:A:6011:BCR:C40	2.94	0.50
2:B:196:HIS:NE2	19:B:1212:CLA:ND	2.59	0.50
19:B:1224:CLA:H3A	19:B:1224:CLA:CGA	2.34	0.50
2:B:451:LYS:HD3	19:B:1230:CLA:O2D	2.10	0.50
2:B:330:ILE:HG13	2:B:330:ILE:O	2.10	0.50
2:B:419:ILE:C	2:B:420:SER:OG	2.50	0.50
2:B:593:TYR:O	2:B:596:TRP:O	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:9022:CLA:C10	21:B:6017:BCR:H19C	2.40	0.50
6:F:173:TRP:CZ3	6:F:211:PHE:N	2.80	0.50
7:G:81:ASN:OD1	7:G:82:PHE:N	2.43	0.50
7:G:87:VAL:O	7:G:88:ALA:CB	2.57	0.50
5:E:127:GLU:OE1	5:E:129:GLU:O	2.28	0.50
14:R:38:UNK:O	14:R:39:UNK:O	2.30	0.50
2:B:247:THR:CA	2:B:250:ALA:HB3	2.20	0.50
12:L:208:ASP:OD2	12:L:209:LEU:O	2.29	0.50
8:H:78:PRO:HG3	19:L:1501:CLA:CMD	2.40	0.50
2:B:6:PRO:HG2	2:B:6:PRO:O	2.12	0.50
6:F:226:LEU:HA	6:F:230:ASN:HD22	1.77	0.50
12:L:166:LEU:O	12:L:167:THR:C	2.45	0.50
19:1:1008:CLA:HBA2	19:1:1008:CLA:CMA	2.42	0.50
2:B:8:PHE:O	2:B:35:ASP:CG	2.50	0.50
22:4:7033:LMU:O2'	22:4:7033:LMU:H6'2	2.12	0.50
16:2:145:TYR:C	16:2:146:PHE:CG	2.85	0.50
19:A:1104:CLA:HBA2	19:A:1104:CLA:HED2	1.93	0.50
1:A:203:LEU:CD2	19:A:1123:CLA:O2D	2.59	0.50
19:A:1112:CLA:CHC	21:A:6002:BCR:H17C	2.31	0.50
1:A:656:PHE:O	1:A:659:ALA:N	2.45	0.50
19:A:9012:CLA:HED1	19:B:9010:CLA:H2	1.94	0.50
19:B:1208:CLA:O2A	19:B:1208:CLA:HBD	2.11	0.50
19:B:1209:CLA:C1	19:B:1209:CLA:H61	2.42	0.50
19:B:1222:CLA:O1A	19:B:1236:CLA:HAA1	2.12	0.50
2:B:175:LEU:HD12	2:B:179:LEU:HD23	1.93	0.50
2:B:292:ARG:HH21	2:B:297:ILE:CA	2.25	0.50
2:B:31:PHE:O	2:B:32:GLU:C	2.50	0.50
2:B:456:GLU:CB	6:F:147:HIS:ND1	2.75	0.50
2:B:354:SER:O	2:B:508:LEU:HD23	2.12	0.50
19:A:9023:CLA:HMC1	2:B:661:PHE:HB2	1.89	0.50
2:B:667:TRP:O	2:B:669:GLY:N	2.44	0.50
2:B:686:PRO:C	2:B:688:ALA:H	2.14	0.50
16:2:219:THR:O	16:2:223:LYS:HB2	2.12	0.50
13:N:155:GLU:O	13:N:157:LYS:CE	2.08	0.50
3:C:29:ILE:HG22	3:C:30:PRO:O	2.12	0.50
11:K:115:ILE:O	11:K:116:ILE:C	2.47	0.50
1:A:23:ASP:OD1	1:A:33:GLN:HG3	2.12	0.50
22:R:7020:LMU:O6B	22:R:7020:LMU:H6E	2.11	0.50
22:H:7032:LMU:H6'2	22:H:7032:LMU:H22	1.93	0.50
2:B:92:TRP:CZ2	9:I:6:SER:HB2	2.47	0.50
1:A:370:ILE:HD13	19:A:1124:CLA:CAD	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1141:CLA:H72	19:A:1141:CLA:H122	1.90	0.50
1:A:148:GLY:O	1:A:152:ILE:CD1	2.57	0.50
1:A:655:ASP:O	1:A:660:GLN:NE2	2.45	0.50
1:A:662:SER:O	1:A:666:GLN:HB2	2.12	0.50
19:B:1221:CLA:HMB2	19:B:1223:CLA:H92	1.93	0.50
2:B:224:PRO:HG3	7:G:153:PHE:HB3	1.94	0.50
2:B:330:ILE:HD12	2:B:333:GLN:HE21	1.77	0.50
2:B:519:VAL:HG11	2:B:593:TYR:HB2	1.94	0.50
1:A:705:GLU:CB	2:B:545:LYS:NZ	2.75	0.50
2:B:626:LEU:O	2:B:627:ASN:CB	2.47	0.50
11:K:51:SER:H	11:K:52:PRO:HD3	1.75	0.50
2:B:685:THR:HG1	19:L:1130:CLA:H3A	1.73	0.50
17:3:109:ALA:O	17:3:111:LEU:CD2	2.60	0.50
4:D:140:LEU:HD22	4:D:144:LEU:HD11	1.92	0.50
6:F:88:SER:HG	6:F:91:PHE:CB	2.25	0.50
1:A:578:ARG:O	1:A:579:PHE:O	2.30	0.50
1:A:425:THR:HG1	1:A:428:TYR:HH	1.59	0.50
15:1:168:PHE:O	15:1:168:PHE:HD1	1.95	0.50
8:H:55:LEU:O	8:H:56:GLU:C	2.50	0.50
4:D:184:VAL:HG12	4:D:185:GLY:H	1.76	0.50
18:4:188:ILE:HG22	18:4:189:PHE:HD2	1.77	0.50
4:D:147:LYS:CA	4:D:148:TYR:CD1	2.93	0.50
2:B:163:PRO:C	2:B:164:SER:OG	2.48	0.50
19:1:1005:CLA:CHA	19:1:1005:CLA:HBA1	2.42	0.50
17:3:246:LEU:HB3	17:3:248:THR:HG23	1.92	0.50
18:4:122:ASN:HB3	18:4:124:PRO:CD	2.36	0.50
18:4:120:ILE:HD11	18:4:226:LYS:HG3	0.51	0.50
22:4:7034:LMU:C10	22:4:7052:LMU:C3'	2.90	0.50
1:A:431:LEU:N	1:A:434:ARG:HE	2.10	0.50
2:B:431:PHE:HE2	19:B:1229:CLA:CED	2.25	0.50
2:B:348:VAL:HG21	19:B:1225:CLA:HHD	1.94	0.50
2:B:420:SER:O	2:B:424:TRP:N	2.36	0.50
2:B:508:LEU:HB2	2:B:509:PHE:HD2	1.76	0.50
2:B:693:TRP:CD1	19:B:1238:CLA:CMD	2.94	0.50
7:G:89:LYS:C	7:G:90:GLN:CG	2.78	0.50
12:L:70:GLU:OE2	12:L:75:SER:OG	2.19	0.50
16:2:224:ASN:C	16:2:227:LEU:H	2.15	0.50
13:N:139:LYS:C	13:N:142:LYS:NZ	2.64	0.50
17:3:104:ILE:CG2	19:3:3004:CLA:C2D	2.90	0.50
17:3:111:LEU:C	17:3:113:ALA:N	2.62	0.50
14:R:34:UNK:O	14:R:36:UNK:O	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:103:THR:OG1	4:D:153:GLN:HB2	2.11	0.50
16:2:249:ASN:OD1	16:2:250:LEU:O	2.30	0.50
6:F:105:SER:O	6:F:107:LYS:N	2.45	0.50
15:1:150:HIS:O	15:1:153:SER:HB3	2.12	0.50
14:R:8:UNK:CB	19:R:1144:CLA:CED	2.90	0.50
13:N:168:TRP:CZ3	13:N:170:TRP:HB3	2.47	0.50
13:N:90:GLU:OE1	13:N:91:TYR:CD1	2.65	0.50
22:H:7002:LMU:O6B	22:H:7002:LMU:C1B	2.58	0.50
18:4:161:LYS:HZ1	18:4:162:ASN:HD21	1.58	0.50
18:4:167:ASN:O	18:4:168:GLN:HB2	2.12	0.50
1:A:167:THR:HG22	19:A:1112:CLA:CAA	2.23	0.50
1:A:240:LYS:O	1:A:240:LYS:HG3	2.12	0.50
1:A:302:HIS:CD2	19:A:1116:CLA:NB	2.78	0.50
1:A:344:LYS:C	1:A:346:LEU:N	2.60	0.50
1:A:348:GLU:O	1:A:351:THR:CG2	2.60	0.50
1:A:348:GLU:O	1:A:351:THR:HG22	2.12	0.50
19:B:1202:CLA:H162	19:B:1210:CLA:OBD	2.12	0.50
19:B:1239:CLA:HMC1	19:B:1239:CLA:CBC	2.35	0.50
2:B:23:PHE:O	2:B:24:GLY:C	2.49	0.50
2:B:317:ARG:NH1	2:B:405:ASP:C	2.58	0.50
2:B:338:LEU:O	2:B:339:ALA:HB3	2.11	0.50
2:B:472:TYR:O	2:B:472:TYR:HD1	1.95	0.50
2:B:620:LEU:CA	2:B:624:LEU:HD23	2.32	0.50
2:B:707:LEU:HD11	2:B:711:VAL:HG21	1.93	0.50
2:B:732:LYS:CG	2:B:734:GLY:CA	2.88	0.50
6:F:169:TYR:C	6:F:169:TYR:CD2	2.85	0.50
11:K:53:THR:HA	11:K:56:ILE:HB	1.94	0.50
12:L:112:GLY:N	12:L:113:PRO:CD	2.75	0.50
12:L:138:VAL:HG21	12:L:194:ILE:HG13	1.94	0.50
13:N:132:THR:HG21	13:N:139:LYS:HD3	0.66	0.50
15:1:133:THR:C	15:1:137:ILE:HD13	2.31	0.50
15:1:137:ILE:O	15:1:141:GLU:CG	2.49	0.50
17:3:109:ALA:HA	17:3:111:LEU:HB3	1.60	0.50
14:R:35:UNK:O	14:R:36:UNK:O	2.30	0.50
17:3:108:PHE:HD2	19:3:3013:CLA:H43	1.77	0.50
16:2:161:GLY:O	16:2:162:TRP:C	2.50	0.50
6:F:129:ARG:NH1	6:F:132:ASN:OD1	2.45	0.50
11:K:116:ILE:HG23	11:K:117:GLY:H	1.74	0.50
19:J:1308:CLA:HBD	19:J:1308:CLA:CGA	2.42	0.50
1:A:255:LEU:O	1:A:256:ALA:C	2.49	0.50
15:1:77:GLU:HG3	15:1:80:LYS:CE	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:4:1004:CLA:OBD	19:4:1004:CLA:O2D	2.29	0.49
18:4:170:PRO:HG2	18:4:171:ILE:HG13	1.94	0.49
19:A:1126:CLA:H72	21:A:6011:BCR:H371	1.94	0.49
1:A:378:SER:OG	19:A:1125:CLA:HBC2	2.12	0.49
1:A:499:ALA:HB3	1:A:500:PRO:CD	2.42	0.49
1:A:744:ALA:HB2	21:A:6011:BCR:H391	0.69	0.49
1:A:701:GLN:NE2	1:A:701:GLN:HA	2.26	0.49
19:B:1225:CLA:H142	21:B:6006:BCR:C10	2.42	0.49
2:B:275:HIS:O	2:B:278:LEU:HB3	2.11	0.49
2:B:306:GLU:CG	2:B:307:ALA:H	2.00	0.49
2:B:434:LEU:O	2:B:438:VAL:HG13	2.12	0.49
2:B:46:ILE:HG21	19:B:1202:CLA:HBC3	1.94	0.49
2:B:592:PHE:HA	2:B:721:TYR:OH	2.12	0.49
7:G:102:ALA:CA	7:G:104:ASP:OD2	2.59	0.49
5:E:76:ILE:O	5:E:84:TYR:O	2.30	0.49
14:R:38:UNK:O	14:R:42:UNK:O	2.30	0.49
16:2:171:ILE:CG1	16:2:172:LEU:H	2.23	0.49
17:3:192:LYS:HZ3	17:3:192:LYS:C	2.15	0.49
4:D:132:ALA:CB	4:D:136:GLN:HE22	2.21	0.49
17:3:161:GLU:CA	17:3:164:LEU:HG	2.39	0.49
2:B:69:ALA:HB1	2:B:135:LEU:CD1	2.37	0.49
22:R:7007:LMU:H1B	22:R:7007:LMU:O6B	2.12	0.49
22:H:7032:LMU:H2B	22:H:7032:LMU:H31	1.93	0.49
7:G:144:THR:CG2	7:G:147:ASN:O	2.58	0.49
1:A:382:TYR:HE2	19:A:1127:CLA:HED3	1.75	0.49
19:A:1132:CLA:CMC	19:A:1132:CLA:HBC3	2.41	0.49
19:A:1141:CLA:O1A	19:A:1141:CLA:O2D	2.29	0.49
1:A:150:PHE:H	1:A:153:TRP:CB	2.19	0.49
1:A:217:SER:HG	21:A:6002:BCR:H17C	1.76	0.49
1:A:233:LEU:O	1:A:235:ALA:N	2.30	0.49
21:A:6011:BCR:H353	19:A:9012:CLA:H41	1.94	0.49
1:A:692:PHE:CE2	1:A:733:VAL:HG11	2.46	0.49
19:B:1205:CLA:H42	19:B:1205:CLA:CHD	2.42	0.49
2:B:91:ILE:HG21	19:B:1206:CLA:HMD1	1.95	0.49
19:B:1222:CLA:H72	19:B:1236:CLA:C3D	2.41	0.49
2:B:244:PHE:CD2	2:B:244:PHE:O	2.58	0.49
2:B:396:ARG:NH1	19:B:1226:CLA:HED2	2.27	0.49
19:B:1225:CLA:H62	21:B:6006:BCR:HC7	1.94	0.49
19:B:1235:CLA:C12	21:F:6016:BCR:C31	2.90	0.49
19:H:1207:CLA:HBB2	9:I:13:GLY:O	2.11	0.49
19:2:2002:CLA:H42	19:2:2002:CLA:C4C	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:127:GLU:C	5:E:128:VAL:CG2	2.77	0.49
13:N:147:SER:O	13:N:148:ASP:CG	2.50	0.49
3:C:5:VAL:CG2	3:C:65:VAL:HG21	2.35	0.49
3:C:7:ILE:C	3:C:8:TYR:O	2.50	0.49
1:A:262:PHE:O	1:A:265:GLY:N	2.44	0.49
11:K:127:ILE:CA	11:K:129:ALA:HA	2.40	0.49
2:B:393:PHE:CZ	2:B:398:TYR:CD2	3.01	0.49
17:3:197:SER:OG	17:3:205:GLY:C	2.50	0.49
22:R:7020:LMU:H5'	22:R:7020:LMU:O2'	2.12	0.49
15:1:207:ALA:C	15:1:209:PRO:CD	2.79	0.49
4:D:105:ASP:HB2	4:D:151:LYS:HB2	1.94	0.49
22:K:7042:LMU:H5'	22:K:7042:LMU:C2B	2.41	0.49
13:N:90:GLU:OE1	13:N:91:TYR:CE2	2.65	0.49
1:A:686:TRP:O	1:A:689:SER:OG	2.19	0.49
12:L:124:GLU:HG3	12:L:124:GLU:O	2.13	0.49
15:1:158:PRO:CD	15:1:159:GLU:H	2.24	0.49
18:4:174:GLN:C	18:4:195:ALA:H	2.15	0.49
19:A:1141:CLA:O2A	19:A:1141:CLA:HMA2	2.11	0.49
1:A:130:GLU:O	1:A:130:GLU:OE1	2.29	0.49
1:A:284:ARG:CZ	1:A:284:ARG:CA	2.88	0.49
1:A:539:PHE:HD2	1:A:539:PHE:O	1.95	0.49
2:B:10:GLN:O	2:B:11:GLY:C	2.49	0.49
2:B:222:LEU:HB3	19:B:1212:CLA:CAD	2.43	0.49
7:G:116:SER:OG	7:G:119:PRO:HG2	2.12	0.49
12:L:137:LEU:C	12:L:137:LEU:CD2	2.64	0.49
3:C:17:CYS:SG	3:C:18:VAL:N	2.86	0.49
17:3:99:ALA:C	17:3:101:GLY:N	2.64	0.49
4:D:95:GLN:NE2	4:D:96:VAL:N	2.60	0.49
22:E:7048:LMU:O4'	22:F:7036:LMU:C6'	2.60	0.49
1:A:267:THR:HG21	1:A:269:PHE:HE2	1.67	0.49
17:3:164:LEU:C	17:3:164:LEU:HD12	2.33	0.49
15:1:125:LEU:N	15:1:125:LEU:HD22	2.13	0.49
22:4:7052:LMU:H52	22:4:7052:LMU:H12	1.93	0.49
19:A:1115:CLA:CMC	19:A:1115:CLA:CBC	2.82	0.49
1:A:372:VAL:HG22	19:A:1117:CLA:C4	2.42	0.49
1:A:159:THR:C	1:A:160:SER:OG	2.50	0.49
1:A:312:ILE:O	1:A:313:ALA:HB2	2.11	0.49
1:A:369:THR:HG21	1:A:402:ILE:CG2	2.42	0.49
1:A:432:LEU:O	1:A:435:VAL:N	2.45	0.49
1:A:462:ILE:HG21	19:A:1132:CLA:HMC3	1.95	0.49
19:A:1119:CLA:C9	21:A:6007:BCR:C37	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1223:CLA:C7	19:B:1223:CLA:H41	2.32	0.49
2:B:123:TRP:CA	2:B:126:THR:HB	2.37	0.49
2:B:312:GLY:O	2:B:314:ARG:N	2.36	0.49
2:B:330:ILE:CD1	19:B:1202:CLA:H193	2.43	0.49
1:A:673:SER:OG	2:B:445:ALA:O	2.16	0.49
2:B:462:TRP:HZ3	19:B:1231:CLA:CBC	2.10	0.49
2:B:500:ALA:HB3	2:B:507:SER:O	2.13	0.49
19:B:1217:CLA:HBB2	7:G:74:LEU:HD22	1.94	0.49
7:G:89:LYS:O	7:G:90:GLN:HB2	2.11	0.49
10:J:10:VAL:HG13	10:J:11:ALA:H	1.76	0.49
12:L:76:SER:O	12:L:78:LEU:N	2.45	0.49
13:N:150:LEU:O	13:N:151:ASP:CB	2.60	0.49
1:A:251:ASN:OD1	17:3:137:PHE:CD1	2.45	0.49
6:F:89:LYS:O	6:F:90:GLN:C	2.47	0.49
17:3:204:GLY:C	17:3:206:PRO:HD2	2.33	0.49
19:1:1008:CLA:CGA	19:1:1008:CLA:H43	2.42	0.49
16:2:211:PRO:O	16:2:212:GLN:HB3	2.11	0.49
4:D:105:ASP:HB2	4:D:151:LYS:CB	2.42	0.49
15:1:157:ASP:OD1	15:1:157:ASP:O	2.29	0.49
19:A:1102:CLA:HBA2	19:A:1109:CLA:C6	2.41	0.49
1:A:401:TRP:HB3	19:A:1126:CLA:HMC3	1.94	0.49
1:A:598:VAL:HG12	1:A:598:VAL:O	2.13	0.49
19:B:1205:CLA:H2	19:B:1205:CLA:H71	1.95	0.49
19:B:1214:CLA:H12	19:B:1214:CLA:C1A	2.42	0.49
2:B:396:ARG:HH11	19:B:1226:CLA:HED2	1.78	0.49
2:B:172:GLU:C	2:B:176:ASN:HB2	2.29	0.49
2:B:646:TRP:CZ2	2:B:726:ILE:HG21	2.48	0.49
19:B:1229:CLA:HBB2	21:F:6014:BCR:H23C	1.94	0.49
7:G:62:LEU:HB3	7:G:65:SER:CB	2.16	0.49
7:G:89:LYS:HZ1	7:G:89:LYS:CA	2.19	0.49
8:H:99:LYS:O	8:H:102:ILE:N	2.42	0.49
13:N:133:GLY:CA	13:N:134:CYS:CB	2.89	0.49
16:2:182:ILE:HD13	16:2:190:GLY:CA	2.34	0.49
4:D:206:GLN:O	4:D:208:TYR:N	2.45	0.49
16:2:200:TRP:HB3	16:2:202:ASP:OD1	2.12	0.49
12:L:164:LEU:HD13	12:L:165:THR:OG1	2.12	0.49
18:4:232:LEU:HB3	18:4:236:ILE:CD1	2.42	0.49
22:H:7011:LMU:C2B	22:H:7011:LMU:C6'	2.90	0.49
13:N:89:GLU:CD	13:N:89:GLU:O	2.51	0.49
18:4:239:PRO:HD2	18:4:240:TRP:H	1.78	0.49
18:4:203:LYS:NZ	19:4:4002:CLA:CAD	2.71	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:SER:C	1:A:106:TYR:N	2.66	0.49
1:A:126:ILE:O	1:A:126:ILE:HG13	2.11	0.49
1:A:385:LEU:O	1:A:386:ALA:HB3	2.12	0.49
1:A:503:THR:HB	19:A:1134:CLA:CBA	2.43	0.49
21:A:6002:BCR:C34	21:A:6002:BCR:C12	2.84	0.49
2:B:224:PRO:C	2:B:227:THR:CB	2.81	0.49
2:B:639:VAL:CG2	2:B:640:CYS:H	2.23	0.49
7:G:76:ARG:HH11	7:G:120:VAL:HB	1.78	0.49
3:C:62:PHE:CE1	5:E:80:GLU:CG	2.93	0.49
1:A:571:ASP:O	1:A:574:ASN:ND2	2.46	0.49
17:3:107:ARG:CZ	17:3:233:LEU:N	2.75	0.49
15:1:186:LYS:O	15:1:189:LYS:HG2	2.12	0.49
2:B:160:LYS:HG3	2:B:161:TRP:H	1.75	0.49
11:K:111:VAL:C	11:K:114:HIS:HB2	2.27	0.49
16:2:200:TRP:HD1	16:2:200:TRP:H	1.61	0.49
2:B:131:THR:CG2	2:B:134:ASP:N	2.55	0.49
1:A:623:ASP:O	1:A:624:VAL:HB	2.12	0.49
15:1:97:ILE:HD12	15:1:98:LEU:CD2	2.32	0.49
1:A:218:TRP:HZ3	19:A:1112:CLA:HMB3	1.77	0.49
1:A:377:TYR:CD1	1:A:616:PHE:CE1	2.99	0.49
1:A:462:ILE:HD13	19:A:9022:CLA:H93	1.95	0.49
1:A:446:LEU:CD2	1:A:554:LEU:HA	2.38	0.49
1:A:216:LEU:HD12	21:A:6002:BCR:C35	2.43	0.49
1:A:397:THR:HG21	1:A:613:ILE:CG1	2.41	0.49
1:A:618:TRP:CH2	1:A:655:ASP:HB2	2.48	0.49
1:A:618:TRP:O	1:A:618:TRP:CD1	2.66	0.49
1:A:656:PHE:O	1:A:658:TRP:N	2.46	0.49
1:A:88:ILE:O	1:A:92:TRP:HB2	2.13	0.49
2:B:311:PRO:HG3	19:B:1301:CLA:C4C	2.42	0.49
2:B:197:VAL:O	2:B:198:ALA:CB	2.60	0.49
2:B:270:LEU:HD12	2:B:271:THR:CA	2.43	0.49
2:B:321:GLY:O	2:B:322:LEU:C	2.49	0.49
2:B:471:THR:O	2:B:472:TYR:C	2.48	0.49
19:B:1205:CLA:CMC	21:B:6017:BCR:C28	2.91	0.49
2:B:618:GLY:CA	2:B:621:ARG:H	2.26	0.49
6:F:204:SER:O	6:F:205:SER:C	2.51	0.49
9:I:11:LEU:CD1	21:I:6021:BCR:C10	2.81	0.49
16:2:218:ARG:HH12	19:2:2001:CLA:HBB2	1.78	0.49
19:3:2009:CLA:H52	19:3:2009:CLA:H92	0.60	0.49
3:C:39:ILE:O	3:C:40:ALA:CB	2.61	0.49
13:N:156:GLY:CA	13:N:157:LYS:CE	2.91	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:156:GLY:HA2	13:N:157:LYS:CD	2.38	0.49
3:C:66:ARG:CB	3:C:66:ARG:NH2	2.75	0.49
3:C:29:ILE:HD11	4:D:180:GLY:O	2.12	0.49
17:3:206:PRO:HG2	17:3:208:PHE:CD2	2.47	0.49
6:F:224:GLY:O	6:F:226:LEU:O	2.30	0.49
12:L:52:PRO:O	12:L:53:THR:C	2.50	0.49
22:E:7037:LMU:O2B	22:E:7037:LMU:H5B	2.12	0.49
2:B:399:ASN:O	2:B:402:GLN:N	2.45	0.49
15:1:158:PRO:HA	15:1:175:LYS:CB	2.42	0.49
15:1:177:PRO:CD	15:1:180:LEU:CA	2.89	0.49
15:1:73:PRO:CD	15:1:74:ALA:N	2.72	0.49
15:1:85:ILE:N	15:1:88:ARG:HG3	2.27	0.49
19:A:1126:CLA:O1D	19:A:1126:CLA:H2A	2.12	0.49
19:A:1138:CLA:HBC3	21:F:6014:BCR:H332	1.93	0.49
1:A:110:LEU:C	1:A:113:PRO:HD3	2.32	0.49
1:A:184:PHE:CE2	19:A:1108:CLA:C2D	2.96	0.49
1:A:75:SER:CB	1:A:354:TRP:HZ2	2.24	0.49
1:A:89:ILE:O	1:A:93:LEU:CD2	2.61	0.49
2:B:103:ALA:HB2	2:B:105:THR:O	2.13	0.49
2:B:527:LEU:HD23	19:B:1222:CLA:C1D	2.43	0.49
2:B:718:ILE:HD13	19:B:1224:CLA:HMC2	1.95	0.49
2:B:707:LEU:HD11	19:B:1226:CLA:C9	2.42	0.49
2:B:129:LEU:CD1	19:B:1211:CLA:HMA2	2.43	0.49
2:B:216:LEU:HD21	2:B:221:GLY:CA	2.42	0.49
2:B:492:ILE:O	2:B:493:TRP:HB2	2.13	0.49
2:B:257:ILE:HG22	2:B:495:PRO:HG2	1.95	0.49
19:B:1222:CLA:HMB3	21:B:6010:BCR:H352	1.93	0.49
2:B:614:THR:O	2:B:614:THR:HG23	2.12	0.49
2:B:87:ILE:O	2:B:121:TYR:HE2	1.96	0.49
10:J:20:GLY:O	10:J:21:ALA:HB3	2.11	0.49
11:K:78:ARG:HB3	11:K:79:LYS:H	1.49	0.49
12:L:111:VAL:C	12:L:113:PRO:HD2	2.32	0.49
12:L:137:LEU:HD23	12:L:138:VAL:N	2.28	0.49
3:C:28:MET:HB3	4:D:176:LYS:O	2.13	0.49
3:C:73:THR:OG1	3:C:76:SER:OG	1.76	0.49
16:2:149:THR:O	16:2:152:LEU:CD1	2.61	0.49
17:3:150:TYR:C	17:3:151:TRP:CD1	2.77	0.49
16:2:95:ASP:CB	17:3:85:ASP:OD2	2.50	0.49
2:B:394:PHE:CE2	2:B:412:LEU:HD21	2.48	0.49
1:A:23:ASP:OD1	1:A:24:ARG:CD	2.56	0.49
19:H:1145:CLA:C14	19:H:1145:CLA:H193	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:476:ILE:O	2:B:476:ILE:CG2	2.58	0.49
13:N:126:LYS:HB3	13:N:126:LYS:HZ3	1.77	0.49
2:B:506:ASN:CG	2:B:506:ASN:O	2.51	0.49
15:1:223:ASP:CB	15:1:224:PRO:HD2	2.43	0.49
15:1:84:LEU:N	15:1:84:LEU:HD12	2.28	0.49
18:4:170:PRO:O	18:4:171:ILE:C	2.50	0.49
18:4:177:LEU:HD22	18:4:178:PRO:CB	2.43	0.49
18:4:177:LEU:CD2	18:4:178:PRO:N	2.68	0.49
18:4:202:GLU:HA	18:4:205:ILE:CG2	2.42	0.49
19:A:1107:CLA:HBA2	19:A:1107:CLA:HBD	1.93	0.49
1:A:370:ILE:CD1	19:A:1124:CLA:C3D	2.90	0.49
1:A:740:LEU:CD2	19:A:1140:CLA:HMA1	2.41	0.49
1:A:223:VAL:O	1:A:228:PRO:HD3	2.13	0.49
1:A:312:ILE:O	1:A:313:ALA:CB	2.60	0.49
1:A:355:HIS:O	1:A:358:LEU:HG	2.12	0.49
1:A:705:GLU:CB	2:B:545:LYS:HZ2	2.26	0.49
2:B:175:LEU:HD21	19:B:1216:CLA:HMA1	1.95	0.49
2:B:223:GLY:O	2:B:225:LEU:HB3	2.13	0.49
2:B:232:LEU:HD12	2:B:235:GLN:HG3	1.78	0.49
2:B:326:ILE:O	2:B:326:ILE:CG1	2.60	0.49
2:B:469:LYS:HG3	2:B:470:THR:OG1	2.12	0.49
2:B:622:ASP:CB	2:B:626:LEU:HG	2.40	0.49
6:F:149:ILE:HG22	6:F:151:SER:H	1.78	0.49
7:G:119:PRO:HB2	7:G:120:VAL:HG23	1.95	0.49
7:G:61:ALA:O	7:G:63:VAL:CG1	2.61	0.49
1:A:244:LEU:CD1	1:A:247:GLU:OE2	2.56	0.49
19:2:2002:CLA:CHD	19:2:2002:CLA:CBC	2.90	0.49
18:4:87:ASN:OD1	18:4:90:TRP:CD2	2.66	0.49
16:2:149:THR:OG1	16:2:150:THR:N	2.46	0.49
16:2:182:ILE:HG21	16:2:187:LYS:HE2	1.95	0.49
12:L:101:GLU:HG3	19:L:1501:CLA:C1A	2.43	0.49
17:3:206:PRO:O	17:3:206:PRO:CD	2.61	0.49
1:A:487:VAL:CG1	1:A:489:ALA:N	2.55	0.49
17:3:171:ARG:O	17:3:172:ARG:C	2.49	0.49
15:1:204:GLN:HE21	19:1:1003:CLA:CBB	2.26	0.49
19:R:1144:CLA:HBD	19:R:1144:CLA:HBA2	1.95	0.49
13:N:127:PHE:HD1	13:N:128:PRO:HA	1.78	0.49
15:1:158:PRO:CD	15:1:159:GLU:N	2.76	0.49
19:A:1138:CLA:NC	19:A:1138:CLA:H52	2.27	0.49
1:A:224:HIS:HE1	19:A:1113:CLA:CHD	2.26	0.49
1:A:226:SER:O	1:A:230:ASN:ND2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:HIS:HE1	19:A:1117:CLA:C1B	2.25	0.49
1:A:532:ILE:O	1:A:532:ILE:HG12	2.13	0.49
1:A:723:ARG:H	19:A:1139:CLA:CBB	2.17	0.49
19:A:9022:CLA:H142	19:B:1206:CLA:HBB2	1.94	0.49
19:A:9022:CLA:C12	19:A:9022:CLA:H71	2.41	0.49
2:B:120:VAL:O	2:B:123:TRP:CD1	2.64	0.49
19:B:1221:CLA:CMB	19:B:1223:CLA:H92	2.43	0.49
2:B:590:VAL:O	2:B:593:TYR:HB3	2.13	0.49
2:B:649:MET:SD	2:B:723:ALA:HB2	2.53	0.49
19:A:1138:CLA:CMD	21:F:6014:BCR:HC41	2.36	0.49
7:G:83:GLN:OE1	19:G:1242:CLA:C2D	2.60	0.49
8:H:98:LEU:O	8:H:99:LYS:O	2.30	0.49
6:F:199:ASP:CA	10:J:9:SER:HA	2.42	0.49
11:K:63:LEU:O	11:K:64:MET:C	2.50	0.49
12:L:81:TRP:C	12:L:83:LEU:H	2.17	0.49
16:2:125:PHE:CA	16:2:127:THR:CG2	2.60	0.49
13:N:148:ASP:H	13:N:149:ASP:CA	2.26	0.49
13:N:164:SER:CA	13:N:165:ASN:C	2.77	0.49
2:B:549:ASP:HB2	3:C:63:LEU:HD12	1.95	0.49
1:A:575:LEU:HD11	1:A:579:PHE:CB	2.40	0.49
17:3:157:LEU:O	17:3:160:LEU:HB3	2.12	0.49
17:3:167:PHE:O	17:3:168:ALA:C	2.50	0.49
18:4:112:PRO:CA	18:4:117:SER:OG	2.61	0.49
12:L:54:TYR:CD1	12:L:57:ILE:HG23	2.47	0.49
1:A:628:ILE:CD1	1:A:629:ASN:O	2.61	0.49
15:1:85:ILE:CA	15:1:88:ARG:CG	2.72	0.48
1:A:246:HIS:NE2	19:3:1147:CLA:O1D	2.46	0.48
19:A:1131:CLA:H101	19:A:1131:CLA:H143	1.94	0.48
1:A:378:SER:OG	1:A:512:SER:OG	2.29	0.48
1:A:366:GLY:O	1:A:403:GLY:HA2	2.13	0.48
1:A:412:ALA:O	1:A:415:ALA:HB3	2.13	0.48
1:A:488:PHE:CD1	1:A:535:GLY:N	2.81	0.48
19:B:1225:CLA:H62	21:B:6006:BCR:C32	2.42	0.48
2:B:427:LEU:HB3	19:B:1229:CLA:HED1	1.95	0.48
2:B:421:HIS:O	19:B:1236:CLA:HMC3	2.13	0.48
2:B:438:VAL:O	2:B:442:VAL:N	2.44	0.48
2:B:454:LEU:HD13	2:B:514:PRO:CG	2.43	0.48
2:B:507:SER:O	2:B:508:LEU:CB	2.60	0.48
19:F:1302:CLA:C3B	19:F:1305:CLA:HAC2	2.41	0.48
7:G:116:SER:OG	7:G:119:PRO:HB2	2.13	0.48
22:G:7026:LMU:H11	22:G:7026:LMU:H3'	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:99:HIS:O	7:G:101:GLU:CA	2.61	0.48
19:A:1132:CLA:O1D	12:L:119:PRO:O	2.31	0.48
16:2:226:ARG:CG	16:2:226:ARG:NH1	2.67	0.48
13:N:146:LEU:HD21	13:N:148:ASP:O	2.12	0.48
17:3:100:TYR:HA	17:3:229:LYS:HE2	1.94	0.48
17:3:238:ILE:HD12	19:3:3003:CLA:HMC2	1.87	0.48
16:2:153:PHE:CD2	16:2:157:LEU:CD2	2.96	0.48
1:A:423:ASP:H	1:A:424:PRO:HD3	1.76	0.48
19:J:1311:CLA:C14	19:J:1311:CLA:O1A	2.59	0.48
2:B:143:LEU:C	2:B:145:LEU:N	2.66	0.48
18:4:107:ALA:O	18:4:110:LEU:HB3	2.13	0.48
2:B:85:ARG:NH1	2:B:85:ARG:HG2	2.04	0.48
21:1:6023:BCR:HC8	21:1:6023:BCR:C2	2.42	0.48
1:A:39:HIS:HA	1:A:44:ILE:CG2	2.43	0.48
2:B:657:TRP:O	2:B:660:GLY:N	2.34	0.48
17:3:182:MET:HG2	17:3:183:GLY:N	2.28	0.48
18:4:123:VAL:O	18:4:123:VAL:HG22	2.13	0.48
19:A:1123:CLA:C14	19:A:1123:CLA:HMD2	2.41	0.48
19:A:1151:CLA:CED	19:A:1151:CLA:CBA	2.91	0.48
1:A:552:THR:O	1:A:553:VAL:HB	2.13	0.48
1:A:618:TRP:HB2	1:A:656:PHE:CE1	2.48	0.48
1:A:679:PHE:O	1:A:683:HIS:CB	2.61	0.48
2:B:317:ARG:HH12	2:B:410:ARG:HG2	1.75	0.48
19:A:1237:CLA:HMD2	21:B:6017:BCR:H313	1.95	0.48
19:A:9022:CLA:CAD	19:B:9010:CLA:HMB3	2.42	0.48
5:E:83:TRP:CH2	5:E:116:SER:OG	2.63	0.48
7:G:100:PHE:HD2	7:G:100:PHE:O	1.96	0.48
7:G:120:VAL:O	7:G:120:VAL:CG1	2.57	0.48
17:3:108:PHE:CD2	19:3:3013:CLA:H43	2.48	0.48
16:2:150:THR:C	16:2:152:LEU:HD13	2.33	0.48
16:2:189:THR:O	16:2:190:GLY:C	2.50	0.48
2:B:4:ARG:O	2:B:4:ARG:CZ	2.60	0.48
1:A:439:ARG:HG2	1:A:562:PHE:CE2	2.47	0.48
1:A:258:LEU:HG	1:A:280:PHE:CD1	2.47	0.48
1:A:464:ASN:O	1:A:468:SER:N	2.42	0.48
10:J:14:VAL:O	10:J:14:VAL:CG1	2.59	0.48
18:4:239:PRO:HD2	18:4:240:TRP:N	2.28	0.48
19:A:1139:CLA:C3	19:A:1139:CLA:O1A	2.62	0.48
1:A:309:LEU:HA	1:A:312:ILE:O	2.13	0.48
1:A:350:LEU:HD23	1:A:350:LEU:HA	1.37	0.48
1:A:382:TYR:HB2	1:A:385:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:ALA:HA	1:A:444:SER:HB3	1.95	0.48
21:A:6007:BCR:C23	21:A:6007:BCR:C38	2.85	0.48
1:A:665:ILE:HD13	2:B:621:ARG:HG3	1.95	0.48
19:B:1218:CLA:HMA3	19:B:1219:CLA:C3D	2.43	0.48
19:B:1222:CLA:HED1	19:B:1223:CLA:HMD2	1.95	0.48
2:B:361:ILE:O	2:B:362:ALA:O	2.31	0.48
2:B:373:THR:O	2:B:377:TYR:N	2.36	0.48
2:B:404:ALA:O	2:B:405:ASP:OD1	2.30	0.48
10:J:21:ALA:O	10:J:23:ALA:N	2.46	0.48
16:2:122:ILE:CD1	19:2:2002:CLA:HMB1	2.42	0.48
3:C:43:PRO:HA	4:D:182:GLN:CG	2.43	0.48
12:L:205:TYR:O	12:L:205:TYR:CG	2.65	0.48
4:D:140:LEU:CB	4:D:143:ARG:HB2	2.40	0.48
17:3:205:GLY:H	17:3:206:PRO:HD2	1.76	0.48
11:K:115:ILE:CG1	11:K:122:LEU:HD12	2.43	0.48
6:F:220:GLU:HG3	6:F:220:GLU:O	2.13	0.48
2:B:70:TRP:CB	2:B:136:TYR:HH	2.25	0.48
15:1:199:VAL:HG12	15:1:200:GLY:N	2.28	0.48
1:A:39:HIS:O	1:A:40:PHE:HB3	2.12	0.48
1:A:482:ILE:O	1:A:482:ILE:HG23	2.13	0.48
18:4:179:ALA:O	18:4:180:GLY:C	2.49	0.48
2:B:165:VAL:O	2:B:166:SER:C	2.50	0.48
6:F:78:ASP:OD1	6:F:154:GLN:NE2	2.39	0.48
15:1:223:ASP:O	15:1:225:TRP:HB2	2.13	0.48
18:4:206:ALA:C	18:4:208:GLY:N	2.66	0.48
19:A:1103:CLA:H141	19:A:1103:CLA:H161	1.68	0.48
1:A:370:ILE:HD11	19:A:1124:CLA:CAD	2.41	0.48
19:A:1128:CLA:H192	21:A:6011:BCR:H20C	1.95	0.48
19:A:1122:CLA:ND	21:A:6007:BCR:H19C	2.27	0.48
1:A:619:LYS:O	1:A:621:GLN:N	2.46	0.48
19:B:1202:CLA:HAC1	19:B:1226:CLA:HMA1	1.94	0.48
19:B:1231:CLA:HMC3	19:B:1234:CLA:H2	1.94	0.48
19:B:1234:CLA:HBC3	19:B:1234:CLA:CMC	2.35	0.48
2:B:314:ARG:CZ	15:1:67:LEU:CD2	2.77	0.48
2:B:666:SER:CB	2:B:671:TRP:HE1	2.13	0.48
2:B:707:LEU:HD13	23:B:7101:LMG:H301	1.96	0.48
2:B:98:GLN:HB2	2:B:99:PRO:HD2	1.96	0.48
9:I:19:VAL:O	9:I:23:SER:N	2.46	0.48
10:J:21:ALA:O	10:J:22:LEU:C	2.51	0.48
13:N:147:SER:O	13:N:151:ASP:CG	2.52	0.48
2:B:560:ASP:CG	3:C:66:ARG:CZ	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:173:TYR:O	4:D:173:TYR:CG	2.62	0.48
1:A:250:LEU:H	17:3:136:TRP:HH2	1.60	0.48
1:A:249:ILE:HG23	17:3:137:PHE:CE2	2.49	0.48
16:2:169:ALA:O	16:2:170:ASP:HB3	2.13	0.48
16:2:184:PRO:N	16:2:187:LYS:HD2	2.28	0.48
16:2:160:ILE:CB	19:2:2012:CLA:HBB1	2.37	0.48
13:N:110:THR:O	13:N:112:ALA:O	2.31	0.48
11:K:125:LYS:CG	11:K:128:GLY:HA2	2.43	0.48
1:A:420:ARG:CB	1:A:420:ARG:CZ	2.91	0.48
15:1:68:GLY:HA2	15:1:72:VAL:HB	1.93	0.48
15:1:83:GLU:CA	15:1:83:GLU:OE2	2.55	0.48
18:4:169:ASP:HA	18:4:173:LYS:C	2.33	0.48
18:4:207:ASN:ND2	19:4:4002:CLA:C1A	2.72	0.48
19:A:1128:CLA:HAA1	19:A:1128:CLA:HBD	1.96	0.48
19:A:1138:CLA:HBC3	19:A:1138:CLA:HHD	1.96	0.48
1:A:130:GLU:OE1	1:A:133:ASN:HB3	2.13	0.48
1:A:502:THR:CB	1:A:504:ALA:H	2.25	0.48
19:A:1119:CLA:H162	21:A:6008:BCR:H271	1.96	0.48
1:A:681:GLY:C	1:A:683:HIS:H	2.16	0.48
1:A:733:VAL:HG21	19:A:1140:CLA:HMD3	1.94	0.48
2:B:697:PRO:CG	19:B:1238:CLA:HBC3	2.44	0.48
2:B:230:TRP:CE3	19:B:1213:CLA:HAA2	2.49	0.48
2:B:374:HIS:HB2	19:B:1224:CLA:C4B	2.42	0.48
6:F:83:THR:CB	6:F:84:PRO:CD	2.91	0.48
7:G:84:ARG:NH1	7:G:89:LYS:H	2.11	0.48
8:H:113:SER:OG	19:H:1207:CLA:H2	2.12	0.48
13:N:139:LYS:O	13:N:140:GLN:C	2.51	0.48
13:N:143:VAL:HG11	13:N:155:GLU:OE1	2.14	0.48
2:B:560:ASP:CG	2:B:561:GLY:N	2.66	0.48
3:C:7:ILE:HG21	3:C:54:CYS:SG	2.54	0.48
6:F:230:ASN:C	6:F:231:PHE:O	2.51	0.48
15:1:163:TYR:N	15:1:164:PRO:CD	2.76	0.48
22:K:7042:LMU:H71	22:K:7042:LMU:C2	2.43	0.48
16:2:145:TYR:C	16:2:146:PHE:CD1	2.87	0.48
19:A:1119:CLA:HAA2	19:A:1123:CLA:HBB2	1.95	0.48
1:A:182:GLY:C	19:A:1109:CLA:HAC1	2.33	0.48
1:A:282:THR:O	1:A:283:PHE:C	2.52	0.48
1:A:390:ALA:HA	1:A:393:LEU:CD2	2.44	0.48
1:A:691:MET:CE	20:A:5001:PQN:H2M2	2.44	0.48
1:A:680:LEU:HD21	2:B:617:MET:CE	2.43	0.48
1:A:73:GLU:O	1:A:76:ARG:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1140:CLA:H102	19:A:9013:CLA:H152	1.95	0.48
19:B:1214:CLA:H112	19:B:1232:CLA:H3A	1.96	0.48
2:B:22:TRP:HE1	19:B:1238:CLA:CAB	2.17	0.48
2:B:620:LEU:O	2:B:621:ARG:C	2.50	0.48
2:B:709:GLY:O	2:B:710:LEU:CB	2.59	0.48
7:G:98:THR:OG1	7:G:100:PHE:N	2.47	0.48
7:G:73:PHE:O	7:G:76:ARG:CB	2.56	0.48
7:G:89:LYS:C	7:G:90:GLN:HG2	2.34	0.48
12:L:148:TYR:C	12:L:150:ILE:H	2.16	0.48
3:C:61:ASP:CG	5:E:118:ASN:HD21	2.14	0.48
13:N:144:PRO:C	13:N:151:ASP:OD1	2.52	0.48
3:C:73:THR:HG23	3:C:76:SER:CB	2.42	0.48
13:N:118:TYR:C	13:N:119:THR:OG1	2.52	0.48
4:D:123:ARG:NH2	22:D:7050:LMU:H4B	1.98	0.48
19:1:1007:CLA:HAA1	22:4:7008:LMU:O3'	2.13	0.48
22:R:7020:LMU:C6B	22:R:7020:LMU:H6E	2.42	0.48
2:B:138:GLY:O	2:B:139:ALA:C	2.50	0.48
8:H:111:TYR:CD1	8:H:112:LEU:HD23	2.48	0.48
4:D:148:TYR:C	4:D:148:TYR:CD2	2.86	0.48
22:1:7013:LMU:O6B	22:1:7013:LMU:C1B	2.58	0.48
15:1:58:ALA:CB	19:1:1015:CLA:C2B	2.91	0.48
15:1:74:ALA:HB3	15:1:75:ASN:CG	2.34	0.48
18:4:168:GLN:O	18:4:172:PHE:CD1	2.66	0.48
18:4:209:ARG:O	18:4:212:LEU:CA	2.61	0.48
19:A:1105:CLA:CGA	19:A:1107:CLA:H12	2.43	0.48
1:A:402:ILE:HD11	19:A:1127:CLA:CBB	2.44	0.48
1:A:462:ILE:HG21	19:A:1132:CLA:CMC	2.43	0.48
19:A:1133:CLA:C2B	21:A:6008:BCR:H333	2.44	0.48
1:A:87:SER:HB3	1:A:178:MET:O	2.14	0.48
19:A:9011:CLA:CBB	19:A:9012:CLA:HED1	2.43	0.48
1:A:98:PHE:O	1:A:100:GLY:CA	2.62	0.48
2:B:103:ALA:HA	2:B:105:THR:CA	2.43	0.48
2:B:103:ALA:CB	2:B:105:THR:O	2.61	0.48
19:B:1202:CLA:H43	21:B:6005:BCR:C31	2.38	0.48
19:B:1224:CLA:O1D	19:B:1225:CLA:CMA	2.54	0.48
2:B:389:HIS:HE1	19:B:1226:CLA:NC	2.11	0.48
2:B:183:PHE:HE1	19:B:1210:CLA:H71	1.79	0.48
2:B:305:LEU:HD23	19:B:1220:CLA:O1D	2.14	0.48
2:B:326:ILE:HG13	2:B:332:PHE:HB3	1.96	0.48
2:B:649:MET:CE	21:B:6017:BCR:H272	2.44	0.48
2:B:98:GLN:CB	2:B:99:PRO:HD2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:L:1502:CLA:CMC	19:L:1502:CLA:HBC3	2.44	0.48
4:D:86:SER:CA	12:L:69:LEU:HD21	2.43	0.48
13:N:139:LYS:CG	13:N:142:LYS:HE2	2.41	0.48
13:N:155:GLU:OE2	13:N:157:LYS:O	2.32	0.48
2:B:559:CYS:SG	2:B:560:ASP:N	2.86	0.48
16:2:157:LEU:HA	16:2:157:LEU:HD12	1.59	0.48
8:H:86:THR:HG23	8:H:89:ALA:HB2	1.94	0.48
16:2:233:MET:SD	16:2:236:TRP:CD1	3.07	0.48
11:K:116:ILE:CG2	11:K:117:GLY:H	2.26	0.48
17:3:191:GLU:O	17:3:192:LYS:CD	2.62	0.48
2:B:131:THR:C	2:B:135:LEU:CD2	2.80	0.48
2:B:436:LEU:O	2:B:437:TYR:CB	2.61	0.48
19:A:1110:CLA:C4D	19:A:1111:CLA:HMC3	2.43	0.48
1:A:281:LEU:CB	19:A:1115:CLA:HED2	2.44	0.48
1:A:188:LYS:HD2	1:A:188:LYS:O	2.14	0.48
1:A:547:PHE:HE2	19:A:9023:CLA:O1A	1.97	0.48
19:A:9023:CLA:HBC2	19:A:9023:CLA:HMC1	1.96	0.48
1:A:93:LEU:H	1:A:96:MET:H	1.60	0.48
2:B:382:ILE:HD11	19:B:1203:CLA:H142	1.95	0.48
2:B:493:TRP:HB2	19:B:1232:CLA:HED2	1.96	0.48
1:A:690:LEU:HD21	2:B:661:PHE:HE1	1.78	0.48
3:C:1:MET:SD	3:C:4:SER:CB	3.02	0.48
6:F:82:LEU:HG	6:F:83:THR:OG1	2.14	0.48
11:K:48:PHE:HB2	11:K:50:GLY:H	1.79	0.48
16:2:229:MET:CE	16:2:230:LEU:HD13	2.43	0.48
13:N:133:GLY:CA	13:N:134:CYS:HB2	2.44	0.48
13:N:148:ASP:N	13:N:149:ASP:CA	2.76	0.48
13:N:157:LYS:CB	13:N:159:LYS:N	2.57	0.48
3:C:66:ARG:HB3	3:C:66:ARG:CZ	2.44	0.48
15:1:189:LYS:CE	15:1:189:LYS:N	2.77	0.48
19:K:1142:CLA:HBD	19:K:1142:CLA:HAA2	1.94	0.48
22:N:7049:LMU:C4	22:N:7049:LMU:O1'	2.61	0.48
1:A:316:MET:HA	1:A:317:TYR:HD1	1.79	0.48
1:A:316:MET:CA	1:A:317:TYR:HD1	2.27	0.48
18:4:243:THR:CG2	18:4:244:ILE:O	2.53	0.48
2:B:7:ARG:CB	2:B:7:ARG:NH1	2.69	0.48
6:F:142:SER:C	6:F:144:GLY:H	2.17	0.48
15:1:77:GLU:CG	15:1:80:LYS:CD	2.78	0.48
15:1:92:LEU:N	15:1:95:PRO:HD3	2.26	0.48
18:4:177:LEU:CD1	18:4:178:PRO:CD	2.59	0.48
19:A:1119:CLA:H43	19:A:1122:CLA:H2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1136:CLA:H71	19:A:1136:CLA:H112	1.60	0.48
19:A:1140:CLA:H62	19:A:9013:CLA:H171	1.96	0.48
1:A:390:ALA:CB	1:A:754:ILE:HD13	2.43	0.48
19:A:9011:CLA:C1A	19:B:9010:CLA:HBB2	2.44	0.48
2:B:405:ASP:C	2:B:405:ASP:OD1	2.52	0.48
2:B:500:ALA:CB	2:B:503:GLU:OE2	2.60	0.48
2:B:594:TRP:CD2	2:B:598:HIS:CE1	3.02	0.48
2:B:685:THR:HG22	2:B:685:THR:O	2.14	0.48
6:F:204:SER:O	6:F:207:LEU:HB3	2.14	0.48
16:2:128:LYS:HB3	16:2:131:ILE:CG1	2.35	0.48
13:N:132:THR:CB	13:N:137:LEU:O	2.62	0.48
4:D:165:TYR:CD2	4:D:168:PRO:HG2	2.49	0.48
14:R:38:UNK:O	14:R:39:UNK:C	2.62	0.48
6:F:194:LYS:N	6:F:195:GLU:OE2	2.47	0.48
1:A:249:ILE:HG22	17:3:137:PHE:CE2	2.49	0.48
19:L:1148:CLA:HED3	19:L:1148:CLA:H72	1.96	0.48
16:2:184:PRO:CG	16:2:185:ASN:N	2.77	0.48
11:K:125:LYS:CD	11:K:128:GLY:HA2	2.44	0.48
15:1:162:LYS:CG	15:1:163:TYR:H	2.24	0.48
3:C:36:ALA:C	3:C:37:LYS:HG2	2.34	0.48
18:4:131:LYS:N	18:4:131:LYS:CD	2.69	0.48
22:B:7038:LMU:O6'	22:B:7038:LMU:C1B	2.62	0.48
2:B:62:SER:OG	2:B:63:GLY:N	2.47	0.48
22:4:7019:LMU:H32	22:4:7019:LMU:O2'	2.13	0.48
15:1:94:VAL:O	15:1:98:LEU:HB2	2.14	0.48
19:A:1112:CLA:CBA	19:3:1147:CLA:HMC3	2.42	0.48
1:A:348:GLU:O	1:A:349:ILE:C	2.52	0.48
1:A:358:LEU:O	1:A:361:ASN:HB3	2.14	0.48
1:A:493:GLN:HG2	1:A:516:GLY:H	1.79	0.48
1:A:588:GLY:N	2:B:668:ARG:NH1	2.60	0.48
1:A:664:VAL:HG23	1:A:665:ILE:HG23	1.95	0.48
1:A:701:GLN:NE2	1:A:724:ALA:H	2.12	0.48
1:A:733:VAL:HG22	19:A:1140:CLA:CAD	2.43	0.48
19:B:1231:CLA:HMB3	19:B:1234:CLA:HED3	1.96	0.48
2:B:172:GLU:OE1	2:B:301:ILE:HG13	2.14	0.48
2:B:469:LYS:C	2:B:501:ILE:CA	2.68	0.48
2:B:618:GLY:HA2	2:B:621:ARG:CB	2.40	0.48
6:F:207:LEU:N	6:F:207:LEU:HD13	2.28	0.48
7:G:80:PHE:CE1	7:G:83:GLN:O	2.67	0.48
12:L:85:ASN:O	12:L:92:ALA:CB	2.55	0.48
19:2:2001:CLA:HBA2	19:2:2001:CLA:H3A	1.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:133:GLY:HA2	13:N:134:CYS:HB2	1.96	0.48
17:3:96:ARG:NH1	17:3:100:TYR:OH	2.43	0.48
1:A:426:THR:HG23	1:A:428:TYR:CE2	2.45	0.48
1:A:316:MET:CA	1:A:317:TYR:CB	2.91	0.48
13:N:96:LYS:HG3	13:N:97:THR:HG1	1.75	0.48
2:B:416:GLU:H	2:B:416:GLU:CD	2.16	0.48
22:4:7034:LMU:C11	22:4:7052:LMU:O3'	2.61	0.47
18:4:142:PHE:O	18:4:143:VAL:C	2.51	0.47
18:4:169:ASP:OD1	18:4:174:GLN:CA	2.62	0.47
18:4:177:LEU:HD13	18:4:178:PRO:HD2	1.95	0.47
18:4:209:ARG:HA	18:4:212:LEU:HD12	1.95	0.47
19:A:1128:CLA:H152	19:A:1128:CLA:H101	1.96	0.47
19:A:1124:CLA:H43	19:A:1136:CLA:CBA	2.39	0.47
1:A:211:LEU:HB3	1:A:310:PHE:CD2	2.49	0.47
1:A:545:HIS:ND1	19:A:1135:CLA:CBB	2.76	0.47
19:A:1126:CLA:C7	21:A:6011:BCR:H371	2.44	0.47
1:A:63:ASP:CA	19:A:1128:CLA:HED2	2.43	0.47
1:A:93:LEU:CA	1:A:96:MET:N	2.69	0.47
2:B:377:TYR:O	2:B:378:ILE:HB	2.14	0.47
2:B:586:THR:C	2:B:588:GLY:N	2.56	0.47
2:B:658:ALA:O	2:B:661:PHE:HD2	1.96	0.47
19:A:9022:CLA:OBD	19:B:9010:CLA:HMB3	2.14	0.47
6:F:208:PHE:O	6:F:209:ARG:C	2.48	0.47
12:L:112:GLY:C	19:L:1503:CLA:HMC3	2.34	0.47
16:2:128:LYS:HD2	16:2:128:LYS:HA	1.61	0.47
13:N:132:THR:CB	13:N:139:LYS:CD	2.90	0.47
15:1:93:ALA:CA	19:1:1006:CLA:C4B	2.91	0.47
4:D:97:GLU:HB2	4:D:98:GLU:HG2	1.96	0.47
8:H:81:SER:O	8:H:83:LEU:HD22	2.14	0.47
19:K:1143:CLA:HAC2	22:K:7001:LMU:H3O1	1.66	0.47
6:F:121:ALA:HB1	6:F:125:LYS:HB3	1.95	0.47
2:B:542:ARG:CG	2:B:542:ARG:NH1	2.41	0.47
19:1:1303:CLA:HMC1	19:4:1304:CLA:CMB	2.40	0.47
19:H:1145:CLA:HED2	19:H:1145:CLA:HAA1	1.93	0.47
1:A:70:ASP:C	1:A:72:GLU:HG2	2.34	0.47
4:D:149:LYS:HE3	4:D:149:LYS:HB3	1.28	0.47
15:1:114:TRP:HH2	15:1:121:GLN:CA	2.27	0.47
18:4:225:GLY:HA2	18:4:226:LYS:NZ	2.24	0.47
1:A:122:VAL:O	19:A:1105:CLA:HED2	2.14	0.47
19:A:1106:CLA:ND	19:A:1126:CLA:H42	2.29	0.47
19:A:1117:CLA:HBC1	21:A:6003:BCR:H12C	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:TRP:CZ3	1:A:728:VAL:HG13	2.50	0.47
19:B:1227:CLA:HBA2	19:B:1227:CLA:H3A	1.50	0.47
19:B:1214:CLA:H8	19:B:1232:CLA:HMA1	1.96	0.47
2:B:167:TRP:CZ2	19:B:1210:CLA:CAC	2.97	0.47
2:B:203:ARG:O	2:B:245:GLY:C	2.53	0.47
2:B:495:PRO:HD2	2:B:497:TRP:HB2	1.95	0.47
2:B:607:SER:HA	2:B:610:ASN:ND2	2.29	0.47
2:B:668:ARG:CG	2:B:699:ALA:O	2.62	0.47
12:L:79:ILE:HD12	19:L:1504:CLA:HMA2	1.95	0.47
3:C:11:CYS:SG	24:C:8003:SF4:S3	3.12	0.47
15:1:145:ILE:O	15:1:148:VAL:HG13	2.14	0.47
1:A:252:ARG:O	1:A:252:ARG:CZ	2.62	0.47
1:A:261:SER:C	1:A:263:ALA:N	2.66	0.47
16:2:184:PRO:CD	16:2:185:ASN:HA	2.44	0.47
18:4:138:SER:O	18:4:139:SER:CB	2.61	0.47
1:A:258:LEU:O	1:A:259:TYR:HD2	1.96	0.47
12:L:52:PRO:HB2	12:L:55:GLN:C	2.32	0.47
12:L:161:ALA:N	12:L:162:PRO:CD	2.77	0.47
15:1:58:ALA:HB3	15:1:59:PRO:HD3	1.96	0.47
18:4:214:PHE:O	18:4:215:LEU:O	2.32	0.47
1:A:91:LEU:O	19:A:1105:CLA:HMC3	2.13	0.47
1:A:350:LEU:O	1:A:350:LEU:HD22	2.14	0.47
1:A:362:LEU:HG	1:A:406:LEU:HG	1.96	0.47
1:A:438:HIS:HB2	1:A:441:ALA:CB	2.44	0.47
1:A:50:THR:HG22	1:A:52:THR:N	2.27	0.47
1:A:651:GLY:O	1:A:655:ASP:N	2.41	0.47
1:A:697:ARG:C	1:A:699:TYR:H	2.17	0.47
1:A:64:PHE:CG	1:A:74:ILE:HD13	2.49	0.47
19:B:1206:CLA:HAA1	19:B:1206:CLA:H12	1.97	0.47
2:B:198:ALA:H	2:B:200:PRO:HG2	1.80	0.47
2:B:19:ARG:O	2:B:23:PHE:HB2	2.15	0.47
2:B:183:PHE:HB3	2:B:284:PHE:CD2	2.48	0.47
2:B:292:ARG:HH12	2:B:295:PHE:N	2.13	0.47
2:B:469:LYS:C	2:B:501:ILE:HA	2.34	0.47
2:B:55:ALA:HB1	2:B:150:LEU:HD12	1.97	0.47
2:B:587:ILE:HA	2:B:587:ILE:HD13	1.72	0.47
21:B:6006:BCR:HC8	21:B:6006:BCR:C33	2.39	0.47
1:A:653:LEU:HD13	19:B:9010:CLA:HBC2	1.96	0.47
11:K:47:ASP:N	11:K:51:SER:CB	2.77	0.47
11:K:75:SER:O	11:K:76:ALA:CB	2.61	0.47
12:L:83:LEU:HD13	12:L:88:ALA:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:168:TRP:NE1	16:2:171:ILE:HG21	2.21	0.47
12:L:209:LEU:CG	12:L:210:PRO:CD	2.92	0.47
6:F:127:LYS:O	6:F:129:ARG:CA	2.60	0.47
6:F:99:LEU:O	6:F:102:LEU:CG	2.30	0.47
13:N:120:VAL:HG12	13:N:122:PHE:CD2	2.49	0.47
16:2:212:GLN:CG	16:2:213:LYS:N	2.74	0.47
1:A:220:ARG:O	1:A:221:HIS:CB	2.62	0.47
6:F:85:CYS:O	6:F:86:LYS:C	2.52	0.47
18:4:176:SER:OG	18:4:177:LEU:HD13	2.14	0.47
1:A:126:ILE:CD1	19:A:1107:CLA:CMA	2.86	0.47
19:A:1126:CLA:HAA1	19:A:1126:CLA:HBD	1.95	0.47
1:A:405:PHE:O	19:A:1128:CLA:HMC1	2.15	0.47
1:A:349:ILE:O	1:A:351:THR:N	2.47	0.47
1:A:619:LYS:HG2	1:A:642:PHE:CE1	2.50	0.47
2:B:375:HIS:CE1	19:B:1225:CLA:NC	2.82	0.47
2:B:693:TRP:HD1	19:B:1238:CLA:C3D	2.27	0.47
2:B:98:GLN:CB	2:B:99:PRO:CD	2.92	0.47
12:L:143:LEU:N	12:L:145:LEU:N	2.60	0.47
12:L:91:THR:HA	12:L:98:ARG:NH1	2.22	0.47
1:A:27:ILE:O	1:A:28:LYS:CD	2.62	0.47
13:N:157:LYS:HG2	13:N:159:LYS:CG	2.44	0.47
6:F:192:THR:O	6:F:193:GLN:HG3	2.14	0.47
17:3:124:LYS:CG	17:3:124:LYS:O	2.62	0.47
19:J:1311:CLA:C15	19:2:2014:CLA:HMB1	2.43	0.47
4:D:132:ALA:HB3	4:D:136:GLN:NE2	2.21	0.47
19:H:1145:CLA:HAA1	19:H:1145:CLA:HED1	1.96	0.47
17:3:159:VAL:O	17:3:161:GLU:C	2.53	0.47
1:A:483:GLN:CB	1:A:485:GLN:CD	2.79	0.47
2:B:130:ARG:NH1	2:B:130:ARG:CG	2.71	0.47
1:A:629:ASN:CG	1:A:630:ASP:N	2.68	0.47
16:2:261:THR:C	16:2:262:ILE:HG23	2.35	0.47
1:A:44:ILE:HG22	1:A:45:ALA:H	1.79	0.47
12:L:181:GLY:O	12:L:184:LYS:HG2	2.14	0.47
18:4:159:ASP:OD2	18:4:163:PRO:CA	2.60	0.47
18:4:161:LYS:NZ	18:4:162:ASN:HD21	2.12	0.47
18:4:214:PHE:O	18:4:218:ILE:HG13	2.15	0.47
19:A:1102:CLA:H12	19:A:1109:CLA:C6	2.20	0.47
19:A:1106:CLA:ND	19:A:1126:CLA:C4	2.77	0.47
19:A:1138:CLA:H122	19:A:1138:CLA:HBB1	1.97	0.47
1:A:130:GLU:O	1:A:131:ILE:C	2.51	0.47
1:A:143:ILE:HG23	1:A:143:ILE:HD12	1.64	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:LEU:CD1	19:A:1115:CLA:CBB	2.93	0.47
1:A:330:ILE:O	1:A:330:ILE:HG22	2.13	0.47
1:A:454:GLY:N	1:A:457:SER:HB3	2.07	0.47
1:A:73:GLU:O	1:A:76:ARG:CB	2.62	0.47
19:A:9012:CLA:H152	19:A:9012:CLA:H101	1.94	0.47
2:B:224:PRO:CB	2:B:227:THR:OG1	2.62	0.47
2:B:544:SER:O	2:B:546:LEU:N	2.48	0.47
2:B:365:PHE:HD1	2:B:602:TRP:NE1	2.12	0.47
2:B:73:ASN:ND2	2:B:73:ASN:N	2.61	0.47
19:A:1237:CLA:HMB2	19:L:1502:CLA:CBC	2.42	0.47
12:L:59:PRO:O	12:L:60:ILE:HB	2.14	0.47
16:2:123:PRO:O	16:2:124:GLU:C	2.50	0.47
8:H:120:ILE:O	8:H:121:LEU:O	2.31	0.47
2:B:157:LEU:HB3	2:B:158:GLN:HG2	1.96	0.47
6:F:97:GLN:O	6:F:99:LEU:N	2.47	0.47
6:F:185:ILE:O	6:F:186:ARG:CG	2.37	0.47
22:R:7014:LMU:H3'	22:R:7014:LMU:H1B	1.27	0.47
9:I:4:LEU:HG	9:I:4:LEU:O	2.15	0.47
15:1:155:GLU:OE1	15:1:156:LYS:N	2.45	0.47
15:1:65:ASP:OD1	15:1:66:PRO:HG3	2.14	0.47
19:A:1133:CLA:H3A	19:A:1133:CLA:HBA2	1.58	0.47
1:A:159:THR:CA	1:A:163:GLN:HE22	2.27	0.47
1:A:246:HIS:C	1:A:248:PHE:H	2.15	0.47
1:A:279:ASP:O	1:A:281:LEU:HD11	2.12	0.47
1:A:310:PHE:H	1:A:313:ALA:HB3	1.79	0.47
1:A:308:ILE:O	1:A:311:LEU:HB2	2.14	0.47
1:A:452:PHE:O	1:A:456:HIS:ND1	2.35	0.47
19:B:1201:CLA:HMC1	19:B:1201:CLA:HBC2	1.97	0.47
19:B:1214:CLA:HMC2	19:B:1214:CLA:H141	1.97	0.47
2:B:411:MET:HE3	19:B:1220:CLA:HMC2	1.96	0.47
2:B:527:LEU:CD2	19:B:1222:CLA:C4D	2.92	0.47
19:A:1237:CLA:HMC3	19:B:1238:CLA:C1D	2.45	0.47
2:B:124:TRP:HD1	2:B:124:TRP:O	1.98	0.47
2:B:493:TRP:O	2:B:495:PRO:CG	2.62	0.47
6:F:207:LEU:HD22	6:F:208:PHE:CG	2.49	0.47
12:L:114:PHE:HD1	12:L:114:PHE:H	1.61	0.47
3:C:28:MET:SD	4:D:176:LYS:C	2.93	0.47
16:2:168:TRP:CD1	16:2:171:ILE:HG23	2.19	0.47
10:J:31:ARG:NH2	19:J:1311:CLA:CHC	2.77	0.47
14:R:46:UNK:CB	14:R:47:UNK:CA	2.92	0.47
15:1:129:VAL:HG12	15:1:130:PRO:CG	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:130:TRP:O	7:G:134:GLY:CA	2.55	0.47
2:B:260:GLY:O	2:B:262:HIS:NE2	2.47	0.47
1:A:709:TRP:CH2	2:B:417:ALA:HB2	2.50	0.47
22:4:7052:LMU:H111	22:4:7052:LMU:H82	1.67	0.47
18:4:217:PHE:HE1	18:4:221:HIS:CG	2.31	0.47
18:4:99:GLY:O	18:4:103:MET:HG3	2.14	0.47
19:A:1104:CLA:CED	19:A:1104:CLA:HBA2	2.45	0.47
1:A:270:PHE:CZ	19:A:1141:CLA:C2	2.97	0.47
1:A:167:THR:CG2	19:A:1112:CLA:CAA	2.87	0.47
1:A:296:LEU:HD12	1:A:297:THR:CG2	2.31	0.47
1:A:309:LEU:C	1:A:309:LEU:HD23	2.35	0.47
1:A:346:LEU:HD11	19:A:1122:CLA:HBC3	1.97	0.47
1:A:346:LEU:CD2	1:A:347:TYR:HB2	2.45	0.47
1:A:466:THR:CG2	2:B:648:TRP:HE1	2.28	0.47
19:B:1206:CLA:H43	21:I:6018:BCR:H21C	1.96	0.47
2:B:503:GLU:O	2:B:503:GLU:HG2	2.13	0.47
2:B:732:LYS:HG2	2:B:734:GLY:H	1.58	0.47
7:G:100:PHE:CD2	7:G:100:PHE:C	2.87	0.47
10:J:25:LEU:HA	10:J:28:GLU:HB2	1.97	0.47
21:J:6012:BCR:C23	21:J:6012:BCR:C39	2.83	0.47
19:A:1129:CLA:HMB2	19:L:1130:CLA:C3D	2.45	0.47
18:4:172:PHE:CD1	18:4:176:SER:O	2.68	0.47
18:4:211:MET:CE	19:4:4002:CLA:CBB	2.92	0.47
19:A:1102:CLA:O1A	19:A:1109:CLA:HBA2	2.15	0.47
19:A:1106:CLA:H111	21:J:6012:BCR:C10	2.45	0.47
19:A:1120:CLA:OBD	19:A:1120:CLA:O2D	2.33	0.47
19:A:1121:CLA:HAA1	11:K:78:ARG:NH1	2.29	0.47
19:A:1138:CLA:C4C	19:A:1138:CLA:H52	2.45	0.47
1:A:201:SER:O	1:A:204:ASN:CB	2.58	0.47
1:A:223:VAL:CG1	1:A:224:HIS:N	2.77	0.47
1:A:281:LEU:CD2	19:A:1115:CLA:HED2	2.37	0.47
1:A:390:ALA:HA	1:A:393:LEU:HD23	1.96	0.47
1:A:51:THR:HG21	1:A:723:ARG:H	1.80	0.47
1:A:599:PHE:CD2	1:A:735:VAL:HG21	2.49	0.47
19:A:1122:CLA:C1B	21:A:6007:BCR:C15	2.93	0.47
1:A:661:ALA:O	1:A:665:ILE:HG13	2.15	0.47
1:A:89:ILE:O	1:A:92:TRP:CB	2.55	0.47
19:B:1201:CLA:HBB2	19:B:1203:CLA:C4D	2.45	0.47
2:B:197:VAL:O	2:B:197:VAL:HG12	2.15	0.47
2:B:224:PRO:O	2:B:227:THR:N	2.43	0.47
2:B:34:HIS:O	2:B:37:ILE:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:497:TRP:C	2:B:499:ASN:N	2.62	0.47
2:B:655:LEU:HD21	19:B:1239:CLA:CBB	2.37	0.47
2:B:710:LEU:HA	2:B:713:PHE:HB3	1.97	0.47
19:H:1207:CLA:HHD	21:I:6018:BCR:H342	1.96	0.47
10:J:19:PHE:O	10:J:23:ALA:HB3	2.14	0.47
1:A:25:ASP:OD1	1:A:26:PRO:CD	2.62	0.47
3:C:62:PHE:CE1	5:E:80:GLU:OE1	2.68	0.47
13:N:146:LEU:O	13:N:147:SER:O	2.33	0.47
15:1:133:THR:O	15:1:135:PRO:HD2	2.15	0.47
2:B:564:ARG:NH2	3:C:66:ARG:NH1	2.63	0.47
1:A:584:PRO:HB2	3:C:67:VAL:HA	1.96	0.47
17:3:101:GLY:O	17:3:102:GLU:C	2.53	0.47
4:D:100:TYR:OH	4:D:134:LYS:HE3	2.14	0.47
4:D:100:TYR:CE2	4:D:156:ARG:HG3	2.50	0.47
16:2:150:THR:CG2	16:2:151:THR:N	2.76	0.47
4:D:114:MET:CG	4:D:115:PRO:N	2.78	0.47
12:L:105:ALA:HB2	19:L:1501:CLA:HMA1	1.97	0.47
15:1:186:LYS:O	15:1:187:GLU:C	2.49	0.47
2:B:154:TRP:O	2:B:158:GLN:HG2	2.14	0.47
6:F:123:MET:O	6:F:125:LYS:N	2.48	0.47
16:2:269:LYS:O	16:2:269:LYS:HE3	2.15	0.47
11:K:101:PHE:O	11:K:104:ALA:HB3	2.15	0.47
1:A:581:CYS:HB3	1:A:590:CYS:O	2.14	0.47
12:L:104:LEU:HD12	12:L:196:GLY:HA2	1.97	0.47
19:3:3017:CLA:H3A	19:3:3017:CLA:HBA1	1.29	0.47
22:1:7013:LMU:H41	22:1:7013:LMU:H1'	1.97	0.47
15:1:216:ASN:O	15:1:217:LEU:HB2	2.12	0.47
18:4:81:LEU:O	18:4:83:GLU:OE2	2.33	0.47
6:F:168:LEU:HA	6:F:168:LEU:HD13	1.75	0.47
19:A:1105:CLA:H3A	19:A:1105:CLA:HBA2	1.49	0.47
19:A:1136:CLA:H11	19:A:1136:CLA:ND	2.29	0.47
1:A:207:LEU:HA	1:A:211:LEU:CB	2.44	0.47
1:A:369:THR:HG21	1:A:402:ILE:HG22	1.96	0.47
19:A:9013:CLA:CMA	19:A:9013:CLA:H2	2.44	0.47
19:A:9023:CLA:CMB	19:A:9023:CLA:H41	2.45	0.47
19:B:1219:CLA:HBA2	19:B:1219:CLA:H3A	1.51	0.47
2:B:172:GLU:CD	2:B:301:ILE:HG13	2.35	0.47
2:B:312:GLY:O	19:B:1301:CLA:CAD	2.62	0.47
19:A:9011:CLA:CMC	2:B:624:LEU:HG	2.44	0.47
2:B:666:SER:O	2:B:667:TRP:HB2	2.14	0.47
3:C:69:LEU:HD12	3:C:70:TRP:H	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:100:ARG:N	16:2:101:TRP:HB2	2.29	0.47
16:2:122:ILE:O	16:2:126:LEU:CD2	2.62	0.47
19:2:2002:CLA:OBD	19:2:2002:CLA:O2D	2.33	0.47
3:C:10:THR:CG2	5:E:101:TYR:CG	2.98	0.47
13:N:157:LYS:CB	13:N:158:ASP:HA	2.42	0.47
1:A:252:ARG:NE	1:A:252:ARG:O	2.48	0.47
4:D:99:PHE:C	4:D:100:TYR:HD2	2.18	0.47
4:D:162:GLU:C	4:D:163:VAL:CG2	2.81	0.47
16:2:172:LEU:HD12	16:2:172:LEU:O	2.15	0.47
10:J:5:LYS:CE	16:2:178:ASN:OD1	2.63	0.47
1:A:644:GLN:HG3	1:A:644:GLN:O	2.15	0.47
4:D:135:GLU:O	4:D:139:ALA:HB2	2.13	0.47
22:4:7008:LMU:C6'	22:4:7008:LMU:H1B	2.45	0.47
6:F:100:LYS:HD3	6:F:100:LYS:HA	1.30	0.47
2:B:611:GLU:OE1	6:F:143:ASP:OD2	2.33	0.47
11:K:81:THR:CG2	11:K:83:GLY:N	2.49	0.47
19:2:2014:CLA:O2D	19:2:2014:CLA:OBD	2.32	0.47
22:1:7013:LMU:H42	22:1:7013:LMU:H11	1.81	0.47
11:K:86:LEU:O	11:K:87:GLU:CB	2.62	0.47
6:F:172:GLY:O	6:F:176:TRP:CB	2.61	0.47
16:2:142:GLU:O	16:2:143:GLN:HG2	2.15	0.47
2:B:30:ASP:O	2:B:30:ASP:CG	2.53	0.47
18:4:140:THR:O	18:4:144:ILE:HD12	2.15	0.47
1:A:281:LEU:HD21	19:A:1115:CLA:HED1	1.94	0.47
19:A:1119:CLA:H61	21:A:6008:BCR:H19C	1.96	0.47
19:A:1124:CLA:HBD	19:A:1124:CLA:HAA1	1.97	0.47
19:A:1126:CLA:H193	19:A:1126:CLA:H162	1.77	0.47
1:A:736:THR:HG21	19:A:1128:CLA:H91	1.96	0.47
19:A:1140:CLA:H3A	19:A:1140:CLA:HBA2	1.47	0.47
1:A:370:ILE:CG2	1:A:403:GLY:HA3	2.26	0.47
1:A:532:ILE:HD13	19:A:1135:CLA:CMD	2.45	0.47
1:A:594:ALA:O	1:A:598:VAL:HG23	2.14	0.47
21:A:6011:BCR:H333	19:B:1230:CLA:HBB2	1.95	0.47
2:B:124:TRP:C	2:B:124:TRP:HD1	2.17	0.47
2:B:225:LEU:HD11	2:B:233:TYR:OH	2.06	0.47
2:B:459:PHE:CD2	19:B:1235:CLA:HMD1	2.45	0.47
2:B:679:ALA:HB1	2:B:683:GLU:OE2	2.15	0.47
7:G:136:VAL:O	7:G:137:VAL:CG2	2.63	0.47
10:J:15:SER:HA	10:J:18:TRP:HB3	1.96	0.47
16:2:215:LYS:CG	16:2:215:LYS:O	2.60	0.47
13:N:142:LYS:HB3	13:N:143:VAL:H	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:560:ASP:OD1	3:C:66:ARG:HB3	2.15	0.47
17:3:94:GLU:CB	17:3:95:PRO:HD3	2.45	0.47
14:R:34:UNK:CB	14:R:35:UNK:CA	2.80	0.47
12:L:206:VAL:O	12:L:207:LEU:O	2.33	0.47
2:B:4:ARG:HB2	2:B:4:ARG:HE	1.46	0.47
16:2:155:VAL:HA	16:2:158:VAL:HG13	1.97	0.47
18:4:144:ILE:HA	18:4:147:ILE:HD13	1.97	0.47
18:4:209:ARG:O	18:4:212:LEU:HB2	2.15	0.47
19:A:1115:CLA:C14	19:A:1115:CLA:C17	2.75	0.47
19:A:1119:CLA:HBC2	19:A:1119:CLA:HMC1	1.96	0.47
19:A:1133:CLA:C3D	19:A:1134:CLA:CAC	2.92	0.47
1:A:360:ILE:HD11	19:A:1123:CLA:HMB2	1.97	0.47
21:A:6003:BCR:C8	21:A:6003:BCR:H311	2.44	0.47
1:A:603:PHE:CE2	2:B:665:ILE:HG21	2.50	0.47
19:B:1205:CLA:HBB2	19:B:1205:CLA:C9	2.29	0.47
19:B:1210:CLA:H192	19:B:1215:CLA:OBD	2.15	0.47
2:B:343:VAL:HG11	19:B:1223:CLA:H2	1.96	0.47
2:B:224:PRO:CB	2:B:227:THR:HG21	2.45	0.47
2:B:235:GLN:O	2:B:236:ASN:C	2.53	0.47
2:B:290:MET:HG3	19:B:1218:CLA:C2C	2.45	0.47
2:B:555:TYR:CE2	2:B:573:TRP:HA	2.50	0.47
21:B:6017:BCR:C33	21:B:6017:BCR:HC8	2.45	0.47
5:E:110:VAL:O	5:E:111:ASN:CB	2.61	0.47
6:F:207:LEU:HD21	6:F:208:PHE:CG	2.48	0.47
7:G:124:ILE:CG2	7:G:125:VAL:H	2.26	0.47
8:H:108:THR:O	8:H:109:LEU:O	2.33	0.47
10:J:2:ARG:NH1	10:J:8:LEU:HB2	2.30	0.47
11:K:55:LEU:O	11:K:58:VAL:HB	2.15	0.47
11:K:78:ARG:N	11:K:78:ARG:CZ	2.78	0.47
12:L:79:ILE:HD12	19:L:1504:CLA:HMA1	1.97	0.47
3:C:11:CYS:O	3:C:13:GLY:N	2.48	0.47
3:C:12:ILE:O	3:C:38:GLN:CG	2.62	0.47
4:D:177:VAL:HG23	4:D:178:ASN:C	2.35	0.47
17:3:107:ARG:NH1	17:3:229:LYS:O	2.47	0.47
17:3:109:ALA:O	17:3:111:LEU:HD23	2.14	0.47
4:D:99:PHE:HB3	4:D:157:VAL:HG12	1.95	0.47
2:B:154:TRP:O	2:B:155:LEU:C	2.52	0.47
17:3:161:GLU:O	17:3:162:MET:C	2.50	0.47
22:H:7032:LMU:O2'	22:H:7032:LMU:H12	2.15	0.47
22:R:7021:LMU:O3'	22:R:7021:LMU:H1B	2.13	0.47
18:4:83:GLU:O	18:4:84:ASP:CG	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:145:TYR:O	16:2:146:PHE:HB2	2.15	0.47
16:2:264:ALA:O	16:2:265:ALA:CB	2.63	0.47
2:B:605:ASN:OD1	2:B:605:ASN:C	2.53	0.47
15:1:77:GLU:CD	15:1:80:LYS:NZ	2.69	0.46
18:4:178:PRO:O	18:4:194:PHE:CZ	2.67	0.46
18:4:173:LYS:CE	18:4:201:LYS:HG3	2.43	0.46
1:A:126:ILE:CD1	19:A:1107:CLA:HMA3	2.42	0.46
19:A:1119:CLA:CAA	19:A:1123:CLA:HBB2	2.45	0.46
19:A:1124:CLA:H111	19:A:1124:CLA:H162	1.96	0.46
19:A:1138:CLA:HAA1	19:A:1138:CLA:HBD	1.95	0.46
1:A:358:LEU:C	1:A:358:LEU:HD12	2.35	0.46
1:A:739:LEU:O	1:A:743:ILE:HG13	2.15	0.46
1:A:84:GLY:O	1:A:88:ILE:HD12	2.15	0.46
19:A:1237:CLA:HMC3	19:B:1238:CLA:ND	2.30	0.46
2:B:15:ASP:O	2:B:20:ARG:HG3	2.15	0.46
2:B:290:MET:HG3	19:B:1218:CLA:HMC3	1.97	0.46
2:B:487:ASN:OD1	2:B:487:ASN:C	2.53	0.46
2:B:649:MET:HE2	21:B:6017:BCR:H272	1.96	0.46
8:H:98:LEU:O	8:H:98:LEU:CG	2.63	0.46
11:K:56:ILE:CA	11:K:59:THR:CG2	2.81	0.46
12:L:131:SER:O	12:L:132:LEU:HB3	2.15	0.46
12:L:82:TYR:OH	19:L:1502:CLA:HBA2	2.15	0.46
16:2:229:MET:CE	16:2:230:LEU:CD1	2.94	0.46
3:C:62:PHE:CD1	4:D:191:ILE:CG2	2.92	0.46
13:N:160:TYR:O	13:N:164:SER:O	2.33	0.46
15:1:133:THR:O	15:1:136:THR:CG2	2.53	0.46
6:F:192:THR:O	6:F:193:GLN:CB	2.63	0.46
1:A:263:ALA:O	1:A:264:GLU:HG3	2.13	0.46
16:2:174:PRO:CD	16:2:189:THR:OG1	2.61	0.46
4:D:123:ARG:HH21	22:D:7050:LMU:C6B	2.17	0.46
12:L:178:THR:HG22	12:L:179:ALA:N	2.30	0.46
6:F:121:ALA:C	6:F:123:MET:N	2.69	0.46
11:K:115:ILE:O	11:K:118:VAL:CG2	2.60	0.46
22:H:7030:LMU:H32	22:H:7030:LMU:H61	1.62	0.46
1:A:581:CYS:HB2	1:A:590:CYS:O	2.14	0.46
1:A:592:VAL:HG23	1:A:593:SER:H	1.80	0.46
19:H:1505:CLA:HBD	19:H:1505:CLA:HAA2	1.96	0.46
18:4:238:ASP:OD2	18:4:238:ASP:N	2.47	0.46
19:1:1001:CLA:HBA1	19:1:1001:CLA:CMA	2.44	0.46
19:1:1001:CLA:HBA2	19:1:1001:CLA:H3A	1.30	0.46
15:1:179:LYS:HG2	15:1:180:LEU:C	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:ILE:CG2	19:A:1115:CLA:C11	2.94	0.46
19:A:1101:CLA:H42	19:A:1140:CLA:H8	1.97	0.46
1:A:124:TRP:HA	1:A:124:TRP:CE3	2.50	0.46
1:A:129:GLN:NE2	19:A:1107:CLA:NB	2.64	0.46
1:A:185:HIS:O	1:A:186:TYR:C	2.54	0.46
1:A:187:HIS:HE1	19:A:1109:CLA:C1A	2.06	0.46
1:A:245:PRO:O	1:A:248:PHE:HE2	1.93	0.46
1:A:473:PRO:O	1:A:475:ASP:N	2.48	0.46
1:A:536:THR:O	1:A:537:ALA:CB	2.63	0.46
19:B:1222:CLA:H11	19:B:1236:CLA:CB	2.46	0.46
2:B:320:LYS:HG3	2:B:321:GLY:H	1.80	0.46
2:B:471:THR:O	2:B:472:TYR:HD1	1.92	0.46
2:B:353:TYR:CB	2:B:594:TRP:CZ3	2.98	0.46
2:B:645:VAL:HG21	19:B:1206:CLA:HMD2	1.96	0.46
2:B:668:ARG:NH1	2:B:672:GLN:HG2	2.30	0.46
3:C:79:LEU:HD22	3:C:81:TYR:O	2.15	0.46
6:F:169:TYR:OH	6:F:211:PHE:HA	2.15	0.46
10:J:26:LEU:HA	10:J:29:ILE:HG22	1.97	0.46
19:A:1105:CLA:C4B	21:J:6012:BCR:H333	2.45	0.46
11:K:48:PHE:C	11:K:52:PRO:HD3	2.34	0.46
16:2:128:LYS:HB2	16:2:131:ILE:HG12	1.96	0.46
17:3:187:PHE:CE1	17:3:188:LEU:HB2	2.51	0.46
2:B:564:ARG:CZ	3:C:64:SER:H	2.28	0.46
4:D:172:VAL:CG1	4:D:173:TYR:N	2.78	0.46
2:B:80:ASP:HA	2:B:81:PRO:HD3	1.75	0.46
22:H:7032:LMU:O1'	22:H:7032:LMU:H1B	2.15	0.46
1:A:564:ARG:HA	1:A:573:ALA:HB2	1.97	0.46
22:R:7021:LMU:H41	22:R:7021:LMU:O6'	2.16	0.46
14:R:6:UNK:CB	14:R:10:UNK:CB	2.92	0.46
2:B:488:ALA:HB2	19:B:1233:CLA:C3C	2.45	0.46
19:B:1233:CLA:H3A	19:B:1233:CLA:HBA2	1.71	0.46
15:1:66:PRO:CD	15:1:67:LEU:H	2.06	0.46
1:A:393:LEU:HD11	1:A:750:PHE:CD1	2.51	0.46
2:B:38:THR:HG23	2:B:41:ARG:NH1	2.30	0.46
2:B:469:LYS:HZ3	2:B:471:THR:N	2.07	0.46
2:B:596:TRP:CD1	2:B:623:TYR:HB2	2.50	0.46
2:B:595:HIS:HD2	2:B:623:TYR:OH	1.99	0.46
2:B:693:TRP:HD1	19:B:1238:CLA:C1D	2.18	0.46
7:G:123:ASN:O	7:G:124:ILE:C	2.52	0.46
9:I:8:PHE:CE1	21:I:6021:BCR:HC7	2.50	0.46
10:J:2:ARG:HB3	10:J:7:TYR:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:92:ALA:N	12:L:98:ARG:HH22	2.12	0.46
16:2:218:ARG:NH1	19:2:2001:CLA:HBB2	2.30	0.46
3:C:18:VAL:HB	3:C:58:CYS:HB2	1.97	0.46
5:E:73:LYS:HG3	5:E:128:VAL:CG1	2.46	0.46
19:1:1010:CLA:C3D	19:1:1010:CLA:O1D	2.54	0.46
16:2:184:PRO:CD	16:2:185:ASN:CA	2.93	0.46
13:N:115:ALA:O	13:N:116:ARG:C	2.49	0.46
4:D:140:LEU:HD22	4:D:144:LEU:HG	1.96	0.46
22:N:7049:LMU:H4'	22:N:7049:LMU:O6B	2.15	0.46
21:3:6022:BCR:C23	21:3:6022:BCR:C39	2.63	0.46
15:1:103:LEU:N	15:1:103:LEU:CD2	2.71	0.46
19:A:1149:CLA:O1D	19:A:1149:CLA:HBA2	2.14	0.46
4:D:147:LYS:C	4:D:148:TYR:CD1	2.88	0.46
16:2:267:THR:HG23	16:2:267:THR:O	2.14	0.46
22:K:7047:LMU:H6E	22:K:7047:LMU:O2B	2.16	0.46
15:1:157:ASP:OD1	15:1:157:ASP:C	2.53	0.46
15:1:75:ASN:O	15:1:76:LEU:O	2.34	0.46
19:4:4014:CLA:HBC2	19:4:4014:CLA:CHD	2.34	0.46
19:A:1102:CLA:HBB2	19:A:1104:CLA:C3D	2.46	0.46
19:A:1138:CLA:H191	6:F:181:TYR:CG	2.51	0.46
19:A:1140:CLA:H43	19:A:1140:CLA:ND	2.30	0.46
19:B:1225:CLA:H62	21:B:6006:BCR:H321	1.97	0.46
19:B:1220:CLA:C9	19:B:1227:CLA:CBC	2.94	0.46
2:B:655:LEU:HD22	19:B:1239:CLA:CBB	2.45	0.46
2:B:294:ASN:ND2	7:G:93:GLU:C	2.66	0.46
2:B:310:PRO:HD2	2:B:311:PRO:HD2	1.97	0.46
19:A:9023:CLA:HMC1	2:B:661:PHE:HB3	1.98	0.46
5:E:111:ASN:CG	5:E:112:TYR:N	2.68	0.46
1:A:244:LEU:CB	1:A:247:GLU:CD	2.81	0.46
13:N:159:LYS:O	13:N:160:TYR:C	2.54	0.46
2:B:247:THR:O	2:B:250:ALA:N	2.49	0.46
4:D:114:MET:SD	4:D:115:PRO:HD2	2.55	0.46
6:F:133:TYR:N	6:F:133:TYR:CD1	2.83	0.46
19:J:1311:CLA:C15	19:J:1311:CLA:O1A	2.64	0.46
12:L:172:GLU:CG	12:L:173:PRO:N	2.73	0.46
11:K:97:ASP:O	11:K:97:ASP:OD1	2.32	0.46
1:A:389:TYR:HD1	1:A:625:TRP:CG	2.32	0.46
18:4:112:PRO:O	18:4:115:PHE:O	2.34	0.46
4:D:147:LYS:O	4:D:148:TYR:CD2	2.68	0.46
17:3:182:MET:CG	17:3:183:GLY:N	2.78	0.46
18:4:176:SER:C	18:4:178:PRO:HD2	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:93:GLN:O	18:4:97:VAL:HG23	2.15	0.46
19:A:1237:CLA:H201	12:L:110:LEU:CD2	2.34	0.46
1:A:130:GLU:C	1:A:132:LEU:N	2.65	0.46
1:A:163:GLN:HG2	1:A:164:LEU:H	1.74	0.46
1:A:313:ALA:C	1:A:315:HIS:H	2.19	0.46
20:A:5001:PQN:H212	20:A:5001:PQN:H243	1.76	0.46
1:A:539:PHE:HE2	1:A:543:HIS:CE1	2.34	0.46
19:A:1124:CLA:HMB3	21:A:6008:BCR:C18	2.45	0.46
1:A:692:PHE:CD2	1:A:733:VAL:CG1	2.97	0.46
1:A:725:LEU:HD21	19:A:1140:CLA:CMD	2.46	0.46
19:B:1217:CLA:HMA1	7:G:77:PHE:CG	2.51	0.46
2:B:15:ASP:O	2:B:20:ARG:CG	2.63	0.46
2:B:594:TRP:CD1	2:B:595:HIS:N	2.84	0.46
2:B:377:TYR:CD1	2:B:718:ILE:HD12	2.51	0.46
9:I:9:VAL:H	9:I:10:PRO:CD	2.28	0.46
9:I:12:VAL:HG12	9:I:13:GLY:N	2.31	0.46
10:J:2:ARG:HH22	10:J:8:LEU:HD22	1.80	0.46
12:L:109:LEU:HG	12:L:110:LEU:H	1.81	0.46
12:L:113:PRO:O	12:L:117:ALA:HB3	2.16	0.46
12:L:96:LEU:HG	12:L:97:LEU:HD23	1.97	0.46
1:A:586:ARG:HA	3:C:77:MET:O	2.15	0.46
17:3:94:GLU:CD	17:3:94:GLU:O	2.54	0.46
17:3:94:GLU:OE2	17:3:94:GLU:CA	2.63	0.46
16:2:189:THR:CG2	16:2:193:VAL:O	2.61	0.46
22:E:7048:LMU:H3'	22:E:7048:LMU:O5B	2.15	0.46
19:J:1308:CLA:H93	19:J:1308:CLA:H61	1.70	0.46
18:4:107:ALA:O	18:4:109:MET:O	2.33	0.46
1:A:42:ARG:O	1:A:44:ILE:HG13	2.15	0.46
1:A:626:GLY:O	1:A:627:THR:CG2	2.64	0.46
1:A:392:GLN:CG	1:A:392:GLN:O	2.64	0.46
18:4:237:SER:O	18:4:238:ASP:C	2.50	0.46
15:1:84:LEU:HA	15:1:87:CYS:HB3	1.97	0.46
19:A:1104:CLA:H12	19:A:1104:CLA:HED2	1.97	0.46
1:A:430:ASP:HA	1:A:434:ARG:HH21	1.80	0.46
19:A:9013:CLA:HMC1	19:A:9013:CLA:HBC2	1.98	0.46
19:B:1220:CLA:CHB	19:B:1220:CLA:H42	2.43	0.46
2:B:321:GLY:O	2:B:325:THR:HG22	2.15	0.46
2:B:450:GLU:C	2:B:452:GLN:H	2.18	0.46
21:B:6004:BCR:H343	7:G:77:PHE:CE1	2.50	0.46
6:F:152:GLY:HA2	6:F:157:TRP:CE3	2.51	0.46
19:2:2001:CLA:O1A	19:2:2001:CLA:NA	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:132:THR:CB	13:N:139:LYS:NZ	2.57	0.46
15:1:138:LEU:O	15:1:139:ALA:C	2.53	0.46
3:C:51:CYS:SG	3:C:53:ARG:N	2.89	0.46
19:3:3013:CLA:O2D	19:3:3013:CLA:OBD	2.33	0.46
16:2:172:LEU:HB3	16:2:173:ASN:HD21	1.73	0.46
16:2:177:VAL:HG13	16:2:178:ASN:OD1	2.14	0.46
16:2:184:PRO:HG2	16:2:185:ASN:CA	2.45	0.46
17:3:150:TYR:CE2	17:3:151:TRP:CE2	2.99	0.46
6:F:95:GLU:OE1	6:F:129:ARG:O	2.33	0.46
1:A:426:THR:N	1:A:428:TYR:CZ	2.84	0.46
2:B:139:ALA:O	2:B:141:PHE:N	2.49	0.46
12:L:175:GLN:O	12:L:176:LEU:CB	2.55	0.46
1:A:497:ALA:HB2	1:A:510:SER:OG	2.14	0.46
14:R:1:UNK:O	14:R:2:UNK:O	2.34	0.46
18:4:154:ILE:HD12	19:4:1009:CLA:HMD1	1.98	0.46
19:A:1135:CLA:H2	19:A:1135:CLA:O1A	2.16	0.46
1:A:284:ARG:HH12	1:A:507:ALA:HB2	1.10	0.46
1:A:309:LEU:HD21	19:A:1119:CLA:HMC3	1.97	0.46
1:A:409:GLY:C	1:A:411:ALA:H	2.19	0.46
1:A:467:MET:HB3	1:A:467:MET:HE3	1.69	0.46
19:A:1117:CLA:HBC1	21:A:6003:BCR:C12	2.46	0.46
21:A:6003:BCR:H402	21:A:6003:BCR:C23	2.44	0.46
1:A:697:ARG:NH1	1:A:724:ALA:HB3	2.30	0.46
2:B:435:GLY:HA3	19:B:1230:CLA:HBB1	1.97	0.46
19:B:1235:CLA:CBB	19:B:1235:CLA:C9	2.66	0.46
2:B:21:ILE:O	2:B:22:TRP:C	2.54	0.46
2:B:536:LYS:O	2:B:537:GLY:C	2.54	0.46
2:B:587:ILE:CG2	2:B:587:ILE:O	2.62	0.46
2:B:623:TYR:O	2:B:624:LEU:CB	2.64	0.46
3:C:69:LEU:H	3:C:69:LEU:HG	1.20	0.46
6:F:180:SER:O	6:F:182:LEU:N	2.38	0.46
6:F:167:PHE:CD1	21:F:6014:BCR:H23C	2.51	0.46
7:G:131:GLY:C	7:G:136:VAL:HB	2.35	0.46
19:L:1130:CLA:H72	19:L:1504:CLA:HBA1	1.98	0.46
16:2:114:MET:O	16:2:117:ALA:HB3	2.16	0.46
16:2:122:ILE:HG13	16:2:126:LEU:CD2	2.46	0.46
5:E:124:GLU:HB2	5:E:126:VAL:HG13	1.97	0.46
1:A:584:PRO:HB2	3:C:67:VAL:CA	2.45	0.46
6:F:190:LYS:HA	6:F:191:PRO:HD3	1.54	0.46
22:3:7005:LMU:C2B	22:3:7005:LMU:H3'	2.46	0.46
8:H:86:THR:HA	8:H:92:THR:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:76:TYR:HH	12:L:90:ARG:NE	1.83	0.46
6:F:132:ASN:O	6:F:132:ASN:CG	2.54	0.46
19:3:3016:CLA:H143	19:3:3016:CLA:H102	1.90	0.46
14:R:8:UNK:CB	19:R:1144:CLA:HED1	2.46	0.46
7:G:134:GLY:O	7:G:135:HIS:CE1	2.69	0.46
2:B:605:ASN:O	2:B:605:ASN:OD1	2.34	0.46
15:1:83:GLU:HA	15:1:86:HIS:CD2	2.51	0.46
15:1:97:ILE:HD11	15:1:98:LEU:HD22	1.97	0.46
18:4:206:ALA:O	18:4:207:ASN:C	2.54	0.46
18:4:98:ASN:HB3	18:4:212:LEU:CD2	2.45	0.46
19:A:1109:CLA:C4A	19:A:1109:CLA:CBA	2.92	0.46
1:A:284:ARG:CB	1:A:295:TRP:CG	2.99	0.46
1:A:402:ILE:CD1	19:A:1127:CLA:CBB	2.94	0.46
1:A:655:ASP:O	1:A:659:ALA:HB3	2.16	0.46
1:A:708:VAL:HA	1:A:711:HIS:HD2	1.80	0.46
2:B:196:HIS:CE1	19:B:1212:CLA:C4D	2.98	0.46
2:B:217:PRO:HD2	19:B:1212:CLA:HED1	1.98	0.46
2:B:53:GLN:O	2:B:55:ALA:N	2.41	0.46
19:B:1235:CLA:C6	21:F:6016:BCR:H323	2.46	0.46
12:L:131:SER:HA	12:L:197:VAL:CG1	2.45	0.46
19:L:1504:CLA:H62	19:L:1504:CLA:H41	1.62	0.46
17:3:184:LYS:HD3	19:3:2009:CLA:H61	1.60	0.46
19:3:2009:CLA:O1A	19:3:2009:CLA:CBD	2.44	0.46
3:C:7:ILE:O	3:C:60:THR:HA	2.16	0.46
19:2:4009:CLA:H111	19:2:4009:CLA:H71	1.68	0.46
4:D:141:GLY:O	4:D:142:THR:O	2.34	0.46
12:L:155:GLU:HG2	12:L:155:GLU:H	1.15	0.46
11:K:124:LEU:HD12	11:K:124:LEU:C	2.36	0.46
6:F:96:LYS:C	6:F:97:GLN:O	2.53	0.46
22:L:7029:LMU:C3	22:L:7029:LMU:H1'	2.23	0.46
15:1:201:PHE:CE1	15:1:204:GLN:OE1	2.69	0.46
4:D:90:LEU:O	12:L:66:ILE:HG23	2.16	0.46
1:A:341:GLN:HB2	1:A:341:GLN:HE21	1.56	0.46
1:A:199:VAL:CG1	1:A:199:VAL:O	2.58	0.46
11:K:95:THR:HG22	11:K:95:THR:O	2.16	0.46
15:1:224:PRO:HA	15:1:225:TRP:C	2.36	0.46
18:4:103:MET:HG2	18:4:211:MET:HB2	1.96	0.46
18:4:154:ILE:O	18:4:155:ARG:C	2.54	0.46
19:A:1117:CLA:H71	19:A:1117:CLA:CAB	2.46	0.46
1:A:112:ASP:N	1:A:113:PRO:CD	2.78	0.46
19:A:1237:CLA:CGA	19:A:1237:CLA:C1A	2.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:PHE:N	1:A:196:PHE:CD2	2.76	0.46
1:A:431:LEU:H	1:A:434:ARG:HE	1.62	0.46
1:A:473:PRO:O	1:A:474:GLN:C	2.54	0.46
1:A:555:ILE:HD11	19:A:9023:CLA:CAD	2.41	0.46
19:A:1126:CLA:H71	21:A:6011:BCR:C37	2.45	0.46
2:B:100:ALA:O	2:B:102:GLU:O	2.33	0.46
2:B:29:HIS:NE2	19:B:1202:CLA:HBB1	2.31	0.46
19:B:1222:CLA:H52	19:B:1236:CLA:CBD	2.45	0.46
2:B:21:ILE:CD1	19:B:1238:CLA:HMA1	2.43	0.46
2:B:255:LEU:N	2:B:271:THR:HG21	2.31	0.46
2:B:330:ILE:HD12	2:B:333:GLN:NE2	2.30	0.46
5:E:93:VAL:O	5:E:93:VAL:HG12	2.15	0.46
6:F:177:VAL:CA	6:F:180:SER:OG	2.57	0.46
7:G:82:PHE:CB	7:G:83:GLN:HG2	2.46	0.46
7:G:98:THR:OG1	7:G:99:HIS:C	2.55	0.46
9:I:12:VAL:HG13	21:I:6018:BCR:H271	1.97	0.46
19:L:1130:CLA:H142	19:L:1504:CLA:H43	1.97	0.46
5:E:73:LYS:CG	5:E:128:VAL:HG11	2.44	0.46
5:E:73:LYS:CG	5:E:73:LYS:O	2.64	0.46
16:2:157:LEU:O	16:2:161:GLY:N	2.39	0.46
1:A:715:LYS:CD	6:F:230:ASN:ND2	2.48	0.46
1:A:71:LEU:HD12	1:A:72:GLU:C	2.36	0.46
16:2:206:TRP:O	16:2:208:SER:CB	2.62	0.46
6:F:153:ASP:N	6:F:153:ASP:OD1	2.47	0.46
15:1:91:MET:O	15:1:94:VAL:HB	2.16	0.46
1:A:105:ASN:HA	1:A:140:PHE:HE2	1.81	0.46
1:A:308:ILE:HD11	19:A:1115:CLA:C4B	2.46	0.46
1:A:308:ILE:HG21	19:A:1115:CLA:C11	2.46	0.46
1:A:654:ARG:HG3	1:A:655:ASP:N	2.30	0.46
1:A:701:GLN:OE1	5:E:112:TYR:CE1	2.69	0.46
19:A:9022:CLA:H91	19:A:9023:CLA:C9	2.43	0.46
19:B:1208:CLA:H12	19:B:1208:CLA:HAA2	1.98	0.46
19:B:1234:CLA:O2D	19:B:1234:CLA:OBD	2.34	0.46
2:B:25:ILE:HG21	21:L:6019:BCR:C28	2.45	0.46
2:B:317:ARG:HH22	2:B:410:ARG:CB	2.28	0.46
2:B:646:TRP:CH2	2:B:726:ILE:HD13	2.50	0.46
6:F:139:LEU:O	6:F:140:CYS:O	2.32	0.46
8:H:91:PHE:HB3	12:L:187:GLY:CA	2.46	0.46
5:E:108:ASN:OD1	5:E:109:LYS:N	2.49	0.46
13:N:156:GLY:CA	13:N:157:LYS:CD	2.94	0.46
4:D:95:GLN:HE21	4:D:96:VAL:CB	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:80:SER:HB2	4:D:127:ASN:H	1.80	0.46
6:F:184:ALA:C	6:F:185:ILE:CG2	2.84	0.46
15:1:201:PHE:CD1	15:1:204:GLN:OE1	2.69	0.46
22:H:7011:LMU:H111	22:H:7011:LMU:C6	2.46	0.46
22:E:7037:LMU:C5	22:E:7037:LMU:C1	2.92	0.46
18:4:83:GLU:C	18:4:84:ASP:CG	2.74	0.46
1:A:520:LEU:HB3	22:A:7044:LMU:H2'	1.62	0.46
11:K:94:GLN:CD	11:K:94:GLN:N	2.69	0.46
18:4:121:ILE:HG12	18:4:122:ASN:H	1.81	0.45
15:1:156:LYS:HB3	15:1:158:PRO:CD	2.46	0.45
18:4:223:VAL:C	18:4:224:THR:HG23	2.36	0.45
1:A:451:ILE:HD13	19:A:1131:CLA:CED	2.35	0.45
1:A:120:ALA:HB3	19:A:1106:CLA:HED3	1.98	0.45
1:A:183:TRP:O	1:A:185:HIS:N	2.49	0.45
1:A:240:LYS:H	1:A:243:PRO:CD	2.24	0.45
1:A:502:THR:HG22	1:A:503:THR:N	2.32	0.45
1:A:660:GLN:O	1:A:661:ALA:HB3	2.16	0.45
1:A:90:PHE:O	1:A:91:LEU:C	2.52	0.45
2:B:95:HIS:CE1	19:B:1206:CLA:HMB3	2.52	0.45
19:B:1229:CLA:HBB2	21:F:6014:BCR:C26	2.46	0.45
2:B:199:ILE:CG2	2:B:270:LEU:HD11	2.43	0.45
2:B:407:VAL:C	2:B:409:ALA:O	2.55	0.45
2:B:447:GLY:C	2:B:449:PRO:HD3	2.37	0.45
2:B:551:LYS:HE3	2:B:551:LYS:HB3	1.55	0.45
2:B:65:LEU:HD11	21:B:6006:BCR:HC42	1.97	0.45
2:B:377:TYR:OH	2:B:717:TYR:HE1	1.99	0.45
21:F:6016:BCR:H24C	21:F:6016:BCR:H371	1.75	0.45
2:B:229:GLN:NE2	7:G:154:PHE:CE1	2.79	0.45
17:3:109:ALA:HA	17:3:111:LEU:HD13	1.97	0.45
17:3:238:ILE:HA	17:3:241:TYR:CZ	2.50	0.45
18:4:89:ARG:CD	18:4:89:ARG:N	2.79	0.45
4:D:103:THR:C	4:D:104:TRP:HD1	2.19	0.45
2:B:5:ILE:CG2	2:B:6:PRO:N	2.75	0.45
2:B:394:PHE:C	2:B:542:ARG:HD3	2.36	0.45
22:R:7020:LMU:H92	22:R:7020:LMU:H62	1.54	0.45
1:A:70:ASP:CB	1:A:72:GLU:HG2	2.46	0.45
11:K:98:PRO:CD	11:K:99:ALA:N	2.64	0.45
1:A:592:VAL:O	1:A:597:HIS:CD2	2.69	0.45
17:3:209:ASN:HD22	17:3:209:ASN:HA	1.55	0.45
15:1:155:GLU:O	15:1:156:LYS:CB	2.61	0.45
15:1:181:GLU:O	15:1:182:GLU:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1122:CLA:HBC1	21:A:6007:BCR:C39	2.46	0.45
19:A:1101:CLA:C1	19:A:1140:CLA:H2	2.47	0.45
2:B:240:SER:O	2:B:242:HIS:N	2.49	0.45
2:B:463:ILE:O	2:B:464:GLN:CG	2.64	0.45
2:B:50:HIS:HB2	2:B:53:GLN:HB2	1.98	0.45
19:A:1237:CLA:CMD	21:B:6017:BCR:H313	2.46	0.45
19:A:1237:CLA:CMD	21:B:6017:BCR:HC31	2.39	0.45
2:B:683:GLU:OE1	4:D:91:LEU:HD13	2.16	0.45
8:H:94:ARG:CZ	8:H:97:LEU:O	2.65	0.45
11:K:50:GLY:CA	11:K:52:PRO:HD2	2.45	0.45
1:A:252:ARG:CZ	1:A:261:SER:OG	2.64	0.45
2:B:636:THR:CG2	2:B:636:THR:O	2.64	0.45
22:2:7006:LMU:O5B	22:2:7006:LMU:C5'	2.50	0.45
8:H:86:THR:O	8:H:88:ALA:N	2.49	0.45
17:3:192:LYS:O	17:3:193:GLY:C	2.54	0.45
1:A:23:ASP:HA	1:A:24:ARG:HE	1.81	0.45
22:4:7053:LMU:C5B	22:4:7053:LMU:O2B	2.60	0.45
16:2:266:PHE:CD1	16:2:267:THR:O	2.68	0.45
22:E:7037:LMU:H4B	22:E:7037:LMU:H1B	1.54	0.45
22:G:7039:LMU:H4B	22:G:7039:LMU:H1B	1.64	0.45
13:N:90:GLU:OE2	13:N:91:TYR:CG	2.69	0.45
4:D:78:THR:N	4:D:79:PRO:CD	2.79	0.45
13:N:127:PHE:CD1	13:N:128:PRO:HA	2.51	0.45
15:1:64:PHE:CD1	15:1:65:ASP:CB	2.99	0.45
19:A:1132:CLA:H172	19:A:1136:CLA:C20	2.46	0.45
1:A:164:LEU:HA	1:A:167:THR:OG1	2.17	0.45
1:A:462:ILE:CG2	19:A:1132:CLA:CMC	2.94	0.45
1:A:596:ASP:HA	1:A:599:PHE:CB	2.38	0.45
19:A:9011:CLA:HBB2	19:A:9012:CLA:HED1	1.98	0.45
19:A:9012:CLA:HBB2	19:A:9013:CLA:C2B	2.47	0.45
19:A:9023:CLA:H141	19:A:9023:CLA:H161	1.72	0.45
19:B:1223:CLA:C7	19:B:1223:CLA:C4	2.94	0.45
2:B:451:LYS:CD	19:B:1230:CLA:O2D	2.65	0.45
2:B:224:PRO:CA	2:B:227:THR:OG1	2.64	0.45
3:C:69:LEU:HD12	3:C:70:TRP:O	2.11	0.45
7:G:76:ARG:NH1	7:G:120:VAL:CA	2.80	0.45
11:K:66:PHE:HE2	11:K:102:THR:HG22	1.82	0.45
16:2:127:THR:OG1	16:2:129:LEU:N	2.49	0.45
5:E:85:LYS:O	5:E:87:THR:CG2	2.64	0.45
3:C:28:MET:HA	3:C:29:ILE:O	2.17	0.45
22:D:7050:LMU:H82	22:D:7050:LMU:C4	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:126:ASN:O	11:K:126:ASN:OD1	2.34	0.45
6:F:99:LEU:CA	6:F:102:LEU:CD2	2.89	0.45
1:A:23:ASP:OD1	1:A:24:ARG:N	2.50	0.45
4:D:121:ILE:HG13	4:D:121:ILE:O	2.17	0.45
18:4:135:PHE:H	18:4:136:ALA:HB2	1.81	0.45
7:G:70:LEU:HG	7:G:70:LEU:O	2.16	0.45
18:4:124:PRO:O	18:4:125:LYS:CG	2.63	0.45
18:4:124:PRO:O	18:4:125:LYS:HB2	2.17	0.45
18:4:217:PHE:CE1	18:4:221:HIS:CG	3.04	0.45
1:A:107:GLU:HA	1:A:110:LEU:CD2	2.46	0.45
1:A:149:PHE:O	1:A:150:PHE:CB	2.36	0.45
1:A:492:ILE:O	1:A:495:THR:HG22	2.17	0.45
1:A:553:VAL:O	1:A:557:LEU:HB2	2.16	0.45
1:A:95:GLY:O	1:A:96:MET:C	2.52	0.45
19:B:1223:CLA:C4	19:B:1223:CLA:H72	2.45	0.45
2:B:339:ALA:O	2:B:340:SER:CB	2.64	0.45
2:B:261:PHE:CE2	2:B:499:ASN:C	2.76	0.45
2:B:97:GLY:O	2:B:100:ALA:HB2	2.17	0.45
19:L:1502:CLA:HBA1	19:L:1502:CLA:CHA	2.47	0.45
17:3:186:TYR:HD2	17:3:188:LEU:O	1.99	0.45
5:E:99:THR:CG2	5:E:100:ARG:N	2.42	0.45
15:1:145:ILE:H	15:1:145:ILE:HG13	1.52	0.45
2:B:564:ARG:CZ	3:C:64:SER:N	2.80	0.45
2:B:564:ARG:HH21	3:C:66:ARG:NH1	2.14	0.45
17:3:101:GLY:C	17:3:103:VAL:N	2.65	0.45
17:3:233:LEU:HA	17:3:236:LEU:CB	2.44	0.45
4:D:116:THR:O	4:D:117:GLY:O	2.34	0.45
4:D:123:ARG:O	4:D:124:GLU:CB	2.63	0.45
19:1:1007:CLA:HHD	19:1:1007:CLA:HBC3	1.96	0.45
1:A:165:TYR:HD2	1:A:165:TYR:O	1.97	0.45
6:F:224:GLY:CA	6:F:227:VAL:CG1	2.94	0.45
1:A:70:ASP:O	1:A:72:GLU:HB2	2.16	0.45
1:A:421:ASP:OD1	1:A:422:TYR:HE1	1.92	0.45
22:4:7033:LMU:H1B	22:4:7033:LMU:H5'	1.73	0.45
1:A:43:THR:HG22	1:A:43:THR:O	2.17	0.45
18:4:170:PRO:C	18:4:173:LYS:N	2.70	0.45
1:A:379:MET:HE1	19:A:1125:CLA:CHC	2.43	0.45
1:A:532:ILE:HG12	1:A:619:LYS:HZ1	1.82	0.45
21:A:6003:BCR:C8	21:A:6003:BCR:C31	2.95	0.45
19:B:1230:CLA:HED2	19:B:1230:CLA:H2A	1.98	0.45
19:B:1231:CLA:H3A	19:B:1231:CLA:HBA2	1.53	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:336:LEU:HD13	19:B:1221:CLA:CBB	2.46	0.45
2:B:395:ILE:HD13	2:B:555:TYR:H	1.81	0.45
2:B:498:LEU:HD23	2:B:498:LEU:O	2.16	0.45
2:B:533:ILE:CD1	2:B:579:ALA:HA	2.46	0.45
2:B:646:TRP:O	2:B:649:MET:HB3	2.17	0.45
2:B:73:ASN:HD22	2:B:73:ASN:H	1.59	0.45
19:B:9010:CLA:H161	19:B:9010:CLA:H193	1.74	0.45
6:F:157:TRP:CE3	19:F:1305:CLA:HMC2	2.49	0.45
5:E:123:ASP:HA	5:E:124:GLU:HA	1.57	0.45
3:C:63:LEU:HD23	3:C:63:LEU:C	2.37	0.45
6:F:103:GLN:OE1	6:F:104:ALA:N	2.50	0.45
19:4:1304:CLA:O2D	19:4:1304:CLA:HAA2	2.13	0.45
12:L:167:THR:OG1	12:L:168:GLY:N	2.47	0.45
22:R:7014:LMU:C1	22:R:7014:LMU:H62	2.25	0.45
22:R:7007:LMU:O5B	22:R:7007:LMU:H6D	2.17	0.45
17:3:176:TRP:O	17:3:178:LYS:HG3	2.16	0.45
16:2:158:VAL:O	16:2:159:PHE:C	2.52	0.45
13:N:90:GLU:OE1	13:N:91:TYR:CD2	2.69	0.45
12:L:158:PRO:O	12:L:159:SER:HB3	2.16	0.45
2:B:505:SER:OG	2:B:506:ASN:N	2.49	0.45
18:4:172:PHE:CD2	18:4:172:PHE:N	2.82	0.45
18:4:215:LEU:O	18:4:218:ILE:N	2.49	0.45
19:4:4001:CLA:HBD	19:4:4001:CLA:HAA2	1.99	0.45
1:A:109:TRP:O	1:A:112:ASP:CA	2.65	0.45
19:A:1101:CLA:HMB1	19:A:1109:CLA:H18	1.99	0.45
1:A:401:TRP:HD1	19:A:1126:CLA:CHC	2.30	0.45
1:A:136:VAL:HG23	1:A:140:PHE:O	2.15	0.45
1:A:210:LEU:N	1:A:213:LEU:H	2.15	0.45
1:A:362:LEU:HD11	19:A:1128:CLA:CBB	2.45	0.45
1:A:496:HIS:O	1:A:499:ALA:HB2	2.17	0.45
1:A:708:VAL:O	1:A:711:HIS:HB2	2.17	0.45
19:B:1203:CLA:H193	19:B:1203:CLA:H161	1.78	0.45
2:B:57:ILE:HG12	19:B:1203:CLA:HMC2	1.97	0.45
19:B:1230:CLA:HBA1	19:B:1230:CLA:H3A	1.70	0.45
2:B:305:LEU:O	2:B:308:HIS:CB	2.65	0.45
2:B:469:LYS:CG	2:B:470:THR:OG1	2.65	0.45
6:F:200:VAL:HG12	10:J:7:TYR:C	2.36	0.45
8:H:113:SER:HG	19:H:1207:CLA:H61	1.76	0.45
12:L:143:LEU:HA	12:L:146:THR:N	2.18	0.45
16:2:215:LYS:HB2	16:2:217:LEU:HG	1.98	0.45
5:E:89:SER:CB	5:E:106:ARG:NH1	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:136:ASP:O	13:N:137:LEU:CD2	2.51	0.45
1:A:569:ILE:HG22	1:A:571:ASP:N	2.32	0.45
17:3:98:LEU:O	17:3:101:GLY:HA3	2.16	0.45
1:A:252:ARG:HE	1:A:252:ARG:HB2	1.34	0.45
17:3:108:PHE:CD2	19:3:3013:CLA:C4	2.99	0.45
19:3:3006:CLA:C3B	19:3:3013:CLA:H11	2.46	0.45
12:L:206:VAL:HG22	12:L:206:VAL:O	2.17	0.45
4:D:104:TRP:NE1	4:D:127:ASN:OD1	2.48	0.45
11:K:125:LYS:CB	11:K:128:GLY:H	2.26	0.45
6:F:124:GLU:N	6:F:127:LYS:HB2	2.32	0.45
6:F:128:LYS:O	6:F:129:ARG:CD	2.64	0.45
16:2:241:TYR:CD2	16:2:242:THR:N	2.84	0.45
8:H:115:THR:O	8:H:116:ALA:CB	2.58	0.45
2:B:141:PHE:O	2:B:144:PHE:N	2.50	0.45
17:3:176:TRP:C	17:3:178:LYS:N	2.67	0.45
2:B:7:ARG:HD2	2:B:7:ARG:N	2.31	0.45
22:K:7042:LMU:H6D	22:K:7042:LMU:C3	2.44	0.45
2:B:515:GLY:HA3	2:B:613:SER:CB	2.39	0.45
15:1:114:TRP:CZ3	15:1:121:GLN:CA	2.96	0.45
22:2:7031:LMU:H52	22:2:7031:LMU:H21	1.56	0.45
1:A:105:ASN:HD22	1:A:105:ASN:HA	1.55	0.45
19:A:1110:CLA:HBD	19:A:1110:CLA:HAA1	1.98	0.45
19:A:1115:CLA:H93	19:A:1115:CLA:H61	1.81	0.45
19:A:1116:CLA:H62	19:A:1116:CLA:C4C	2.47	0.45
19:A:1138:CLA:HBC2	19:A:1139:CLA:NC	2.32	0.45
1:A:185:HIS:O	1:A:188:LYS:N	2.49	0.45
1:A:443:ILE:CG2	2:B:674:LEU:CD1	2.95	0.45
1:A:691:MET:O	20:A:5001:PQN:O1	2.35	0.45
1:A:685:VAL:O	1:A:688:PHE:HB3	2.17	0.45
19:A:9012:CLA:H62	19:A:9012:CLA:H41	1.80	0.45
2:B:302:LYS:HZ3	7:G:103:GLY:HA3	1.78	0.45
2:B:315:LEU:CD1	2:B:316:GLY:C	2.85	0.45
2:B:444:LEU:C	2:B:446:PHE:N	2.68	0.45
2:B:606:VAL:O	2:B:608:GLN:N	2.49	0.45
2:B:608:GLN:HG3	2:B:608:GLN:O	2.16	0.45
1:A:555:ILE:HG23	2:B:670:TYR:CE2	2.51	0.45
5:E:111:ASN:CG	5:E:116:SER:CB	2.85	0.45
10:J:22:LEU:O	10:J:23:ALA:C	2.55	0.45
3:C:12:ILE:CG2	3:C:39:ILE:HA	2.47	0.45
19:3:3006:CLA:HHC	19:3:3013:CLA:H11	1.98	0.45
16:2:167:ARG:NE	16:2:168:TRP:H	2.10	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:4:1304:CLA:O1A	19:4:1304:CLA:C2	2.64	0.45
19:H:1145:CLA:HBA1	19:H:1145:CLA:H3A	1.35	0.45
17:3:154:ASN:O	17:3:158:PHE:CZ	2.70	0.45
22:N:7049:LMU:H41	22:N:7049:LMU:H5'	1.98	0.45
1:A:525:ASN:HD22	1:A:526:LYS:CE	2.24	0.45
1:A:421:ASP:OD1	1:A:422:TYR:CD1	2.70	0.45
4:D:101:VAL:O	4:D:101:VAL:HG23	2.15	0.45
4:D:74:LEU:CD1	12:L:58:GLN:OE1	2.64	0.45
15:1:205:GLN:HE21	15:1:205:GLN:HB2	1.62	0.45
15:1:183:LEU:O	15:1:184:LYS:C	2.54	0.45
15:1:68:GLY:O	15:1:73:PRO:CD	2.65	0.45
19:A:1106:CLA:H3A	19:A:1106:CLA:HBA2	1.35	0.45
19:A:1104:CLA:O1A	19:A:1128:CLA:HMB2	2.16	0.45
1:A:170:GLY:C	1:A:173:VAL:HG22	2.37	0.45
1:A:213:LEU:HD12	1:A:311:LEU:HD21	1.97	0.45
1:A:413:HIS:ND1	1:A:416:ILE:HD12	2.32	0.45
1:A:668:TYR:HA	2:B:445:ALA:HB1	1.98	0.45
1:A:708:VAL:HA	1:A:711:HIS:CD2	2.52	0.45
1:A:75:SER:HB3	1:A:354:TRP:CE2	2.52	0.45
2:B:175:LEU:HD13	19:B:1221:CLA:O2D	2.16	0.45
2:B:182:LEU:O	2:B:186:SER:HB2	2.17	0.45
2:B:29:HIS:CG	19:B:1202:CLA:CBB	2.99	0.45
19:B:1203:CLA:H41	23:B:7101:LMG:H321	1.98	0.45
2:B:726:ILE:C	2:B:728:SER:H	2.19	0.45
5:E:111:ASN:HB3	5:E:116:SER:HG	1.78	0.45
19:G:1242:CLA:HHD	19:G:1242:CLA:HBC3	1.97	0.45
19:H:1207:CLA:HMA2	19:H:1207:CLA:C1	2.46	0.45
21:L:6019:BCR:H331	21:L:6019:BCR:C8	2.46	0.45
19:2:2007:CLA:CGA	19:2:2007:CLA:C1A	2.95	0.45
1:A:569:ILE:CG1	1:A:586:ARG:NH1	2.80	0.45
3:C:72:GLU:CB	3:C:77:MET:HE2	2.45	0.45
3:C:44:ARG:CD	4:D:182:GLN:NE2	2.80	0.45
16:2:160:ILE:HG22	16:2:161:GLY:N	2.32	0.45
10:J:5:LYS:CE	16:2:178:ASN:CG	2.85	0.45
16:2:249:ASN:O	16:2:250:LEU:C	2.47	0.45
6:F:129:ARG:HD2	6:F:129:ARG:HA	1.61	0.45
15:1:151:GLN:N	15:1:151:GLN:NE2	2.56	0.45
19:3:3008:CLA:O1D	19:3:3008:CLA:CGA	2.64	0.45
19:4:1304:CLA:H122	19:4:1304:CLA:H161	1.38	0.45
1:A:254:LEU:HA	1:A:254:LEU:HD13	1.41	0.45
12:L:54:TYR:HE1	12:L:57:ILE:CG2	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:ALA:O	1:A:640:GLY:C	2.53	0.45
7:G:109:GLU:O	7:G:109:GLU:HG3	2.17	0.45
18:4:201:LYS:O	18:4:205:ILE:HG23	2.17	0.45
19:A:1117:CLA:HAC2	21:A:6003:BCR:H352	1.98	0.45
1:A:119:SER:CA	1:A:145:ILE:HD12	2.47	0.45
1:A:284:ARG:N	1:A:298:ASP:OD1	2.49	0.45
1:A:536:THR:HA	1:A:539:PHE:CB	2.46	0.45
1:A:74:ILE:O	1:A:76:ARG:N	2.50	0.45
2:B:167:TRP:CZ2	19:B:1210:CLA:HAC2	2.52	0.45
19:B:1223:CLA:H202	19:B:1223:CLA:H162	1.80	0.45
2:B:255:LEU:HA	2:B:271:THR:OG1	2.16	0.45
2:B:284:PHE:CE1	19:B:1216:CLA:HHC	2.52	0.45
2:B:370:ALA:HB2	2:B:725:LEU:HD11	1.99	0.45
2:B:503:GLU:O	2:B:504:ASN:C	2.55	0.45
2:B:637:PRO:O	2:B:639:VAL:N	2.44	0.45
19:F:1302:CLA:HMA1	21:F:6016:BCR:C5	2.47	0.45
6:F:181:TYR:CD2	6:F:181:TYR:C	2.90	0.45
7:G:101:GLU:HA	7:G:105:THR:HG21	1.12	0.45
7:G:137:VAL:CG2	7:G:137:VAL:O	2.60	0.45
19:A:1126:CLA:H171	21:J:6012:BCR:H351	1.98	0.45
11:K:58:VAL:CG1	11:K:59:THR:N	2.76	0.45
12:L:148:TYR:O	12:L:151:SER:HB3	2.17	0.45
16:2:120:ILE:CG1	16:2:121:PHE:H	2.24	0.45
13:N:155:GLU:CA	13:N:157:LYS:H	2.19	0.45
3:C:44:ARG:HG3	3:C:44:ARG:O	2.17	0.45
1:A:249:ILE:HG22	17:3:137:PHE:HE2	1.82	0.45
16:2:152:LEU:N	16:2:152:LEU:HD13	2.32	0.45
16:2:164:GLU:HG2	16:2:167:ARG:HD3	1.98	0.45
12:L:207:LEU:HD23	12:L:208:ASP:C	2.37	0.45
4:D:113:GLU:O	4:D:114:MET:CB	2.59	0.45
13:N:114:PHE:HE2	13:N:116:ARG:CD	2.29	0.45
12:L:156:GLY:N	12:L:178:THR:HG21	2.32	0.45
7:G:149:TYR:CG	7:G:150:ASP:OD1	2.70	0.45
6:F:123:MET:C	6:F:127:LYS:HB2	2.37	0.45
19:J:1311:CLA:H152	19:J:1311:CLA:O1A	2.16	0.45
16:2:244:THR:O	16:2:245:GLY:C	2.55	0.45
12:L:54:TYR:O	12:L:55:GLN:CB	2.65	0.45
1:A:421:ASP:H	1:A:422:TYR:HD1	1.64	0.45
1:A:418:MET:O	1:A:564:ARG:HD2	2.16	0.45
3:C:36:ALA:O	3:C:37:LYS:CG	2.65	0.45
1:A:42:ARG:O	1:A:44:ILE:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:156:HIS:O	2:B:163:PRO:HB3	2.17	0.45
22:A:7010:LMU:O5'	22:K:7047:LMU:H122	2.17	0.45
13:N:90:GLU:OE1	13:N:91:TYR:CG	2.70	0.45
19:4:4006:CLA:HMA1	22:4:7034:LMU:C6	2.28	0.45
15:1:178:LYS:HD2	15:1:178:LYS:O	2.17	0.45
1:A:98:PHE:HZ	19:A:1105:CLA:HMD3	1.79	0.45
19:A:1119:CLA:HMB2	19:A:1125:CLA:H92	1.99	0.45
19:A:1138:CLA:HBC1	21:F:6014:BCR:C33	2.47	0.45
1:A:159:THR:O	1:A:163:GLN:OE1	2.35	0.45
1:A:196:PHE:HD2	1:A:196:PHE:N	2.07	0.45
1:A:531:PRO:O	1:A:532:ILE:CB	2.65	0.45
1:A:217:SER:CB	21:A:6002:BCR:H351	2.46	0.45
19:A:1106:CLA:C4	21:A:6011:BCR:H383	2.46	0.45
19:B:1202:CLA:H62	19:B:1202:CLA:H2	1.37	0.45
2:B:355:LEU:HD11	19:B:1223:CLA:HMC2	1.99	0.45
2:B:129:LEU:HA	19:B:1211:CLA:HED3	1.99	0.45
2:B:172:GLU:HG3	2:B:301:ILE:CG1	2.47	0.45
2:B:193:HIS:HD2	19:B:1211:CLA:NC	2.15	0.45
2:B:289:LEU:O	19:B:1218:CLA:HAC1	2.16	0.45
6:F:199:ASP:HB2	10:J:7:TYR:O	2.17	0.45
7:G:99:HIS:CA	7:G:100:PHE:CB	2.62	0.45
11:K:55:LEU:O	11:K:58:VAL:CB	2.65	0.45
12:L:131:SER:CB	12:L:201:TYR:HE2	2.05	0.45
12:L:92:ALA:H	12:L:98:ARG:HH22	1.59	0.45
16:2:227:LEU:HD21	19:2:2004:CLA:C4B	2.46	0.45
19:L:1148:CLA:CED	19:L:1148:CLA:HAA1	2.46	0.45
18:4:89:ARG:CD	18:4:90:TRP:N	2.45	0.45
16:2:250:LEU:HD23	16:2:251:PHE:CD1	2.52	0.45
12:L:169:ARG:CZ	12:L:169:ARG:HA	2.47	0.45
12:L:168:GLY:O	12:L:170:LYS:O	2.34	0.45
15:1:161:LYS:C	15:1:161:LYS:CD	2.85	0.45
16:2:211:PRO:O	16:2:212:GLN:HB2	2.17	0.45
22:K:7041:LMU:H4B	22:K:7041:LMU:H1B	1.67	0.45
6:F:80:ALA:O	6:F:81:GLY:C	2.55	0.45
15:1:70:GLY:N	15:1:73:PRO:CD	2.80	0.44
18:4:168:GLN:O	18:4:172:PHE:HD1	2.00	0.44
19:A:1116:CLA:C4A	19:A:1116:CLA:H12	2.47	0.44
19:A:1132:CLA:H172	19:A:1136:CLA:H202	1.99	0.44
19:A:1132:CLA:HBA1	19:A:1132:CLA:H3A	1.78	0.44
1:A:239:PRO:O	1:A:240:LYS:HB3	2.17	0.44
2:B:255:LEU:HD13	2:B:275:HIS:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:292:ARG:NH1	2:B:295:PHE:N	2.65	0.44
2:B:382:ILE:O	2:B:385:GLY:N	2.48	0.44
2:B:38:THR:OG1	2:B:41:ARG:HB2	2.17	0.44
2:B:420:SER:H	2:B:422:LEU:H	1.65	0.44
2:B:535:VAL:CG1	2:B:536:LYS:N	2.79	0.44
2:B:580:VAL:HG11	2:B:710:LEU:HD11	1.98	0.44
2:B:593:TYR:CZ	19:B:1234:CLA:HBC2	2.52	0.44
2:B:697:PRO:CB	19:B:1238:CLA:HBC3	2.48	0.44
5:E:82:TYR:CB	5:E:83:TRP:HE3	2.20	0.44
21:A:6011:BCR:H322	21:J:6012:BCR:H391	1.97	0.44
12:L:112:GLY:HA2	12:L:115:VAL:HG22	1.99	0.44
12:L:69:LEU:HA	12:L:69:LEU:HD23	1.80	0.44
5:E:89:SER:O	5:E:105:VAL:CA	2.65	0.44
8:H:61:THR:C	8:H:62:THR:HG23	2.25	0.44
15:1:138:LEU:HA	15:1:141:GLU:HG3	1.99	0.44
4:D:95:GLN:HE21	4:D:96:VAL:N	2.16	0.44
22:3:7005:LMU:C2	22:3:7005:LMU:O5'	2.64	0.44
4:D:140:LEU:CD2	4:D:144:LEU:CG	2.96	0.44
7:G:151:PRO:O	7:G:151:PRO:CD	2.65	0.44
4:D:131:LEU:HD13	4:D:136:GLN:HB3	1.99	0.44
1:A:629:ASN:CG	1:A:630:ASP:H	2.21	0.44
22:4:7033:LMU:H31	22:4:7033:LMU:H61	1.83	0.44
15:1:58:ALA:HB3	15:1:59:PRO:HD2	1.99	0.44
4:D:77:ASN:C	4:D:79:PRO:CD	2.86	0.44
22:H:7028:LMU:O6'	22:H:7028:LMU:C1'	2.65	0.44
15:1:177:PRO:O	15:1:178:LYS:HG3	2.17	0.44
15:1:68:GLY:CA	15:1:72:VAL:HB	2.47	0.44
15:1:73:PRO:O	15:1:74:ALA:C	2.54	0.44
18:4:173:LYS:CD	18:4:201:LYS:HG3	2.46	0.44
19:A:1120:CLA:C2D	19:A:1121:CLA:HMB3	2.47	0.44
1:A:163:GLN:CA	1:A:166:CYS:HG	2.27	0.44
1:A:209:GLY:C	1:A:213:LEU:HB2	2.37	0.44
1:A:331:LEU:HD22	1:A:343:HIS:O	2.15	0.44
1:A:431:LEU:N	1:A:434:ARG:HB2	2.32	0.44
1:A:499:ALA:HB1	19:A:1133:CLA:O2D	2.14	0.44
1:A:59:ALA:O	1:A:61:ALA:N	2.50	0.44
1:A:555:ILE:HD11	19:A:9023:CLA:CMD	2.48	0.44
2:B:120:VAL:CA	2:B:123:TRP:NE1	2.71	0.44
2:B:279:ALA:HA	19:B:1213:CLA:HMA1	1.99	0.44
2:B:718:ILE:HD11	19:B:1224:CLA:HHC	1.97	0.44
19:B:1226:CLA:C20	19:B:1239:CLA:HBA1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:256:THR:OG1	2:B:257:ILE:N	2.50	0.44
2:B:261:PHE:HE2	2:B:499:ASN:O	2.00	0.44
2:B:378:ILE:HG22	2:B:379:ALA:N	2.32	0.44
2:B:458:ILE:N	19:B:1235:CLA:HMD1	2.32	0.44
2:B:493:TRP:HB3	2:B:494:LEU:H	1.54	0.44
2:B:584:LEU:HD11	2:B:714:SER:OG	2.18	0.44
2:B:597:LYS:HG2	19:B:1234:CLA:HBC1	1.99	0.44
2:B:644:SER:O	2:B:645:VAL:C	2.54	0.44
7:G:76:ARG:HH12	7:G:120:VAL:N	2.16	0.44
7:G:119:PRO:HB3	19:G:1242:CLA:CBC	2.47	0.44
7:G:64:ILE:CG1	7:G:68:THR:HG23	2.45	0.44
12:L:182:TRP:O	12:L:186:THR:HG23	2.17	0.44
16:2:131:ILE:C	16:2:133:ASN:H	2.20	0.44
5:E:127:GLU:HA	5:E:128:VAL:O	2.13	0.44
5:E:85:LYS:HB3	5:E:85:LYS:HE3	1.67	0.44
13:N:132:THR:HA	13:N:137:LEU:O	2.18	0.44
4:D:145:ARG:NH1	4:D:173:TYR:HE1	2.12	0.44
6:F:190:LYS:HZ2	6:F:192:THR:HG21	0.48	0.44
17:3:124:LYS:NZ	17:3:148:TYR:N	2.65	0.44
19:L:1501:CLA:HBA2	19:L:1501:CLA:H3A	1.57	0.44
11:K:111:VAL:HA	11:K:114:HIS:ND1	2.30	0.44
1:A:567:ARG:HH11	4:D:89:GLY:N	2.15	0.44
2:B:131:THR:O	2:B:135:LEU:N	2.49	0.44
15:1:202:CYS:SG	15:1:202:CYS:O	2.71	0.44
22:4:7053:LMU:H51	22:4:7053:LMU:H21	1.57	0.44
7:G:144:THR:OG1	7:G:147:ASN:C	2.56	0.44
11:K:86:LEU:O	11:K:87:GLU:HB2	2.16	0.44
6:F:154:GLN:OE1	6:F:154:GLN:C	2.55	0.44
22:4:7052:LMU:H12	22:4:7052:LMU:C5	2.47	0.44
15:1:177:PRO:HG2	15:1:180:LEU:CA	2.47	0.44
1:A:106:TYR:O	1:A:110:LEU:CD2	2.50	0.44
19:A:1103:CLA:H202	19:A:1103:CLA:H161	1.62	0.44
19:A:1103:CLA:HMB3	19:A:1104:CLA:HAA1	1.99	0.44
19:A:1112:CLA:C4B	21:A:6002:BCR:C20	2.94	0.44
19:A:1140:CLA:H43	19:A:1140:CLA:C4C	2.46	0.44
1:A:488:PHE:N	1:A:488:PHE:CD1	2.83	0.44
1:A:493:GLN:HE21	1:A:515:TRP:HA	1.82	0.44
1:A:499:ALA:HB3	1:A:500:PRO:HD2	1.99	0.44
1:A:502:THR:CG2	1:A:503:THR:N	2.81	0.44
1:A:85:GLN:O	1:A:89:ILE:HG13	2.18	0.44
19:B:1220:CLA:H161	19:B:1220:CLA:H141	1.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:244:PHE:HD2	2:B:245:GLY:N	2.15	0.44
2:B:292:ARG:CZ	2:B:297:ILE:O	2.65	0.44
6:F:200:VAL:CG2	6:F:203:ALA:C	2.85	0.44
7:G:75:GLY:C	7:G:77:PHE:H	2.20	0.44
7:G:84:ARG:NE	7:G:89:LYS:CD	2.80	0.44
10:J:26:LEU:HD23	10:J:26:LEU:O	2.17	0.44
19:2:2006:CLA:H71	19:2:2006:CLA:H112	1.72	0.44
3:C:44:ARG:O	3:C:44:ARG:CG	2.65	0.44
17:3:224:LYS:O	17:3:226:LYS:N	2.50	0.44
16:2:171:ILE:HG12	16:2:172:LEU:N	2.26	0.44
17:3:151:TRP:CG	17:3:152:ALA:N	2.84	0.44
4:D:80:SER:HB2	4:D:127:ASN:CA	2.47	0.44
19:4:1304:CLA:CAA	19:4:1304:CLA:O2D	2.65	0.44
17:3:200:PRO:O	17:3:201:ALA:C	2.54	0.44
15:1:116:ALA:HA	15:1:117:LEU:HD22	1.99	0.44
14:R:5:UNK:O	14:R:6:UNK:CB	2.65	0.44
1:A:359:SER:OG	1:A:414:ALA:HB2	2.16	0.44
15:1:68:GLY:O	15:1:72:VAL:CA	2.64	0.44
1:A:308:ILE:CG1	19:A:1115:CLA:CBB	2.96	0.44
1:A:432:LEU:HB3	1:A:433:ASP:H	1.71	0.44
1:A:539:PHE:HE2	1:A:543:HIS:HE1	1.65	0.44
1:A:549:ILE:O	1:A:552:THR:O	2.34	0.44
1:A:615:HIS:ND1	19:A:1135:CLA:HBC3	2.32	0.44
19:B:1217:CLA:NA	19:B:1217:CLA:O2A	2.51	0.44
19:B:1229:CLA:H162	19:B:1229:CLA:H143	1.84	0.44
2:B:120:VAL:CB	2:B:123:TRP:NE1	2.80	0.44
2:B:316:GLY:O	2:B:317:ARG:CD	2.64	0.44
1:A:669:GLY:CA	2:B:445:ALA:HA	2.44	0.44
2:B:495:PRO:HB2	2:B:496:GLY:H	1.40	0.44
6:F:149:ILE:O	6:F:150:VAL:CG1	2.64	0.44
16:2:113:ALA:CA	16:2:114:MET:HE3	2.45	0.44
3:C:11:CYS:C	3:C:13:GLY:N	2.71	0.44
4:D:173:TYR:CZ	4:D:175:GLU:OE2	2.70	0.44
13:N:104:LYS:HB3	13:N:105:LYS:H	1.53	0.44
19:3:3011:CLA:CAC	19:3:3012:CLA:C2A	2.78	0.44
17:3:93:ILE:HA	17:3:95:PRO:HD2	1.99	0.44
16:2:183:PHE:O	16:2:184:PRO:C	2.55	0.44
12:L:205:TYR:CD2	12:L:205:TYR:N	2.84	0.44
4:D:199:GLU:O	4:D:200:VAL:C	2.56	0.44
17:3:164:LEU:HD12	17:3:165:MET:SD	2.58	0.44
17:3:190:LEU:HA	17:3:190:LEU:HD23	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:GLU:CD	1:A:161:GLU:CG	2.85	0.44
19:A:1107:CLA:CBD	19:A:1107:CLA:HBA2	2.47	0.44
1:A:218:TRP:CA	19:A:1112:CLA:HBB2	2.48	0.44
19:A:1125:CLA:CBA	21:A:6008:BCR:H12C	2.45	0.44
19:A:1140:CLA:H71	19:A:9013:CLA:H171	1.98	0.44
1:A:122:VAL:HG13	1:A:133:ASN:HD21	1.83	0.44
1:A:190:ALA:HA	1:A:191:PRO:HD3	1.77	0.44
1:A:227:LEU:O	1:A:231:GLN:HB2	2.18	0.44
1:A:680:LEU:HB3	19:A:9012:CLA:C2	2.48	0.44
1:A:684:PHE:CD2	1:A:685:VAL:N	2.78	0.44
1:A:98:PHE:CD1	1:A:99:HIS:N	2.77	0.44
19:B:1229:CLA:CBB	21:F:6014:BCR:C23	2.96	0.44
2:B:167:TRP:CZ2	19:B:1210:CLA:HAC1	2.53	0.44
2:B:33:SER:H	2:B:37:ILE:CD1	2.30	0.44
2:B:469:LYS:CD	2:B:470:THR:CA	2.60	0.44
2:B:664:LEU:C	2:B:667:TRP:CZ3	2.76	0.44
2:B:697:PRO:HB3	19:B:1238:CLA:HBC3	1.99	0.44
7:G:116:SER:O	7:G:119:PRO:N	2.50	0.44
8:H:97:LEU:HG	8:H:98:LEU:N	2.32	0.44
11:K:49:ILE:CA	11:K:52:PRO:HG2	2.23	0.44
12:L:108:TYR:C	12:L:109:LEU:O	2.52	0.44
12:L:114:PHE:CD1	12:L:114:PHE:N	2.85	0.44
12:L:146:THR:C	12:L:148:TYR:N	2.69	0.44
12:L:138:VAL:CG2	12:L:194:ILE:HG13	2.47	0.44
16:2:226:ARG:HG2	16:2:226:ARG:NH1	2.33	0.44
3:C:10:THR:HG23	5:E:101:TYR:HD2	1.67	0.44
17:3:226:LYS:O	17:3:226:LYS:HG2	2.18	0.44
4:D:99:PHE:O	4:D:99:PHE:CD1	2.71	0.44
16:2:156:GLU:OE2	19:2:2013:CLA:HHD	2.11	0.44
16:2:184:PRO:N	16:2:187:LYS:CG	2.74	0.44
17:3:151:TRP:HD1	17:3:152:ALA:N	1.97	0.44
13:N:113:ASN:C	13:N:113:ASN:OD1	2.56	0.44
4:D:141:GLY:N	4:D:143:ARG:N	2.66	0.44
1:A:23:ASP:CG	1:A:24:ARG:HD2	2.37	0.44
16:2:195:TYR:HD1	16:2:196:PRO:N	2.14	0.44
2:B:75:GLU:O	2:B:79:GLN:HG2	2.17	0.44
1:A:389:TYR:HD1	1:A:625:TRP:CD2	2.36	0.44
16:2:97:GLU:OE1	16:2:97:GLU:N	2.51	0.44
12:L:56:VAL:HG23	12:L:56:VAL:O	2.17	0.44
15:1:73:PRO:HD2	15:1:74:ALA:H	1.82	0.44
18:4:158:GLN:HB3	19:4:1004:CLA:HMA3	0.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1119:CLA:HBA1	19:A:1123:CLA:CBB	2.46	0.44
1:A:729:GLN:HE21	19:A:1140:CLA:HMD1	1.83	0.44
1:A:148:GLY:C	1:A:149:PHE:O	2.51	0.44
1:A:450:CYS:O	1:A:453:LEU:O	2.35	0.44
1:A:51:THR:CG2	1:A:723:ARG:HB2	2.47	0.44
1:A:723:ARG:CG	1:A:723:ARG:NH1	2.57	0.44
19:A:1140:CLA:C6	19:A:9013:CLA:H193	2.45	0.44
2:B:55:ALA:HB1	2:B:150:LEU:HD11	2.00	0.44
2:B:182:LEU:HD13	19:B:1210:CLA:HHB	1.99	0.44
2:B:387:PHE:HB2	2:B:534:LEU:HD13	1.98	0.44
19:A:1139:CLA:C4	6:F:198:ILE:HD13	2.45	0.44
7:G:79:PHE:CE2	7:G:80:PHE:HB2	2.53	0.44
9:I:12:VAL:CG1	21:I:6018:BCR:H271	2.48	0.44
12:L:83:LEU:HD13	12:L:88:ALA:HB3	1.98	0.44
16:2:128:LYS:HG3	16:2:131:ILE:HG23	1.98	0.44
3:C:62:PHE:CD1	5:E:80:GLU:CB	3.00	0.44
3:C:9:ASP:OD1	3:C:61:ASP:HB2	2.17	0.44
5:E:122:LEU:O	5:E:124:GLU:C	2.56	0.44
5:E:128:VAL:C	5:E:129:GLU:O	2.56	0.44
17:3:96:ARG:NH2	17:3:100:TYR:OH	2.51	0.44
16:2:164:GLU:HB3	19:2:2012:CLA:CHB	2.47	0.44
22:3:7005:LMU:C5	22:3:7005:LMU:O1'	2.63	0.44
12:L:208:ASP:OD2	12:L:208:ASP:C	2.55	0.44
8:H:89:ALA:HB3	8:H:90:PRO:HD3	1.99	0.44
17:3:164:LEU:O	17:3:167:PHE:HB2	2.18	0.44
22:R:7022:LMU:H111	22:R:7022:LMU:H81	1.72	0.44
18:4:232:LEU:HB3	18:4:236:ILE:HD13	1.99	0.44
8:H:112:LEU:HA	8:H:112:LEU:HD22	1.74	0.44
4:D:148:TYR:O	4:D:149:LYS:NZ	2.44	0.44
4:D:151:LYS:HB3	4:D:151:LYS:HE2	1.72	0.44
22:A:7023:LMU:H92	22:A:7023:LMU:H41	1.99	0.44
1:A:527:VAL:CB	1:A:626:GLY:HA3	2.41	0.44
22:K:7042:LMU:C5'	22:K:7042:LMU:O2B	2.59	0.44
13:N:90:GLU:OE2	13:N:91:TYR:N	2.51	0.44
18:4:170:PRO:C	18:4:173:LYS:H	2.21	0.44
1:A:370:ILE:HD11	19:A:1124:CLA:O1D	2.17	0.44
1:A:132:LEU:O	1:A:671:SER:C	2.52	0.44
1:A:358:LEU:HD11	1:A:413:HIS:CD2	2.48	0.44
1:A:538:ASP:O	1:A:542:HIS:CD2	2.71	0.44
1:A:648:THR:C	1:A:650:ASN:H	2.21	0.44
1:A:93:LEU:HA	1:A:96:MET:CG	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:10:GLN:HE21	2:B:10:GLN:HB2	1.53	0.44
19:B:1229:CLA:HBA1	19:B:1229:CLA:HBD	1.98	0.44
2:B:510:LEU:CD2	2:B:597:LYS:HD2	2.47	0.44
1:A:588:GLY:HA3	2:B:668:ARG:HB3	1.99	0.44
2:B:707:LEU:HD13	23:B:7101:LMG:H331	1.98	0.44
5:E:81:SER:OG	5:E:120:TYR:CE1	2.68	0.44
6:F:207:LEU:C	6:F:209:ARG:H	2.21	0.44
2:B:294:ASN:CB	7:G:94:GLN:CG	2.96	0.44
12:L:76:SER:H	12:L:79:ILE:HG22	1.83	0.44
15:1:138:LEU:HA	15:1:141:GLU:CD	2.38	0.44
1:A:49:ASP:HA	6:F:193:GLN:OE1	2.18	0.44
4:D:83:PHE:CZ	4:D:114:MET:HE3	2.51	0.44
4:D:110:GLN:O	4:D:122:MET:HG3	2.18	0.44
12:L:153:PHE:CG	12:L:155:GLU:OE1	2.71	0.44
12:L:155:GLU:CA	12:L:178:THR:HG21	2.43	0.44
2:B:160:LYS:NZ	2:B:161:TRP:HB3	2.32	0.44
11:K:110:GLY:O	11:K:114:HIS:CG	2.70	0.44
19:3:3008:CLA:CBC	19:3:3008:CLA:CMC	2.86	0.44
18:4:242:ASN:O	18:4:243:THR:CB	2.66	0.44
16:2:137:TRP:CD1	16:2:139:THR:HG22	2.53	0.44
7:G:144:THR:CG2	7:G:144:THR:O	2.66	0.44
2:B:488:ALA:HB2	19:B:1233:CLA:C2C	2.48	0.44
13:N:126:LYS:HB3	13:N:126:LYS:NZ	2.32	0.44
1:A:357:GLN:O	1:A:357:GLN:OE1	2.36	0.44
15:1:223:ASP:HB3	15:1:224:PRO:HD2	1.99	0.44
19:A:1119:CLA:HMB2	19:A:1123:CLA:HMA3	1.98	0.44
19:A:1126:CLA:H171	19:A:1126:CLA:H122	2.00	0.44
19:A:1131:CLA:HBB2	19:A:1132:CLA:H2	2.00	0.44
19:A:1141:CLA:H41	19:A:1141:CLA:H62	1.48	0.44
1:A:159:THR:O	1:A:163:GLN:CD	2.56	0.44
1:A:406:LEU:HD11	19:A:1104:CLA:HMB3	1.99	0.44
1:A:89:ILE:O	1:A:92:TRP:C	2.54	0.44
19:B:1206:CLA:C4	21:I:6018:BCR:H21C	2.48	0.44
19:B:1218:CLA:HBA2	19:B:1219:CLA:O1A	2.18	0.44
19:B:1220:CLA:C4	19:B:1220:CLA:HAA1	2.33	0.44
2:B:444:LEU:O	2:B:445:ALA:CB	2.62	0.44
2:B:535:VAL:HG13	2:B:536:LYS:H	1.83	0.44
2:B:37:ILE:HG13	4:D:202:PHE:HD2	1.83	0.44
6:F:84:PRO:HA	6:F:138:LEU:O	2.18	0.44
12:L:68:SER:O	12:L:70:GLU:N	2.50	0.44
16:2:122:ILE:CD1	19:2:2002:CLA:C2B	2.89	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:59:PRO:HB3	3:C:61:ASP:OD2	2.18	0.44
13:N:131:PHE:HA	13:N:133:GLY:H	1.83	0.44
14:R:34:UNK:C	14:R:36:UNK:O	2.66	0.44
15:1:189:LYS:CG	19:1:1007:CLA:CMC	2.53	0.44
19:K:1143:CLA:H43	19:K:1143:CLA:O2A	2.18	0.44
6:F:128:LYS:C	6:F:129:ARG:HD3	2.37	0.44
16:2:241:TYR:O	16:2:242:THR:C	2.52	0.44
17:3:204:GLY:HA3	17:3:207:PHE:O	2.17	0.44
17:3:155:TYR:HB2	17:3:157:LEU:HG	1.99	0.44
19:3:3016:CLA:CMC	19:3:3016:CLA:CBC	2.87	0.44
15:1:161:LYS:HG3	15:1:162:LYS:N	2.33	0.44
1:A:620:MET:HG3	1:A:625:TRP:CE2	2.52	0.44
2:B:163:PRO:O	2:B:164:SER:CB	2.66	0.44
12:L:100:ILE:HG22	12:L:188:GLY:O	2.18	0.44
18:4:83:GLU:C	18:4:84:ASP:OD1	2.56	0.44
19:H:1505:CLA:C10	19:H:1505:CLA:H41	2.47	0.44
22:B:7012:LMU:H3'	22:B:7012:LMU:H1B	1.36	0.44
18:4:172:PHE:O	18:4:194:PHE:CD2	2.71	0.44
19:A:1124:CLA:HAA2	19:A:1125:CLA:OBD	2.18	0.44
1:A:109:TRP:O	1:A:112:ASP:C	2.56	0.44
1:A:119:SER:OG	1:A:136:VAL:HG11	2.18	0.44
1:A:701:GLN:OE1	5:E:112:TYR:CZ	2.71	0.44
2:B:586:THR:O	2:B:590:VAL:HG12	2.17	0.44
6:F:83:THR:CB	6:F:84:PRO:HD2	2.41	0.44
3:C:61:ASP:O	3:C:62:PHE:CD2	2.71	0.44
19:3:3011:CLA:H142	19:3:3011:CLA:H92	1.99	0.44
16:2:112:TRP:CZ3	16:2:164:GLU:CG	2.97	0.44
11:K:127:ILE:HA	11:K:130:LEU:CD2	2.42	0.44
6:F:102:LEU:HD12	6:F:103:GLN:N	2.33	0.44
11:K:84:LEU:HG	11:K:85:LYS:N	2.33	0.44
19:H:1145:CLA:CAA	19:H:1145:CLA:HED1	2.44	0.44
12:L:173:PRO:CD	12:L:173:PRO:O	2.65	0.44
12:L:164:LEU:C	12:L:165:THR:HG22	2.37	0.44
2:B:214:ASP:OD1	2:B:214:ASP:O	2.36	0.44
7:G:138:ALA:O	7:G:140:TYR:N	2.50	0.44
15:1:114:TRP:CH2	15:1:121:GLN:CG	2.95	0.44
15:1:114:TRP:HZ3	15:1:121:GLN:HA	1.76	0.44
22:4:7034:LMU:H92	22:4:7052:LMU:C1	2.47	0.43
18:4:158:GLN:O	19:4:1004:CLA:HMA2	2.13	0.43
18:4:204:GLU:O	18:4:205:ILE:C	2.54	0.43
18:4:220:GLN:CD	19:4:1306:CLA:CAC	2.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1115:CLA:H61	19:A:1115:CLA:H41	1.68	0.43
1:A:398:HIS:HD2	19:A:1126:CLA:ND	2.15	0.43
19:A:1138:CLA:OBD	2:B:427:LEU:HD22	2.18	0.43
1:A:133:ASN:HA	1:A:142:GLY:O	2.18	0.43
1:A:181:ALA:HA	1:A:184:PHE:HB3	1.99	0.43
1:A:473:PRO:C	1:A:475:ASP:N	2.71	0.43
1:A:711:HIS:O	1:A:716:VAL:HG22	2.18	0.43
2:B:31:PHE:CD1	19:B:1202:CLA:HMC2	2.53	0.43
19:B:1206:CLA:H93	19:B:1206:CLA:H61	1.83	0.43
2:B:14:GLN:O	2:B:15:ASP:C	2.56	0.43
2:B:170:ASN:O	2:B:171:ALA:HB3	2.18	0.43
2:B:304:ILE:O	2:B:308:HIS:CD2	2.71	0.43
2:B:309:ILE:HG22	2:B:319:HIS:HD2	1.82	0.43
2:B:310:PRO:HD2	2:B:311:PRO:CD	2.48	0.43
2:B:337:ALA:O	2:B:339:ALA:O	2.35	0.43
2:B:388:ALA:HA	2:B:391:PRO:CG	2.48	0.43
2:B:529:THR:O	2:B:532:LEU:HG	2.17	0.43
19:B:1223:CLA:C10	21:B:6010:BCR:H14C	2.48	0.43
2:B:454:LEU:HD11	6:F:146:PRO:O	2.18	0.43
19:A:1139:CLA:OBD	6:F:182:LEU:HD11	2.18	0.43
8:H:109:LEU:HD23	19:H:1207:CLA:C6	2.47	0.43
12:L:125:ILE:HG23	12:L:128:GLN:H	1.82	0.43
12:L:76:SER:OG	12:L:78:LEU:HD11	2.17	0.43
16:2:101:TRP:N	16:2:103:VAL:CB	2.66	0.43
3:C:12:ILE:HG21	3:C:39:ILE:CA	2.47	0.43
8:H:65:TRP:N	8:H:66:ASP:CA	2.74	0.43
2:B:549:ASP:HB2	3:C:63:LEU:HB2	2.00	0.43
16:2:182:ILE:HG22	16:2:187:LYS:CD	2.48	0.43
16:2:182:ILE:CD1	16:2:187:LYS:O	2.64	0.43
11:K:125:LYS:HD2	11:K:128:GLY:CA	2.48	0.43
17:3:204:GLY:CA	17:3:207:PHE:HA	2.48	0.43
14:R:50:UNK:HA	14:R:51:UNK:HA	1.70	0.43
14:R:27:UNK:O	14:R:29:UNK:C	2.65	0.43
19:1:1303:CLA:CMC	19:4:1304:CLA:HMB3	2.43	0.43
19:H:1145:CLA:C3A	19:H:1145:CLA:CGA	2.95	0.43
2:B:513:GLY:O	2:B:516:ASP:OD1	2.36	0.43
19:A:1131:CLA:CBC	19:A:1136:CLA:HBC2	2.48	0.43
1:A:188:LYS:CD	1:A:188:LYS:C	2.65	0.43
1:A:336:GLY:HA3	19:A:1151:CLA:CMC	2.37	0.43
1:A:662:SER:HA	1:A:665:ILE:HD11	2.00	0.43
19:B:1208:CLA:C1	19:B:1208:CLA:HBD	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1205:CLA:H193	19:B:1224:CLA:H192	1.99	0.43
19:B:1205:CLA:C14	19:B:1224:CLA:H91	2.44	0.43
2:B:175:LEU:HD21	19:B:1216:CLA:HMA3	1.99	0.43
2:B:216:LEU:HD11	2:B:221:GLY:HA2	2.00	0.43
2:B:224:PRO:HB3	2:B:227:THR:HG21	2.00	0.43
2:B:317:ARG:CB	2:B:317:ARG:CZ	2.94	0.43
21:B:6010:BCR:C8	21:B:6010:BCR:H311	2.47	0.43
2:B:618:GLY:HA2	2:B:621:ARG:N	2.31	0.43
2:B:98:GLN:H	2:B:99:PRO:HD2	1.82	0.43
16:2:100:ARG:O	16:2:101:TRP:C	2.55	0.43
16:2:226:ARG:HA	16:2:226:ARG:HD3	1.60	0.43
13:N:146:LEU:HD22	17:3:142:ILE:O	2.11	0.43
16:2:147:THR:HG22	16:2:148:ASP:CG	2.35	0.43
22:2:7006:LMU:H3'	22:2:7006:LMU:C5B	2.48	0.43
11:K:113:GLY:O	11:K:114:HIS:O	2.36	0.43
11:K:84:LEU:HD11	11:K:85:LYS:HE3	2.01	0.43
1:A:23:ASP:CG	1:A:24:ARG:CD	2.87	0.43
4:D:133:ARG:N	4:D:136:GLN:HE22	2.09	0.43
4:D:129:LEU:HD13	12:L:65:PHE:CD1	2.53	0.43
13:N:90:GLU:HA	13:N:91:TYR:CD2	2.53	0.43
1:A:36:LYS:HA	1:A:37:PRO:HD3	1.60	0.43
15:1:176:ASP:HB3	15:1:180:LEU:HD11	1.74	0.43
18:4:177:LEU:CD2	18:4:177:LEU:C	2.84	0.43
18:4:220:GLN:HG3	19:4:1306:CLA:CAC	2.42	0.43
1:A:207:LEU:CG	19:A:1119:CLA:HBB2	2.49	0.43
19:A:1124:CLA:H61	19:A:1125:CLA:CED	2.49	0.43
19:A:1136:CLA:H18	19:A:1136:CLA:H151	1.84	0.43
1:A:270:PHE:HE1	19:A:1141:CLA:H2	1.78	0.43
19:B:1201:CLA:HBA2	19:B:1201:CLA:H3A	1.57	0.43
19:B:1215:CLA:C4A	19:B:1215:CLA:CGA	2.96	0.43
2:B:293:THR:O	2:B:295:PHE:CE2	2.72	0.43
2:B:420:SER:HA	2:B:423:SER:OG	2.19	0.43
2:B:532:LEU:HA	2:B:535:VAL:HG12	2.00	0.43
6:F:136:TYR:HD1	6:F:138:LEU:CD1	2.30	0.43
19:B:1235:CLA:H41	21:F:6016:BCR:H323	2.00	0.43
19:B:1201:CLA:CHD	21:I:6021:BCR:H401	2.48	0.43
12:L:110:LEU:HA	12:L:113:PRO:HG3	2.00	0.43
12:L:79:ILE:O	12:L:80:ALA:C	2.56	0.43
1:A:244:LEU:HB3	1:A:247:GLU:HG2	1.92	0.43
13:N:138:ALA:O	13:N:139:LYS:HD2	2.17	0.43
1:A:250:LEU:HD23	1:A:250:LEU:HA	1.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:PHE:C	1:A:262:PHE:CD2	2.91	0.43
16:2:182:ILE:CG2	16:2:187:LYS:HE2	2.48	0.43
11:K:124:LEU:O	11:K:126:ASN:HB3	2.17	0.43
22:A:7016:LMU:H112	22:A:7016:LMU:H71	1.97	0.43
18:4:228:PRO:CG	18:4:228:PRO:O	2.66	0.43
19:2:2014:CLA:H91	19:2:2014:CLA:H151	1.96	0.43
22:L:7029:LMU:C4'	22:L:7029:LMU:C5B	2.82	0.43
12:L:170:LYS:HB2	12:L:170:LYS:HE2	1.65	0.43
18:4:198:LEU:HG	18:4:199:GLU:CA	2.48	0.43
18:4:190:ASN:HA	18:4:191:PRO:HD3	1.74	0.43
19:A:1125:CLA:C14	19:A:1125:CLA:H101	2.44	0.43
19:A:1136:CLA:O1D	19:A:1136:CLA:H2A	2.18	0.43
1:A:400:MET:HG3	1:A:609:ILE:HG23	2.00	0.43
1:A:411:ALA:O	1:A:412:ALA:C	2.57	0.43
1:A:599:PHE:CE2	1:A:735:VAL:CG2	3.00	0.43
1:A:401:TRP:CZ3	1:A:609:ILE:HB	2.52	0.43
1:A:707:ILE:H	1:A:707:ILE:HG12	1.49	0.43
2:B:493:TRP:CZ2	19:B:1214:CLA:C12	3.01	0.43
2:B:285:LEU:HD11	19:B:1217:CLA:HBC2	2.00	0.43
19:B:1216:CLA:C2	19:B:1221:CLA:H92	2.49	0.43
2:B:304:ILE:O	2:B:308:HIS:CG	2.72	0.43
2:B:469:LYS:CG	2:B:470:THR:CB	2.97	0.43
2:B:497:TRP:C	2:B:499:ASN:H	2.21	0.43
2:B:620:LEU:O	2:B:625:TRP:HB3	2.18	0.43
2:B:599:ILE:O	2:B:734:GLY:C	2.57	0.43
19:H:1241:CLA:H62	19:H:1241:CLA:H92	1.88	0.43
12:L:97:LEU:O	12:L:98:ARG:C	2.55	0.43
16:2:128:LYS:C	16:2:130:GLY:N	2.66	0.43
1:A:22:VAL:H	1:A:25:ASP:HB2	1.83	0.43
1:A:27:ILE:O	1:A:28:LYS:CB	2.65	0.43
17:3:103:VAL:C	17:3:107:ARG:HD2	2.38	0.43
4:D:100:TYR:CE1	4:D:134:LYS:CD	2.88	0.43
4:D:100:TYR:CE1	4:D:134:LYS:HE2	2.50	0.43
1:A:478:SER:OG	1:A:481:ALA:N	2.45	0.43
6:F:90:GLN:CG	6:F:143:ASP:HA	2.48	0.43
16:2:243:GLY:N	16:2:244:THR:HG23	2.33	0.43
12:L:165:THR:O	12:L:166:LEU:C	2.57	0.43
22:K:7042:LMU:H32	22:K:7042:LMU:C5'	2.49	0.43
22:2:7027:LMU:O2'	22:2:7027:LMU:C1	2.66	0.43
18:4:120:ILE:HD11	18:4:226:LYS:CA	2.48	0.43
15:1:98:LEU:HD22	15:1:98:LEU:HA	1.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:100:ARG:O	18:4:104:LEU:HD13	2.19	0.43
19:A:1102:CLA:HBB2	19:A:1104:CLA:CHA	2.49	0.43
1:A:207:LEU:CB	19:A:1119:CLA:CBB	2.83	0.43
1:A:382:TYR:CD2	19:A:1127:CLA:HED3	2.53	0.43
19:A:1129:CLA:HMB2	19:L:1130:CLA:C4D	2.49	0.43
19:A:1131:CLA:H93	19:A:1131:CLA:H61	1.86	0.43
1:A:457:SER:OG	1:A:544:ILE:HA	2.19	0.43
1:A:479:ASP:CA	1:A:536:THR:CG2	2.90	0.43
19:A:9023:CLA:H162	19:A:9023:CLA:H202	1.85	0.43
19:B:1222:CLA:C2B	21:B:6010:BCR:C35	2.97	0.43
2:B:303:TYR:CA	2:B:306:GLU:CB	2.85	0.43
2:B:471:THR:HG23	2:B:502:ASN:HB2	1.99	0.43
2:B:514:PRO:HG2	6:F:147:HIS:CE1	2.54	0.43
3:C:1:MET:N	3:C:4:SER:N	2.57	0.43
4:D:87:THR:HG23	12:L:69:LEU:CG	2.45	0.43
21:F:6016:BCR:C31	21:F:6016:BCR:HC8	2.40	0.43
7:G:69:GLY:O	7:G:72:LEU:CD1	2.67	0.43
13:N:136:ASP:CG	13:N:137:LEU:N	2.71	0.43
4:D:95:GLN:O	4:D:159:PRO:HG3	2.17	0.43
17:3:149:ASN:HA	17:3:150:TYR:HA	1.40	0.43
8:H:119:ASP:HB3	8:H:121:LEU:CG	2.47	0.43
16:2:269:LYS:C	16:2:269:LYS:CE	2.87	0.43
8:H:114:ALA:O	8:H:115:THR:HG22	2.15	0.43
17:3:211:LEU:HD12	17:3:211:LEU:H	1.84	0.43
1:A:71:LEU:O	1:A:72:GLU:C	2.53	0.43
2:B:110:LEU:HD12	2:B:110:LEU:C	2.34	0.43
18:4:111:LEU:CD1	18:4:112:PRO:HD3	2.48	0.43
22:K:7042:LMU:H52	22:K:7042:LMU:H81	1.52	0.43
10:J:41:PHE:N	10:J:41:PHE:CD1	2.87	0.43
15:1:155:GLU:HB2	15:1:160:LYS:HD2	1.99	0.43
15:1:177:PRO:CD	15:1:180:LEU:N	2.82	0.43
15:1:71:GLU:OE1	15:1:76:LEU:HD11	2.17	0.43
15:1:97:ILE:HD13	15:1:98:LEU:HB2	1.78	0.43
1:A:334:HIS:HB3	19:A:1120:CLA:CMA	2.49	0.43
1:A:372:VAL:O	1:A:374:GLN:N	2.51	0.43
1:A:409:GLY:C	1:A:411:ALA:N	2.72	0.43
1:A:607:ASN:O	1:A:608:SER:C	2.57	0.43
19:B:1201:CLA:HBC3	19:B:1226:CLA:H41	2.00	0.43
2:B:212:PHE:HZ	19:B:1211:CLA:HAC1	1.77	0.43
19:B:1220:CLA:O1D	19:B:1220:CLA:OBD	2.35	0.43
19:B:1222:CLA:H11	19:B:1236:CLA:HBD	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1225:CLA:H162	19:B:1225:CLA:H141	1.91	0.43
2:B:172:GLU:HG3	2:B:301:ILE:HG12	2.00	0.43
2:B:500:ALA:CB	2:B:507:SER:O	2.66	0.43
2:B:568:CYS:HB3	2:B:569:ASP:H	1.65	0.43
6:F:167:PHE:HA	21:F:6014:BCR:C39	2.47	0.43
7:G:89:LYS:CE	7:G:89:LYS:CA	2.47	0.43
11:K:56:ILE:C	11:K:59:THR:HG23	2.39	0.43
19:2:2004:CLA:HBC2	19:2:2004:CLA:HMC1	2.01	0.43
13:N:132:THR:O	13:N:133:GLY:C	2.55	0.43
3:C:47:ASP:OD1	4:D:134:LYS:NZ	2.51	0.43
8:H:76:TYR:HH	12:L:90:ARG:HD3	1.72	0.43
17:3:210:PRO:CD	17:3:211:LEU:HD12	2.48	0.43
19:3:3016:CLA:CMA	19:3:3016:CLA:O1A	2.67	0.43
22:H:7043:LMU:H71	22:H:7043:LMU:H112	2.00	0.43
15:1:117:LEU:H	15:1:117:LEU:HD13	1.78	0.43
15:1:77:GLU:CG	15:1:80:LYS:CE	2.96	0.43
18:4:193:ASN:O	18:4:201:LYS:NZ	2.52	0.43
1:A:113:PRO:C	1:A:114:THR:HG22	2.29	0.43
1:A:338:PHE:CZ	19:A:1151:CLA:HBB1	2.38	0.43
1:A:183:TRP:CZ3	1:A:188:LYS:HB3	2.54	0.43
1:A:295:TRP:HB3	1:A:297:THR:CG2	2.48	0.43
1:A:63:ASP:OD2	1:A:64:PHE:N	2.52	0.43
19:A:9011:CLA:H71	19:A:9011:CLA:H111	1.87	0.43
19:B:1209:CLA:C3C	19:B:1210:CLA:HBB2	2.40	0.43
2:B:188:LEU:HG	2:B:189:ALA:N	2.34	0.43
20:B:5002:PQN:H192	21:B:6017:BCR:C8	2.48	0.43
5:E:81:SER:O	5:E:82:TYR:C	2.53	0.43
6:F:205:SER:C	6:F:207:LEU:CD1	2.86	0.43
7:G:75:GLY:N	7:G:77:PHE:H	2.17	0.43
8:H:98:LEU:C	8:H:99:LYS:O	2.56	0.43
19:A:1105:CLA:HMB2	21:J:6012:BCR:HC7	1.98	0.43
12:L:135:GLY:O	12:L:138:VAL:HG22	2.19	0.43
16:2:119:GLY:O	16:2:123:PRO:HD3	2.14	0.43
13:N:139:LYS:HD2	13:N:139:LYS:HA	1.14	0.43
13:N:145:PHE:N	13:N:145:PHE:CD1	2.80	0.43
15:1:136:THR:O	15:1:137:ILE:C	2.56	0.43
4:D:167:HIS:HD2	4:D:172:VAL:CG2	2.03	0.43
17:3:238:ILE:N	17:3:238:ILE:HD13	2.34	0.43
17:3:150:TYR:C	17:3:152:ALA:CB	2.83	0.43
12:L:204:LEU:CD1	12:L:205:TYR:C	2.85	0.43
4:D:140:LEU:HD13	4:D:144:LEU:CA	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:121:ALA:O	6:F:123:MET:N	2.50	0.43
1:A:575:LEU:C	1:A:575:LEU:HD12	2.32	0.43
1:A:23:ASP:OD2	1:A:33:GLN:HG2	2.16	0.43
19:4:1304:CLA:HBA2	19:4:1304:CLA:H3A	1.19	0.43
6:F:117:LEU:CA	6:F:119:ILE:HG12	2.46	0.43
12:L:171:LYS:O	12:L:173:PRO:CD	2.38	0.43
22:4:7053:LMU:C7	22:4:7053:LMU:C11	2.97	0.43
1:A:40:PHE:O	1:A:44:ILE:HA	2.18	0.43
15:1:114:TRP:HH2	15:1:121:GLN:HG3	1.75	0.43
22:B:7038:LMU:H1B	22:B:7038:LMU:C6'	2.48	0.43
15:1:58:ALA:HB1	19:1:1015:CLA:C2B	2.48	0.43
2:B:689:ASN:OD1	2:B:689:ASN:N	2.52	0.43
1:A:561:LEU:HA	1:A:561:LEU:HD23	1.77	0.43
19:A:1120:CLA:H3A	19:A:1120:CLA:HBA2	1.84	0.43
2:B:29:HIS:CB	19:B:1226:CLA:HBA1	2.49	0.43
19:A:1138:CLA:HBB2	19:B:1229:CLA:H43	2.00	0.43
2:B:224:PRO:CB	2:B:227:THR:CG2	2.96	0.43
2:B:323:TYR:HD2	7:G:104:ASP:H	1.65	0.43
2:B:431:PHE:CE2	19:B:1229:CLA:CED	3.02	0.43
2:B:517:PHE:O	2:B:517:PHE:CG	2.64	0.43
2:B:50:HIS:CA	2:B:53:GLN:HB2	2.49	0.43
2:B:557:PHE:N	2:B:558:PRO:HD3	2.30	0.43
2:B:596:TRP:NE1	2:B:623:TYR:HB2	2.34	0.43
9:I:24:LEU:HD23	21:L:6019:BCR:H23C	2.01	0.43
12:L:102:VAL:HG22	19:L:1502:CLA:HED2	2.01	0.43
12:L:111:VAL:O	12:L:115:VAL:N	2.52	0.43
8:H:94:ARG:HD2	12:L:183:ALA:HB1	2.00	0.43
17:3:187:PHE:HD1	17:3:188:LEU:N	2.08	0.43
3:C:61:ASP:CG	5:E:118:ASN:ND2	2.72	0.43
16:2:148:ASP:O	16:2:151:THR:N	2.52	0.43
4:D:103:THR:HG22	4:D:128:LEU:CB	2.48	0.43
2:B:161:TRP:O	2:B:162:LYS:C	2.57	0.43
6:F:96:LYS:O	6:F:97:GLN:O	2.36	0.43
12:L:174:ASP:O	12:L:175:GLN:O	2.36	0.43
18:4:198:LEU:CG	18:4:199:GLU:N	2.59	0.43
18:4:245:VAL:HG22	18:4:246:GLN:H	1.82	0.43
19:4:1306:CLA:H92	19:4:1306:CLA:H61	1.87	0.43
1:A:369:THR:O	1:A:372:VAL:HB	2.19	0.43
1:A:711:HIS:CB	1:A:717:ALA:HB2	2.43	0.43
19:B:1203:CLA:H3A	19:B:1203:CLA:HBA1	1.74	0.43
19:B:1214:CLA:H3A	19:B:1214:CLA:HBA2	1.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1220:CLA:C2A	19:B:1220:CLA:CGD	2.96	0.43
2:B:432:HIS:CE1	19:B:1229:CLA:NB	2.72	0.43
2:B:242:HIS:O	2:B:243:LEU:HB2	2.19	0.43
2:B:290:MET:O	2:B:299:HIS:HB2	2.19	0.43
19:B:1209:CLA:HMC2	21:B:6005:BCR:H373	2.01	0.43
2:B:662:MET:O	2:B:663:PHE:C	2.57	0.43
6:F:205:SER:O	6:F:207:LEU:CD1	2.67	0.43
6:F:207:LEU:C	6:F:209:ARG:N	2.69	0.43
9:I:8:PHE:CZ	21:I:6021:BCR:C7	3.02	0.43
11:K:60:SER:O	11:K:63:LEU:CD2	2.67	0.43
5:E:86:GLY:HA3	5:E:109:LYS:NZ	2.33	0.43
16:2:148:ASP:CA	16:2:152:LEU:HB3	2.41	0.43
16:2:186:ASN:O	16:2:187:LYS:CB	2.65	0.43
12:L:207:LEU:HD23	12:L:208:ASP:N	2.33	0.43
4:D:122:MET:O	4:D:123:ARG:HB3	2.19	0.43
11:K:127:ILE:HG23	11:K:130:LEU:CD1	2.46	0.43
17:3:197:SER:CB	17:3:206:PRO:CG	2.97	0.43
21:3:6022:BCR:H14C	21:3:6022:BCR:H11C	1.56	0.43
19:3:3016:CLA:H41	19:3:3016:CLA:H61	1.58	0.43
18:4:85:PRO:HB3	18:4:188:ILE:HA	2.00	0.43
1:A:408:VAL:HG11	1:A:602:LEU:HD23	2.00	0.43
22:2:7046:LMU:H41	22:2:7046:LMU:H6D	2.01	0.43
19:A:1134:CLA:HBD	19:A:1134:CLA:HAA1	2.01	0.43
1:A:615:HIS:CE1	19:A:1135:CLA:CBC	3.00	0.43
1:A:732:ALA:HB1	19:A:1140:CLA:HED2	2.01	0.43
19:A:9013:CLA:HHD	19:A:9013:CLA:HAC1	1.88	0.43
2:B:119:GLY:O	2:B:122:GLN:OE1	2.37	0.43
2:B:222:LEU:HA	19:B:1212:CLA:CMD	2.40	0.43
2:B:444:LEU:HD23	2:B:452:GLN:HE22	1.80	0.43
2:B:496:GLY:O	2:B:499:ASN:HB2	2.19	0.43
2:B:456:GLU:HA	2:B:514:PRO:HG3	2.01	0.43
2:B:98:GLN:CA	2:B:98:GLN:HE21	2.30	0.43
7:G:90:GLN:HB2	7:G:91:VAL:C	2.36	0.43
16:2:156:GLU:OE2	19:2:2013:CLA:C1D	2.67	0.43
16:2:157:LEU:HD11	19:2:2012:CLA:HMC3	2.00	0.43
10:J:5:LYS:HE3	16:2:178:ASN:CG	2.38	0.43
19:K:1143:CLA:C4	19:K:1143:CLA:O2A	2.67	0.43
15:1:171:LEU:CD2	15:1:171:LEU:N	2.81	0.43
22:R:7022:LMU:H1B	22:R:7022:LMU:O2'	2.19	0.43
18:4:110:LEU:HA	18:4:113:GLU:OE2	2.19	0.43
22:H:7011:LMU:C7	22:H:7011:LMU:C11	2.94	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:4:7053:LMU:C1B	22:4:7053:LMU:C6'	2.89	0.43
1:A:119:SER:OG	1:A:143:ILE:C	2.57	0.42
1:A:538:ASP:O	1:A:542:HIS:HD2	2.02	0.42
1:A:682:ALA:HA	1:A:685:VAL:HB	2.01	0.42
1:A:744:ALA:HA	1:A:747:TRP:HB3	2.00	0.42
1:A:600:LEU:HD13	19:A:9023:CLA:HMD3	2.00	0.42
19:B:1222:CLA:HMB3	21:B:6010:BCR:H351	1.99	0.42
2:B:229:GLN:O	7:G:63:VAL:CG1	2.67	0.42
2:B:315:LEU:O	2:B:315:LEU:CD1	2.54	0.42
2:B:390:GLY:HA3	21:B:6010:BCR:HC22	2.01	0.42
2:B:395:ILE:HG21	2:B:554:GLY:HA3	2.00	0.42
2:B:498:LEU:O	2:B:499:ASN:OD1	2.36	0.42
20:B:5002:PQN:H192	21:B:6017:BCR:C10	2.49	0.42
2:B:721:TYR:HA	2:B:724:PHE:HB3	2.00	0.42
3:C:74:THR:CG2	3:C:75:ARG:N	2.81	0.42
7:G:76:ARG:NH1	7:G:120:VAL:CB	2.78	0.42
7:G:96:GLY:O	7:G:97:LEU:HD23	2.18	0.42
8:H:110:ALA:HA	8:H:113:SER:HB2	2.01	0.42
13:N:132:THR:CG2	13:N:139:LYS:CE	2.97	0.42
10:J:5:LYS:HE3	16:2:178:ASN:ND2	2.34	0.42
4:D:124:GLU:OE1	4:D:125:GLY:N	2.52	0.42
1:A:255:LEU:O	1:A:259:TYR:O	2.37	0.42
21:1:6023:BCR:C33	21:1:6023:BCR:H322	2.31	0.42
8:H:70:SER:O	8:H:73:PRO:HD2	2.19	0.42
22:2:7027:LMU:H31	22:2:7027:LMU:H62	1.51	0.42
1:A:498:LEU:HA	1:A:498:LEU:HD23	1.83	0.42
1:A:205:HIS:CG	19:A:1111:CLA:HMC2	2.54	0.42
19:A:1237:CLA:C11	19:A:1237:CLA:H61	2.49	0.42
1:A:154:ARG:HD2	1:A:154:ARG:HA	1.48	0.42
1:A:396:PHE:CE2	1:A:616:PHE:CB	2.99	0.42
1:A:96:MET:O	1:A:99:HIS:HB2	2.18	0.42
2:B:177:HIS:CE1	19:B:1209:CLA:NC	2.86	0.42
2:B:377:TYR:O	2:B:378:ILE:CB	2.66	0.42
2:B:414:HIS:O	2:B:414:HIS:CD2	2.72	0.42
2:B:575:ASP:O	2:B:579:ALA:N	2.49	0.42
2:B:710:LEU:H	2:B:713:PHE:H	1.66	0.42
6:F:207:LEU:CD1	6:F:207:LEU:H	2.32	0.42
19:2:2002:CLA:HBA2	19:2:2002:CLA:H3A	1.76	0.42
19:2:2004:CLA:O1D	19:3:2009:CLA:HBB2	2.19	0.42
3:C:9:ASP:OD1	3:C:61:ASP:CG	2.57	0.42
5:E:88:GLY:HA3	5:E:107:PHE:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:64:GLN:HB2	8:H:67:SER:N	2.23	0.42
17:3:233:LEU:C	17:3:236:LEU:H	2.22	0.42
16:2:150:THR:CA	16:2:152:LEU:CD1	2.97	0.42
16:2:189:THR:OG1	16:2:193:VAL:O	2.36	0.42
17:3:133:ALA:HB3	17:3:134:LEU:CG	2.49	0.42
12:L:209:LEU:HG	12:L:210:PRO:CD	2.49	0.42
4:D:80:SER:HB2	4:D:127:ASN:N	2.34	0.42
6:F:103:GLN:OE1	6:F:103:GLN:C	2.57	0.42
2:B:75:GLU:HB3	2:B:132:ASN:ND2	2.17	0.42
2:B:78:VAL:O	2:B:79:GLN:C	2.56	0.42
17:3:210:PRO:HG2	17:3:211:LEU:N	2.33	0.42
2:B:476:ILE:HG21	2:B:479:SER:OG	2.12	0.42
14:R:8:UNK:CB	19:R:1144:CLA:O2D	2.67	0.42
18:4:122:ASN:OD1	18:4:124:PRO:HA	2.19	0.42
22:4:7034:LMU:C10	22:4:7052:LMU:H2'	2.45	0.42
18:4:144:ILE:HA	18:4:147:ILE:CD1	2.49	0.42
19:A:1119:CLA:C1C	19:A:1125:CLA:H171	2.49	0.42
19:A:1135:CLA:H11	19:A:1136:CLA:O1A	2.19	0.42
19:A:1139:CLA:C4	19:A:1139:CLA:O1A	2.67	0.42
19:A:1141:CLA:O1A	19:A:1141:CLA:H2A	2.08	0.42
1:A:337:PRO:HB2	19:A:1151:CLA:HBB2	2.00	0.42
1:A:159:THR:O	1:A:160:SER:OG	2.34	0.42
1:A:452:PHE:CD1	19:A:1136:CLA:HBB2	2.54	0.42
1:A:551:VAL:HG21	1:A:604:TRP:CZ2	2.53	0.42
19:A:1126:CLA:C7	21:A:6011:BCR:H372	2.49	0.42
19:B:1206:CLA:HED1	19:I:1204:CLA:HMA2	2.00	0.42
19:B:1238:CLA:H172	19:B:1239:CLA:H13	2.02	0.42
2:B:120:VAL:CG1	2:B:123:TRP:CD1	3.01	0.42
2:B:267:SER:OG	2:B:268:LEU:N	2.49	0.42
2:B:289:LEU:HA	19:B:1217:CLA:O1D	2.19	0.42
2:B:449:PRO:O	2:B:452:GLN:CB	2.67	0.42
2:B:463:ILE:CG2	2:B:467:HIS:HE1	2.32	0.42
2:B:493:TRP:CZ3	19:B:1232:CLA:CMA	3.01	0.42
2:B:366:THR:HA	2:B:729:THR:HG21	2.00	0.42
7:G:77:PHE:CE2	7:G:79:PHE:CD2	3.07	0.42
12:L:111:VAL:H	12:L:113:PRO:HD2	1.84	0.42
16:2:224:ASN:HD21	16:2:227:LEU:HD23	1.84	0.42
1:A:27:ILE:O	1:A:27:ILE:CG2	2.54	0.42
1:A:569:ILE:HG22	1:A:572:LYS:N	2.34	0.42
1:A:249:ILE:HG23	17:3:137:PHE:CZ	2.54	0.42
2:B:633:ASN:HB2	2:B:636:THR:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:K:1142:CLA:OBD	19:K:1143:CLA:C1B	2.68	0.42
7:G:150:ASP:N	7:G:151:PRO:HD3	2.33	0.42
1:A:427:ARG:HG2	1:A:428:TYR:HA	2.02	0.42
2:B:490:ARG:NH1	2:B:490:ARG:CG	2.47	0.42
1:A:628:ILE:HD11	1:A:629:ASN:O	2.20	0.42
4:D:101:VAL:HG12	4:D:130:LYS:HB3	1.98	0.42
15:1:116:ALA:CA	15:1:117:LEU:HD22	2.49	0.42
16:2:204:LEU:CD1	16:2:210:SER:O	2.62	0.42
1:A:476:MET:O	1:A:477:PHE:HB2	2.19	0.42
2:B:684:ARG:HA	2:B:684:ARG:HD3	1.76	0.42
18:4:231:ASN:O	18:4:235:HIS:HB3	2.18	0.42
15:1:72:VAL:O	15:1:73:PRO:C	2.54	0.42
19:A:1131:CLA:O1A	19:A:1237:CLA:C1	2.65	0.42
19:A:1132:CLA:H61	19:A:1132:CLA:H41	1.60	0.42
1:A:350:LEU:O	1:A:350:LEU:CD2	2.67	0.42
1:A:645:SER:O	1:A:651:GLY:HA3	2.19	0.42
1:A:733:VAL:HG13	1:A:737:HIS:CE1	2.54	0.42
2:B:299:HIS:CE1	19:B:1219:CLA:OBD	2.73	0.42
2:B:424:TRP:CH2	19:B:1228:CLA:HAC1	2.55	0.42
2:B:310:PRO:HG3	19:B:1220:CLA:CMA	2.33	0.42
2:B:316:GLY:O	2:B:317:ARG:HD2	2.19	0.42
2:B:486:LEU:O	2:B:487:ASN:HB3	2.20	0.42
2:B:50:HIS:HA	2:B:53:GLN:H	1.85	0.42
2:B:674:LEU:O	2:B:678:LEU:HB2	2.19	0.42
2:B:230:TRP:H	7:G:63:VAL:CG2	2.23	0.42
21:I:6018:BCR:H272	21:I:6021:BCR:H352	2.01	0.42
13:N:147:SER:C	13:N:151:ASP:N	2.71	0.42
13:N:104:LYS:O	13:N:105:LYS:C	2.58	0.42
17:3:236:LEU:C	17:3:238:ILE:H	2.17	0.42
22:3:7005:LMU:C5'	22:3:7005:LMU:O2B	2.67	0.42
17:3:132:THR:CG2	17:3:133:ALA:N	2.82	0.42
4:D:123:ARG:HH21	22:D:7050:LMU:C5B	2.13	0.42
4:D:137:CYS:O	4:D:138:LEU:C	2.55	0.42
6:F:88:SER:O	6:F:91:PHE:HB3	2.19	0.42
1:A:427:ARG:HE	1:A:428:TYR:HD1	1.66	0.42
19:J:1308:CLA:CBD	19:J:1308:CLA:CGA	2.97	0.42
19:3:3016:CLA:C3A	19:3:3016:CLA:O1A	2.68	0.42
10:J:36:ALA:O	10:J:37:LEU:HB2	2.18	0.42
18:4:217:PHE:CE1	18:4:221:HIS:CE1	3.08	0.42
18:4:96:LEU:CD1	18:4:100:ARG:NE	2.83	0.42
1:A:331:LEU:CD2	1:A:343:HIS:C	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:GLN:C	1:A:376:MET:N	2.71	0.42
19:A:1138:CLA:HMC1	20:A:5001:PQN:H251	2.01	0.42
1:A:613:ILE:HG23	1:A:750:PHE:HE2	1.83	0.42
1:A:94:SER:OG	1:A:95:GLY:N	2.53	0.42
19:B:1234:CLA:HMC1	19:B:1234:CLA:CBC	2.35	0.42
2:B:256:THR:N	2:B:271:THR:OG1	2.52	0.42
2:B:292:ARG:NE	2:B:292:ARG:HA	2.34	0.42
2:B:408:LEU:O	2:B:411:MET:HB2	2.20	0.42
2:B:596:TRP:CH2	2:B:612:SER:HB3	2.55	0.42
2:B:615:TYR:O	2:B:619:TRP:HD1	2.03	0.42
6:F:138:LEU:HD22	6:F:146:PRO:HB3	2.01	0.42
6:F:181:TYR:C	6:F:181:TYR:HD2	2.22	0.42
19:A:1131:CLA:C15	21:L:6019:BCR:C36	2.97	0.42
12:L:78:LEU:HD12	12:L:79:ILE:H	1.79	0.42
12:L:95:PRO:O	12:L:98:ARG:HG3	2.19	0.42
8:H:66:ASP:C	8:H:68:TYR:N	2.71	0.42
13:N:134:CYS:O	13:N:136:ASP:O	2.37	0.42
13:N:155:GLU:CB	13:N:157:LYS:HA	2.50	0.42
17:3:99:ALA:O	17:3:100:TYR:C	2.58	0.42
1:A:249:ILE:CG2	17:3:137:PHE:CZ	3.03	0.42
16:2:167:ARG:HE	16:2:167:ARG:C	2.22	0.42
13:N:108:ALA:C	13:N:109:THR:HG1	2.23	0.42
13:N:112:ALA:O	13:N:113:ASN:C	2.58	0.42
4:D:139:ALA:O	4:D:142:THR:CG2	2.59	0.42
6:F:130:PHE:O	6:F:131:ASP:C	2.56	0.42
18:4:233:LEU:HG	18:4:233:LEU:H	1.79	0.42
4:D:77:ASN:HB3	4:D:79:PRO:HD3	2.01	0.42
2:B:252:THR:O	2:B:252:THR:HG22	2.19	0.42
18:4:120:ILE:CG2	18:4:121:ILE:N	2.65	0.42
15:1:177:PRO:O	15:1:178:LYS:CB	2.68	0.42
19:A:1101:CLA:C4	19:A:1140:CLA:H8	2.50	0.42
1:A:149:PHE:HB3	1:A:153:TRP:CZ3	2.53	0.42
1:A:652:TRP:O	1:A:656:PHE:HB3	2.19	0.42
1:A:741:GLY:O	1:A:743:ILE:N	2.53	0.42
19:B:1202:CLA:CAB	19:B:1203:CLA:HBA2	2.49	0.42
2:B:429:LEU:HD11	19:B:1235:CLA:HMB3	2.00	0.42
2:B:319:HIS:CE1	2:B:322:LEU:HD11	2.50	0.42
2:B:346:SER:O	2:B:350:GLN:N	2.50	0.42
2:B:450:GLU:O	2:B:451:LYS:HB2	2.19	0.42
5:E:91:VAL:CG1	5:E:92:ALA:H	2.26	0.42
16:2:104:GLN:N	16:2:104:GLN:CD	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:107:LEU:CD1	16:2:108:VAL:HG23	2.49	0.42
3:C:38:GLN:HE21	3:C:38:GLN:HB3	1.65	0.42
17:3:95:PRO:C	17:3:96:ARG:CG	2.85	0.42
14:R:38:UNK:C	14:R:42:UNK:CA	2.97	0.42
18:4:89:ARG:N	18:4:89:ARG:HD3	2.33	0.42
6:F:97:GLN:HE21	6:F:97:GLN:HB3	1.52	0.42
16:2:195:TYR:CD2	16:2:198:GLY:CA	2.93	0.42
22:L:7029:LMU:H11	22:L:7029:LMU:O2'	2.20	0.42
1:A:68:THR:HG22	1:A:70:ASP:O	2.20	0.42
17:3:174:GLN:HE21	17:3:174:GLN:HB2	1.47	0.42
18:4:189:PHE:CD2	18:4:189:PHE:N	2.88	0.42
4:D:204:GLY:C	4:D:205:LYS:HE2	2.40	0.42
12:L:104:LEU:HA	12:L:192:GLY:O	2.19	0.42
2:B:488:ALA:CB	19:B:1233:CLA:C1C	2.96	0.42
18:4:121:ILE:O	18:4:122:ASN:HB3	2.20	0.42
19:A:1103:CLA:HBA1	19:A:1103:CLA:H3A	1.71	0.42
1:A:119:SER:HA	1:A:145:ILE:CD1	2.50	0.42
2:B:225:LEU:CA	2:B:227:THR:O	2.67	0.42
2:B:278:LEU:O	2:B:279:ALA:C	2.58	0.42
2:B:556:SER:CA	2:B:558:PRO:HD2	2.50	0.42
7:G:83:GLN:O	7:G:84:ARG:CB	2.67	0.42
19:A:1136:CLA:H203	19:L:1130:CLA:HBB2	2.02	0.42
12:L:150:ILE:HD12	12:L:150:ILE:O	2.18	0.42
12:L:82:TYR:HE1	19:L:1130:CLA:H93	1.80	0.42
16:2:114:MET:HG2	16:2:227:LEU:CA	2.36	0.42
15:1:142:PHE:C	15:1:143:LEU:HD12	2.40	0.42
15:1:148:VAL:HG22	15:1:148:VAL:O	2.19	0.42
17:3:238:ILE:HG13	19:3:3003:CLA:HMC2	1.93	0.42
1:A:261:SER:C	1:A:262:PHE:CG	2.93	0.42
16:2:167:ARG:HB3	16:2:169:ALA:H	1.84	0.42
2:B:160:LYS:HE2	2:B:160:LYS:HB2	1.43	0.42
16:2:238:GLN:O	16:2:239:HIS:C	2.57	0.42
11:K:115:ILE:HG12	11:K:122:LEU:HD12	1.99	0.42
15:1:168:PHE:CD1	15:1:168:PHE:O	2.72	0.42
2:B:628:SER:O	2:B:629:SER:O	2.38	0.42
15:1:198:PHE:C	15:1:199:VAL:O	2.57	0.42
2:B:262:HIS:HB2	2:B:265:THR:O	2.20	0.42
1:A:299:ILE:HA	1:A:299:ILE:HD12	1.78	0.42
19:4:4006:CLA:HED2	19:4:4006:CLA:H2A	2.01	0.42
15:1:92:LEU:HA	15:1:95:PRO:HD2	1.92	0.42
18:4:162:ASN:HA	18:4:163:PRO:HD3	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:171:ILE:N	18:4:173:LYS:H	2.17	0.42
19:A:1119:CLA:HBC3	19:A:1119:CLA:HMC1	1.99	0.42
1:A:733:VAL:CG2	19:A:1140:CLA:C2D	2.87	0.42
1:A:335:LYS:HG2	1:A:336:GLY:N	2.35	0.42
1:A:534:LEU:HB2	1:A:538:ASP:HB3	2.02	0.42
1:A:53:TRP:O	1:A:56:ASN:O	2.38	0.42
1:A:60:ASP:OD1	1:A:60:ASP:O	2.38	0.42
1:A:660:GLN:O	1:A:661:ALA:HB2	2.17	0.42
1:A:93:LEU:O	1:A:97:TYR:CD2	2.70	0.42
2:B:202:SER:C	2:B:204:GLY:N	2.58	0.42
2:B:126:THR:HG21	2:B:358:TYR:CE1	2.54	0.42
2:B:350:GLN:HG3	2:B:372:TYR:HE1	1.85	0.42
2:B:431:PHE:CE2	19:B:1229:CLA:HED3	2.55	0.42
2:B:445:ALA:N	2:B:447:GLY:H	2.17	0.42
5:E:111:ASN:CB	5:E:116:SER:OG	2.54	0.42
6:F:205:SER:CA	6:F:207:LEU:HD12	2.49	0.42
7:G:76:ARG:HH12	7:G:120:VAL:H	1.66	0.42
10:J:9:SER:HB2	10:J:10:VAL:H	1.67	0.42
12:L:145:LEU:O	12:L:182:TRP:HZ3	2.02	0.42
12:L:78:LEU:HD22	19:L:1504:CLA:CED	2.42	0.42
16:2:118:ALA:CB	16:2:121:PHE:CE2	2.96	0.42
15:1:148:VAL:CG2	15:1:148:VAL:O	2.65	0.42
3:C:8:TYR:HB2	3:C:41:SER:OG	2.18	0.42
17:3:107:ARG:HG2	17:3:232:ARG:HB2	2.01	0.42
12:L:209:LEU:HG	12:L:210:PRO:N	2.33	0.42
13:N:112:ALA:O	13:N:113:ASN:O	2.37	0.42
16:2:238:GLN:HA	16:2:241:TYR:CE2	2.54	0.42
19:J:1311:CLA:H152	19:2:2014:CLA:CMB	2.48	0.42
2:B:631:LEU:HG	2:B:632:ILE:N	2.34	0.42
2:B:715:VAL:O	2:B:719:PHE:N	2.42	0.42
4:D:130:LYS:HG3	4:D:130:LYS:O	2.19	0.42
22:H:7002:LMU:H5'	22:H:7002:LMU:O2'	2.19	0.42
1:A:271:THR:HG22	1:A:271:THR:O	2.20	0.42
18:4:142:PHE:CA	18:4:145:GLU:OE1	2.63	0.42
18:4:192:LEU:CD1	18:4:193:ASN:H	2.33	0.42
19:A:1138:CLA:CED	19:A:1138:CLA:H2A	2.35	0.42
1:A:457:SER:O	1:A:544:ILE:CD1	2.64	0.42
1:A:488:PHE:HD1	1:A:535:GLY:CA	2.33	0.42
1:A:554:LEU:HD11	2:B:674:LEU:HD21	2.01	0.42
1:A:555:ILE:HD11	19:A:9023:CLA:C3D	2.49	0.42
19:B:1201:CLA:O1D	19:B:1201:CLA:H2A	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1208:CLA:H51	19:B:1208:CLA:H8	1.75	0.42
19:B:1220:CLA:H11	19:B:1220:CLA:H203	2.02	0.42
2:B:655:LEU:HD22	19:B:1239:CLA:CAB	2.50	0.42
2:B:123:TRP:HB3	2:B:126:THR:HG21	1.99	0.42
2:B:182:LEU:HG	2:B:183:PHE:N	2.34	0.42
2:B:310:PRO:HG2	2:B:311:PRO:HD2	1.99	0.42
2:B:387:PHE:CB	2:B:534:LEU:HD13	2.50	0.42
20:B:5002:PQN:H111	20:B:5002:PQN:H2M1	1.78	0.42
2:B:430:GLY:CA	2:B:525:LEU:CD1	2.88	0.42
2:B:648:TRP:HZ3	21:B:6017:BCR:H383	1.84	0.42
2:B:694:ARG:HE	12:L:151:SER:HA	1.85	0.42
2:B:692:ARG:NH2	2:B:694:ARG:HH22	2.10	0.42
7:G:102:ALA:N	7:G:104:ASP:OD2	2.53	0.42
7:G:125:VAL:O	7:G:129:ALA:CB	2.67	0.42
7:G:123:ASN:C	7:G:126:ASP:OD2	2.58	0.42
9:I:20:ALA:O	9:I:24:LEU:N	2.52	0.42
10:J:18:TRP:CZ2	10:J:22:LEU:HD22	2.55	0.42
11:K:48:PHE:O	11:K:52:PRO:CD	2.57	0.42
16:2:133:ASN:ND2	16:2:134:THR:OG1	2.50	0.42
16:2:226:ARG:HD3	16:2:229:MET:HB3	2.01	0.42
13:N:133:GLY:CA	13:N:134:CYS:C	2.86	0.42
13:N:146:LEU:HA	13:N:146:LEU:HD12	1.72	0.42
17:3:98:LEU:CD2	19:3:3012:CLA:C2D	2.94	0.42
17:3:94:GLU:N	17:3:95:PRO:CD	2.83	0.42
1:A:250:LEU:HD12	17:3:136:TRP:CZ2	2.49	0.42
16:2:184:PRO:CD	16:2:186:ASN:C	2.87	0.42
11:K:125:LYS:HD2	11:K:128:GLY:HA3	2.01	0.42
6:F:100:LYS:NZ	6:F:103:GLN:HB2	2.35	0.42
19:J:1308:CLA:C2A	19:J:1308:CLA:O2A	2.53	0.42
2:B:74:PHE:C	2:B:76:ALA:N	2.73	0.42
2:B:144:PHE:HD2	2:B:144:PHE:O	2.02	0.42
1:A:68:THR:CG2	1:A:69:SER:N	2.79	0.42
1:A:389:TYR:CE2	1:A:526:LYS:HD3	2.45	0.42
4:D:101:VAL:O	4:D:101:VAL:CG2	2.67	0.42
2:B:331:HIS:CE1	2:B:392:ILE:CG2	2.97	0.42
22:A:7045:LMU:H21	22:A:7045:LMU:H1'	1.69	0.42
2:B:399:ASN:OD1	2:B:402:GLN:HB2	2.20	0.42
13:N:92:LEU:HD12	13:N:92:LEU:HA	1.68	0.42
15:1:155:GLU:CD	15:1:156:LYS:N	2.73	0.42
18:4:193:ASN:C	18:4:194:PHE:CG	2.87	0.42
18:4:157:TRP:HE3	19:4:4012:CLA:HMA2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1115:CLA:H51	19:A:1115:CLA:H11	1.74	0.42
19:A:1139:CLA:H3A	19:A:1139:CLA:HBA1	1.69	0.42
1:A:132:LEU:O	1:A:143:ILE:HD11	2.20	0.42
1:A:288:ASP:HB2	1:A:291:THR:O	2.19	0.42
1:A:378:SER:O	1:A:512:SER:OG	2.29	0.42
1:A:580:PRO:HA	1:A:728:VAL:HG23	2.01	0.42
19:A:1122:CLA:ND	21:A:6007:BCR:C19	2.83	0.42
1:A:651:GLY:O	1:A:655:ASP:HB2	2.20	0.42
1:A:92:TRP:O	1:A:93:LEU:CG	2.68	0.42
2:B:343:VAL:HG12	19:B:1223:CLA:H2	2.02	0.42
19:B:1229:CLA:H51	21:F:6016:BCR:H403	2.01	0.42
2:B:202:SER:CB	2:B:270:LEU:HD22	2.46	0.42
2:B:273:VAL:O	2:B:277:HIS:CD2	2.65	0.42
2:B:292:ARG:HH12	2:B:295:PHE:H	1.66	0.42
2:B:623:TYR:HH	2:B:721:TYR:HH	1.68	0.42
3:C:1:MET:H2	3:C:3:HIS:H	1.66	0.42
19:H:1207:CLA:H152	19:H:1207:CLA:H102	2.02	0.42
8:H:98:LEU:HD23	12:L:146:THR:CG2	2.41	0.42
19:A:1129:CLA:HHB	19:L:1130:CLA:CAD	2.50	0.42
12:L:79:ILE:HG22	12:L:80:ALA:N	2.30	0.42
16:2:226:ARG:CA	16:2:226:ARG:NH1	2.83	0.42
5:E:79:LYS:CA	5:E:84:TYR:CD1	2.90	0.42
13:N:146:LEU:HD11	13:N:148:ASP:O	2.20	0.42
1:A:584:PRO:HG3	2:B:559:CYS:SG	2.59	0.42
17:3:136:TRP:N	17:3:139:THR:HG1	2.17	0.42
16:2:149:THR:HG1	16:2:150:THR:N	2.18	0.42
2:B:398:TYR:CD1	2:B:400:PRO:HD3	2.55	0.42
15:1:173:TYR:O	15:1:174:SER:OG	2.29	0.42
19:4:1304:CLA:H202	19:4:1304:CLA:C15	2.40	0.42
17:3:158:PHE:HA	17:3:159:VAL:C	2.40	0.42
6:F:117:LEU:CD1	6:F:120:LYS:HB2	2.49	0.42
18:4:122:ASN:O	18:4:123:VAL:CG1	2.59	0.41
15:1:177:PRO:CG	15:1:180:LEU:N	2.79	0.41
18:4:173:LYS:CB	18:4:194:PHE:CD2	2.87	0.41
19:A:1101:CLA:H12	19:A:1140:CLA:C6	2.49	0.41
1:A:75:SER:CB	1:A:354:TRP:CZ2	2.98	0.41
1:A:363:ALA:N	1:A:410:ALA:CB	2.83	0.41
1:A:448:TRP:HD1	19:A:1131:CLA:CED	2.32	0.41
1:A:701:GLN:HE21	1:A:724:ALA:HB2	1.85	0.41
1:A:64:PHE:CZ	1:A:74:ILE:HG23	2.52	0.41
1:A:93:LEU:HA	1:A:96:MET:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:VAL:CG2	2:B:123:TRP:NE1	2.57	0.41
19:B:1211:CLA:C2B	21:B:6006:BCR:H11C	2.50	0.41
2:B:344:ILE:HD13	19:B:1215:CLA:H71	2.02	0.41
2:B:42:LEU:O	2:B:45:ASN:N	2.53	0.41
2:B:645:VAL:HG13	21:B:6017:BCR:H282	2.02	0.41
2:B:661:PHE:HA	2:B:664:LEU:HB2	2.02	0.41
6:F:140:CYS:H	6:F:146:PRO:HA	1.85	0.41
7:G:124:ILE:CD1	7:G:128:LEU:CD1	2.98	0.41
12:L:92:ALA:HB3	12:L:98:ARG:CZ	2.50	0.41
19:2:2004:CLA:H2	19:2:2007:CLA:HMD3	2.02	0.41
5:E:122:LEU:HD12	5:E:122:LEU:HA	1.57	0.41
8:H:58:LEU:HG	8:H:61:THR:HB	1.93	0.41
1:A:252:ARG:NE	1:A:252:ARG:CA	2.77	0.41
19:3:3013:CLA:H12	19:3:3013:CLA:H51	1.83	0.41
4:D:196:SER:HA	4:D:197:PRO:HD3	1.33	0.41
17:3:204:GLY:HA3	17:3:207:PHE:CA	2.49	0.41
6:F:184:ALA:O	6:F:185:ILE:CG2	2.68	0.41
1:A:485:GLN:CA	1:A:485:GLN:OE1	2.67	0.41
1:A:525:ASN:CB	1:A:526:LYS:CG	2.90	0.41
15:1:130:PRO:HB2	15:1:131:TRP:H	1.63	0.41
15:1:201:PHE:CA	15:1:204:GLN:HB2	2.48	0.41
4:D:203:THR:CG2	4:D:205:LYS:HG2	2.50	0.41
22:4:7033:LMU:H1B	22:4:7033:LMU:H3'	1.73	0.41
18:4:120:ILE:HD11	18:4:226:LYS:CD	2.29	0.41
15:1:158:PRO:HD2	15:1:159:GLU:O	2.20	0.41
18:4:202:GLU:O	18:4:205:ILE:HD13	2.19	0.41
1:A:240:LYS:HA	1:A:243:PRO:HD2	2.01	0.41
1:A:293:GLY:O	1:A:380:PRO:O	2.37	0.41
1:A:349:ILE:CG2	1:A:350:LEU:HA	2.45	0.41
1:A:488:PHE:CD1	1:A:535:GLY:CA	3.03	0.41
1:A:400:MET:HE3	1:A:612:VAL:HG11	2.01	0.41
19:B:1229:CLA:C5	21:F:6016:BCR:H403	2.49	0.41
2:B:314:ARG:HH22	15:1:67:LEU:CG	2.28	0.41
2:B:37:ILE:C	2:B:37:ILE:HD12	2.41	0.41
2:B:431:PHE:HE2	19:B:1229:CLA:HED3	1.85	0.41
19:A:1131:CLA:H191	20:B:5002:PQN:H303	2.02	0.41
2:B:365:PHE:CD1	2:B:602:TRP:CD1	3.08	0.41
2:B:621:ARG:C	2:B:625:TRP:HB3	2.35	0.41
5:E:82:TYR:CD2	5:E:83:TRP:CE3	3.08	0.41
19:F:1305:CLA:HBD	19:F:1305:CLA:HAA2	2.02	0.41
6:F:173:TRP:CZ3	6:F:211:PHE:CA	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:90:GLN:CB	7:G:92:PRO:N	2.83	0.41
12:L:114:PHE:HD1	12:L:114:PHE:N	2.17	0.41
12:L:73:VAL:CB	19:L:1504:CLA:HMA3	2.50	0.41
16:2:103:VAL:HG13	16:2:104:GLN:N	2.35	0.41
17:3:241:TYR:OH	19:3:3003:CLA:CHC	2.68	0.41
22:3:7003:LMU:C2B	22:3:7005:LMU:C6B	2.96	0.41
13:N:114:PHE:CD2	13:N:116:ARG:HD2	2.55	0.41
2:B:4:ARG:HH21	2:B:5:ILE:N	2.19	0.41
6:F:224:GLY:O	6:F:227:VAL:HG12	2.14	0.41
17:3:243:ILE:CG1	19:3:3005:CLA:C4C	2.79	0.41
2:B:141:PHE:O	2:B:142:LEU:C	2.58	0.41
2:B:110:LEU:CG	2:B:111:GLY:N	2.83	0.41
4:D:187:ASN:HB2	4:D:188:PHE:H	1.60	0.41
1:A:564:ARG:HB2	1:A:564:ARG:CZ	2.49	0.41
22:K:7041:LMU:O2'	22:K:7041:LMU:H5'	2.20	0.41
5:E:66:ILE:HG13	5:E:67:GLY:N	2.36	0.41
1:A:105:ASN:HB2	1:A:140:PHE:HZ	1.86	0.41
19:A:1117:CLA:H3A	19:A:1117:CLA:HBA2	1.62	0.41
19:A:1119:CLA:C2C	19:A:1125:CLA:H171	2.50	0.41
19:A:1103:CLA:HMC3	19:A:1128:CLA:HMA1	2.01	0.41
19:A:1131:CLA:HED1	19:A:1237:CLA:O1A	2.20	0.41
1:A:121:GLN:NE2	19:A:1107:CLA:HMD1	2.35	0.41
1:A:158:ILE:O	1:A:159:THR:CB	2.68	0.41
1:A:210:LEU:HD12	19:A:1111:CLA:CMB	2.48	0.41
1:A:443:ILE:N	1:A:443:ILE:HD12	2.35	0.41
1:A:553:VAL:CG2	21:A:6008:BCR:H401	2.50	0.41
19:A:9011:CLA:H162	19:A:9011:CLA:H122	1.68	0.41
2:B:323:TYR:CD1	19:B:1221:CLA:HBC1	2.54	0.41
19:A:9023:CLA:C9	19:B:1239:CLA:HBB2	2.48	0.41
2:B:212:PHE:HE1	19:B:1211:CLA:CMD	2.33	0.41
2:B:583:MET:O	2:B:587:ILE:HB	2.20	0.41
21:B:6017:BCR:C38	21:B:6017:BCR:C23	2.97	0.41
2:B:661:PHE:O	2:B:665:ILE:N	2.52	0.41
6:F:170:ILE:CG2	21:F:6014:BCR:H371	2.32	0.41
8:H:97:LEU:HD11	8:H:101:LEU:H	1.85	0.41
16:2:125:PHE:C	16:2:127:THR:N	2.60	0.41
19:2:2001:CLA:H43	19:2:2001:CLA:O2A	2.20	0.41
19:2:2004:CLA:HED2	19:3:2009:CLA:CAB	2.50	0.41
16:2:192:ASP:OD2	16:2:194:GLY:CA	2.65	0.41
19:L:1501:CLA:C4D	19:L:1501:CLA:H11	2.50	0.41
17:3:208:PHE:HD1	17:3:208:PHE:HA	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:115:ILE:CD1	11:K:122:LEU:H	2.32	0.41
2:B:75:GLU:HB2	2:B:132:ASN:HD22	1.63	0.41
12:L:171:LYS:CA	12:L:173:PRO:HD3	2.48	0.41
12:L:164:LEU:HG	12:L:164:LEU:H	1.53	0.41
22:4:7034:LMU:H81	22:4:7052:LMU:H2'	0.42	0.41
1:A:123:VAL:HG23	1:A:124:TRP:O	2.19	0.41
1:A:218:TRP:NE1	1:A:222:GLN:OE1	2.54	0.41
1:A:365:LEU:O	1:A:369:THR:HG23	2.21	0.41
2:B:87:ILE:C	2:B:115:ASN:HA	2.40	0.41
2:B:718:ILE:CD1	19:B:1224:CLA:HMC2	2.50	0.41
2:B:497:TRP:O	2:B:498:LEU:HB3	2.21	0.41
1:A:443:ILE:CG2	2:B:674:LEU:HD11	2.47	0.41
19:F:1305:CLA:CAD	19:F:1305:CLA:CED	2.97	0.41
19:B:1229:CLA:CBB	21:F:6014:BCR:C26	2.99	0.41
16:2:123:PRO:HA	16:2:126:LEU:HG	2.00	0.41
17:3:135:ALA:HB1	17:3:139:THR:HG21	1.98	0.41
17:3:137:PHE:CD2	17:3:137:PHE:N	2.88	0.41
17:3:204:GLY:O	17:3:206:PRO:C	2.59	0.41
11:K:112:VAL:O	11:K:114:HIS:N	2.53	0.41
1:A:578:ARG:HB3	1:A:578:ARG:NH1	2.32	0.41
2:B:77:TRP:O	2:B:81:PRO:HB3	2.20	0.41
22:H:7032:LMU:H5'	22:H:7032:LMU:H1B	1.84	0.41
1:A:158:ILE:CD1	19:A:1112:CLA:HED3	2.40	0.41
19:A:1138:CLA:HBC3	19:A:1138:CLA:CHD	2.50	0.41
19:A:1139:CLA:O2A	19:A:1139:CLA:H42	2.19	0.41
1:A:336:GLY:HA2	19:A:1151:CLA:HMC3	2.00	0.41
1:A:214:GLY:HA3	21:A:6003:BCR:C15	2.51	0.41
1:A:656:PHE:O	1:A:657:LEU:C	2.58	0.41
2:B:104:PHE:HZ	2:B:645:VAL:HG23	1.84	0.41
19:B:1211:CLA:H111	19:B:1211:CLA:H71	1.47	0.41
2:B:193:HIS:CD2	19:B:1211:CLA:NB	2.88	0.41
19:B:1225:CLA:HBA2	19:B:1225:CLA:H3A	1.62	0.41
19:B:1228:CLA:HBC3	19:B:1228:CLA:CHD	2.41	0.41
2:B:268:LEU:O	2:B:269:TRP:C	2.58	0.41
2:B:502:ASN:C	2:B:502:ASN:OD1	2.59	0.41
2:B:430:GLY:N	2:B:525:LEU:CD1	2.83	0.41
2:B:580:VAL:HG11	2:B:710:LEU:HD21	2.02	0.41
2:B:594:TRP:HD1	2:B:595:HIS:N	2.17	0.41
2:B:645:VAL:HA	19:B:1206:CLA:HAC1	2.03	0.41
2:B:724:PHE:CE1	19:B:9010:CLA:HMD1	2.55	0.41
6:F:157:TRP:HZ3	19:F:1302:CLA:CMC	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:127:VAL:O	7:G:128:LEU:C	2.57	0.41
16:2:117:ALA:HB1	16:2:230:LEU:HD12	2.01	0.41
19:2:2004:CLA:C3	19:3:2009:CLA:HBC3	2.50	0.41
19:1:1006:CLA:HHC	19:1:1013:CLA:HBC1	2.02	0.41
4:D:140:LEU:CD1	4:D:141:GLY:CA	2.80	0.41
6:F:118:ALA:O	6:F:121:ALA:O	2.38	0.41
1:A:258:LEU:HG	1:A:280:PHE:HE1	1.82	0.41
2:B:715:VAL:O	2:B:719:PHE:HB2	2.20	0.41
6:F:188:GLU:HB3	6:F:189:LYS:H	1.23	0.41
16:2:264:ALA:O	16:2:265:ALA:HB3	2.20	0.41
15:1:77:GLU:OE1	15:1:80:LYS:HE3	2.20	0.41
19:A:1106:CLA:H2A	19:A:1106:CLA:O2D	2.21	0.41
19:A:1107:CLA:CHA	19:A:1107:CLA:CBA	2.98	0.41
19:A:1116:CLA:HHD	19:A:1116:CLA:HAC2	1.96	0.41
1:A:123:VAL:HB	1:A:124:TRP:O	2.21	0.41
1:A:119:SER:C	1:A:145:ILE:HD12	2.41	0.41
1:A:109:TRP:HH2	1:A:154:ARG:HD3	1.83	0.41
1:A:328:LYS:HZ2	1:A:345:GLY:N	2.17	0.41
1:A:355:HIS:ND1	1:A:416:ILE:HG22	2.31	0.41
1:A:431:LEU:O	1:A:435:VAL:CG1	2.61	0.41
1:A:685:VAL:HG22	19:A:1140:CLA:CBB	2.48	0.41
1:A:79:PHE:CE1	19:A:1111:CLA:HED1	2.55	0.41
19:B:1203:CLA:C2A	19:B:1203:CLA:O1D	2.60	0.41
2:B:192:GLY:HA2	19:B:1212:CLA:CHC	2.51	0.41
19:B:1210:CLA:C15	19:B:1225:CLA:HMD2	2.35	0.41
2:B:152:ALA:HB2	19:B:1208:CLA:C2C	2.50	0.41
2:B:217:PRO:HB2	2:B:218:TYR:HD1	1.85	0.41
2:B:443:MET:CG	2:B:451:LYS:O	2.68	0.41
2:B:67:HIS:CD2	2:B:89:HIS:HB2	2.55	0.41
7:G:116:SER:O	7:G:119:PRO:CD	2.68	0.41
7:G:97:LEU:O	7:G:98:THR:O	2.39	0.41
8:H:109:LEU:HD21	19:H:1207:CLA:C5	2.50	0.41
3:C:12:ILE:HG21	3:C:39:ILE:C	2.40	0.41
13:N:146:LEU:HD22	17:3:142:ILE:CA	2.50	0.41
19:1:1014:CLA:H102	19:1:1014:CLA:C5	2.18	0.41
17:3:107:ARG:NH1	17:3:233:LEU:N	2.69	0.41
19:3:3013:CLA:H3A	19:3:3013:CLA:HBA2	1.87	0.41
12:L:210:PRO:O	12:L:211:TYR:HB3	2.18	0.41
2:B:397:ASP:O	2:B:398:TYR:HB3	2.20	0.41
17:3:197:SER:OG	17:3:198:GLY:N	2.53	0.41
19:1:1002:CLA:CGA	19:1:1002:CLA:HMA2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:THR:O	1:A:428:TYR:CE1	2.73	0.41
14:R:27:UNK:C	14:R:29:UNK:C	2.98	0.41
18:4:110:LEU:HA	18:4:113:GLU:CD	2.40	0.41
15:1:115:ALA:O	15:1:116:ALA:CB	2.69	0.41
2:B:93:ASP:HA	2:B:94:PRO:HD2	1.48	0.41
2:B:680:TRP:O	2:B:684:ARG:HB2	2.20	0.41
12:L:63:ASP:OD1	12:L:63:ASP:C	2.59	0.41
19:F:1305:CLA:H12	19:4:1306:CLA:HAA1	2.02	0.41
18:4:158:GLN:CD	19:4:1004:CLA:C2A	2.89	0.41
18:4:210:LEU:HD23	19:4:4002:CLA:CAB	2.51	0.41
1:A:110:LEU:O	1:A:111:ASN:C	2.57	0.41
1:A:417:PHE:CD1	1:A:417:PHE:C	2.94	0.41
1:A:537:ALA:O	1:A:642:PHE:HE2	2.04	0.41
19:A:1122:CLA:CBC	21:A:6007:BCR:H393	2.51	0.41
1:A:691:MET:CE	20:A:5001:PQN:C2M	2.98	0.41
1:A:708:VAL:N	1:A:711:HIS:HD2	2.19	0.41
2:B:98:GLN:NE2	2:B:101:VAL:HG23	2.36	0.41
19:B:1239:CLA:H2	20:B:5002:PQN:H251	2.02	0.41
2:B:289:LEU:HD22	21:B:6004:BCR:H352	2.02	0.41
2:B:294:ASN:HB2	7:G:94:GLN:CG	2.45	0.41
2:B:573:TRP:CZ3	2:B:703:VAL:HG13	2.55	0.41
2:B:91:ILE:HG21	2:B:91:ILE:HD13	1.78	0.41
2:B:98:GLN:N	2:B:99:PRO:CD	2.81	0.41
2:B:458:ILE:HD11	6:F:149:ILE:HG13	2.02	0.41
10:J:19:PHE:C	10:J:19:PHE:CD2	2.94	0.41
19:A:1126:CLA:C11	21:J:6012:BCR:H353	2.48	0.41
12:L:83:LEU:HA	12:L:86:LEU:HD13	2.02	0.41
19:2:2006:CLA:H72	19:2:2006:CLA:H41	2.02	0.41
3:C:58:CYS:HA	3:C:59:PRO:HD2	1.57	0.41
5:E:77:LEU:C	5:E:78:ARG:HD2	2.40	0.41
5:E:76:ILE:CB	5:E:84:TYR:O	2.53	0.41
19:1:1014:CLA:H91	19:1:1014:CLA:C12	2.50	0.41
15:1:138:LEU:O	15:1:141:GLU:HG3	2.21	0.41
2:B:549:ASP:CB	3:C:63:LEU:HB2	2.51	0.41
1:A:249:ILE:HG12	17:3:136:TRP:HH2	1.85	0.41
2:B:160:LYS:NZ	2:B:161:TRP:N	2.69	0.41
22:E:7048:LMU:O4'	22:F:7036:LMU:H6E	2.15	0.41
16:2:202:ASP:C	16:2:202:ASP:OD2	2.58	0.41
19:2:2014:CLA:C15	19:2:2014:CLA:C9	2.84	0.41
1:A:389:TYR:HE2	1:A:526:LYS:CD	2.29	0.41
19:1:1008:CLA:CMC	19:1:1008:CLA:HBC3	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:K:7041:LMU:H111	22:K:7041:LMU:H82	1.95	0.41
16:2:155:VAL:CA	16:2:158:VAL:HG13	2.50	0.41
15:1:85:ILE:HG12	15:1:88:ARG:NE	2.26	0.41
18:4:154:ILE:HD13	19:4:1009:CLA:HMD1	2.03	0.41
18:4:169:ASP:OD1	18:4:174:GLN:N	2.54	0.41
18:4:175:TYR:CB	18:4:194:PHE:CD1	2.90	0.41
1:A:109:TRP:HD1	1:A:116:ILE:HB	1.84	0.41
1:A:349:ILE:CG2	1:A:350:LEU:CA	2.95	0.41
1:A:479:ASP:CB	1:A:536:THR:CG2	2.99	0.41
1:A:514:THR:HA	1:A:530:LEU:O	2.21	0.41
1:A:57:LEU:HD22	1:A:58:HIS:CD2	2.54	0.41
1:A:547:PHE:CE2	19:A:9023:CLA:O1A	2.73	0.41
2:B:410:ARG:HD2	2:B:410:ARG:HA	1.49	0.41
2:B:353:TYR:CB	2:B:594:TRP:CH2	3.01	0.41
2:B:622:ASP:CA	2:B:626:LEU:HD12	2.48	0.41
9:I:8:PHE:CD1	19:I:1204:CLA:H12	2.56	0.41
11:K:47:ASP:C	11:K:51:SER:H	2.24	0.41
12:L:91:THR:OG1	12:L:91:THR:O	2.34	0.41
16:2:110:SER:HB3	16:2:227:LEU:HD13	2.02	0.41
13:N:164:SER:HA	13:N:165:ASN:O	2.18	0.41
19:3:3011:CLA:H11	19:3:3011:CLA:HBA2	1.88	0.41
12:L:210:PRO:HB2	12:L:211:TYR:CE2	2.55	0.41
4:D:114:MET:HG2	4:D:115:PRO:O	1.98	0.41
22:K:7001:LMU:H102	22:K:7001:LMU:H42	2.01	0.41
11:K:127:ILE:O	11:K:130:LEU:CA	2.69	0.41
22:A:7016:LMU:H1'	22:A:7016:LMU:H6D	1.76	0.41
19:2:2014:CLA:H91	19:2:2014:CLA:C16	2.51	0.41
19:J:1308:CLA:H93	19:2:2014:CLA:O1D	2.13	0.41
19:J:1311:CLA:H3A	19:J:1311:CLA:HBA2	1.27	0.41
15:1:200:GLY:HA3	19:1:1003:CLA:HBB2	2.02	0.41
15:1:201:PHE:HA	15:1:204:GLN:CB	2.49	0.41
3:C:33:GLY:HA2	3:C:37:LYS:HB3	2.02	0.41
13:N:127:PHE:CG	13:N:128:PRO:HD3	2.55	0.41
2:B:52:GLY:O	2:B:56:ILE:HG12	2.21	0.41
1:A:709:TRP:CZ3	2:B:417:ALA:HA	2.55	0.41
2:B:208:ARG:HA	2:B:208:ARG:HD2	1.98	0.41
18:4:121:ILE:C	18:4:123:VAL:N	2.71	0.41
15:1:65:ASP:CG	15:1:66:PRO:CA	2.83	0.41
18:4:95:GLU:HG3	18:4:96:LEU:N	2.35	0.41
19:A:1126:CLA:C17	19:A:1126:CLA:H122	2.50	0.41
1:A:173:VAL:O	1:A:175:ALA:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ASP:O	1:A:292:GLY:HA2	2.20	0.41
1:A:378:SER:OG	1:A:378:SER:O	2.35	0.41
1:A:604:TRP:O	1:A:605:MET:C	2.59	0.41
1:A:663:GLN:HB3	1:A:752:ALA:O	2.21	0.41
2:B:439:HIS:HB2	19:B:1230:CLA:C1C	2.50	0.41
2:B:355:LEU:HD21	2:B:508:LEU:CD2	2.51	0.41
2:B:395:ILE:H	2:B:395:ILE:HG13	1.75	0.41
2:B:729:THR:CG2	2:B:729:THR:O	2.61	0.41
2:B:724:PHE:CD1	19:B:9010:CLA:HMD1	2.56	0.41
9:I:11:LEU:O	9:I:16:PHE:N	2.51	0.41
12:L:111:VAL:HG23	12:L:112:GLY:H	1.86	0.41
19:4:1004:CLA:H52	19:4:1004:CLA:H11	1.83	0.41
19:A:1102:CLA:CHD	19:A:1102:CLA:HBC3	2.50	0.41
1:A:212:GLY:C	1:A:214:GLY:H	2.23	0.41
1:A:288:ASP:OD1	1:A:295:TRP:CD2	2.74	0.41
1:A:580:PRO:HB3	1:A:727:ILE:CG2	2.51	0.41
2:B:88:ALA:HB1	19:B:1205:CLA:O2D	2.20	0.41
19:B:1214:CLA:NA	19:B:1214:CLA:H12	2.36	0.41
2:B:73:ASN:C	2:B:121:TYR:OH	2.48	0.41
2:B:305:LEU:HD22	19:B:1220:CLA:O1D	2.18	0.41
2:B:175:LEU:HD13	19:B:1221:CLA:CED	2.51	0.41
19:B:1229:CLA:H13	19:B:1229:CLA:HMD2	2.03	0.41
1:A:466:THR:HG22	2:B:648:TRP:CE2	2.56	0.41
8:H:113:SER:HG	19:H:1207:CLA:C6	2.31	0.41
11:K:50:GLY:N	11:K:52:PRO:HD2	2.33	0.41
16:2:106:GLU:HG2	19:2:2004:CLA:HBC2	2.02	0.41
3:C:39:ILE:CG1	3:C:40:ALA:H	2.32	0.41
5:E:127:GLU:HB3	5:E:129:GLU:C	2.32	0.41
5:E:106:ARG:CZ	5:E:106:ARG:O	2.67	0.41
15:1:135:PRO:HD2	15:1:136:THR:N	2.32	0.41
17:3:111:LEU:CD2	17:3:112:GLY:H	2.21	0.41
22:3:7005:LMU:H42	22:3:7005:LMU:H71	1.79	0.41
4:D:110:GLN:O	4:D:122:MET:CG	2.69	0.41
16:2:94:SER:O	16:2:95:ASP:CB	2.62	0.41
2:B:4:ARG:C	2:B:5:ILE:HG12	2.41	0.41
2:B:4:ARG:NH2	2:B:5:ILE:N	2.69	0.41
6:F:101:LYS:O	6:F:104:ALA:HB3	2.21	0.41
22:E:7048:LMU:H4'	22:E:7048:LMU:H1'	1.79	0.41
19:1:1303:CLA:CMC	19:1:1303:CLA:CBC	2.86	0.41
2:B:142:LEU:O	2:B:145:LEU:HB3	2.21	0.41
6:F:116:ALA:O	6:F:119:ILE:HD13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:214:PRO:C	6:F:215:VAL:CG2	2.86	0.41
17:3:178:LYS:HB3	17:3:179:PRO:HD3	2.03	0.41
17:3:178:LYS:HB3	17:3:179:PRO:CD	2.49	0.41
2:B:7:ARG:CD	2:B:7:ARG:H	2.32	0.41
8:H:111:TYR:CB	8:H:112:LEU:HD23	2.51	0.41
8:H:111:TYR:CG	8:H:112:LEU:HD23	2.56	0.41
8:H:107:SER:O	8:H:111:TYR:CB	2.68	0.41
2:B:478:LEU:CG	2:B:478:LEU:O	2.68	0.41
12:L:103:GLY:HA3	12:L:192:GLY:HA3	2.02	0.41
22:K:7042:LMU:H121	22:K:7042:LMU:H91	1.75	0.41
16:2:266:PHE:CD2	16:2:267:THR:O	2.74	0.41
22:H:7017:LMU:H1B	22:H:7017:LMU:H6'2	1.72	0.41
15:1:68:GLY:O	15:1:73:PRO:N	2.55	0.41
19:4:1306:CLA:CBC	19:4:1306:CLA:CMC	2.79	0.41
19:A:1104:CLA:H11	19:A:1128:CLA:O2A	2.21	0.41
19:A:1106:CLA:H142	21:J:6012:BCR:C13	2.50	0.41
19:A:1106:CLA:CBB	19:A:1107:CLA:C3D	2.95	0.41
1:A:281:LEU:CD2	19:A:1115:CLA:HED3	2.22	0.41
19:A:1119:CLA:H112	19:A:1119:CLA:H91	1.83	0.41
1:A:684:PHE:HB2	19:A:9012:CLA:HAA1	2.02	0.41
2:B:334:LEU:HD22	19:B:1202:CLA:CHD	2.51	0.41
2:B:366:THR:O	2:B:366:THR:HG22	2.21	0.41
6:F:201:PRO:O	6:F:202:LEU:HB2	2.21	0.41
7:G:87:VAL:O	7:G:90:GLN:O	2.38	0.41
16:2:107:LEU:HD11	16:2:108:VAL:HG23	2.03	0.41
19:2:2004:CLA:C4	19:3:2009:CLA:HBC3	2.51	0.41
19:1:1014:CLA:H121	19:1:1014:CLA:C9	2.51	0.41
1:A:720:THR:O	1:A:720:THR:CG2	2.65	0.41
4:D:93:LYS:HG3	4:D:96:VAL:HG11	1.99	0.41
16:2:184:PRO:CD	16:2:186:ASN:N	2.83	0.41
11:K:92:GLY:O	11:K:93:LEU:CB	2.66	0.41
22:E:7048:LMU:O2'	22:E:7048:LMU:H6'2	2.21	0.41
17:3:156:THR:C	17:3:158:PHE:N	2.69	0.41
17:3:157:LEU:O	17:3:160:LEU:CA	2.69	0.41
2:B:131:THR:O	2:B:135:LEU:CD2	2.62	0.41
1:A:484:LEU:CA	1:A:485:GLN:NE2	2.84	0.41
4:D:185:GLY:O	4:D:186:GLN:HB2	2.19	0.41
1:A:236:GLY:O	1:A:237:VAL:CB	2.69	0.41
22:K:7041:LMU:H4'	22:K:7041:LMU:H2B	1.79	0.41
22:A:7010:LMU:H2O1	22:A:7010:LMU:H3'	1.83	0.41
22:E:7037:LMU:O2B	22:E:7037:LMU:C5B	2.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:G:7039:LMU:H112	22:G:7039:LMU:H82	1.61	0.41
19:4:4006:CLA:HBA2	19:4:4006:CLA:CBD	2.51	0.40
15:1:68:GLY:C	15:1:69:LEU:O	2.56	0.40
1:A:127:VAL:CG2	19:A:1107:CLA:HBB2	2.39	0.40
1:A:201:SER:O	1:A:204:ASN:CA	2.69	0.40
1:A:208:ALA:HA	1:A:310:PHE:C	2.37	0.40
1:A:375:HIS:N	1:A:375:HIS:ND1	2.69	0.40
1:A:539:PHE:CD2	1:A:539:PHE:C	2.94	0.40
1:A:648:THR:O	1:A:649:ILE:HG22	2.21	0.40
19:B:1235:CLA:HBC1	6:F:160:PHE:CE1	2.48	0.40
2:B:169:LYS:O	2:B:170:ASN:O	2.39	0.40
2:B:15:ASP:HA	2:B:16:PRO:HD3	1.89	0.40
2:B:289:LEU:O	19:B:1218:CLA:HMC1	2.22	0.40
2:B:29:HIS:HB3	19:B:1226:CLA:HBA1	2.03	0.40
2:B:373:THR:C	2:B:375:HIS:H	2.24	0.40
20:B:5002:PQN:H161	20:B:5002:PQN:H141	1.60	0.40
2:B:535:VAL:CG1	2:B:536:LYS:H	2.34	0.40
3:C:70:TRP:O	3:C:71:HIS:C	2.59	0.40
7:G:136:VAL:C	7:G:137:VAL:HG22	2.41	0.40
11:K:50:GLY:N	11:K:52:PRO:HD3	2.36	0.40
12:L:145:LEU:CG	21:L:6019:BCR:HC7	2.41	0.40
13:N:155:GLU:CB	13:N:157:LYS:NZ	2.82	0.40
4:D:134:LYS:HE2	4:D:166:LEU:HD11	2.03	0.40
19:3:3013:CLA:HBC2	19:3:3013:CLA:HHD	2.02	0.40
13:N:118:TYR:O	13:N:119:THR:OG1	2.39	0.40
4:D:125:GLY:HA2	4:D:127:ASN:H	1.85	0.40
17:3:85:ASP:HA	17:3:86:PRO:HD3	1.40	0.40
6:F:102:LEU:O	6:F:103:GLN:O	2.39	0.40
1:A:23:ASP:C	1:A:23:ASP:OD1	2.59	0.40
22:F:7036:LMU:H1'	22:F:7036:LMU:O6'	2.21	0.40
17:3:201:ALA:O	17:3:202:TYR:CD2	2.74	0.40
18:4:180:GLY:O	18:4:183:GLY:N	2.54	0.40
18:4:126:TRP:HA	19:4:4006:CLA:HMD3	2.02	0.40
18:4:149:SER:OG	18:4:150:HIS:N	2.54	0.40
18:4:153:GLU:OE2	19:4:4012:CLA:HHC	2.17	0.40
1:A:284:ARG:O	1:A:285:GLY:C	2.56	0.40
1:A:363:ALA:N	1:A:410:ALA:HB2	2.36	0.40
1:A:434:ARG:HA	1:A:437:ARG:HD2	2.03	0.40
21:A:6011:BCR:H323	21:J:6012:BCR:C39	2.49	0.40
19:A:9023:CLA:C3A	19:A:9023:CLA:O2A	2.65	0.40
2:B:310:PRO:CG	2:B:311:PRO:HD2	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:320:LYS:HG3	2:B:321:GLY:N	2.37	0.40
2:B:593:TYR:CD1	19:B:1234:CLA:HMC2	2.57	0.40
2:B:285:LEU:HD12	21:B:6004:BCR:C17	2.50	0.40
19:B:1232:CLA:CBB	21:B:6010:BCR:C28	2.99	0.40
7:G:131:GLY:HA2	7:G:136:VAL:CB	2.50	0.40
7:G:90:GLN:HB2	7:G:92:PRO:N	2.37	0.40
11:K:56:ILE:HG12	11:K:59:THR:CG2	2.50	0.40
12:L:182:TRP:CZ3	12:L:186:THR:HG21	2.56	0.40
12:L:194:ILE:O	12:L:195:SER:HB3	2.21	0.40
5:E:108:ASN:O	5:E:109:LYS:C	2.57	0.40
15:1:140:ILE:CD1	15:1:140:ILE:N	2.72	0.40
1:A:586:ARG:HB2	1:A:589:THR:OG1	2.22	0.40
4:D:155:TYR:CD1	4:D:168:PRO:HG3	2.57	0.40
17:3:108:PHE:HD2	19:3:3013:CLA:C4	2.34	0.40
18:4:88:LEU:O	18:4:90:TRP:CB	2.59	0.40
16:2:95:ASP:HA	16:2:96:PRO:HD3	1.93	0.40
2:B:631:LEU:O	2:B:634:GLY:N	2.53	0.40
6:F:116:ALA:O	6:F:119:ILE:HG12	2.20	0.40
2:B:475:ASP:CG	2:B:480:SER:HA	2.35	0.40
18:4:243:THR:HG23	18:4:244:ILE:N	2.36	0.40
18:4:108:GLY:O	18:4:109:MET:O	2.39	0.40
18:4:232:LEU:HD12	18:4:234:GLN:N	2.36	0.40
19:1:1003:CLA:HED1	19:1:1008:CLA:HMB1	2.04	0.40
22:K:7042:LMU:H22	22:K:7042:LMU:C7	2.50	0.40
22:G:7039:LMU:H3'	22:G:7039:LMU:C6B	2.49	0.40
6:F:113:SER:C	6:F:115:PRO:HD3	2.42	0.40
1:A:177:LEU:C	1:A:179:LEU:N	2.75	0.40
4:D:169:LYS:HB2	4:D:169:LYS:HZ3	1.85	0.40
4:D:169:LYS:NZ	4:D:169:LYS:HB2	2.36	0.40
15:1:177:PRO:HG2	15:1:180:LEU:HA	2.03	0.40
18:4:217:PHE:O	18:4:220:GLN:HB2	2.21	0.40
1:A:98:PHE:C	1:A:100:GLY:N	2.68	0.40
19:A:1120:CLA:C1A	19:A:1120:CLA:CGA	2.99	0.40
19:A:1119:CLA:CGA	19:A:1123:CLA:HBB2	2.51	0.40
1:A:492:ILE:HD13	19:A:1133:CLA:CHC	2.50	0.40
1:A:170:GLY:O	1:A:173:VAL:CG2	2.64	0.40
1:A:352:THR:HG22	19:A:1123:CLA:H201	2.03	0.40
1:A:409:GLY:O	1:A:411:ALA:N	2.55	0.40
1:A:472:ARG:HH22	12:L:120:LEU:HD13	1.85	0.40
19:A:9013:CLA:H91	19:A:9013:CLA:H112	1.78	0.40
1:A:94:SER:O	1:A:95:GLY:C	2.58	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1205:CLA:H162	19:B:1224:CLA:H192	2.03	0.40
21:B:6004:BCR:H351	21:B:6004:BCR:H15C	1.88	0.40
20:B:5002:PQN:H141	21:B:6017:BCR:H331	2.04	0.40
2:B:653:GLY:HA3	2:B:720:THR:OG1	2.20	0.40
21:F:6014:BCR:C33	21:F:6014:BCR:HC8	2.52	0.40
7:G:66:LEU:HD23	7:G:69:GLY:HA3	2.03	0.40
13:N:123:GLY:O	13:N:124:SER:O	2.39	0.40
1:A:569:ILE:HG12	1:A:586:ARG:NH1	2.36	0.40
19:3:3011:CLA:H62	19:3:3011:CLA:H41	1.80	0.40
16:2:160:ILE:HG21	19:2:2012:CLA:CAB	2.41	0.40
16:2:172:LEU:HD12	16:2:172:LEU:HA	1.75	0.40
10:J:5:LYS:CG	16:2:178:ASN:HA	2.52	0.40
4:D:140:LEU:HD22	4:D:144:LEU:CG	2.49	0.40
19:K:1143:CLA:CBC	22:K:7001:LMU:C3B	2.91	0.40
17:3:197:SER:HB3	17:3:206:PRO:CG	2.51	0.40
8:H:103:LEU:O	8:H:107:SER:HB3	2.22	0.40
1:A:631:GLN:O	1:A:631:GLN:HG2	2.21	0.40
1:A:39:HIS:ND1	1:A:39:HIS:C	2.75	0.40
22:B:7040:LMU:H3O2	22:B:7040:LMU:C1B	2.34	0.40
22:4:7009:LMU:C3'	22:4:7009:LMU:H5B	2.52	0.40
2:B:262:HIS:HB2	2:B:265:THR:OG1	2.21	0.40
1:A:755:ILE:H	1:A:755:ILE:HG13	1.62	0.40
2:B:700:LEU:HD23	2:B:700:LEU:N	2.36	0.40
19:3:1147:CLA:H3A	19:3:1147:CLA:HBA2	1.72	0.40
18:4:169:ASP:HB3	19:4:4001:CLA:CMB	2.43	0.40
18:4:212:LEU:O	18:4:213:ALA:CB	2.70	0.40
19:A:1107:CLA:CMC	19:A:1107:CLA:HBC3	2.52	0.40
19:A:1119:CLA:H101	19:A:1122:CLA:H93	2.02	0.40
19:A:1124:CLA:H172	21:A:6007:BCR:C33	2.46	0.40
1:A:397:THR:OG1	19:A:1126:CLA:CMB	2.70	0.40
19:A:1138:CLA:H202	19:A:1139:CLA:H41	2.03	0.40
19:A:1138:CLA:HMC3	19:A:1139:CLA:ND	2.36	0.40
1:A:295:TRP:CB	1:A:297:THR:HG23	2.51	0.40
1:A:334:HIS:HB3	19:A:1120:CLA:HMA1	2.04	0.40
1:A:368:LEU:HD12	19:A:1125:CLA:C6	2.52	0.40
19:A:1119:CLA:H8	21:A:6008:BCR:H19C	2.03	0.40
19:B:1235:CLA:H121	21:F:6016:BCR:H311	1.98	0.40
2:B:178:HIS:C	2:B:180:SER:N	2.72	0.40
2:B:440:ASN:OD1	2:B:452:GLN:CD	2.60	0.40
2:B:569:ASP:HB3	2:B:574:ASP:HB3	2.04	0.40
2:B:586:THR:O	2:B:589:TRP:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:596:TRP:CZ2	2:B:612:SER:HB3	2.56	0.40
19:B:1235:CLA:C12	21:F:6016:BCR:H311	2.51	0.40
9:I:15:LEU:HD12	9:I:18:ALA:HB3	2.03	0.40
12:L:195:SER:C	12:L:197:VAL:H	2.25	0.40
19:2:2006:CLA:OBD	19:2:2006:CLA:HED2	2.22	0.40
16:2:222:ILE:O	16:2:226:ARG:N	2.51	0.40
19:2:2004:CLA:HED2	19:3:2009:CLA:CBB	2.51	0.40
19:1:1006:CLA:CAB	19:1:1013:CLA:HHD	2.51	0.40
17:3:111:LEU:CD2	17:3:112:GLY:N	2.83	0.40
1:A:261:SER:O	1:A:262:PHE:CE1	2.73	0.40
2:B:635:ILE:O	2:B:636:THR:O	2.38	0.40
17:3:124:LYS:CG	17:3:149:ASN:HB3	2.49	0.40
12:L:210:PRO:CB	12:L:211:TYR:CD2	3.03	0.40
13:N:114:PHE:C	13:N:117:ALA:HB3	2.39	0.40
19:1:1007:CLA:H51	19:1:1007:CLA:H11	1.92	0.40
11:K:123:GLY:HA3	11:K:124:LEU:HA	1.82	0.40
11:K:127:ILE:CB	11:K:129:ALA:HB1	2.33	0.40
6:F:130:PHE:O	6:F:132:ASN:O	2.39	0.40
6:F:230:ASN:O	6:F:231:PHE:O	2.40	0.40
4:D:148:TYR:O	4:D:149:LYS:HB3	2.21	0.40
7:G:140:TYR:CG	7:G:141:ILE:N	2.86	0.40
22:E:7037:LMU:H32	22:E:7037:LMU:C7	2.51	0.40
6:F:154:GLN:OE1	6:F:155:ARG:N	2.55	0.40
22:4:7034:LMU:H71	22:4:7052:LMU:C1	2.38	0.40
15:1:155:GLU:CD	15:1:155:GLU:H	2.19	0.40
15:1:65:ASP:HA	15:1:69:LEU:CD1	2.49	0.40
15:1:94:VAL:C	15:1:96:GLY:N	2.73	0.40
19:A:1101:CLA:H12	19:A:1140:CLA:H61	2.02	0.40
19:A:1104:CLA:H12	19:A:1104:CLA:HBA2	1.79	0.40
1:A:146:THR:HA	1:A:391:THR:HG22	2.03	0.40
1:A:195:TRP:CZ2	19:A:1108:CLA:HMA2	2.52	0.40
1:A:222:GLN:O	1:A:227:LEU:HG	2.21	0.40
1:A:286:GLY:O	1:A:295:TRP:NE1	2.55	0.40
1:A:447:ASN:ND2	2:B:678:LEU:CD2	2.82	0.40
1:A:672:LEU:C	1:A:674:ALA:H	2.16	0.40
1:A:697:ARG:C	1:A:699:TYR:N	2.74	0.40
19:B:1202:CLA:HMC3	19:B:1226:CLA:H3A	2.02	0.40
2:B:649:MET:HE1	19:B:1205:CLA:HBC3	2.04	0.40
19:B:1218:CLA:CBA	19:B:1219:CLA:O1A	2.70	0.40
2:B:421:HIS:CE1	19:B:1228:CLA:C4D	3.04	0.40
2:B:120:VAL:CB	2:B:123:TRP:CD1	3.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:185:VAL:HA	2:B:188:LEU:HB3	2.04	0.40
2:B:463:ILE:HD12	19:B:1234:CLA:CGA	2.51	0.40
1:A:705:GLU:HG2	2:B:545:LYS:HZ2	1.86	0.40
2:B:557:PHE:O	2:B:557:PHE:CD2	2.74	0.40
21:B:6005:BCR:HC7	21:B:6005:BCR:H321	1.87	0.40
2:B:668:ARG:HG3	2:B:699:ALA:C	2.42	0.40
22:G:7026:LMU:C8	22:G:7026:LMU:C4	2.96	0.40
19:A:9022:CLA:C14	19:H:1207:CLA:HBC3	2.52	0.40
8:H:91:PHE:CZ	8:H:98:LEU:HD13	2.56	0.40
19:2:2002:CLA:H72	19:2:2002:CLA:H41	2.04	0.40
16:2:170:ASP:C	16:2:172:LEU:N	2.67	0.40
19:K:1143:CLA:CMC	19:K:1143:CLA:HBC2	2.52	0.40
6:F:103:GLN:O	6:F:105:SER:N	2.54	0.40
6:F:123:MET:O	6:F:127:LYS:N	2.54	0.40
6:F:121:ALA:HA	6:F:124:GLU:HB3	2.04	0.40
17:3:197:SER:CB	17:3:206:PRO:HG3	2.52	0.40
19:2:2014:CLA:CAD	19:2:2014:CLA:HED3	2.50	0.40
15:1:173:TYR:HA	15:1:173:TYR:HD2	1.49	0.40
12:L:52:PRO:O	12:L:54:TYR:N	2.55	0.40
15:1:192:ARG:CG	15:1:193:LEU:N	2.82	0.40
13:N:91:TYR:HD2	13:N:91:TYR:HA	1.68	0.40
2:B:488:ALA:CB	19:B:1233:CLA:C2C	3.00	0.40

All (130) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:173:TYR:OH	16:2:132:LEU:C[2_646]	0.71	1.49
6:F:130:PHE:CG	12:L:170:LYS:NZ[2_556]	0.72	1.48
2:B:205:GLU:OE2	11:K:69:ARG:NH1[1_554]	0.79	1.41
12:L:123:THR:O	18:4:180:GLY:CA[1_455]	0.88	1.32
15:1:171:LEU:N	16:2:132:LEU:N[2_646]	0.98	1.22
15:1:173:TYR:OH	16:2:132:LEU:CA[2_646]	1.01	1.19
12:L:203:LEU:C	18:4:184:TYR:OH[1_455]	1.02	1.18
12:L:205:TYR:OH	18:4:181:GLU:O[1_455]	1.02	1.18
12:L:124:GLU:OE1	18:4:172:PHE:CE2[1_455]	1.06	1.14
15:1:171:LEU:CD2	16:2:131:ILE:C[2_646]	1.07	1.13
15:1:171:LEU:CD2	16:2:131:ILE:O[2_646]	1.08	1.12
12:L:124:GLU:OE1	18:4:172:PHE:CZ[1_455]	1.09	1.11
12:L:124:GLU:CD	18:4:172:PHE:CE2[1_455]	1.11	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:GLN:NE2	19:K:3009:CLA:C2C[1_554]	1.11	1.09
15:1:173:TYR:CE1	16:2:132:LEU:O[2_646]	1.13	1.07
12:L:124:GLU:CD	18:4:172:PHE:CZ[1_455]	1.15	1.05
15:1:118:PRO:O	17:3:89:THR:CG2[1_554]	1.17	1.03
6:F:130:PHE:CD2	12:L:170:LYS:NZ[2_556]	1.18	1.02
6:F:130:PHE:CE1	12:L:170:LYS:CE[2_556]	1.18	1.02
2:B:205:GLU:OE2	11:K:69:ARG:CZ[1_554]	1.19	1.01
15:1:170:PRO:O	16:2:132:LEU:CB[2_646]	1.20	1.00
12:L:203:LEU:O	18:4:184:TYR:CE2[1_455]	1.27	0.93
15:1:170:PRO:O	16:2:132:LEU:CA[2_646]	1.30	0.90
6:F:130:PHE:CD1	12:L:170:LYS:NZ[2_556]	1.32	0.88
6:F:131:ASP:OD2	12:L:170:LYS:CD[2_556]	1.32	0.88
1:A:348:GLU:OE2	7:G:147:ASN:OD1[1_556]	1.33	0.87
15:1:173:TYR:CZ	16:2:132:LEU:O[2_646]	1.37	0.83
6:F:131:ASP:OD1	12:L:170:LYS:CG[2_556]	1.38	0.82
2:B:205:GLU:CD	11:K:69:ARG:NH1[1_554]	1.39	0.81
4:D:160:ASN:CG	6:F:101:LYS:NZ[2_546]	1.39	0.81
12:L:203:LEU:O	18:4:184:TYR:CZ[1_455]	1.40	0.80
2:B:248:GLN:NE2	19:K:3009:CLA:CMC[1_554]	1.40	0.80
12:L:122:ASN:ND2	18:4:181:GLU:OE1[1_455]	1.46	0.74
15:1:173:TYR:CZ	16:2:132:LEU:C[2_646]	1.47	0.73
2:B:248:GLN:NE2	19:K:3009:CLA:C1C[1_554]	1.49	0.71
6:F:131:ASP:CG	12:L:170:LYS:CD[2_556]	1.49	0.71
12:L:123:THR:O	18:4:180:GLY:N[1_455]	1.50	0.70
12:L:124:GLU:OE2	18:4:172:PHE:CZ[1_455]	1.50	0.70
8:H:81:SER:OG	18:4:240:TRP:CZ3[2_546]	1.51	0.69
12:L:124:GLU:OE2	18:4:172:PHE:CE1[1_455]	1.52	0.68
6:F:130:PHE:CZ	12:L:170:LYS:CE[2_556]	1.53	0.67
12:L:124:GLU:N	18:4:177:LEU:O[1_455]	1.54	0.66
15:1:171:LEU:CG	16:2:131:ILE:CA[2_646]	1.55	0.65
12:L:205:TYR:OH	18:4:181:GLU:C[1_455]	1.55	0.65
6:F:130:PHE:CD1	12:L:170:LYS:CE[2_556]	1.56	0.64
12:L:203:LEU:O	18:4:184:TYR:OH[1_455]	1.58	0.62
15:1:170:PRO:C	16:2:132:LEU:N[2_646]	1.58	0.62
15:1:173:TYR:CZ	16:2:132:LEU:CA[2_646]	1.59	0.61
12:L:122:ASN:CG	18:4:181:GLU:OE1[1_455]	1.60	0.60
12:L:202:PHE:O	18:4:184:TYR:OH[1_455]	1.61	0.59
15:1:171:LEU:CG	16:2:131:ILE:C[2_646]	1.62	0.58
6:F:131:ASP:OD1	12:L:170:LYS:CD[2_556]	1.62	0.58
12:L:122:ASN:OD1	18:4:181:GLU:OE1[1_455]	1.64	0.56
12:L:124:GLU:OE2	18:4:176:SER:O[1_455]	1.65	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:173:TYR:OH	16:2:132:LEU:O[2_646]	1.66	0.54
15:1:118:PRO:C	17:3:89:THR:CG2[1_554]	1.67	0.53
12:L:203:LEU:CA	18:4:184:TYR:OH[1_455]	1.68	0.52
15:1:171:LEU:CG	16:2:131:ILE:N[2_646]	1.68	0.52
2:B:205:GLU:OE2	11:K:69:ARG:NH2[1_554]	1.70	0.50
19:K:1142:CLA:O2A	19:1:1008:CLA:O2D[1_456]	1.70	0.50
15:1:173:TYR:OH	16:2:133:ASN:N[2_646]	1.71	0.49
15:1:171:LEU:CD1	16:2:131:ILE:CB[2_646]	1.72	0.48
4:D:160:ASN:ND2	6:F:101:LYS:NZ[2_546]	1.72	0.48
15:1:173:TYR:OH	16:2:132:LEU:CB[2_646]	1.72	0.48
6:F:120:LYS:NZ	12:L:155:GLU:CG[2_556]	1.73	0.47
15:1:171:LEU:CA	16:2:132:LEU:N[2_646]	1.73	0.47
12:L:124:GLU:OE2	18:4:172:PHE:CE2[1_455]	1.74	0.46
12:L:204:LEU:N	18:4:184:TYR:OH[1_455]	1.75	0.45
12:L:203:LEU:C	18:4:184:TYR:CZ[1_455]	1.76	0.44
12:L:124:GLU:OE2	18:4:172:PHE:CD1[1_455]	1.76	0.44
15:1:170:PRO:C	16:2:132:LEU:CA[2_646]	1.81	0.39
15:1:170:PRO:O	16:2:132:LEU:CG[2_646]	1.83	0.37
12:L:205:TYR:CZ	18:4:181:GLU:O[1_455]	1.83	0.37
1:A:348:GLU:OE2	7:G:147:ASN:CG[1_556]	1.84	0.36
6:F:120:LYS:NZ	12:L:155:GLU:CD[2_556]	1.85	0.35
6:F:130:PHE:CE2	12:L:170:LYS:NZ[2_556]	1.85	0.35
8:H:81:SER:OG	18:4:240:TRP:CH2[2_546]	1.86	0.34
1:A:200:GLU:OE1	2:B:220:GLN:NE2[1_556]	1.86	0.34
15:1:171:LEU:CD2	16:2:132:LEU:N[2_646]	1.88	0.32
6:F:130:PHE:CE1	12:L:170:LYS:CD[2_556]	1.88	0.32
6:F:130:PHE:CD1	12:L:170:LYS:CD[2_556]	1.89	0.31
12:L:122:ASN:OD1	18:4:181:GLU:CD[1_455]	1.91	0.29
6:F:120:LYS:CE	12:L:155:GLU:CG[2_556]	1.92	0.28
2:B:248:GLN:NE2	19:K:3009:CLA:CHC[1_554]	1.92	0.28
12:L:204:LEU:CD2	18:4:185:PRO:O[1_455]	1.92	0.28
15:1:171:LEU:CG	16:2:132:LEU:N[2_646]	1.93	0.27
12:L:124:GLU:OE2	18:4:172:PHE:CD2[1_455]	1.95	0.25
7:G:85:GLU:OE2	22:K:7047:LMU:C7[2_546]	1.96	0.24
15:1:171:LEU:CD2	16:2:133:ASN:N[2_646]	1.96	0.24
15:1:173:TYR:CE2	16:2:132:LEU:CA[2_646]	1.97	0.23
2:B:205:GLU:OE1	11:K:69:ARG:NH1[1_554]	1.97	0.23
12:L:124:GLU:OE2	18:4:172:PHE:CG[1_455]	1.97	0.23
15:1:171:LEU:CB	16:2:132:LEU:N[2_646]	1.97	0.23
6:F:130:PHE:CE1	12:L:170:LYS:NZ[2_556]	1.98	0.22
2:B:248:GLN:CD	19:K:3009:CLA:CMC[1_554]	1.99	0.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:GLN:CD	19:K:3009:CLA:C2C[1_554]	1.99	0.21
2:B:5:ILE:CD1	6:F:111:ASP:OD1[2_546]	2.00	0.20
15:1:170:PRO:O	16:2:132:LEU:N[2_646]	2.01	0.19
6:F:131:ASP:CG	12:L:170:LYS:CG[2_556]	2.01	0.19
12:L:122:ASN:O	18:4:179:ALA:N[1_455]	2.02	0.18
12:L:203:LEU:N	18:4:184:TYR:OH[1_455]	2.02	0.18
12:L:202:PHE:C	18:4:184:TYR:OH[1_455]	2.03	0.17
4:D:160:ASN:OD1	6:F:101:LYS:NZ[2_546]	2.03	0.17
15:1:171:LEU:N	16:2:132:LEU:CA[2_646]	2.03	0.17
4:D:160:ASN:CB	6:F:101:LYS:NZ[2_546]	2.04	0.16
1:A:348:GLU:OE2	7:G:147:ASN:ND2[1_556]	2.04	0.16
2:B:239:SER:OG	19:K:3009:CLA:CAA[1_554]	2.04	0.16
6:F:120:LYS:NZ	12:L:155:GLU:OE2[2_556]	2.05	0.15
15:1:171:LEU:N	16:2:131:ILE:C[2_646]	2.06	0.14
7:G:85:GLU:OE2	22:K:7047:LMU:C9[2_546]	2.07	0.13
15:1:171:LEU:CD2	16:2:131:ILE:CA[2_646]	2.10	0.10
1:A:348:GLU:CD	7:G:147:ASN:OD1[1_556]	2.10	0.10
12:L:123:THR:C	18:4:180:GLY:CA[1_455]	2.11	0.09
6:F:130:PHE:CE2	12:L:170:LYS:CE[2_556]	2.11	0.09
12:L:124:GLU:CD	18:4:172:PHE:CD2[1_455]	2.12	0.08
1:A:474:GLN:O	18:4:175:TYR:OH[1_455]	2.12	0.08
12:L:209:LEU:CD2	18:4:189:PHE:CE1[1_455]	2.13	0.07
15:1:173:TYR:CE1	16:2:132:LEU:C[2_646]	2.13	0.07
6:F:130:PHE:CG	12:L:170:LYS:CE[2_556]	2.14	0.06
15:1:171:LEU:CD1	16:2:131:ILE:N[2_646]	2.14	0.06
12:L:204:LEU:CD2	18:4:185:PRO:C[1_455]	2.14	0.06
12:L:204:LEU:N	18:4:184:TYR:CZ[1_455]	2.15	0.05
15:1:171:LEU:CG	16:2:131:ILE:CB[2_646]	2.15	0.05
6:F:130:PHE:CZ	12:L:170:LYS:NZ[2_556]	2.15	0.05
12:L:203:LEU:C	18:4:184:TYR:CE2[1_455]	2.16	0.04
12:L:123:THR:C	18:4:180:GLY:N[1_455]	2.17	0.03
12:L:124:GLU:CD	18:4:172:PHE:CE1[1_455]	2.18	0.02
6:F:112:ASP:OD2	9:I:30:LYS:NZ[2_556]	2.18	0.02
12:L:202:PHE:O	18:4:184:TYR:CZ[1_455]	2.19	0.01
15:1:171:LEU:CD1	16:2:131:ILE:CA[2_646]	2.19	0.01

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	726/738 (98%)	483 (66%)	139 (19%)	104 (14%)	0	1
2	B	731/733 (100%)	527 (72%)	111 (15%)	93 (13%)	0	2
3	C	79/81 (98%)	42 (53%)	18 (23%)	19 (24%)	0	0
4	D	136/138 (99%)	94 (69%)	24 (18%)	18 (13%)	0	2
5	E	62/64 (97%)	44 (71%)	11 (18%)	7 (11%)	0	3
6	F	152/154 (99%)	105 (69%)	27 (18%)	20 (13%)	0	2
7	G	93/95 (98%)	60 (64%)	22 (24%)	11 (12%)	0	3
8	H	67/69 (97%)	49 (73%)	9 (13%)	9 (13%)	0	2
9	I	28/30 (93%)	11 (39%)	9 (32%)	8 (29%)	0	0
10	J	40/42 (95%)	19 (48%)	11 (28%)	10 (25%)	0	0
11	K	82/84 (98%)	66 (80%)	9 (11%)	7 (8%)	1	7
12	L	159/161 (99%)	110 (69%)	23 (14%)	26 (16%)	0	1
13	N	83/85 (98%)	50 (60%)	19 (23%)	14 (17%)	0	1
15	1	161/170 (95%)	119 (74%)	28 (17%)	14 (9%)	1	7
16	2	174/176 (99%)	129 (74%)	26 (15%)	19 (11%)	0	4
17	3	148/172 (86%)	111 (75%)	20 (14%)	17 (12%)	0	3
18	4	164/166 (99%)	129 (79%)	21 (13%)	14 (8%)	1	7
All	All	3085/3158 (98%)	2148 (70%)	527 (17%)	410 (13%)	0	2

All (410) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	LYS
1	A	41	SER
1	A	98	PHE
1	A	99	HIS
1	A	158	ILE

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Mol	Chain	Res	Type
1	A	164	LEU
1	A	175	ALA
1	A	205	HIS
1	A	221	HIS
1	A	237	VAL
1	A	268	PRO
1	A	279	ASP
1	A	283	PHE
1	A	307	ALA
1	A	310	PHE
1	A	317	TYR
1	A	329	ASP
1	A	333	ALA
1	A	346	LEU
1	A	361	ASN
1	A	386	ALA
1	A	389	TYR
1	A	424	PRO
1	A	431	LEU
1	A	433	ASP
1	A	473	PRO
1	A	474	GLN
1	A	477	PHE
1	A	509	ALA
1	A	523	VAL
1	A	532	ILE
1	A	553	VAL
1	A	594	ALA
1	A	643	ALA
1	A	657	LEU
1	A	673	SER
1	A	679	PHE
1	A	727	ILE
1	A	735	VAL
1	A	750	PHE
1	A	751	LEU
1	A	752	ALA
1	A	757	VAL
2	B	35	ASP
2	B	80	ASP
2	B	83	HIS
2	B	99	PRO

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Mol	Chain	Res	Type
2	B	105	THR
2	B	142	LEU
2	B	160	LYS
2	B	170	ASN
2	B	182	LEU
2	B	187	SER
2	B	198	ALA
2	B	208	ARG
2	B	231	ASN
2	B	267	SER
2	B	308	HIS
2	B	321	GLY
2	B	378	ILE
2	B	382	ILE
2	B	383	MET
2	B	420	SER
2	B	490	ARG
2	B	495	PRO
2	B	506	ASN
2	B	512	ILE
2	B	545	LYS
2	B	554	GLY
2	B	555	TYR
2	B	569	ASP
2	B	587	ILE
2	B	599	ILE
2	B	629	SER
2	B	639	VAL
2	B	661	PHE
2	B	662	MET
2	B	668	ARG
2	B	681	ALA
2	B	710	LEU
2	B	733	PHE
3	C	8	TYR
3	C	21	CYS
3	C	32	GLY
3	C	49	VAL
3	C	56	SER
3	C	59	PRO
3	C	62	PHE
3	C	65	VAL

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Mol	Chain	Res	Type
4	D	107	PRO
4	D	124	GLU
4	D	132	ALA
4	D	151	LYS
4	D	173	TYR
4	D	186	GLN
4	D	193	LYS
4	D	207	PRO
5	E	73	LYS
5	E	92	ALA
5	E	102	PRO
5	E	103	VAL
5	E	128	VAL
6	F	84	PRO
6	F	119	ILE
6	F	124	GLU
6	F	191	PRO
6	F	193	GLN
7	G	84	ARG
7	G	92	PRO
7	G	98	THR
7	G	130	TRP
7	G	142	LEU
7	G	150	ASP
8	H	62	THR
8	H	99	LYS
9	I	22	ALA
9	I	23	SER
10	J	5	LYS
10	J	6	THR
10	J	10	VAL
10	J	22	LEU
10	J	26	LEU
10	J	38	ILE
11	K	87	GLU
11	K	93	LEU
12	L	60	ILE
12	L	73	VAL
12	L	83	LEU
12	L	121	ARG
12	L	122	ASN
12	L	143	LEU

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Mol	Chain	Res	Type
12	L	169	ARG
12	L	195	SER
13	N	97	THR
13	N	125	CYS
13	N	134	CYS
13	N	146	LEU
13	N	148	ASP
13	N	149	ASP
15	1	65	ASP
15	1	97	ILE
15	1	130	PRO
15	1	156	LYS
15	1	169	ASP
15	1	170	PRO
15	1	177	PRO
15	1	217	LEU
15	1	225	TRP
16	2	139	THR
16	2	174	PRO
16	2	183	PHE
16	2	207	GLY
16	2	212	GLN
16	2	246	PRO
16	2	257	PRO
16	2	265	ALA
17	3	92	PHE
17	3	129	PRO
17	3	151	TRP
17	3	160	LEU
17	3	178	LYS
17	3	254	GLN
18	4	85	PRO
18	4	109	MET
18	4	120	ILE
18	4	134	TYR
1	A	22	VAL
1	A	35	ALA
1	A	57	LEU
1	A	160	SER
1	A	163	GLN
1	A	210	LEU
1	A	215	SER

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Mol	Chain	Res	Type
1	A	247	GLU
1	A	249	ILE
1	A	250	LEU
1	A	294	LEU
1	A	308	ILE
1	A	313	ALA
1	A	347	TYR
1	A	373	ALA
1	A	400	MET
1	A	439	ARG
1	A	446	LEU
1	A	476	MET
1	A	592	VAL
1	A	624	VAL
1	A	640	GLY
1	A	649	ILE
1	A	661	ALA
1	A	671	SER
1	A	717	ALA
2	B	26	ALA
2	B	153	GLY
2	B	178	HIS
2	B	179	LEU
2	B	188	LEU
2	B	330	ILE
2	B	371	LEU
2	B	375	HIS
2	B	379	ALA
2	B	437	TYR
2	B	501	ILE
2	B	505	SER
2	B	528	HIS
2	B	657	TRP
2	B	664	LEU
2	B	707	LEU
2	B	731	GLY
2	B	732	LYS
3	C	10	THR
3	C	12	ILE
3	C	28	MET
3	C	40	ALA
3	C	66	ARG

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Mol	Chain	Res	Type
4	D	76	PRO
4	D	81	PRO
4	D	119	ALA
4	D	149	LYS
4	D	164	GLN
5	E	110	VAL
5	E	111	ASN
6	F	128	LYS
6	F	135	LYS
6	F	138	LEU
6	F	140	CYS
6	F	205	SER
7	G	62	LEU
7	G	141	ILE
8	H	64	GLN
8	H	100	PHE
8	H	116	ALA
9	I	25	PHE
10	J	37	LEU
11	K	86	LEU
11	K	114	HIS
11	K	126	ASN
12	L	68	SER
12	L	200	ALA
13	N	109	THR
13	N	119	THR
13	N	147	SER
15	1	59	PRO
16	2	104	GLN
16	2	133	ASN
16	2	146	PHE
16	2	248	ASP
17	3	152	ALA
17	3	250	VAL
17	3	252	PRO
18	4	192	LEU
1	A	127	VAL
1	A	184	PHE
1	A	213	LEU
1	A	243	PRO
1	A	421	ASP
1	A	498	LEU

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Mol	Chain	Res	Type
1	A	742	GLY
2	B	42	LEU
2	B	81	PRO
2	B	141	PHE
2	B	189	ALA
2	B	273	VAL
2	B	335	GLY
2	B	362	ALA
2	B	470	THR
2	B	558	PRO
2	B	592	PHE
3	C	23	THR
3	C	52	LYS
4	D	88	GLY
4	D	175	GLU
4	D	184	VAL
6	F	102	LEU
6	F	103	GLN
6	F	121	ALA
6	F	186	ARG
8	H	98	LEU
10	J	9	SER
10	J	23	ALA
10	J	39	PHE
12	L	193	GLY
13	N	110	THR
13	N	132	THR
13	N	142	LYS
13	N	159	LYS
15	1	224	PRO
16	2	168	TRP
17	3	112	GLY
18	4	173	LYS
18	4	201	LYS
18	4	228	PRO
18	4	230	ASP
1	A	67	HIS
1	A	186	TYR
1	A	234	ASN
1	A	259	TYR
1	A	306	ILE
1	A	404	GLY

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Mol	Chain	Res	Type
1	A	574	ASN
1	A	701	GLN
2	B	41	ARG
2	B	43	TYR
2	B	69	ALA
2	B	164	SER
2	B	281	ALA
2	B	309	ILE
2	B	474	PHE
2	B	476	ILE
2	B	593	TYR
2	B	595	HIS
6	F	97	GLN
6	F	115	PRO
6	F	123	MET
6	F	160	PHE
8	H	69	GLY
8	H	117	SER
9	I	2	ILE
9	I	5	PRO
9	I	9	VAL
12	L	56	VAL
12	L	57	ILE
12	L	59	PRO
12	L	131	SER
12	L	159	SER
12	L	181	GLY
15	1	220	HIS
16	2	203	PRO
17	3	140	GLY
17	3	156	THR
17	3	248	THR
1	A	151	GLN
1	A	179	LEU
1	A	230	ASN
1	A	472	ARG
1	A	580	PRO
1	A	718	PRO
2	B	172	GLU
2	B	265	THR
2	B	278	LEU
2	B	311	PRO

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Mol	Chain	Res	Type
2	B	391	PRO
2	B	398	TYR
2	B	457	PRO
2	B	514	PRO
2	B	596	TRP
2	B	623	TYR
2	B	730	SER
3	C	55	GLU
3	C	58	CYS
4	D	202	PHE
7	G	90	GLN
7	G	149	TYR
8	H	120	ILE
11	K	48	PHE
11	K	80	ALA
12	L	55	GLN
12	L	175	GLN
15	1	119	GLY
16	2	95	ASP
16	2	206	TRP
17	3	202	TYR
17	3	230	ASN
17	3	234	ALA
18	4	179	ALA
18	4	223	VAL
18	4	243	THR
1	A	36	LYS
1	A	130	GLU
1	A	225	VAL
1	A	289	PRO
1	A	542	HIS
1	A	721	GLN
2	B	598	HIS
3	C	71	HIS
6	F	214	PRO
16	2	135	PRO
18	4	195	ALA
1	A	223	VAL
1	A	584	PRO
2	B	557	PHE
2	B	711	VAL
2	B	716	GLY

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Mol	Chain	Res	Type
3	C	22	PRO
4	D	89	GLY
15	1	223	ASP
1	A	112	ASP
1	A	125	PRO
1	A	229	ILE
1	A	754	ILE
2	B	708	VAL
12	L	192	GLY
16	2	196	PRO
17	3	245	GLY
2	B	219	PRO
12	L	107	GLY
12	L	118	GLY
12	L	158	PRO
1	A	124	TRP
1	A	190	ALA
6	F	215	VAL
7	G	78	VAL
9	I	12	VAL
12	L	99	GLY
13	N	166	VAL
16	2	130	GLY
18	4	163	PRO
9	I	10	PRO
12	L	62	GLY
12	L	115	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	590/599 (98%)	475 (80%)	115 (20%)	2	7
2	B	597/599 (100%)	468 (78%)	129 (22%)	1	5
3	C	70/70 (100%)	60 (86%)	10 (14%)	4	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	117/117 (100%)	83 (71%)	34 (29%)	0	1
5	E	56/56 (100%)	42 (75%)	14 (25%)	1	3
6	F	127/127 (100%)	91 (72%)	36 (28%)	0	2
7	G	78/79 (99%)	60 (77%)	18 (23%)	1	4
8	H	55/55 (100%)	42 (76%)	13 (24%)	1	3
9	I	26/26 (100%)	23 (88%)	3 (12%)	7	29
10	J	35/36 (97%)	26 (74%)	9 (26%)	0	2
11	K	62/62 (100%)	45 (73%)	17 (27%)	0	2
12	L	127/127 (100%)	105 (83%)	22 (17%)	2	11
13	N	74/74 (100%)	49 (66%)	25 (34%)	0	1
15	1	126/134 (94%)	76 (60%)	50 (40%)	0	0
16	2	139/142 (98%)	91 (66%)	48 (34%)	0	1
17	3	113/129 (88%)	74 (66%)	39 (34%)	0	1
18	4	136/140 (97%)	107 (79%)	29 (21%)	1	5
All	All	2528/2572 (98%)	1917 (76%)	611 (24%)	1	3

All (611) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASP
1	A	24	ARG
1	A	25	ASP
1	A	31	PHE
1	A	34	TRP
1	A	39	HIS
1	A	55	TRP
1	A	57	LEU
1	A	60	ASP
1	A	62	HIS
1	A	63	ASP
1	A	68	THR
1	A	78	VAL
1	A	93	LEU
1	A	103	PHE
1	A	104	SER
1	A	105	ASN
1	A	110	LEU

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Mol	Chain	Res	Type
1	A	124	TRP
1	A	129	GLN
1	A	132	LEU
1	A	153	TRP
1	A	159	THR
1	A	160	SER
1	A	172	LEU
1	A	180	PHE
1	A	187	HIS
1	A	188	LYS
1	A	195	TRP
1	A	196	PHE
1	A	224	HIS
1	A	232	PHE
1	A	233	LEU
1	A	246	HIS
1	A	248	PHE
1	A	250	LEU
1	A	252	ARG
1	A	254	LEU
1	A	255	LEU
1	A	270	PHE
1	A	277	TYR
1	A	284	ARG
1	A	296	LEU
1	A	297	THR
1	A	298	ASP
1	A	317	TYR
1	A	328	LYS
1	A	331	LEU
1	A	334	HIS
1	A	338	PHE
1	A	341	GLN
1	A	350	LEU
1	A	351	THR
1	A	353	SER
1	A	357	GLN
1	A	368	LEU
1	A	369	THR
1	A	375	HIS
1	A	377	TYR
1	A	384	TYR

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Mol	Chain	Res	Type
1	A	392	GLN
1	A	393	LEU
1	A	400	MET
1	A	402	ILE
1	A	405	PHE
1	A	408	VAL
1	A	420	ARG
1	A	421	ASP
1	A	422	TYR
1	A	426	THR
1	A	427	ARG
1	A	433	ASP
1	A	434	ARG
1	A	435	VAL
1	A	438	HIS
1	A	439	ARG
1	A	444	SER
1	A	462	ILE
1	A	464	ASN
1	A	477	PHE
1	A	484	LEU
1	A	485	GLN
1	A	488	PHE
1	A	490	GLN
1	A	498	LEU
1	A	519	ASP
1	A	523	VAL
1	A	538	ASP
1	A	539	PHE
1	A	553	VAL
1	A	558	LYS
1	A	561	LEU
1	A	564	ARG
1	A	577	PHE
1	A	578	ARG
1	A	579	PHE
1	A	590	CYS
1	A	591	GLN
1	A	605	MET
1	A	637	ILE
1	A	642	PHE
1	A	646	SER

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Mol	Chain	Res	Type
1	A	654	ARG
1	A	660	GLN
1	A	662	SER
1	A	684	PHE
1	A	689	SER
1	A	691	MET
1	A	697	ARG
1	A	707	ILE
1	A	715	LYS
1	A	723	ARG
1	A	726	SER
1	A	727	ILE
1	A	754	ILE
2	B	4	ARG
2	B	6	PRO
2	B	7	ARG
2	B	8	PHE
2	B	10	GLN
2	B	12	ILE
2	B	19	ARG
2	B	20	ARG
2	B	46	ILE
2	B	50	HIS
2	B	51	PHE
2	B	67	HIS
2	B	70	TRP
2	B	73	ASN
2	B	78	VAL
2	B	83	HIS
2	B	85	ARG
2	B	87	ILE
2	B	96	PHE
2	B	98	GLN
2	B	106	ARG
2	B	113	VAL
2	B	115	ASN
2	B	121	TYR
2	B	123	TRP
2	B	124	TRP
2	B	129	LEU
2	B	130	ARG
2	B	131	THR

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Mol	Chain	Res	Type
2	B	135	LEU
2	B	144	PHE
2	B	154	TRP
2	B	158	GLN
2	B	160	LYS
2	B	161	TRP
2	B	165	VAL
2	B	177	HIS
2	B	178	HIS
2	B	188	LEU
2	B	195	VAL
2	B	206	TYR
2	B	212	PHE
2	B	229	GLN
2	B	233	TYR
2	B	241	ASN
2	B	244	PHE
2	B	247	THR
2	B	248	GLN
2	B	262	HIS
2	B	267	SER
2	B	269	TRP
2	B	285	LEU
2	B	291	TYR
2	B	292	ARG
2	B	295	PHE
2	B	299	HIS
2	B	317	ARG
2	B	319	HIS
2	B	320	LYS
2	B	332	PHE
2	B	347	LEU
2	B	348	VAL
2	B	350	GLN
2	B	353	TYR
2	B	361	ILE
2	B	365	PHE
2	B	367	THR
2	B	374	HIS
2	B	382	ILE
2	B	393	PHE
2	B	395	ILE

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Mol	Chain	Res	Type
2	B	396	ARG
2	B	410	ARG
2	B	420	SER
2	B	422	LEU
2	B	428	PHE
2	B	437	TYR
2	B	438	VAL
2	B	440	ASN
2	B	443	MET
2	B	448	THR
2	B	451	LYS
2	B	455	ILE
2	B	464	GLN
2	B	469	LYS
2	B	472	TYR
2	B	474	PHE
2	B	490	ARG
2	B	492	ILE
2	B	497	TRP
2	B	509	PHE
2	B	516	ASP
2	B	521	HIS
2	B	528	HIS
2	B	542	ARG
2	B	545	LYS
2	B	555	TYR
2	B	564	ARG
2	B	577	TYR
2	B	580	VAL
2	B	583	MET
2	B	587	ILE
2	B	592	PHE
2	B	594	TRP
2	B	596	TRP
2	B	608	GLN
2	B	613	SER
2	B	614	THR
2	B	615	TYR
2	B	617	MET
2	B	620	LEU
2	B	622	ASP
2	B	629	SER

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Mol	Chain	Res	Type
2	B	630	GLN
2	B	662	MET
2	B	670	TYR
2	B	677	THR
2	B	682	HIS
2	B	685	THR
2	B	690	LEU
2	B	692	ARG
2	B	694	ARG
2	B	696	LYS
2	B	701	SER
2	B	710	LEU
2	B	712	HIS
2	B	719	PHE
2	B	732	LYS
2	B	733	PHE
3	C	18	VAL
3	C	24	ASP
3	C	28	MET
3	C	38	GLN
3	C	45	THR
3	C	48	CYS
3	C	52	LYS
3	C	58	CYS
3	C	66	ARG
3	C	70	TRP
4	D	75	ASP
4	D	78	THR
4	D	80	SER
4	D	82	ILE
4	D	83	PHE
4	D	92	ARG
4	D	95	GLN
4	D	97	GLU
4	D	99	PHE
4	D	100	TYR
4	D	101	VAL
4	D	104	TRP
4	D	105	ASP
4	D	112	PHE
4	D	122	MET
4	D	124	GLU

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Mol	Chain	Res	Type
4	D	130	LYS
4	D	133	ARG
4	D	135	GLU
4	D	140	LEU
4	D	147	LYS
4	D	149	LYS
4	D	152	TYR
4	D	162	GLU
4	D	165	TYR
4	D	169	LYS
4	D	176	LYS
4	D	177	VAL
4	D	187	ASN
4	D	188	PHE
4	D	198	ILE
4	D	200	VAL
4	D	201	LYS
4	D	205	LYS
5	E	66	ILE
5	E	69	LYS
5	E	70	ARG
5	E	77	LEU
5	E	78	ARG
5	E	79	LYS
5	E	83	TRP
5	E	93	VAL
5	E	106	ARG
5	E	111	ASN
5	E	114	ASN
5	E	126	VAL
5	E	128	VAL
5	E	129	GLU
6	F	79	ILE
6	F	86	LYS
6	F	89	LYS
6	F	91	PHE
6	F	94	ARG
6	F	97	GLN
6	F	100	LYS
6	F	103	GLN
6	F	106	LEU
6	F	107	LYS

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Mol	Chain	Res	Type
6	F	125	LYS
6	F	128	LYS
6	F	129	ARG
6	F	131	ASP
6	F	136	TYR
6	F	138	LEU
6	F	151	SER
6	F	154	GLN
6	F	156	HIS
6	F	160	PHE
6	F	165	ILE
6	F	168	LEU
6	F	170	ILE
6	F	173	TRP
6	F	177	VAL
6	F	181	TYR
6	F	183	ILE
6	F	188	GLU
6	F	200	VAL
6	F	207	LEU
6	F	208	PHE
6	F	213	TRP
6	F	218	TYR
6	F	219	ARG
6	F	221	LEU
6	F	231	PHE
7	G	66	LEU
7	G	73	PHE
7	G	76	ARG
7	G	80	PHE
7	G	87	VAL
7	G	89	LYS
7	G	90	GLN
7	G	94	GLN
7	G	95	ASN
7	G	97	LEU
7	G	98	THR
7	G	101	GLU
7	G	104	ASP
7	G	116	SER
7	G	125	VAL
7	G	144	THR

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Mol	Chain	Res	Type
7	G	147	ASN
7	G	149	TYR
8	H	66	ASP
8	H	76	TYR
8	H	79	LEU
8	H	80	GLN
8	H	93	LYS
8	H	94	ARG
8	H	99	LYS
8	H	100	PHE
8	H	109	LEU
8	H	111	TYR
8	H	112	LEU
8	H	113	SER
8	H	119	ASP
9	I	3	ASN
9	I	7	LEU
9	I	11	LEU
10	J	2	ARG
10	J	3	ASP
10	J	5	LYS
10	J	9	SER
10	J	16	THR
10	J	19	PHE
10	J	35	ASP
10	J	37	LEU
10	J	41	PHE
11	K	51	SER
11	K	53	THR
11	K	58	VAL
11	K	59	THR
11	K	63	LEU
11	K	65	LEU
11	K	66	PHE
11	K	70	PHE
11	K	77	ASN
11	K	78	ARG
11	K	89	ARG
11	K	102	THR
11	K	103	LEU
11	K	114	HIS
11	K	122	LEU

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Mol	Chain	Res	Type
11	K	125	LYS
11	K	130	LEU
12	L	51	LYS
12	L	54	TYR
12	L	86	LEU
12	L	96	LEU
12	L	114	PHE
12	L	116	LYS
12	L	122	ASN
12	L	128	GLN
12	L	141	LEU
12	L	142	SER
12	L	145	LEU
12	L	151	SER
12	L	153	PHE
12	L	155	GLU
12	L	171	LYS
12	L	172	GLU
12	L	182	TRP
12	L	186	THR
12	L	191	PHE
12	L	201	TYR
12	L	205	TYR
12	L	211	TYR
13	N	90	GLU
13	N	91	TYR
13	N	94	LYS
13	N	96	LYS
13	N	104	LYS
13	N	105	LYS
13	N	106	ARG
13	N	110	THR
13	N	114	PHE
13	N	118	TYR
13	N	122	PHE
13	N	126	LYS
13	N	127	PHE
13	N	135	GLN
13	N	139	LYS
13	N	142	LYS
13	N	145	PHE
13	N	150	LEU

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Mol	Chain	Res	Type
13	N	157	LYS
13	N	160	TYR
13	N	161	LYS
13	N	162	CYS
13	N	167	PHE
13	N	168	TRP
13	N	170	TRP
15	1	62	PHE
15	1	71	GLU
15	1	76	LEU
15	1	77	GLU
15	1	81	GLU
15	1	86	HIS
15	1	87	CYS
15	1	91	MET
15	1	92	LEU
15	1	94	VAL
15	1	97	ILE
15	1	98	LEU
15	1	101	GLU
15	1	103	LEU
15	1	117	LEU
15	1	124	TYR
15	1	125	LEU
15	1	131	TRP
15	1	133	THR
15	1	136	THR
15	1	137	ILE
15	1	138	LEU
15	1	141	GLU
15	1	145	ILE
15	1	147	PHE
15	1	149	GLU
15	1	150	HIS
15	1	151	GLN
15	1	155	GLU
15	1	161	LYS
15	1	163	TYR
15	1	168	PHE
15	1	169	ASP
15	1	170	PRO
15	1	171	LEU

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Mol	Chain	Res	Type
15	1	173	TYR
15	1	175	LYS
15	1	178	LYS
15	1	181	GLU
15	1	189	LYS
15	1	193	LEU
15	1	198	PHE
15	1	199	VAL
15	1	203	VAL
15	1	205	GLN
15	1	206	SER
15	1	211	THR
15	1	214	LEU
15	1	225	TRP
15	1	226	HIS
16	2	99	LEU
16	2	101	TRP
16	2	104	GLN
16	2	114	MET
16	2	121	PHE
16	2	128	LYS
16	2	133	ASN
16	2	138	TYR
16	2	139	THR
16	2	144	GLU
16	2	145	TYR
16	2	150	THR
16	2	152	LEU
16	2	154	ILE
16	2	156	GLU
16	2	157	LEU
16	2	159	PHE
16	2	167	ARG
16	2	168	TRP
16	2	173	ASN
16	2	183	PHE
16	2	185	ASN
16	2	187	LYS
16	2	188	LEU
16	2	189	THR
16	2	192	ASP
16	2	195	TYR

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Mol	Chain	Res	Type
16	2	200	TRP
16	2	201	PHE
16	2	202	ASP
16	2	215	LYS
16	2	217	LEU
16	2	219	THR
16	2	220	LYS
16	2	222	ILE
16	2	226	ARG
16	2	229	MET
16	2	230	LEU
16	2	232	VAL
16	2	237	PHE
16	2	241	TYR
16	2	242	THR
16	2	244	THR
16	2	251	PHE
16	2	254	LEU
16	2	256	ASP
16	2	259	HIS
16	2	269	LYS
17	3	87	GLU
17	3	92	PHE
17	3	93	ILE
17	3	94	GLU
17	3	96	ARG
17	3	97	TRP
17	3	107	ARG
17	3	108	PHE
17	3	111	LEU
17	3	124	LYS
17	3	134	LEU
17	3	136	TRP
17	3	137	PHE
17	3	138	GLN
17	3	151	TRP
17	3	153	ASP
17	3	155	TYR
17	3	156	THR
17	3	158	PHE
17	3	161	GLU
17	3	165	MET

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Mol	Chain	Res	Type
17	3	167	PHE
17	3	173	PHE
17	3	174	GLN
17	3	175	ASP
17	3	181	SER
17	3	185	GLN
17	3	187	PHE
17	3	192	LYS
17	3	202	TYR
17	3	207	PHE
17	3	208	PHE
17	3	209	ASN
17	3	215	LYS
17	3	229	LYS
17	3	232	ARG
17	3	235	MET
17	3	242	PHE
17	3	253	TYR
18	4	86	GLU
18	4	89	ARG
18	4	90	TRP
18	4	95	GLU
18	4	96	LEU
18	4	101	TRP
18	4	115	PHE
18	4	118	ILE
18	4	131	LYS
18	4	139	SER
18	4	141	LEU
18	4	143	VAL
18	4	146	PHE
18	4	151	TYR
18	4	157	TRP
18	4	161	LYS
18	4	165	SER
18	4	172	PHE
18	4	175	TYR
18	4	177	LEU
18	4	192	LEU
18	4	201	LYS
18	4	214	PHE
18	4	226	LYS

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Mol	Chain	Res	Type
18	4	234	GLN
18	4	238	ASP
18	4	240	TRP
18	4	241	HIS
18	4	245	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
1	A	82	HIS
1	A	115	HIS
1	A	129	GLN
1	A	163	GLN
1	A	224	HIS
1	A	303	HIS
1	A	341	GLN
1	A	398	HIS
1	A	464	ASN
1	A	485	GLN
1	A	493	GLN
1	A	525	ASN
1	A	542	HIS
1	A	545	HIS
1	A	591	GLN
1	A	607	ASN
1	A	636	HIS
1	A	644	GLN
1	A	660	GLN
1	A	683	HIS
1	A	711	HIS
1	A	729	GLN
2	B	10	GLN
2	B	50	HIS
2	B	53	GLN
2	B	67	HIS
2	B	73	ASN
2	B	98	GLN
2	B	158	GLN
2	B	178	HIS
2	B	193	HIS
2	B	231	ASN

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Mol	Chain	Res	Type
2	B	277	HIS
2	B	294	ASN
2	B	319	HIS
2	B	331	HIS
2	B	333	GLN
2	B	375	HIS
2	B	403	ASN
2	B	432	HIS
2	B	452	GLN
2	B	464	GLN
2	B	502	ASN
2	B	521	HIS
2	B	528	HIS
2	B	595	HIS
2	B	610	ASN
2	B	633	ASN
2	B	712	HIS
3	C	71	HIS
4	D	95	GLN
4	D	110	GLN
4	D	136	GLN
4	D	182	GLN
4	D	187	ASN
4	D	206	GLN
5	E	111	ASN
6	F	97	GLN
6	F	193	GLN
8	H	77	ASN
8	H	80	GLN
11	K	77	ASN
11	K	114	HIS
12	L	85	ASN
12	L	122	ASN
13	N	113	ASN
13	N	130	ASN
15	1	86	HIS
15	1	112	GLN
15	1	151	GLN
15	1	190	ASN
15	1	204	GLN
15	1	205	GLN
15	1	226	HIS

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Mol	Chain	Res	Type
16	2	133	ASN
16	2	173	ASN
16	2	238	GLN
17	3	149	ASN
17	3	174	GLN
17	3	209	ASN
17	3	254	GLN
18	4	158	GLN
18	4	190	ASN
18	4	246	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

252 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
19	CLA	1	1001	-	36,54,73	2.57	13 (36%)	41,90,113	5.06	22 (53%)
19	CLA	1	1002	-	37,55,73	2.37	10 (27%)	42,91,113	4.01	19 (45%)
19	CLA	1	1003	-	37,55,73	2.36	10 (27%)	42,91,113	5.21	19 (45%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	1	1005	-	36,54,73	2.80	11 (30%)	41,90,113	4.64	16 (39%)
19	CLA	1	1006	-	24,44,73	2.93	8 (33%)	28,78,113	4.61	13 (46%)
19	CLA	1	1007	-	51,69,73	2.11	10 (19%)	56,108,113	3.86	17 (30%)
19	CLA	1	1008	-	41,59,73	2.43	14 (34%)	44,96,113	4.94	20 (45%)
19	CLA	1	1010	-	36,54,73	2.46	12 (33%)	41,90,113	5.24	20 (48%)
19	CLA	1	1011	-	24,44,73	2.90	9 (37%)	28,78,113	5.29	14 (50%)
19	CLA	1	1012	-	24,44,73	2.74	8 (33%)	28,78,113	4.32	12 (42%)
19	CLA	1	1013	-	41,59,73	2.67	16 (39%)	44,96,113	4.85	20 (45%)
19	CLA	1	1014	-	51,69,73	2.12	11 (21%)	56,108,113	4.06	15 (26%)
19	CLA	1	1015	-	16,32,73	1.75	4 (25%)	21,54,113	3.13	11 (52%)
19	CLA	1	1303	-	41,59,73	2.47	13 (31%)	44,96,113	5.78	18 (40%)
19	CLA	1	1310	-	16,32,73	1.71	2 (12%)	21,54,113	3.48	12 (57%)
21	BCR	1	6023	-	41,41,41	1.72	3 (7%)	56,56,56	6.27	31 (55%)
22	LMU	1	7004	-	36,36,36	0.64	1 (2%)	47,47,47	0.85	1 (2%)
22	LMU	1	7013	-	36,36,36	0.69	0	47,47,47	1.06	1 (2%)
19	CLA	2	1307	-	16,32,73	1.76	3 (18%)	21,54,113	3.26	11 (52%)
19	CLA	2	2001	-	41,59,73	2.26	10 (24%)	44,96,113	4.63	17 (38%)
19	CLA	2	2002	-	46,64,73	2.18	11 (23%)	50,102,113	4.27	20 (40%)
19	CLA	2	2003	-	16,32,73	1.73	3 (18%)	21,54,113	3.13	11 (52%)
19	CLA	2	2004	-	40,58,73	2.25	10 (25%)	44,95,113	4.64	16 (36%)
19	CLA	2	2005	-	16,32,73	1.72	3 (18%)	21,54,113	3.21	11 (52%)
19	CLA	2	2006	-	55,73,73	2.02	11 (20%)	61,113,113	4.28	15 (24%)
19	CLA	2	2007	-	55,73,73	1.97	10 (18%)	61,113,113	3.70	19 (31%)
19	CLA	2	2008	-	16,32,73	1.69	3 (18%)	21,54,113	3.13	11 (52%)
19	CLA	2	2010	-	16,32,73	1.75	4 (25%)	21,54,113	2.85	8 (38%)
19	CLA	2	2011	-	16,32,73	1.73	3 (18%)	21,54,113	3.19	12 (57%)
19	CLA	2	2012	16	40,58,73	2.30	9 (22%)	44,95,113	4.11	18 (40%)
19	CLA	2	2013	-	40,58,73	2.31	10 (25%)	44,95,113	4.91	18 (40%)
19	CLA	2	2014	-	51,69,73	1.99	11 (21%)	56,108,113	4.35	21 (37%)
19	CLA	2	4009	-	55,73,73	1.98	11 (20%)	61,113,113	4.47	20 (32%)
22	LMU	2	7006	-	36,36,36	0.62	0	47,47,47	0.76	0
22	LMU	2	7027	-	36,36,36	0.79	1 (2%)	47,47,47	1.76	11 (23%)
22	LMU	2	7031	-	36,36,36	1.19	2 (5%)	47,47,47	1.42	6 (12%)
22	LMU	2	7046	-	36,36,36	0.69	1 (2%)	47,47,47	0.90	3 (6%)
19	CLA	3	1118	-	24,44,73	2.78	8 (33%)	28,78,113	4.68	13 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	3	1147	-	36,54,73	2.50	12 (33%)	41,90,113	5.07	23 (56%)
19	CLA	3	2009	-	46,64,73	2.23	13 (28%)	50,102,113	4.62	19 (38%)
19	CLA	3	3001	-	16,32,73	1.83	4 (25%)	21,54,113	3.27	12 (57%)
19	CLA	3	3002	-	16,32,73	1.77	3 (18%)	21,54,113	2.94	11 (52%)
19	CLA	3	3003	-	24,44,73	2.73	8 (33%)	28,78,113	4.21	13 (46%)
19	CLA	3	3004	-	16,32,73	1.75	5 (31%)	21,54,113	3.14	11 (52%)
19	CLA	3	3005	-	16,32,73	1.79	3 (18%)	21,54,113	3.18	12 (57%)
19	CLA	3	3006	-	16,32,73	1.83	5 (31%)	21,54,113	3.23	12 (57%)
19	CLA	3	3007	-	32,50,73	2.36	8 (25%)	36,85,113	5.51	17 (47%)
19	CLA	3	3008	-	40,58,73	2.28	11 (27%)	44,95,113	5.19	18 (40%)
19	CLA	3	3010	-	16,32,73	1.60	3 (18%)	21,54,113	3.04	11 (52%)
19	CLA	3	3011	-	55,73,73	1.91	10 (18%)	61,113,113	3.96	19 (31%)
19	CLA	3	3012	-	16,32,73	1.82	4 (25%)	21,54,113	3.43	12 (57%)
19	CLA	3	3013	-	55,73,73	2.04	12 (21%)	61,113,113	4.68	17 (27%)
19	CLA	3	3014	-	16,32,73	1.77	4 (25%)	21,54,113	3.49	12 (57%)
19	CLA	3	3015	-	16,32,73	1.76	4 (25%)	21,54,113	2.93	11 (52%)
19	CLA	3	3016	-	55,73,73	1.97	10 (18%)	61,113,113	4.11	20 (32%)
19	CLA	3	3017	-	40,58,73	2.27	10 (25%)	44,95,113	4.76	23 (52%)
21	BCR	3	6022	-	41,41,41	1.33	4 (9%)	56,56,56	4.91	26 (46%)
22	LMU	3	7003	-	36,36,36	0.78	0	47,47,47	1.48	7 (14%)
22	LMU	3	7005	-	36,36,36	0.70	0	47,47,47	2.17	14 (29%)
19	CLA	4	1004	-	45,63,73	2.30	15 (33%)	49,101,113	4.82	19 (38%)
19	CLA	4	1009	-	24,44,73	2.88	9 (37%)	28,78,113	4.66	14 (50%)
19	CLA	4	1304	-	55,73,73	2.07	11 (20%)	61,113,113	4.34	22 (36%)
19	CLA	4	1306	-	45,63,73	2.17	9 (20%)	49,101,113	4.17	17 (34%)
19	CLA	4	4001	-	40,58,73	2.37	10 (25%)	44,95,113	4.83	15 (34%)
19	CLA	4	4002	18	42,60,73	2.32	14 (33%)	45,97,113	5.27	26 (57%)
19	CLA	4	4003	-	45,63,73	2.21	10 (22%)	49,101,113	4.36	18 (36%)
19	CLA	4	4004	-	16,32,73	1.78	3 (18%)	21,54,113	3.31	12 (57%)
19	CLA	4	4005	-	16,32,73	1.81	4 (25%)	21,54,113	3.14	11 (52%)
19	CLA	4	4006	-	45,63,73	2.22	9 (20%)	49,101,113	4.27	17 (34%)
19	CLA	4	4007	-	42,60,73	2.29	10 (23%)	45,97,113	4.11	20 (44%)
19	CLA	4	4010	-	16,32,73	1.72	3 (18%)	21,54,113	3.11	11 (52%)
19	CLA	4	4011	-	16,32,73	1.69	3 (18%)	21,54,113	3.21	12 (57%)
19	CLA	4	4012	-	24,44,73	2.74	7 (29%)	28,78,113	5.01	15 (53%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	4	4013	18	16,32,73	1.70	4 (25%)	21,54,113	2.71	11 (52%)
19	CLA	4	4014	-	37,55,73	2.26	12 (32%)	42,91,113	5.52	19 (45%)
19	CLA	4	4015	-	36,54,73	2.41	12 (33%)	41,90,113	5.01	14 (34%)
22	LMU	4	7008	-	36,36,36	0.56	0	47,47,47	0.92	2 (4%)
22	LMU	4	7009	-	35,35,36	1.31	2 (5%)	46,46,47	1.34	3 (6%)
22	LMU	4	7018	-	36,36,36	0.72	1 (2%)	47,47,47	1.13	3 (6%)
22	LMU	4	7019	-	36,36,36	0.79	1 (2%)	47,47,47	1.40	9 (19%)
22	LMU	4	7033	-	36,36,36	0.73	0	47,47,47	1.60	9 (19%)
22	LMU	4	7034	-	36,36,36	0.60	0	47,47,47	0.74	0
22	LMU	4	7052	-	36,36,36	1.20	4 (11%)	47,47,47	1.92	8 (17%)
22	LMU	4	7053	-	35,35,36	0.68	1 (2%)	46,46,47	1.31	6 (13%)
19	CLA	A	1101	-	40,58,73	2.30	11 (27%)	44,95,113	4.46	19 (43%)
19	CLA	A	1102	19	45,63,73	2.22	11 (24%)	49,101,113	3.77	19 (38%)
19	CLA	A	1103	-	55,73,73	2.00	12 (21%)	61,113,113	3.83	18 (29%)
19	CLA	A	1104	-	47,65,73	2.10	10 (21%)	50,103,113	4.57	19 (38%)
19	CLA	A	1105	-	36,54,73	2.31	10 (27%)	41,90,113	5.55	18 (43%)
19	CLA	A	1106	-	55,73,73	1.93	12 (21%)	61,113,113	3.30	19 (31%)
19	CLA	A	1107	-	45,63,73	2.10	10 (22%)	49,101,113	3.94	21 (42%)
19	CLA	A	1108	-	32,53,73	2.43	9 (28%)	37,89,113	4.44	17 (45%)
19	CLA	A	1109	19	55,73,73	2.00	11 (20%)	61,113,113	3.65	21 (34%)
19	CLA	A	1110	-	44,62,73	2.19	10 (22%)	47,99,113	4.12	16 (34%)
19	CLA	A	1111	-	44,62,73	2.12	10 (22%)	47,99,113	4.35	17 (36%)
19	CLA	A	1112	-	32,53,73	2.51	10 (31%)	37,89,113	4.70	15 (40%)
19	CLA	A	1113	-	40,58,73	2.37	10 (25%)	44,95,113	4.57	18 (40%)
19	CLA	A	1115	-	55,73,73	1.97	11 (20%)	61,113,113	4.09	19 (31%)
19	CLA	A	1116	-	42,60,73	2.33	11 (26%)	45,97,113	4.95	16 (35%)
19	CLA	A	1117	-	55,73,73	1.99	11 (20%)	61,113,113	3.63	19 (31%)
19	CLA	A	1119	-	55,73,73	1.99	11 (20%)	61,113,113	4.13	18 (29%)
19	CLA	A	1120	-	41,59,73	2.29	11 (26%)	44,96,113	4.66	18 (40%)
19	CLA	A	1121	1	32,50,73	2.49	10 (31%)	36,85,113	5.14	15 (41%)
19	CLA	A	1122	-	45,63,73	2.20	11 (24%)	49,101,113	4.54	18 (36%)
19	CLA	A	1123	-	55,73,73	1.88	11 (20%)	61,113,113	3.52	19 (31%)
19	CLA	A	1124	-	55,73,73	1.95	11 (20%)	61,113,113	3.94	18 (29%)
19	CLA	A	1125	-	55,73,73	1.95	11 (20%)	61,113,113	3.68	16 (26%)
19	CLA	A	1126	-	55,73,73	1.97	10 (18%)	61,113,113	3.95	17 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	A	1127	-	45,63,73	2.20	11 (24%)	49,101,113	4.23	17 (34%)
19	CLA	A	1128	-	55,73,73	1.97	12 (21%)	61,113,113	3.50	21 (34%)
19	CLA	A	1129	-	40,58,73	2.26	11 (27%)	44,95,113	4.97	21 (47%)
19	CLA	A	1131	-	55,73,73	1.97	11 (20%)	61,113,113	4.14	17 (27%)
19	CLA	A	1132	-	55,73,73	1.96	11 (20%)	61,113,113	4.21	22 (36%)
19	CLA	A	1133	-	40,58,73	2.27	11 (27%)	44,95,113	4.74	17 (38%)
19	CLA	A	1134	1	32,53,73	2.40	10 (31%)	37,89,113	5.53	16 (43%)
19	CLA	A	1135	-	41,59,73	2.29	10 (24%)	44,96,113	4.58	18 (40%)
19	CLA	A	1136	-	55,73,73	1.94	11 (20%)	61,113,113	4.24	18 (29%)
19	CLA	A	1137	-	37,55,73	2.38	12 (32%)	42,91,113	5.12	16 (38%)
19	CLA	A	1138	-	55,73,73	1.98	10 (18%)	61,113,113	4.15	18 (29%)
19	CLA	A	1139	-	41,59,73	2.30	10 (24%)	44,96,113	4.81	18 (40%)
19	CLA	A	1140	-	55,73,73	1.93	10 (18%)	61,113,113	4.16	17 (27%)
19	CLA	A	1141	-	55,73,73	1.97	10 (18%)	61,113,113	4.21	19 (31%)
19	CLA	A	1149	-	36,54,73	2.74	12 (33%)	42,90,113	4.74	26 (61%)
19	CLA	A	1151	-	40,58,73	2.31	10 (25%)	44,95,113	4.74	17 (38%)
19	CLA	A	1237	-	55,73,73	1.96	11 (20%)	61,113,113	4.39	17 (27%)
19	CLA	A	1309	-	16,32,73	1.74	4 (25%)	21,54,113	2.97	11 (52%)
20	PQN	A	5001	-	34,34,34	1.51	2 (5%)	44,45,45	1.34	6 (13%)
21	BCR	A	6002	-	41,41,41	1.83	5 (12%)	56,56,56	4.63	34 (60%)
21	BCR	A	6003	-	41,41,41	1.47	3 (7%)	56,56,56	4.11	29 (51%)
21	BCR	A	6007	-	41,41,41	1.51	4 (9%)	56,56,56	3.83	32 (57%)
21	BCR	A	6008	-	41,41,41	1.35	4 (9%)	56,56,56	4.09	27 (48%)
21	BCR	A	6011	-	41,41,41	1.33	5 (12%)	56,56,56	4.19	31 (55%)
22	LMU	A	7010	-	36,36,36	1.25	2 (5%)	47,47,47	1.27	5 (10%)
22	LMU	A	7016	-	36,36,36	0.66	0	47,47,47	1.49	6 (12%)
22	LMU	A	7023	-	36,36,36	0.58	0	47,47,47	1.25	4 (8%)
22	LMU	A	7035	-	36,36,36	0.59	0	47,47,47	1.61	10 (21%)
22	LMU	A	7044	-	36,36,36	0.84	1 (2%)	47,47,47	1.71	9 (19%)
22	LMU	A	7045	-	36,36,36	0.73	1 (2%)	47,47,47	1.56	8 (17%)
24	SF4	A	8001	1,2	0,12,12	0.00	-	0,24,24	0.00	-
19	CLA	A	9011	-	55,73,73	2.01	11 (20%)	61,113,113	4.02	19 (31%)
19	CLA	A	9012	-	55,73,73	2.01	12 (21%)	61,113,113	4.13	20 (32%)
19	CLA	A	9013	-	55,73,73	2.09	11 (20%)	61,113,113	4.29	17 (27%)
19	CLA	A	9022	-	55,73,73	2.00	11 (20%)	61,113,113	4.10	20 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	A	9023	-	55,73,73	2.03	10 (18%)	61,113,113	3.95	17 (27%)
19	CLA	B	1201	-	32,53,73	2.42	10 (31%)	37,89,113	4.68	15 (40%)
19	CLA	B	1202	-	55,73,73	1.98	10 (18%)	61,113,113	4.36	20 (32%)
19	CLA	B	1203	-	55,73,73	1.98	11 (20%)	61,113,113	4.27	25 (40%)
19	CLA	B	1205	-	55,73,73	2.03	11 (20%)	61,113,113	4.23	18 (29%)
19	CLA	B	1206	2	55,73,73	1.89	11 (20%)	61,113,113	3.90	18 (29%)
19	CLA	B	1208	-	44,62,73	2.44	10 (22%)	49,100,113	3.22	18 (36%)
19	CLA	B	1209	-	45,63,73	2.11	11 (24%)	49,101,113	4.10	19 (38%)
19	CLA	B	1210	-	55,73,73	2.00	10 (18%)	61,113,113	4.00	19 (31%)
19	CLA	B	1211	-	55,73,73	2.04	11 (20%)	61,113,113	3.58	17 (27%)
19	CLA	B	1212	-	50,68,73	2.03	10 (20%)	55,107,113	3.93	18 (32%)
19	CLA	B	1213	-	36,54,73	2.42	10 (27%)	41,90,113	4.42	15 (36%)
19	CLA	B	1214	-	49,67,73	2.12	10 (20%)	53,105,113	3.98	17 (32%)
19	CLA	B	1215	-	50,68,73	2.02	11 (22%)	55,107,113	4.46	19 (34%)
19	CLA	B	1216	-	51,69,73	1.97	11 (21%)	56,108,113	4.54	19 (33%)
19	CLA	B	1217	-	40,58,73	2.25	11 (27%)	44,95,113	4.75	18 (40%)
19	CLA	B	1218	-	36,54,73	2.38	11 (30%)	41,90,113	4.88	14 (34%)
19	CLA	B	1219	-	45,63,73	2.30	10 (22%)	49,101,113	4.75	17 (34%)
19	CLA	B	1220	-	55,73,73	2.12	13 (23%)	61,113,113	4.42	16 (26%)
19	CLA	B	1221	-	44,62,73	2.29	13 (29%)	47,99,113	4.45	20 (42%)
19	CLA	B	1222	-	48,66,73	2.13	12 (25%)	52,104,113	4.58	18 (34%)
19	CLA	B	1223	-	55,73,73	1.95	11 (20%)	61,113,113	3.84	16 (26%)
19	CLA	B	1224	-	55,73,73	2.04	11 (20%)	61,113,113	4.18	19 (31%)
19	CLA	B	1225	-	55,73,73	1.96	12 (21%)	61,113,113	3.85	20 (32%)
19	CLA	B	1226	-	55,73,73	1.90	11 (20%)	61,113,113	3.37	18 (29%)
19	CLA	B	1227	-	40,58,73	2.33	10 (25%)	44,95,113	4.44	17 (38%)
19	CLA	B	1228	-	40,58,73	2.26	11 (27%)	44,95,113	5.03	18 (40%)
19	CLA	B	1229	-	55,73,73	2.05	11 (20%)	61,113,113	4.28	17 (27%)
19	CLA	B	1230	-	40,58,73	2.31	12 (30%)	44,95,113	4.13	18 (40%)
19	CLA	B	1231	19	32,53,73	2.55	9 (28%)	37,89,113	4.73	14 (37%)
19	CLA	B	1232	19	32,53,73	2.46	10 (31%)	37,89,113	5.31	15 (40%)
19	CLA	B	1233	-	41,59,73	2.38	9 (21%)	44,96,113	4.92	17 (38%)
19	CLA	B	1234	-	50,68,73	2.06	11 (22%)	55,107,113	4.49	14 (25%)
19	CLA	B	1235	-	55,73,73	1.88	10 (18%)	61,113,113	3.40	17 (27%)
19	CLA	B	1236	-	37,55,73	2.33	11 (29%)	42,91,113	4.41	17 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	B	1238	-	55,73,73	1.95	10 (18%)	61,113,113	3.72	20 (32%)
19	CLA	B	1239	-	55,73,73	1.90	12 (21%)	61,113,113	3.87	18 (29%)
19	CLA	B	1301	-	24,44,73	2.80	9 (37%)	28,78,113	4.82	16 (57%)
20	PQN	B	5002	-	34,34,34	1.40	2 (5%)	44,45,45	1.44	6 (13%)
21	BCR	B	6004	-	41,41,41	1.25	3 (7%)	56,56,56	4.29	30 (53%)
21	BCR	B	6005	-	41,41,41	1.34	4 (9%)	56,56,56	4.75	31 (55%)
21	BCR	B	6006	-	41,41,41	1.49	6 (14%)	56,56,56	4.50	25 (44%)
21	BCR	B	6010	-	41,41,41	1.36	3 (7%)	56,56,56	4.28	30 (53%)
21	BCR	B	6017	-	41,41,41	1.49	5 (12%)	56,56,56	3.97	26 (46%)
21	BCR	B	6020	-	41,41,41	2.17	10 (24%)	56,56,56	4.43	26 (46%)
22	LMU	B	7012	-	26,26,36	0.76	1 (3%)	37,37,47	1.49	8 (21%)
22	LMU	B	7038	-	36,36,36	0.73	0	47,47,47	1.71	11 (23%)
22	LMU	B	7040	-	36,36,36	0.72	1 (2%)	47,47,47	1.66	11 (23%)
23	LMG	B	7101	-	49,49,55	1.00	3 (6%)	57,57,63	1.02	2 (3%)
19	CLA	B	9010	-	55,73,73	1.92	11 (20%)	61,113,113	3.62	18 (29%)
22	LMU	C	7015	-	36,36,36	0.67	1 (2%)	47,47,47	1.35	6 (12%)
24	SF4	C	8002	3	0,12,12	0.00	-	0,24,24	0.00	-
24	SF4	C	8003	3	0,12,12	0.00	-	0,24,24	0.00	-
22	LMU	D	7050	-	36,36,36	0.60	0	47,47,47	0.85	1 (2%)
22	LMU	E	7037	-	36,36,36	0.71	1 (2%)	47,47,47	1.75	11 (23%)
22	LMU	E	7048	-	36,36,36	0.81	1 (2%)	47,47,47	2.09	10 (21%)
19	CLA	F	1240	-	24,44,73	2.63	8 (33%)	28,78,113	3.65	15 (53%)
19	CLA	F	1302	-	30,49,73	2.52	11 (36%)	34,84,113	5.45	16 (47%)
19	CLA	F	1305	-	43,61,73	2.45	15 (34%)	46,98,113	4.15	20 (43%)
21	BCR	F	6014	-	41,41,41	1.29	6 (14%)	56,56,56	4.83	27 (48%)
21	BCR	F	6016	-	41,41,41	1.61	10 (24%)	56,56,56	3.66	27 (48%)
22	LMU	F	7036	-	35,35,36	0.74	1 (2%)	46,46,47	1.55	6 (13%)
19	CLA	G	1242	-	41,59,73	2.33	9 (21%)	44,96,113	4.76	20 (45%)
22	LMU	G	7026	-	36,36,36	0.86	2 (5%)	47,47,47	1.51	6 (12%)
22	LMU	G	7039	-	36,36,36	0.66	0	47,47,47	1.41	4 (8%)
22	LMU	G	7051	-	36,36,36	0.85	1 (2%)	47,47,47	2.16	12 (25%)
19	CLA	H	1145	-	55,73,73	1.91	10 (18%)	61,113,113	4.39	19 (31%)
19	CLA	H	1207	-	55,73,73	2.00	11 (20%)	61,113,113	4.17	18 (29%)
19	CLA	H	1241	-	45,63,73	2.25	9 (20%)	49,101,113	4.51	19 (38%)
19	CLA	H	1505	-	45,63,73	2.22	11 (24%)	49,101,113	4.67	17 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	LMU	H	7002	-	36,36,36	0.59	0	47,47,47	1.56	7 (14%)
22	LMU	H	7011	-	36,36,36	0.76	2 (5%)	47,47,47	1.95	12 (25%)
22	LMU	H	7017	-	36,36,36	0.71	1 (2%)	47,47,47	1.88	11 (23%)
22	LMU	H	7028	-	36,36,36	0.58	0	47,47,47	1.05	2 (4%)
22	LMU	H	7030	-	36,36,36	0.74	2 (5%)	47,47,47	1.24	5 (10%)
22	LMU	H	7032	-	36,36,36	0.70	1 (2%)	47,47,47	1.47	8 (17%)
22	LMU	H	7043	-	36,36,36	0.81	1 (2%)	47,47,47	1.67	10 (21%)
19	CLA	I	1204	-	50,68,73	2.03	11 (22%)	55,107,113	4.80	14 (25%)
21	BCR	I	6018	-	41,41,41	1.44	4 (9%)	56,56,56	4.73	31 (55%)
21	BCR	I	6021	-	41,41,41	2.01	8 (19%)	56,56,56	4.74	31 (55%)
19	CLA	J	1308	-	45,63,73	2.23	12 (26%)	49,101,113	4.81	20 (40%)
19	CLA	J	1311	-	51,69,73	2.03	11 (21%)	56,108,113	4.49	17 (30%)
21	BCR	J	6012	-	41,41,41	1.44	5 (12%)	56,56,56	5.41	24 (42%)
19	CLA	K	1142	-	32,53,73	2.33	9 (28%)	37,89,113	5.18	14 (37%)
19	CLA	K	1143	-	40,58,73	2.27	10 (25%)	44,95,113	4.51	18 (40%)
19	CLA	K	1146	-	40,58,73	2.36	11 (27%)	44,95,113	4.96	21 (47%)
19	CLA	K	3009	-	55,73,73	2.01	9 (16%)	61,113,113	4.24	18 (29%)
22	LMU	K	7001	-	36,36,36	0.80	2 (5%)	47,47,47	1.44	8 (17%)
22	LMU	K	7041	-	36,36,36	0.55	0	47,47,47	1.07	3 (6%)
22	LMU	K	7042	-	36,36,36	0.61	0	47,47,47	1.18	6 (12%)
22	LMU	K	7047	-	36,36,36	0.77	1 (2%)	47,47,47	1.09	5 (10%)
19	CLA	L	1130	-	55,73,73	2.05	11 (20%)	61,113,113	4.09	19 (31%)
19	CLA	L	1148	-	45,63,73	2.26	14 (31%)	49,101,113	4.70	21 (42%)
19	CLA	L	1501	12	40,58,73	2.31	10 (25%)	44,95,113	5.09	14 (31%)
19	CLA	L	1502	-	37,55,73	2.41	10 (27%)	42,91,113	5.12	19 (45%)
19	CLA	L	1503	-	40,58,73	2.47	14 (35%)	44,95,113	5.56	18 (40%)
19	CLA	L	1504	-	45,63,73	2.26	9 (20%)	49,101,113	4.06	19 (38%)
21	BCR	L	6019	-	41,41,41	1.71	10 (24%)	56,56,56	4.30	25 (44%)
22	LMU	L	7029	-	36,36,36	0.66	1 (2%)	47,47,47	0.77	1 (2%)
22	LMU	N	7049	-	36,36,36	0.56	1 (2%)	47,47,47	1.38	4 (8%)
19	CLA	R	1144	-	47,65,73	2.14	11 (23%)	50,103,113	4.62	17 (34%)
19	CLA	R	1150	-	55,73,73	2.15	11 (20%)	61,113,113	4.05	20 (32%)
22	LMU	R	7007	-	36,36,36	0.56	0	47,47,47	0.86	2 (4%)
22	LMU	R	7014	-	36,36,36	0.89	2 (5%)	47,47,47	2.09	9 (19%)
22	LMU	R	7020	-	36,36,36	0.66	0	47,47,47	1.48	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	LMU	R	7021	-	36,36,36	0.73	0	47,47,47	1.40	4 (8%)
22	LMU	R	7022	-	36,36,36	0.70	0	47,47,47	1.35	6 (12%)
22	LMU	R	7024	-	36,36,36	0.74	1 (2%)	47,47,47	1.53	8 (17%)
22	LMU	R	7025	-	36,36,36	0.74	1 (2%)	47,47,47	1.22	5 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	1	1001	-	3/3/16/25	0/15/113/135	0/0/9/9
19	CLA	1	1002	-	3/3/16/25	0/16/114/135	0/0/9/9
19	CLA	1	1003	-	3/3/16/25	0/16/114/135	0/0/9/9
19	CLA	1	1005	-	3/3/16/25	1/15/113/135	0/0/9/9
19	CLA	1	1006	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	1	1007	-	4/4/19/25	0/33/131/135	0/0/9/9
19	CLA	1	1008	-	4/4/17/25	0/21/119/135	0/0/9/9
19	CLA	1	1010	-	3/3/16/25	0/15/113/135	0/0/9/9
19	CLA	1	1011	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	1	1012	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	1	1013	-	4/4/17/25	1/21/119/135	0/0/9/9
19	CLA	1	1014	-	4/4/19/25	0/33/131/135	0/0/9/9
19	CLA	1	1015	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	1	1303	-	5/5/17/25	0/21/119/135	0/0/9/9
19	CLA	1	1310	-	3/3/7/25	0/0/66/135	0/0/8/9
21	BCR	1	6023	-	-	2/29/63/63	0/2/2/2
22	LMU	1	7004	-	-	0/21/61/61	0/2/2/2
22	LMU	1	7013	-	-	0/21/61/61	0/2/2/2
19	CLA	2	1307	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	2	2001	-	3/3/17/25	0/21/119/135	0/0/9/9
19	CLA	2	2002	-	4/4/18/25	0/27/125/135	0/0/9/9
19	CLA	2	2003	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	2	2004	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	2	2005	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	2	2006	-	4/4/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	2	2007	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	2	2008	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	2	2010	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	2	2011	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	2	2012	16	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	2	2013	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	2	2014	-	4/4/19/25	0/33/131/135	0/0/9/9
19	CLA	2	4009	-	4/4/20/25	0/37/135/135	0/0/9/9
22	LMU	2	7006	-	-	0/21/61/61	0/2/2/2
22	LMU	2	7027	-	-	0/21/61/61	0/2/2/2
22	LMU	2	7031	-	-	0/21/61/61	0/2/2/2
22	LMU	2	7046	-	-	0/21/61/61	0/2/2/2
19	CLA	3	1118	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	3	1147	-	3/3/16/25	0/15/113/135	0/0/9/9
19	CLA	3	2009	-	4/4/18/25	0/27/125/135	0/0/9/9
19	CLA	3	3001	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	3002	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	3003	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	3	3004	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	3005	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	3006	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	3007	-	3/3/15/25	0/10/108/135	0/0/9/9
19	CLA	3	3008	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	3	3010	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	3011	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	3	3012	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	3013	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	3	3014	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	3015	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	3016	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	3	3017	-	3/3/17/25	0/19/117/135	0/0/9/9
21	BCR	3	6022	-	-	1/29/63/63	0/2/2/2
22	LMU	3	7003	-	-	0/21/61/61	0/2/2/2
22	LMU	3	7005	-	-	0/21/61/61	0/2/2/2
19	CLA	4	1004	-	4/4/18/25	0/25/123/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	4	1009	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	4	1304	-	5/5/20/25	0/37/135/135	0/0/9/9
19	CLA	4	1306	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	4	4001	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	4	4002	18	4/4/17/25	0/22/120/135	0/0/9/9
19	CLA	4	4003	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	4	4004	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	4	4005	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	4	4006	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	4	4007	-	3/3/17/25	0/22/120/135	0/0/9/9
19	CLA	4	4010	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	4	4011	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	4	4012	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	4	4013	18	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	4	4014	-	3/3/16/25	0/16/114/135	0/0/9/9
19	CLA	4	4015	-	3/3/16/25	0/15/113/135	0/0/9/9
22	LMU	4	7008	-	-	0/21/61/61	0/2/2/2
22	LMU	4	7009	-	-	0/20/60/61	0/2/2/2
22	LMU	4	7018	-	-	0/21/61/61	0/2/2/2
22	LMU	4	7019	-	-	0/21/61/61	0/2/2/2
22	LMU	4	7033	-	-	0/21/61/61	0/2/2/2
22	LMU	4	7034	-	-	0/21/61/61	0/2/2/2
22	LMU	4	7052	-	-	0/21/61/61	0/2/2/2
22	LMU	4	7053	-	-	0/20/60/61	0/2/2/2
19	CLA	A	1101	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	A	1102	19	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	A	1103	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1104	-	4/4/18/25	0/28/126/135	0/0/9/9
19	CLA	A	1105	-	3/3/16/25	0/15/113/135	0/0/9/9
19	CLA	A	1106	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1107	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	A	1108	-	3/3/16/25	0/11/111/135	0/0/9/9
19	CLA	A	1109	19	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1110	-	3/3/17/25	0/24/122/135	0/0/9/9
19	CLA	A	1111	-	3/3/17/25	0/24/122/135	0/0/9/9
19	CLA	A	1112	-	3/3/16/25	0/11/111/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	1113	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	A	1115	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1116	-	3/3/17/25	0/22/120/135	0/0/9/9
19	CLA	A	1117	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1119	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1120	-	3/3/17/25	0/21/119/135	0/0/9/9
19	CLA	A	1121	1	3/3/15/25	0/10/108/135	0/0/9/9
19	CLA	A	1122	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	A	1123	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1124	-	4/4/20/25	1/37/135/135	0/0/9/9
19	CLA	A	1125	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1126	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1127	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	A	1128	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1129	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	A	1131	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1132	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1133	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	A	1134	1	3/3/16/25	0/11/111/135	0/0/9/9
19	CLA	A	1135	-	3/3/17/25	0/21/119/135	0/0/9/9
19	CLA	A	1136	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1137	-	3/3/16/25	0/16/114/135	0/0/9/9
19	CLA	A	1138	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1139	-	3/3/17/25	0/21/119/135	0/0/9/9
19	CLA	A	1140	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1141	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1149	-	5/5/16/25	0/16/112/135	0/0/9/9
19	CLA	A	1151	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	A	1237	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1309	-	3/3/7/25	0/0/66/135	0/0/8/9
20	PQN	A	5001	-	1/1/8/9	0/23/43/43	0/2/2/2
21	BCR	A	6002	-	-	0/29/63/63	0/2/2/2
21	BCR	A	6003	-	-	0/29/63/63	0/2/2/2
21	BCR	A	6007	-	-	0/29/63/63	0/2/2/2
21	BCR	A	6008	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	BCR	A	6011	-	-	0/29/63/63	0/2/2/2
22	LMU	A	7010	-	-	0/21/61/61	0/2/2/2
22	LMU	A	7016	-	-	0/21/61/61	0/2/2/2
22	LMU	A	7023	-	-	0/21/61/61	0/2/2/2
22	LMU	A	7035	-	-	0/21/61/61	0/2/2/2
22	LMU	A	7044	-	-	0/21/61/61	0/2/2/2
22	LMU	A	7045	-	-	0/21/61/61	0/2/2/2
24	SF4	A	8001	1,2	-	0/0/48/48	0/6/5/5
19	CLA	A	9011	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	9012	-	4/4/20/25	1/37/135/135	0/0/9/9
19	CLA	A	9013	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	9022	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	9023	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1201	-	3/3/16/25	0/11/111/135	0/0/9/9
19	CLA	B	1202	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1203	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1205	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1206	2	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1208	-	4/4/18/25	0/25/121/135	0/0/9/9
19	CLA	B	1209	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	B	1210	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1211	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1212	-	4/4/19/25	0/31/129/135	0/0/9/9
19	CLA	B	1213	-	3/3/16/25	0/15/113/135	0/0/9/9
19	CLA	B	1214	-	4/4/18/25	0/30/128/135	0/0/9/9
19	CLA	B	1215	-	4/4/19/25	0/31/129/135	0/0/9/9
19	CLA	B	1216	-	4/4/19/25	0/33/131/135	0/0/9/9
19	CLA	B	1217	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	B	1218	-	3/3/16/25	0/15/113/135	0/0/9/9
19	CLA	B	1219	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	B	1220	-	3/3/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1221	-	3/3/17/25	0/24/122/135	0/0/9/9
19	CLA	B	1222	-	4/4/18/25	1/29/127/135	0/0/9/9
19	CLA	B	1223	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1224	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1225	-	4/4/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	1226	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1227	-	3/3/17/25	1/19/117/135	0/0/9/9
19	CLA	B	1228	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	B	1229	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1230	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	B	1231	19	3/3/16/25	0/11/111/135	0/0/9/9
19	CLA	B	1232	19	3/3/16/25	0/11/111/135	0/0/9/9
19	CLA	B	1233	-	3/3/17/25	0/21/119/135	0/0/9/9
19	CLA	B	1234	-	4/4/19/25	0/31/129/135	0/0/9/9
19	CLA	B	1235	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1236	-	3/3/16/25	0/16/114/135	0/0/9/9
19	CLA	B	1238	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1239	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1301	-	3/3/14/25	0/0/96/135	0/0/9/9
20	PQN	B	5002	-	1/1/8/9	0/23/43/43	0/2/2/2
21	BCR	B	6004	-	-	0/29/63/63	0/2/2/2
21	BCR	B	6005	-	-	0/29/63/63	0/2/2/2
21	BCR	B	6006	-	-	0/29/63/63	0/2/2/2
21	BCR	B	6010	-	-	0/29/63/63	0/2/2/2
21	BCR	B	6017	-	-	0/29/63/63	0/2/2/2
21	BCR	B	6020	-	-	0/29/63/63	0/2/2/2
22	LMU	B	7012	-	-	0/11/51/61	0/2/2/2
22	LMU	B	7038	-	-	0/21/61/61	0/2/2/2
22	LMU	B	7040	-	-	0/21/61/61	0/2/2/2
23	LMG	B	7101	-	-	0/44/64/70	0/1/1/1
19	CLA	B	9010	-	4/4/20/25	0/37/135/135	0/0/9/9
22	LMU	C	7015	-	-	0/21/61/61	0/2/2/2
24	SF4	C	8002	3	-	0/0/48/48	0/6/5/5
24	SF4	C	8003	3	-	0/0/48/48	0/6/5/5
22	LMU	D	7050	-	-	0/21/61/61	0/2/2/2
22	LMU	E	7037	-	-	0/21/61/61	0/2/2/2
22	LMU	E	7048	-	-	0/21/61/61	0/2/2/2
19	CLA	F	1240	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	F	1302	-	3/3/15/25	0/8/106/135	0/0/9/9
19	CLA	F	1305	-	6/6/17/25	1/23/121/135	0/0/9/9
21	BCR	F	6014	-	-	1/29/63/63	0/2/2/2
21	BCR	F	6016	-	-	0/29/63/63	0/2/2/2
22	LMU	F	7036	-	-	1/20/60/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	G	1242	-	3/3/17/25	0/21/119/135	0/0/9/9
22	LMU	G	7026	-	-	0/21/61/61	0/2/2/2
22	LMU	G	7039	-	-	0/21/61/61	0/2/2/2
22	LMU	G	7051	-	-	0/21/61/61	0/2/2/2
19	CLA	H	1145	-	5/5/20/25	0/37/135/135	0/0/9/9
19	CLA	H	1207	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	H	1241	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	H	1505	-	4/4/18/25	0/25/123/135	0/0/9/9
22	LMU	H	7002	-	-	0/21/61/61	0/2/2/2
22	LMU	H	7011	-	-	0/21/61/61	0/2/2/2
22	LMU	H	7017	-	-	0/21/61/61	0/2/2/2
22	LMU	H	7028	-	-	0/21/61/61	0/2/2/2
22	LMU	H	7030	-	-	0/21/61/61	0/2/2/2
22	LMU	H	7032	-	-	0/21/61/61	0/2/2/2
22	LMU	H	7043	-	-	0/21/61/61	0/2/2/2
19	CLA	I	1204	-	4/4/19/25	0/31/129/135	0/0/9/9
21	BCR	I	6018	-	-	0/29/63/63	0/2/2/2
21	BCR	I	6021	-	-	0/29/63/63	0/2/2/2
19	CLA	J	1308	-	4/4/18/25	1/25/123/135	0/0/9/9
19	CLA	J	1311	-	4/4/19/25	1/33/131/135	0/0/9/9
21	BCR	J	6012	-	-	0/29/63/63	0/2/2/2
19	CLA	K	1142	-	3/3/16/25	0/11/111/135	0/0/9/9
19	CLA	K	1143	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	K	1146	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	K	3009	-	4/4/20/25	0/37/135/135	0/0/9/9
22	LMU	K	7001	-	-	0/21/61/61	0/2/2/2
22	LMU	K	7041	-	-	0/21/61/61	0/2/2/2
22	LMU	K	7042	-	-	0/21/61/61	0/2/2/2
22	LMU	K	7047	-	-	0/21/61/61	0/2/2/2
19	CLA	L	1130	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	L	1148	-	5/5/18/25	0/25/123/135	0/0/9/9
19	CLA	L	1501	12	3/3/17/25	1/19/117/135	0/0/9/9
19	CLA	L	1502	-	3/3/16/25	0/16/114/135	0/0/9/9
19	CLA	L	1503	-	4/4/17/25	0/19/117/135	0/0/9/9
19	CLA	L	1504	-	4/4/18/25	1/25/123/135	0/0/9/9
21	BCR	L	6019	-	-	0/29/63/63	0/2/2/2
22	LMU	L	7029	-	-	1/21/61/61	0/2/2/2
22	LMU	N	7049	-	-	0/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	R	1144	-	4/4/18/25	0/28/126/135	0/0/9/9
19	CLA	R	1150	-	4/4/20/25	0/37/135/135	0/0/9/9
22	LMU	R	7007	-	-	0/21/61/61	0/2/2/2
22	LMU	R	7014	-	-	0/21/61/61	0/2/2/2
22	LMU	R	7020	-	-	0/21/61/61	0/2/2/2
22	LMU	R	7021	-	-	0/21/61/61	0/2/2/2
22	LMU	R	7022	-	-	0/21/61/61	0/2/2/2
22	LMU	R	7024	-	-	0/21/61/61	0/2/2/2
22	LMU	R	7025	-	-	0/21/61/61	0/2/2/2

All (1849) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	1011	CLA	CAB-C3B	-9.04	1.33	1.51
19	1	1006	CLA	CAB-C3B	-9.03	1.33	1.51
19	4	1009	CLA	CAB-C3B	-8.69	1.33	1.51
19	B	1208	CLA	CAB-C3B	-8.41	1.34	1.51
19	4	4012	CLA	CAB-C3B	-8.40	1.34	1.51
19	B	1301	CLA	CAB-C3B	-8.34	1.34	1.51
19	1	1012	CLA	CAB-C3B	-8.20	1.34	1.51
19	A	1149	CLA	CAB-C3B	-8.12	1.35	1.51
19	3	1118	CLA	CAB-C3B	-7.92	1.35	1.51
19	3	1147	CLA	C3B-CAB	-7.77	1.31	1.47
19	3	3003	CLA	CAB-C3B	-7.59	1.36	1.51
19	1	1013	CLA	C3B-CAB	-7.51	1.31	1.47
19	B	1220	CLA	C3B-CAB	-7.49	1.31	1.47
19	B	1203	CLA	C3B-CAB	-7.46	1.32	1.47
19	A	9013	CLA	C3B-CAB	-7.46	1.32	1.47
19	B	1205	CLA	C3B-CAB	-7.17	1.32	1.47
19	B	1210	CLA	C3B-CAB	-7.14	1.32	1.47
19	2	2012	CLA	C3B-CAB	-7.12	1.32	1.47
19	A	1139	CLA	C3B-CAB	-7.09	1.32	1.47
19	F	1240	CLA	CAB-C3B	-7.08	1.37	1.51
19	A	9023	CLA	C3B-CAB	-7.02	1.32	1.47
21	B	6020	BCR	C21-C22	-7.00	1.26	1.35
21	1	6023	BCR	C11-C10	-6.98	1.22	1.43
19	A	1138	CLA	C3B-CAB	-6.93	1.33	1.47
19	A	1126	CLA	C3B-CAB	-6.92	1.33	1.47
19	A	1135	CLA	C3B-CAB	-6.91	1.33	1.47
19	B	1221	CLA	C3B-CAB	-6.90	1.33	1.47
19	4	1304	CLA	C3B-CAB	-6.86	1.33	1.47
19	B	1219	CLA	C3B-CAB	-6.84	1.33	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1137	CLA	C3B-CAB	-6.84	1.33	1.47
19	A	1136	CLA	C3B-CAB	-6.83	1.33	1.47
19	J	1308	CLA	C3B-CAB	-6.82	1.33	1.47
19	B	1229	CLA	C3B-CAB	-6.82	1.33	1.47
19	3	3013	CLA	C3B-CAB	-6.80	1.33	1.47
19	B	1235	CLA	C3B-CAB	-6.77	1.33	1.47
19	A	1127	CLA	C3B-CAB	-6.75	1.33	1.47
19	A	1103	CLA	C3B-CAB	-6.75	1.33	1.47
19	A	9022	CLA	C3B-CAB	-6.72	1.33	1.47
19	A	1124	CLA	C3B-CAB	-6.72	1.33	1.47
19	B	1234	CLA	C3B-CAB	-6.71	1.33	1.47
19	A	1125	CLA	C3B-CAB	-6.68	1.33	1.47
19	A	9012	CLA	C3B-CAB	-6.65	1.33	1.47
19	4	4015	CLA	C3B-CAB	-6.64	1.33	1.47
19	R	1150	CLA	C3B-CAB	-6.63	1.33	1.47
19	B	1222	CLA	C3B-CAB	-6.57	1.33	1.47
19	B	1211	CLA	C3B-CAB	-6.57	1.33	1.47
19	B	1231	CLA	C3B-CAB	-6.57	1.33	1.47
19	1	1014	CLA	C3B-CAB	-6.57	1.33	1.47
19	A	1141	CLA	C3B-CAB	-6.57	1.33	1.47
19	3	3016	CLA	C3B-CAB	-6.53	1.34	1.47
19	3	2009	CLA	C3B-CAB	-6.52	1.34	1.47
19	K	1146	CLA	C3B-CAB	-6.52	1.34	1.47
19	L	1130	CLA	C3B-CAB	-6.52	1.34	1.47
19	B	1223	CLA	C3B-CAB	-6.49	1.34	1.47
19	B	1232	CLA	C3B-CAB	-6.49	1.34	1.47
19	F	1305	CLA	C3B-CAB	-6.48	1.34	1.47
19	A	1237	CLA	C3B-CAB	-6.48	1.34	1.47
19	4	4003	CLA	C3B-CAB	-6.46	1.34	1.47
19	F	1302	CLA	C3B-CAB	-6.45	1.34	1.47
19	4	1004	CLA	C3B-CAB	-6.44	1.34	1.47
19	A	1115	CLA	C3B-CAB	-6.42	1.34	1.47
19	B	1227	CLA	C3B-CAB	-6.42	1.34	1.47
19	4	1306	CLA	C3B-CAB	-6.41	1.34	1.47
19	1	1007	CLA	C3B-CAB	-6.40	1.34	1.47
19	B	1225	CLA	C3B-CAB	-6.39	1.34	1.47
19	B	1202	CLA	C3B-CAB	-6.39	1.34	1.47
19	B	1224	CLA	C3B-CAB	-6.39	1.34	1.47
19	3	3008	CLA	C3B-CAB	-6.38	1.34	1.47
19	2	2014	CLA	C3B-CAB	-6.37	1.34	1.47
19	A	1140	CLA	C3B-CAB	-6.36	1.34	1.47
19	A	1132	CLA	C3B-CAB	-6.36	1.34	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1233	CLA	C3B-CAB	-6.36	1.34	1.47
19	L	1503	CLA	C3B-CAB	-6.36	1.34	1.47
19	L	1502	CLA	C3B-CAB	-6.34	1.34	1.47
19	I	1204	CLA	C3B-CAB	-6.34	1.34	1.47
19	A	1131	CLA	C3B-CAB	-6.33	1.34	1.47
21	I	6021	BCR	C30-C25	-6.32	1.44	1.53
19	A	9011	CLA	C3B-CAB	-6.28	1.34	1.47
19	A	1113	CLA	C3B-CAB	-6.28	1.34	1.47
19	H	1145	CLA	C3B-CAB	-6.26	1.34	1.47
19	B	1239	CLA	C3B-CAB	-6.26	1.34	1.47
19	A	1101	CLA	C3B-CAB	-6.24	1.34	1.47
19	A	1107	CLA	C3B-CAB	-6.24	1.34	1.47
19	J	1311	CLA	C3B-CAB	-6.23	1.34	1.47
19	2	2001	CLA	C3B-CAB	-6.23	1.34	1.47
19	2	2006	CLA	C3B-CAB	-6.23	1.34	1.47
19	A	1116	CLA	C3B-CAB	-6.22	1.34	1.47
19	1	1005	CLA	C3B-CAB	-6.21	1.34	1.47
19	A	1134	CLA	C3B-CAB	-6.21	1.34	1.47
19	B	1206	CLA	C3B-CAB	-6.20	1.34	1.47
19	A	1121	CLA	C3B-CAB	-6.20	1.34	1.47
19	B	1216	CLA	C3B-CAB	-6.20	1.34	1.47
19	A	1109	CLA	C3B-CAB	-6.17	1.34	1.47
19	A	1117	CLA	C3B-CAB	-6.15	1.34	1.47
19	1	1303	CLA	C3B-CAB	-6.14	1.34	1.47
19	4	4007	CLA	C3B-CAB	-6.13	1.34	1.47
19	K	1143	CLA	C3B-CAB	-6.13	1.34	1.47
19	H	1241	CLA	C3B-CAB	-6.10	1.34	1.47
19	1	1010	CLA	C3B-CAB	-6.04	1.35	1.47
19	B	1215	CLA	C3B-CAB	-6.03	1.35	1.47
19	K	3009	CLA	C3B-CAB	-6.02	1.35	1.47
19	3	3011	CLA	C3B-CAB	-6.01	1.35	1.47
19	B	1217	CLA	C3B-CAB	-6.01	1.35	1.47
19	3	3017	CLA	C3B-CAB	-6.01	1.35	1.47
19	A	1123	CLA	C3B-CAB	-5.98	1.35	1.47
19	H	1505	CLA	C3B-CAB	-5.97	1.35	1.47
19	L	1501	CLA	C3B-CAB	-5.97	1.35	1.47
19	2	2013	CLA	C3B-CAB	-5.94	1.35	1.47
19	1	1008	CLA	C3B-CAB	-5.93	1.35	1.47
19	A	1122	CLA	C3B-CAB	-5.93	1.35	1.47
19	A	1112	CLA	C3B-CAB	-5.91	1.35	1.47
19	1	1003	CLA	C3B-CAB	-5.91	1.35	1.47
19	B	1214	CLA	C3B-CAB	-5.91	1.35	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	H	1207	CLA	C3B-CAB	-5.90	1.35	1.47
19	A	1133	CLA	C3B-CAB	-5.89	1.35	1.47
19	B	1201	CLA	C3B-CAB	-5.88	1.35	1.47
19	2	4009	CLA	C3B-CAB	-5.88	1.35	1.47
19	A	1151	CLA	C3B-CAB	-5.87	1.35	1.47
19	L	1504	CLA	C3B-CAB	-5.87	1.35	1.47
19	K	1142	CLA	C3B-CAB	-5.84	1.35	1.47
19	B	1238	CLA	C3B-CAB	-5.84	1.35	1.47
19	1	1002	CLA	C3B-CAB	-5.84	1.35	1.47
19	B	1228	CLA	C3B-CAB	-5.81	1.35	1.47
21	1	6023	BCR	C10-C9	-5.81	1.28	1.35
19	B	9010	CLA	C3B-CAB	-5.77	1.35	1.47
19	4	4006	CLA	C3B-CAB	-5.77	1.35	1.47
21	B	6020	BCR	C17-C18	-5.76	1.28	1.35
19	4	4001	CLA	C3B-CAB	-5.74	1.35	1.47
19	3	3007	CLA	C3B-CAB	-5.73	1.35	1.47
19	G	1242	CLA	C3B-CAB	-5.73	1.35	1.47
19	A	1120	CLA	C3B-CAB	-5.72	1.35	1.47
19	A	1104	CLA	C3B-CAB	-5.72	1.35	1.47
19	A	1105	CLA	C3B-CAB	-5.71	1.35	1.47
19	1	1001	CLA	C3B-CAB	-5.70	1.35	1.47
19	B	1220	CLA	C4C-C3C	-5.69	1.34	1.45
19	A	1119	CLA	C3B-CAB	-5.68	1.35	1.47
19	2	2007	CLA	C3B-CAB	-5.65	1.35	1.47
19	B	1212	CLA	C3B-CAB	-5.63	1.35	1.47
19	A	1106	CLA	C3B-CAB	-5.62	1.35	1.47
19	A	1111	CLA	C3B-CAB	-5.60	1.35	1.47
19	B	1236	CLA	C3B-CAB	-5.57	1.36	1.47
19	B	1209	CLA	C3B-CAB	-5.56	1.36	1.47
19	L	1148	CLA	C3B-CAB	-5.56	1.36	1.47
21	L	6019	BCR	C21-C22	-5.56	1.28	1.35
19	B	1213	CLA	C3B-CAB	-5.53	1.36	1.47
19	4	4002	CLA	C4C-C3C	-5.51	1.35	1.45
19	2	2004	CLA	C3B-CAB	-5.49	1.36	1.47
19	B	1230	CLA	C3B-CAB	-5.48	1.36	1.47
19	A	1102	CLA	C3B-CAB	-5.44	1.36	1.47
19	A	1129	CLA	C3B-CAB	-5.44	1.36	1.47
19	R	1144	CLA	C3B-CAB	-5.39	1.36	1.47
21	I	6018	BCR	C10-C9	-5.36	1.28	1.35
19	A	1128	CLA	C3B-CAB	-5.31	1.36	1.47
21	I	6021	BCR	C10-C9	-5.24	1.28	1.35
19	A	1110	CLA	C3B-CAB	-5.23	1.36	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	2002	CLA	C3B-CAB	-5.22	1.36	1.47
19	B	1218	CLA	C3B-CAB	-5.20	1.36	1.47
21	B	6017	BCR	C10-C9	-5.11	1.29	1.35
21	F	6016	BCR	C30-C25	-5.07	1.46	1.53
19	4	4002	CLA	C3B-CAB	-4.98	1.37	1.47
19	1	1010	CLA	C4C-C3C	-4.80	1.36	1.45
19	B	1226	CLA	C3B-CAB	-4.79	1.37	1.47
19	3	3013	CLA	C4C-C3C	-4.78	1.36	1.45
19	3	1147	CLA	C3B-C2B	-4.62	1.34	1.40
19	A	1108	CLA	C3B-CAB	-4.60	1.38	1.47
21	A	6007	BCR	C30-C25	-4.60	1.47	1.53
19	1	1013	CLA	C4C-C3C	-4.58	1.36	1.45
21	B	6010	BCR	C21-C22	-4.48	1.29	1.35
21	A	6008	BCR	C10-C9	-4.33	1.30	1.35
21	B	6020	BCR	C30-C25	-4.29	1.47	1.53
21	A	6007	BCR	C10-C9	-4.28	1.30	1.35
21	B	6005	BCR	C10-C9	-4.25	1.30	1.35
21	A	6008	BCR	C21-C22	-4.25	1.30	1.35
19	4	4002	CLA	C1C-C2C	-4.19	1.36	1.44
19	1	1303	CLA	C3A-C2A	-4.18	1.42	1.54
19	3	1147	CLA	C4C-C3C	-4.15	1.37	1.45
21	F	6016	BCR	C21-C22	-4.13	1.30	1.35
19	1	1011	CLA	C1C-C2C	-4.13	1.36	1.44
19	K	1146	CLA	C1C-C2C	-4.12	1.36	1.44
19	J	1308	CLA	C4C-C3C	-4.10	1.37	1.45
19	1	1013	CLA	C3D-CAD	-4.10	1.34	1.45
21	J	6012	BCR	C21-C22	-4.06	1.30	1.35
19	F	1305	CLA	C3A-C2A	-4.05	1.42	1.54
19	1	1303	CLA	C1C-C2C	-4.00	1.36	1.44
19	4	1304	CLA	C1C-C2C	-3.94	1.36	1.44
21	3	6022	BCR	C30-C25	-3.93	1.48	1.53
19	1	1014	CLA	C4C-C3C	-3.86	1.38	1.45
19	K	1146	CLA	C4C-C3C	-3.86	1.38	1.45
19	A	9011	CLA	C4C-C3C	-3.85	1.38	1.45
19	A	1107	CLA	C1C-C2C	-3.85	1.36	1.44
19	1	1013	CLA	C3B-C2B	-3.82	1.35	1.40
19	A	1117	CLA	C4C-C3C	-3.81	1.38	1.45
19	F	1305	CLA	C3B-C2B	-3.81	1.35	1.40
19	4	1304	CLA	C4C-C3C	-3.80	1.38	1.45
21	I	6018	BCR	C20-C21	-3.79	1.32	1.43
21	B	6004	BCR	C10-C9	-3.77	1.30	1.35
21	B	6010	BCR	C30-C25	-3.76	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	J	6012	BCR	C20-C21	-3.76	1.32	1.43
21	J	6012	BCR	C10-C9	-3.75	1.30	1.35
19	3	3017	CLA	C1C-C2C	-3.75	1.37	1.44
21	A	6011	BCR	C21-C22	-3.73	1.30	1.35
21	B	6020	BCR	C20-C21	-3.73	1.32	1.43
21	A	6002	BCR	C20-C21	-3.71	1.32	1.43
19	F	1305	CLA	C4C-C3C	-3.69	1.38	1.45
21	3	6022	BCR	C21-C22	-3.68	1.30	1.35
21	B	6004	BCR	C21-C22	-3.67	1.30	1.35
19	B	1226	CLA	C4C-C3C	-3.66	1.38	1.45
21	B	6005	BCR	C21-C22	-3.66	1.30	1.35
19	B	1230	CLA	C1C-C2C	-3.65	1.37	1.44
19	4	4015	CLA	C4C-C3C	-3.64	1.38	1.45
19	A	1125	CLA	C4C-C3C	-3.64	1.38	1.45
19	4	4006	CLA	C4C-C3C	-3.64	1.38	1.45
21	L	6019	BCR	C10-C9	-3.63	1.31	1.35
21	B	6006	BCR	C20-C21	-3.62	1.32	1.43
19	A	9023	CLA	C4C-C3C	-3.59	1.38	1.45
19	B	1210	CLA	C4C-C3C	-3.59	1.38	1.45
21	B	6005	BCR	C30-C25	-3.58	1.48	1.53
19	1	1303	CLA	C4C-C3C	-3.57	1.38	1.45
21	B	6017	BCR	C21-C22	-3.57	1.31	1.35
21	3	6022	BCR	C20-C21	-3.56	1.32	1.43
19	B	1203	CLA	C1C-C2C	-3.55	1.37	1.44
19	A	1139	CLA	C4C-C3C	-3.54	1.38	1.45
19	3	2009	CLA	C4C-C3C	-3.52	1.38	1.45
19	1	1001	CLA	C4C-C3C	-3.50	1.38	1.45
19	B	1225	CLA	C4C-C3C	-3.49	1.38	1.45
19	B	1215	CLA	C4C-C3C	-3.49	1.38	1.45
19	A	1134	CLA	C4C-C3C	-3.47	1.38	1.45
19	A	9013	CLA	C4C-C3C	-3.47	1.38	1.45
19	A	1131	CLA	C4C-C3C	-3.46	1.38	1.45
19	1	1008	CLA	C2A-C1A	-3.46	1.45	1.52
21	B	6010	BCR	C10-C9	-3.46	1.31	1.35
19	1	1013	CLA	C1C-C2C	-3.45	1.37	1.44
19	A	1112	CLA	C3B-C2B	-3.45	1.35	1.40
19	3	3013	CLA	C1C-C2C	-3.43	1.37	1.44
19	B	1236	CLA	C4C-C3C	-3.42	1.38	1.45
19	1	1011	CLA	C4C-C3C	-3.42	1.37	1.44
19	B	1231	CLA	C4C-C3C	-3.41	1.38	1.45
19	L	1504	CLA	C4C-C3C	-3.40	1.38	1.45
19	1	1001	CLA	C1C-C2C	-3.39	1.37	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	1304	CLA	C3B-C2B	-3.39	1.35	1.40
19	A	1137	CLA	C4C-C3C	-3.38	1.38	1.45
21	I	6021	BCR	C26-C25	-3.38	1.28	1.34
21	B	6020	BCR	C20-C19	-3.37	1.25	1.34
21	B	6020	BCR	C31-C1	-3.36	1.46	1.53
19	B	1220	CLA	C1C-C2C	-3.36	1.37	1.44
19	B	1220	CLA	C3B-C2B	-3.34	1.35	1.40
19	J	1308	CLA	C1C-C2C	-3.34	1.37	1.44
19	B	1202	CLA	C1C-C2C	-3.32	1.37	1.44
21	B	6017	BCR	C30-C25	-3.31	1.49	1.53
21	F	6014	BCR	C30-C25	-3.31	1.49	1.53
19	1	1010	CLA	C3B-C2B	-3.30	1.36	1.40
19	2	2001	CLA	C4C-C3C	-3.28	1.39	1.45
21	A	6011	BCR	C10-C9	-3.27	1.31	1.35
21	A	6003	BCR	C10-C9	-3.27	1.31	1.35
21	J	6012	BCR	C30-C25	-3.26	1.49	1.53
19	A	1140	CLA	C4C-C3C	-3.25	1.39	1.45
19	A	9023	CLA	C1C-C2C	-3.25	1.38	1.44
19	A	9012	CLA	C4C-C3C	-3.24	1.39	1.45
19	L	1501	CLA	C4C-C3C	-3.24	1.39	1.45
19	A	9011	CLA	C3B-C2B	-3.24	1.36	1.40
19	A	1115	CLA	C4C-C3C	-3.24	1.39	1.45
19	A	1141	CLA	C4C-C3C	-3.23	1.39	1.45
19	A	1136	CLA	C4C-C3C	-3.22	1.39	1.45
19	B	1222	CLA	C4C-C3C	-3.22	1.39	1.45
21	A	6011	BCR	C30-C25	-3.21	1.49	1.53
19	K	1142	CLA	C4C-C3C	-3.21	1.39	1.45
19	J	1311	CLA	C4C-C3C	-3.21	1.39	1.45
19	A	1132	CLA	C1C-C2C	-3.20	1.38	1.44
19	4	4007	CLA	C4C-C3C	-3.20	1.39	1.45
19	B	1229	CLA	C4C-C3C	-3.19	1.39	1.45
19	I	1204	CLA	C4C-C3C	-3.19	1.39	1.45
19	B	1205	CLA	C1C-C2C	-3.19	1.38	1.44
19	A	1138	CLA	C4C-C3C	-3.18	1.39	1.45
19	K	1143	CLA	C4C-C3C	-3.18	1.39	1.45
19	B	1223	CLA	C4C-C3C	-3.18	1.39	1.45
19	L	1148	CLA	C4C-C3C	-3.18	1.39	1.45
19	A	1135	CLA	C4C-C3C	-3.18	1.39	1.45
19	1	1010	CLA	C1C-C2C	-3.16	1.38	1.44
21	F	6016	BCR	C32-C1	-3.16	1.47	1.53
19	K	3009	CLA	C4C-C3C	-3.16	1.39	1.45
19	B	1235	CLA	C4C-C3C	-3.15	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	1008	CLA	C4C-C3C	-3.15	1.39	1.45
19	3	3016	CLA	C4C-C3C	-3.14	1.39	1.45
19	A	1134	CLA	C1C-C2C	-3.14	1.38	1.44
19	H	1207	CLA	C4C-C3C	-3.14	1.39	1.45
19	H	1145	CLA	C4C-C3C	-3.13	1.39	1.45
19	A	1109	CLA	C1C-C2C	-3.13	1.38	1.44
19	B	1218	CLA	C4C-C3C	-3.12	1.39	1.45
19	B	9010	CLA	C4C-C3C	-3.12	1.39	1.45
19	B	1230	CLA	C4C-C3C	-3.11	1.39	1.45
19	4	1306	CLA	C1C-C2C	-3.11	1.38	1.44
19	A	1111	CLA	C1C-C2C	-3.11	1.38	1.44
19	L	1148	CLA	C3A-C2A	-3.11	1.45	1.54
19	A	1106	CLA	C4C-C3C	-3.09	1.39	1.45
19	A	1109	CLA	C4C-C3C	-3.09	1.39	1.45
19	4	4001	CLA	C4C-C3C	-3.09	1.39	1.45
19	A	1101	CLA	C4C-C3C	-3.09	1.39	1.45
21	L	6019	BCR	C17-C18	-3.09	1.31	1.35
19	B	1228	CLA	C4C-C3C	-3.08	1.39	1.45
19	B	1216	CLA	C4C-C3C	-3.08	1.39	1.45
19	L	1503	CLA	C4C-C3C	-3.07	1.39	1.45
21	A	6002	BCR	C21-C22	-3.07	1.31	1.35
19	B	1213	CLA	C1C-C2C	-3.07	1.38	1.44
19	2	2014	CLA	C4C-C3C	-3.06	1.39	1.45
19	4	4015	CLA	C3B-C2B	-3.06	1.36	1.40
19	B	1224	CLA	C4C-C3C	-3.06	1.39	1.45
19	A	1124	CLA	C4C-C3C	-3.05	1.39	1.45
19	A	1117	CLA	C3B-C2B	-3.04	1.36	1.40
19	B	1226	CLA	C1C-C2C	-3.04	1.38	1.44
21	A	6008	BCR	C30-C25	-3.04	1.49	1.53
19	B	1235	CLA	C1C-C2C	-3.03	1.38	1.44
19	2	4009	CLA	C1C-C2C	-3.03	1.38	1.44
19	4	4015	CLA	C1C-C2C	-3.03	1.38	1.44
19	B	1208	CLA	C4C-C3C	-3.03	1.39	1.45
19	3	1147	CLA	C1C-C2C	-3.02	1.38	1.44
19	K	1143	CLA	C1C-C2C	-3.02	1.38	1.44
19	F	1305	CLA	C2A-C1A	-3.02	1.46	1.52
19	B	1217	CLA	C4C-C3C	-3.01	1.39	1.45
19	4	4003	CLA	C4C-C3C	-3.01	1.39	1.45
19	4	1004	CLA	C1C-C2C	-3.01	1.38	1.44
19	A	1131	CLA	C1C-C2C	-3.01	1.38	1.44
21	1	6023	BCR	C11-C12	-3.00	1.26	1.34
19	A	1116	CLA	C4C-C3C	-3.00	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1213	CLA	C4C-C3C	-2.99	1.39	1.45
19	A	1110	CLA	C4C-C3C	-2.99	1.39	1.45
19	1	1014	CLA	C1C-C2C	-2.98	1.38	1.44
19	3	3008	CLA	C4C-C3C	-2.97	1.39	1.45
19	B	1238	CLA	C4C-C3C	-2.97	1.39	1.45
19	G	1242	CLA	C4C-C3C	-2.96	1.39	1.45
21	A	6003	BCR	C30-C25	-2.96	1.49	1.53
19	F	1302	CLA	C4C-C3C	-2.96	1.39	1.45
19	B	1206	CLA	C4C-C3C	-2.96	1.39	1.45
21	I	6018	BCR	C30-C25	-2.95	1.49	1.53
19	A	1103	CLA	C1C-C2C	-2.95	1.38	1.44
19	L	1148	CLA	C3B-C2B	-2.94	1.36	1.40
19	B	1236	CLA	C1C-C2C	-2.94	1.38	1.44
19	B	1209	CLA	C1C-C2C	-2.94	1.38	1.44
19	B	1232	CLA	C4C-C3C	-2.94	1.39	1.45
21	B	6020	BCR	C11-C12	-2.94	1.26	1.34
19	A	9013	CLA	C1C-C2C	-2.93	1.38	1.44
19	A	1104	CLA	C4C-C3C	-2.93	1.39	1.45
19	B	1206	CLA	C1C-C2C	-2.93	1.38	1.44
19	A	1126	CLA	C1C-C2C	-2.92	1.38	1.44
19	B	1203	CLA	C3B-C2B	-2.92	1.36	1.40
19	3	3017	CLA	C4C-C3C	-2.92	1.39	1.45
21	B	6006	BCR	C10-C9	-2.92	1.31	1.35
19	A	1115	CLA	C3B-C2B	-2.92	1.36	1.40
19	2	2004	CLA	C4C-C3C	-2.92	1.39	1.45
19	A	1119	CLA	C1C-C2C	-2.91	1.38	1.44
19	2	2007	CLA	C1C-C2C	-2.91	1.38	1.44
19	4	4003	CLA	C1C-C2C	-2.91	1.38	1.44
19	4	4014	CLA	C1C-C2C	-2.89	1.38	1.44
19	B	1203	CLA	C4C-C3C	-2.89	1.39	1.45
19	B	1202	CLA	C4C-C3C	-2.89	1.39	1.45
19	A	1237	CLA	C4C-C3C	-2.89	1.39	1.45
19	B	1238	CLA	C1C-C2C	-2.88	1.38	1.44
19	A	1135	CLA	C1C-C2C	-2.88	1.38	1.44
21	B	6020	BCR	C2-C1	-2.87	1.47	1.54
19	2	2001	CLA	C1C-C2C	-2.86	1.38	1.44
21	B	6004	BCR	C30-C25	-2.86	1.49	1.53
19	3	1118	CLA	C4C-C3C	-2.86	1.38	1.44
19	A	1136	CLA	C1C-C2C	-2.86	1.38	1.44
19	4	1004	CLA	C4C-C3C	-2.85	1.39	1.45
19	A	1124	CLA	C1C-C2C	-2.85	1.38	1.44
19	2	2006	CLA	C4C-C3C	-2.85	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1205	CLA	C4C-C3C	-2.84	1.39	1.45
19	A	9022	CLA	C4C-C3C	-2.84	1.39	1.45
21	B	6005	BCR	C20-C21	-2.83	1.34	1.43
19	A	1139	CLA	C1C-C2C	-2.83	1.38	1.44
21	3	6022	BCR	C10-C9	-2.82	1.32	1.35
21	F	6014	BCR	C10-C9	-2.81	1.32	1.35
19	A	1110	CLA	C1C-C2C	-2.81	1.38	1.44
19	B	1209	CLA	C4C-C3C	-2.80	1.40	1.45
21	F	6014	BCR	C20-C21	-2.80	1.35	1.43
19	L	1148	CLA	C3D-CAD	-2.80	1.37	1.45
19	3	1118	CLA	C1C-C2C	-2.79	1.39	1.44
19	4	4007	CLA	C1C-C2C	-2.79	1.39	1.44
19	H	1145	CLA	C1C-C2C	-2.78	1.39	1.44
19	A	1137	CLA	C1C-C2C	-2.78	1.39	1.44
19	A	1125	CLA	C1C-C2C	-2.77	1.39	1.44
19	F	1305	CLA	C1C-C2C	-2.77	1.39	1.44
19	A	1115	CLA	C1C-C2C	-2.77	1.39	1.44
19	2	2013	CLA	C4C-C3C	-2.77	1.40	1.45
21	F	6016	BCR	C10-C9	-2.77	1.32	1.35
19	A	1108	CLA	C4C-C3C	-2.77	1.40	1.45
19	B	1226	CLA	C3D-CAD	-2.76	1.38	1.45
19	A	1120	CLA	C4C-C3C	-2.76	1.40	1.45
19	B	1233	CLA	C4C-C3C	-2.76	1.40	1.45
19	A	1102	CLA	C4C-C3C	-2.76	1.40	1.45
19	3	3016	CLA	C1C-C2C	-2.75	1.39	1.44
19	A	1149	CLA	C1C-C2C	-2.75	1.39	1.44
19	4	1009	CLA	C4C-C3C	-2.75	1.39	1.44
19	4	4014	CLA	C4C-C3C	-2.75	1.40	1.45
19	A	1128	CLA	C4C-C3C	-2.75	1.40	1.45
19	1	1005	CLA	C4C-C3C	-2.75	1.40	1.45
21	L	6019	BCR	C31-C1	-2.74	1.47	1.53
19	2	2014	CLA	C1C-C2C	-2.74	1.39	1.44
19	F	1240	CLA	C1C-C2C	-2.74	1.39	1.44
19	F	1305	CLA	CAA-C2A	-2.74	1.48	1.54
19	J	1308	CLA	C3D-CAD	-2.74	1.38	1.45
19	A	1140	CLA	C1C-C2C	-2.74	1.39	1.44
19	2	4009	CLA	C4C-C3C	-2.74	1.40	1.45
19	B	1227	CLA	C1C-C2C	-2.73	1.39	1.44
19	1	1001	CLA	C3D-CAD	-2.73	1.38	1.45
19	A	1138	CLA	C1C-C2C	-2.73	1.39	1.44
19	1	1007	CLA	C4C-C3C	-2.73	1.40	1.45
19	3	2009	CLA	C1C-C2C	-2.72	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	3013	CLA	C3D-CAD	-2.72	1.38	1.45
19	1	1010	CLA	C3D-CAD	-2.72	1.38	1.45
19	B	1223	CLA	C1C-C2C	-2.72	1.39	1.44
19	1	1006	CLA	C1C-C2C	-2.71	1.39	1.44
19	A	1151	CLA	C1C-C2C	-2.71	1.39	1.44
19	A	1127	CLA	C3B-C2B	-2.70	1.36	1.40
19	B	1215	CLA	C1C-C2C	-2.70	1.39	1.44
19	A	1101	CLA	C1C-C2C	-2.70	1.39	1.44
19	A	1121	CLA	C1C-C2C	-2.69	1.39	1.44
19	J	1311	CLA	C1C-C2C	-2.69	1.39	1.44
19	A	1128	CLA	C3B-C2B	-2.69	1.36	1.40
19	B	1212	CLA	C4C-C3C	-2.69	1.40	1.45
19	A	1117	CLA	C1C-C2C	-2.68	1.39	1.44
19	3	3003	CLA	C4C-C3C	-2.68	1.39	1.44
19	B	1220	CLA	C3D-CAD	-2.68	1.38	1.45
19	A	1108	CLA	C1C-C2C	-2.67	1.39	1.44
19	A	1104	CLA	C1C-C2C	-2.67	1.39	1.44
21	I	6021	BCR	C32-C1	-2.67	1.48	1.53
19	1	1005	CLA	C1C-C2C	-2.66	1.39	1.44
19	B	1208	CLA	C1C-C2C	-2.66	1.39	1.44
19	2	2002	CLA	C1C-C2C	-2.65	1.39	1.44
19	B	1219	CLA	C1C-C2C	-2.65	1.39	1.44
19	A	1103	CLA	C3B-C2B	-2.65	1.36	1.40
19	A	1106	CLA	C3B-C2B	-2.65	1.36	1.40
19	A	1141	CLA	C1C-C2C	-2.65	1.39	1.44
19	A	1126	CLA	C4C-C3C	-2.64	1.40	1.45
19	F	1302	CLA	C1C-C2C	-2.64	1.39	1.44
19	3	3008	CLA	C3D-CAD	-2.64	1.38	1.45
19	A	1105	CLA	C4C-C3C	-2.63	1.40	1.45
19	B	1214	CLA	C4C-C3C	-2.62	1.40	1.45
19	B	1221	CLA	C3B-C2B	-2.62	1.36	1.40
19	R	1144	CLA	C4C-C3C	-2.62	1.40	1.45
19	B	1210	CLA	C1C-C2C	-2.61	1.39	1.44
19	A	1122	CLA	C4C-C3C	-2.61	1.40	1.45
19	B	1234	CLA	C3D-CAD	-2.61	1.38	1.45
19	B	1214	CLA	C1C-C2C	-2.61	1.39	1.44
19	1	1007	CLA	C1C-C2C	-2.60	1.39	1.44
19	A	1109	CLA	C3B-C2B	-2.60	1.36	1.40
19	B	1222	CLA	C1C-C2C	-2.59	1.39	1.44
19	A	1129	CLA	C1C-C2C	-2.59	1.39	1.44
19	L	1130	CLA	C4C-C3C	-2.59	1.40	1.45
19	B	1221	CLA	C1C-C2C	-2.58	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1116	CLA	C1C-C2C	-2.58	1.39	1.44
19	B	1201	CLA	C4C-C3C	-2.58	1.40	1.45
19	B	1224	CLA	C1C-C2C	-2.58	1.39	1.44
19	H	1505	CLA	C4C-C3C	-2.58	1.40	1.45
19	A	1122	CLA	C1C-C2C	-2.57	1.39	1.44
21	B	6020	BCR	C14-C13	-2.57	1.32	1.35
19	B	9010	CLA	C1C-C2C	-2.57	1.39	1.44
19	4	4012	CLA	C1C-C2C	-2.56	1.39	1.44
21	I	6021	BCR	C21-C22	-2.56	1.32	1.35
19	1	1006	CLA	C4C-C3C	-2.56	1.39	1.44
19	A	9012	CLA	C1C-C2C	-2.55	1.39	1.44
19	3	2009	CLA	C3D-CAD	-2.55	1.38	1.45
19	B	1201	CLA	C3B-C2B	-2.55	1.37	1.40
19	1	1012	CLA	C4C-C3C	-2.55	1.39	1.44
19	2	2013	CLA	C3D-CAD	-2.55	1.38	1.45
19	1	1011	CLA	C3D-CAD	-2.54	1.38	1.45
19	3	3013	CLA	C1C-NC	-2.54	1.33	1.37
19	L	1502	CLA	C1C-C2C	-2.54	1.39	1.44
19	4	4015	CLA	C3D-CAD	-2.53	1.38	1.45
19	B	1221	CLA	C4C-C3C	-2.53	1.40	1.45
21	A	6007	BCR	C21-C22	-2.51	1.32	1.35
19	1	1013	CLA	C3D-C2D	-2.51	1.34	1.40
19	B	1227	CLA	C4C-C3C	-2.51	1.40	1.45
19	3	1147	CLA	C1C-NC	-2.50	1.33	1.37
19	2	2012	CLA	C1C-C2C	-2.50	1.39	1.44
21	F	6016	BCR	C17-C18	-2.50	1.32	1.35
19	B	1234	CLA	C1C-C2C	-2.50	1.39	1.44
19	A	1127	CLA	C4C-C3C	-2.50	1.40	1.45
21	L	6019	BCR	C20-C21	-2.49	1.36	1.43
19	A	1111	CLA	C4C-C3C	-2.49	1.40	1.45
19	A	1128	CLA	C1C-C2C	-2.49	1.39	1.44
19	A	1113	CLA	C1C-C2C	-2.49	1.39	1.44
19	A	9011	CLA	C1C-C2C	-2.48	1.39	1.44
19	H	1145	CLA	C3D-CAD	-2.48	1.38	1.45
19	A	1121	CLA	C4C-C3C	-2.48	1.40	1.45
19	F	1240	CLA	C4C-C3C	-2.47	1.39	1.44
19	2	2006	CLA	C1C-C2C	-2.47	1.39	1.44
19	3	3008	CLA	C1C-C2C	-2.47	1.39	1.44
19	1	1003	CLA	C3D-CAD	-2.46	1.38	1.45
19	B	1230	CLA	C3D-CAD	-2.46	1.38	1.45
19	B	1211	CLA	C1C-C2C	-2.46	1.39	1.44
19	B	1220	CLA	C1C-NC	-2.46	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	4014	CLA	C3D-CAD	-2.46	1.38	1.45
19	3	3017	CLA	C3D-CAD	-2.46	1.38	1.45
19	A	1112	CLA	C1C-C2C	-2.46	1.39	1.44
19	A	1127	CLA	C1C-C2C	-2.45	1.39	1.44
19	B	1301	CLA	C1C-C2C	-2.45	1.39	1.44
19	K	1142	CLA	C1C-C2C	-2.45	1.39	1.44
19	B	1234	CLA	C4C-C3C	-2.45	1.40	1.45
19	1	1003	CLA	C4C-C3C	-2.44	1.40	1.45
19	3	3003	CLA	C1C-C2C	-2.44	1.39	1.44
19	B	1218	CLA	C3D-CAD	-2.44	1.38	1.45
19	B	1229	CLA	C3D-CAD	-2.44	1.38	1.45
19	H	1207	CLA	C3D-CAD	-2.44	1.38	1.45
19	R	1150	CLA	C4C-C3C	-2.43	1.40	1.45
19	B	9010	CLA	C3B-C2B	-2.43	1.37	1.40
19	A	9022	CLA	C3B-C2B	-2.43	1.37	1.40
19	A	1237	CLA	C1C-C2C	-2.43	1.39	1.44
19	A	1133	CLA	C1C-C2C	-2.43	1.39	1.44
19	B	1231	CLA	C1C-C2C	-2.42	1.39	1.44
19	I	1204	CLA	C3D-CAD	-2.41	1.39	1.45
19	B	1229	CLA	C1C-C2C	-2.40	1.39	1.44
21	F	6014	BCR	C21-C22	-2.39	1.32	1.35
19	B	1219	CLA	C4C-C3C	-2.38	1.40	1.45
19	1	1014	CLA	C3D-CAD	-2.38	1.39	1.45
19	4	1009	CLA	C1C-C2C	-2.38	1.39	1.44
19	B	1225	CLA	C1C-C2C	-2.38	1.39	1.44
21	A	6002	BCR	C30-C25	-2.37	1.50	1.53
19	A	1133	CLA	C4C-C3C	-2.37	1.40	1.45
21	F	6016	BCR	C20-C19	-2.37	1.28	1.34
19	A	1113	CLA	C4C-C3C	-2.37	1.40	1.45
19	4	4002	CLA	C3D-CAD	-2.37	1.39	1.45
19	R	1144	CLA	C3D-CAD	-2.36	1.39	1.45
19	A	1102	CLA	C1C-C2C	-2.36	1.39	1.44
19	4	4002	CLA	C3A-C2A	-2.36	1.47	1.54
19	B	1222	CLA	C3D-CAD	-2.36	1.39	1.45
19	B	1230	CLA	C1C-NC	-2.36	1.33	1.37
21	B	6006	BCR	C30-C25	-2.35	1.50	1.53
19	3	3011	CLA	C4C-C3C	-2.35	1.40	1.45
19	1	1002	CLA	C1C-C2C	-2.35	1.39	1.44
19	2	2002	CLA	C4C-C3C	-2.35	1.40	1.45
19	B	1211	CLA	C3B-C2B	-2.35	1.37	1.40
19	L	1130	CLA	C1C-C2C	-2.35	1.39	1.44
19	L	1148	CLA	C1C-NC	-2.35	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	1012	CLA	C1C-C2C	-2.34	1.39	1.44
21	L	6019	BCR	C20-C19	-2.34	1.28	1.34
19	L	1148	CLA	C1C-C2C	-2.34	1.39	1.44
19	A	1115	CLA	C3D-CAD	-2.33	1.39	1.45
19	3	3011	CLA	C1C-C2C	-2.33	1.39	1.44
21	L	6019	BCR	C2-C1	-2.33	1.48	1.54
19	B	1224	CLA	C3D-CAD	-2.32	1.39	1.45
19	J	1308	CLA	C3B-C2B	-2.32	1.37	1.40
19	A	1149	CLA	C2A-C1A	-2.32	1.47	1.52
19	3	3004	CLA	C2C-C1C	-2.32	1.37	1.43
19	B	1225	CLA	C3B-C2B	-2.32	1.37	1.40
19	A	9022	CLA	C1C-C2C	-2.32	1.39	1.44
21	L	6019	BCR	C30-C25	-2.31	1.50	1.53
21	F	6016	BCR	C1-C6	-2.31	1.50	1.53
19	A	1123	CLA	C1C-C2C	-2.31	1.39	1.44
19	R	1150	CLA	C3B-C2B	-2.30	1.37	1.40
19	1	1011	CLA	C1C-NC	-2.30	1.33	1.37
19	4	4014	CLA	C3B-CAB	-2.30	1.42	1.47
19	A	1128	CLA	C3D-CAD	-2.30	1.39	1.45
19	4	4002	CLA	C2A-C1A	-2.30	1.47	1.52
19	L	1502	CLA	C4C-C3C	-2.29	1.40	1.45
21	I	6021	BCR	C31-C1	-2.29	1.48	1.53
19	1	1303	CLA	C1C-NC	-2.29	1.33	1.37
19	B	1218	CLA	C1C-C2C	-2.28	1.40	1.44
19	A	1237	CLA	C3D-CAD	-2.28	1.39	1.45
19	A	1101	CLA	C3B-C2B	-2.28	1.37	1.40
19	A	1102	CLA	C3B-C2B	-2.28	1.37	1.40
19	B	1206	CLA	C3D-CAD	-2.28	1.39	1.45
19	3	3007	CLA	C1C-C2C	-2.27	1.40	1.44
19	B	1217	CLA	C1C-C2C	-2.27	1.40	1.44
19	A	1120	CLA	C1C-C2C	-2.27	1.40	1.44
19	L	1503	CLA	C3D-CAD	-2.26	1.39	1.45
19	1	1303	CLA	C3B-C2B	-2.26	1.37	1.40
19	A	9012	CLA	C3B-C2B	-2.26	1.37	1.40
19	1	1005	CLA	C3D-CAD	-2.26	1.39	1.45
19	2	4009	CLA	C3D-CAD	-2.25	1.39	1.45
19	B	1211	CLA	C4C-C3C	-2.25	1.41	1.45
19	B	1232	CLA	C1C-C2C	-2.25	1.40	1.44
19	3	3012	CLA	C2C-C1C	-2.25	1.37	1.43
19	A	1107	CLA	C4C-C3C	-2.25	1.41	1.45
19	1	1008	CLA	C3D-CAD	-2.24	1.39	1.45
19	A	1123	CLA	C3D-CAD	-2.24	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1239	CLA	C3B-C2B	-2.24	1.37	1.40
19	B	1228	CLA	C1C-C2C	-2.23	1.40	1.44
19	A	1151	CLA	C4C-C3C	-2.23	1.41	1.45
19	H	1207	CLA	C1C-C2C	-2.22	1.40	1.44
19	A	1149	CLA	C3D-CAD	-2.21	1.39	1.45
19	4	1304	CLA	CBD-CHA	-2.21	1.41	1.52
19	R	1144	CLA	C1C-C2C	-2.21	1.40	1.44
19	B	1221	CLA	C3D-CAD	-2.20	1.39	1.45
19	A	1125	CLA	C3D-CAD	-2.20	1.39	1.45
19	I	1204	CLA	C1C-C2C	-2.20	1.40	1.44
19	B	1239	CLA	C4C-C3C	-2.20	1.41	1.45
19	1	1013	CLA	C1C-NC	-2.20	1.34	1.37
19	2	2004	CLA	C1C-C2C	-2.20	1.40	1.44
19	1	1002	CLA	C4C-C3C	-2.19	1.41	1.45
19	A	1137	CLA	C3B-C2B	-2.19	1.37	1.40
21	F	6014	BCR	C20-C19	-2.19	1.28	1.34
19	4	1004	CLA	C3D-CAD	-2.19	1.39	1.45
19	H	1241	CLA	C1C-C2C	-2.19	1.40	1.44
19	B	1301	CLA	C4C-C3C	-2.18	1.40	1.44
19	1	1010	CLA	C3D-C2D	-2.18	1.34	1.40
19	B	1216	CLA	C1C-C2C	-2.18	1.40	1.44
19	B	1205	CLA	C3B-C2B	-2.17	1.37	1.40
19	B	1215	CLA	C3D-CAD	-2.17	1.39	1.45
19	F	1302	CLA	C3D-CAD	-2.17	1.39	1.45
19	A	1129	CLA	C3D-CAD	-2.17	1.39	1.45
19	A	1119	CLA	C4C-C3C	-2.17	1.41	1.45
19	A	1106	CLA	C1C-C2C	-2.17	1.40	1.44
19	A	1134	CLA	C3D-CAD	-2.16	1.39	1.45
19	A	1123	CLA	C4C-C3C	-2.16	1.41	1.45
19	B	1216	CLA	C3D-CAD	-2.16	1.39	1.45
19	1	1013	CLA	CBD-CGD	-2.16	1.44	1.52
19	2	2006	CLA	C3D-CAD	-2.15	1.39	1.45
19	A	1129	CLA	C4C-C3C	-2.14	1.41	1.45
19	L	1503	CLA	C3B-C2B	-2.14	1.37	1.40
19	1	1008	CLA	C3A-C2A	-2.14	1.48	1.54
19	B	1239	CLA	C3D-CAD	-2.14	1.39	1.45
19	B	1225	CLA	C3D-CAD	-2.14	1.39	1.45
19	B	1212	CLA	C1C-C2C	-2.14	1.40	1.44
19	B	1232	CLA	C3D-CAD	-2.13	1.39	1.45
19	A	1132	CLA	C3D-CAD	-2.13	1.39	1.45
19	1	1008	CLA	C1C-C2C	-2.13	1.40	1.44
19	K	1146	CLA	C3D-CAD	-2.12	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1131	CLA	C3D-CAD	-2.12	1.39	1.45
19	A	1116	CLA	C3D-CAD	-2.12	1.39	1.45
19	B	1228	CLA	C3D-CAD	-2.11	1.39	1.45
19	A	1106	CLA	C3D-CAD	-2.11	1.39	1.45
19	2	2014	CLA	C3D-CAD	-2.11	1.39	1.45
19	A	9012	CLA	C3D-CAD	-2.11	1.39	1.45
19	B	1209	CLA	C3D-CAD	-2.11	1.39	1.45
19	4	4001	CLA	C1C-C2C	-2.10	1.40	1.44
19	A	1124	CLA	C3D-CAD	-2.10	1.39	1.45
19	L	1501	CLA	C1C-C2C	-2.10	1.40	1.44
19	4	4002	CLA	C1C-NC	-2.09	1.34	1.37
19	R	1150	CLA	C1C-C2C	-2.09	1.40	1.44
19	4	1009	CLA	C3D-CAD	-2.09	1.39	1.45
19	3	3004	CLA	C3C-C4C	-2.09	1.38	1.43
19	A	1136	CLA	C3D-CAD	-2.09	1.39	1.45
19	3	2009	CLA	C3B-C2B	-2.08	1.37	1.40
19	A	1103	CLA	C4C-C3C	-2.07	1.41	1.45
19	A	9013	CLA	C3B-C2B	-2.07	1.37	1.40
19	1	1303	CLA	C2A-C1A	-2.07	1.48	1.52
19	B	1201	CLA	C1C-C2C	-2.07	1.40	1.44
19	L	1503	CLA	C1C-C2C	-2.07	1.40	1.44
19	A	1122	CLA	C3D-CAD	-2.07	1.39	1.45
19	4	4002	CLA	CAA-C2A	-2.06	1.50	1.54
19	B	1223	CLA	C3D-CAD	-2.06	1.39	1.45
19	A	1132	CLA	C4C-C3C	-2.06	1.41	1.45
21	I	6018	BCR	C21-C22	-2.06	1.33	1.35
19	H	1505	CLA	C1C-C2C	-2.06	1.40	1.44
19	F	1302	CLA	C3B-C2B	-2.06	1.37	1.40
19	4	4014	CLA	C3B-C2B	-2.06	1.37	1.40
19	J	1311	CLA	C3D-CAD	-2.05	1.40	1.45
19	3	3006	CLA	C3C-C4C	-2.05	1.38	1.43
19	A	1105	CLA	C1C-C2C	-2.05	1.40	1.44
19	H	1505	CLA	C3D-CAD	-2.05	1.40	1.45
19	B	1220	CLA	C2A-C1A	-2.05	1.48	1.52
19	A	1121	CLA	C3B-C2B	-2.05	1.37	1.40
19	B	1217	CLA	C3D-CAD	-2.05	1.40	1.45
19	A	1137	CLA	C3D-CAD	-2.04	1.40	1.45
19	A	1133	CLA	C3D-CAD	-2.03	1.40	1.45
19	4	1004	CLA	C3B-C2B	-2.03	1.37	1.40
21	A	6008	BCR	C40-C30	-2.03	1.49	1.53
19	2	2002	CLA	C3D-CAD	-2.03	1.40	1.45
19	B	1301	CLA	C3D-CAD	-2.03	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	F	6016	BCR	C11-C12	-2.02	1.29	1.34
19	A	1120	CLA	C3D-CAD	-2.02	1.40	1.45
19	A	1112	CLA	C4C-C3C	-2.02	1.41	1.45
21	B	6017	BCR	C39-C30	-2.01	1.49	1.53
21	A	6011	BCR	C31-C1	-2.01	1.49	1.53
19	L	1503	CLA	CBD-CGD	-2.01	1.45	1.52
19	3	3014	CLA	C2C-C1C	-2.01	1.38	1.43
19	F	1305	CLA	C3D-CAD	-2.01	1.40	1.45
19	B	1236	CLA	C3D-CAD	-2.01	1.40	1.45
19	A	1103	CLA	C3D-CAD	-2.01	1.40	1.45
19	A	1119	CLA	C3D-CAD	-2.01	1.40	1.45
19	B	1239	CLA	C1C-C2C	-2.01	1.40	1.44
19	2	2014	CLA	C3A-C2A	-2.00	1.48	1.54
22	2	7031	LMU	O5'-C1'	2.00	1.47	1.41
19	3	3006	CLA	C1B-CHB	2.00	1.47	1.43
22	K	7001	LMU	O1'-C1'	2.00	1.43	1.40
19	4	4005	CLA	C1B-CHB	2.00	1.47	1.43
22	R	7014	LMU	O1'-C1'	2.01	1.43	1.40
23	B	7101	LMG	O1-C1	2.01	1.43	1.40
19	L	1130	CLA	C2-C3	2.02	1.36	1.33
22	4	7053	LMU	O1'-C1'	2.02	1.43	1.40
22	E	7048	LMU	O1'-C1'	2.02	1.43	1.40
19	2	2007	CLA	C2-C3	2.02	1.36	1.33
22	C	7015	LMU	O1'-C1'	2.02	1.43	1.40
19	3	3001	CLA	C1B-CHB	2.03	1.47	1.43
22	H	7017	LMU	O1'-C1'	2.04	1.43	1.40
22	H	7011	LMU	O5B-C1B	2.04	1.47	1.41
22	N	7049	LMU	O1'-C1'	2.04	1.43	1.40
22	H	7011	LMU	O1'-C1'	2.05	1.43	1.40
21	J	6012	BCR	C32-C1	2.05	1.58	1.53
22	1	7004	LMU	O1'-C1'	2.06	1.43	1.40
19	K	1146	CLA	C1B-CHB	2.06	1.45	1.39
19	B	1201	CLA	C1B-CHB	2.06	1.45	1.39
22	H	7030	LMU	O1'-C1'	2.06	1.43	1.40
22	E	7037	LMU	O1'-C1'	2.06	1.43	1.40
21	F	6016	BCR	C11-C10	2.07	1.50	1.43
22	4	7052	LMU	C2-C1	2.07	1.60	1.50
19	4	4011	CLA	CHA-C1A	2.08	1.47	1.41
21	B	6006	BCR	C37-C22	2.09	1.55	1.50
19	3	3011	CLA	C1B-CHB	2.10	1.45	1.39
19	A	1309	CLA	C1B-CHB	2.10	1.48	1.43
19	1	1015	CLA	C1B-CHB	2.10	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	7040	LMU	O1'-C1'	2.11	1.43	1.40
19	1	1002	CLA	C1B-CHB	2.12	1.45	1.39
19	A	1149	CLA	CMA-C3A	2.12	1.58	1.53
19	A	1106	CLA	C1B-CHB	2.14	1.45	1.39
22	F	7036	LMU	O1'-C1'	2.15	1.44	1.40
19	A	1151	CLA	C1B-CHB	2.19	1.45	1.39
22	2	7027	LMU	O1'-C1'	2.20	1.44	1.40
19	4	4005	CLA	CHA-C1A	2.20	1.47	1.41
21	L	6019	BCR	C11-C10	2.22	1.50	1.43
19	2	2010	CLA	C1B-CHB	2.22	1.48	1.43
19	3	3004	CLA	CHA-C1A	2.23	1.47	1.41
22	R	7024	LMU	O1'-C1'	2.23	1.44	1.40
19	2	2013	CLA	C1B-CHB	2.23	1.46	1.39
22	K	7001	LMU	O3B-C3B	2.23	1.48	1.43
19	3	3004	CLA	C4B-CHC	2.23	1.48	1.43
19	B	1218	CLA	C1B-CHB	2.25	1.46	1.39
19	3	1147	CLA	C4B-CHC	2.25	1.46	1.39
19	B	1221	CLA	C1B-CHB	2.26	1.46	1.39
22	A	7010	LMU	C4-C3	2.26	1.64	1.51
19	B	1227	CLA	C1B-CHB	2.27	1.46	1.39
19	1	1008	CLA	C2-C3	2.27	1.37	1.33
19	2	2002	CLA	C1B-CHB	2.28	1.46	1.39
19	F	1240	CLA	C1B-CHB	2.28	1.46	1.39
19	4	4013	CLA	C1B-CHB	2.29	1.48	1.43
19	1	1001	CLA	C1B-CHB	2.29	1.46	1.39
21	I	6021	BCR	C11-C10	2.32	1.50	1.43
19	3	2009	CLA	C4-C3	2.32	1.56	1.50
22	B	7012	LMU	O1'-C1'	2.33	1.44	1.40
19	A	9022	CLA	C1B-CHB	2.33	1.46	1.39
19	B	1238	CLA	C1B-CHB	2.33	1.46	1.39
19	2	2003	CLA	CHA-C1A	2.34	1.48	1.41
19	2	2005	CLA	CHA-C1A	2.35	1.48	1.41
19	J	1308	CLA	C1B-CHB	2.35	1.46	1.39
19	3	1147	CLA	C1B-CHB	2.35	1.46	1.39
19	B	1203	CLA	C1B-CHB	2.35	1.46	1.39
22	A	7045	LMU	O1'-C1'	2.35	1.44	1.40
19	L	1502	CLA	C1B-CHB	2.36	1.46	1.39
19	1	1001	CLA	O1D-CGD	2.38	1.27	1.21
19	B	1206	CLA	C1B-CHB	2.39	1.46	1.39
19	A	9012	CLA	C1B-CHB	2.39	1.46	1.39
22	G	7026	LMU	O1'-C1'	2.39	1.44	1.40
19	A	1309	CLA	CHA-C1A	2.40	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	9013	CLA	C1B-CHB	2.40	1.46	1.39
19	H	1207	CLA	C1B-CHB	2.40	1.46	1.39
19	2	2010	CLA	CHA-C1A	2.40	1.48	1.41
22	H	7030	LMU	O6B-C6B	2.41	1.52	1.42
22	4	7018	LMU	O1'-C1'	2.41	1.44	1.40
19	B	1210	CLA	C1B-CHB	2.42	1.46	1.39
22	R	7014	LMU	O2B-C2B	2.43	1.48	1.43
19	A	1102	CLA	C1B-CHB	2.44	1.46	1.39
21	F	6016	BCR	C39-C30	2.44	1.59	1.53
19	4	4010	CLA	CHA-C1A	2.44	1.48	1.41
19	A	1110	CLA	C1B-CHB	2.44	1.46	1.39
22	K	7047	LMU	O1'-C1'	2.45	1.44	1.40
22	G	7026	LMU	O3B-C3B	2.45	1.48	1.43
22	H	7043	LMU	O1'-C1'	2.45	1.44	1.40
19	B	1220	CLA	C1B-CHB	2.46	1.46	1.39
19	A	1141	CLA	C1B-CHB	2.46	1.46	1.39
19	B	1221	CLA	C2-C3	2.47	1.37	1.33
19	3	3015	CLA	C1B-CHB	2.47	1.48	1.43
19	3	3016	CLA	C1B-CHB	2.48	1.46	1.39
19	B	1202	CLA	C1B-CHB	2.48	1.46	1.39
19	3	3014	CLA	CHA-C1A	2.48	1.48	1.41
22	4	7009	LMU	O6'-C6'	2.50	1.53	1.42
19	A	1123	CLA	C1B-CHB	2.50	1.46	1.39
19	A	1126	CLA	C1B-CHB	2.50	1.46	1.39
22	L	7029	LMU	O1'-C1'	2.50	1.44	1.40
19	4	4012	CLA	C1B-CHB	2.51	1.46	1.39
19	A	1122	CLA	C1B-CHB	2.51	1.46	1.39
19	4	1004	CLA	C5-C3	2.51	1.56	1.51
19	A	9023	CLA	C1B-CHB	2.51	1.46	1.39
19	A	1133	CLA	C1B-CHB	2.52	1.46	1.39
19	B	1222	CLA	CBC-CAC	2.52	1.63	1.51
19	2	2001	CLA	C1B-CHB	2.53	1.46	1.39
19	A	1120	CLA	C1B-CHB	2.53	1.46	1.39
19	3	2009	CLA	C1B-CHB	2.54	1.46	1.39
19	3	3002	CLA	CHA-C1A	2.54	1.48	1.41
19	B	1229	CLA	C1B-CHB	2.54	1.46	1.39
19	B	1211	CLA	C1B-CHB	2.54	1.46	1.39
22	2	7046	LMU	O1'-C1'	2.54	1.44	1.40
19	2	1307	CLA	CHA-C1A	2.54	1.48	1.41
22	4	7052	LMU	O1'-C1	2.55	1.50	1.42
19	A	1131	CLA	C1B-CHB	2.55	1.46	1.39
19	L	1503	CLA	C1B-CHB	2.55	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	1004	CLA	C1B-CHB	2.56	1.46	1.39
19	3	1147	CLA	O2A-CGA	2.56	1.41	1.32
19	K	1142	CLA	C1B-CHB	2.57	1.46	1.39
19	A	1104	CLA	C1B-CHB	2.57	1.46	1.39
19	B	1219	CLA	C1B-CHB	2.57	1.46	1.39
19	F	1302	CLA	C1B-CHB	2.57	1.46	1.39
19	A	1134	CLA	C1B-CHB	2.57	1.46	1.39
19	3	3008	CLA	C1B-CHB	2.58	1.47	1.39
19	B	1205	CLA	C1B-CHB	2.58	1.47	1.39
22	R	7025	LMU	O1'-C1'	2.59	1.44	1.40
19	1	1013	CLA	C2-C3	2.59	1.38	1.33
19	4	4004	CLA	CHA-C1A	2.59	1.49	1.41
19	2	2011	CLA	CHA-C1A	2.60	1.49	1.41
19	3	3015	CLA	CHA-C1A	2.60	1.49	1.41
19	4	1009	CLA	C1B-CHB	2.60	1.47	1.39
19	3	3010	CLA	CHA-C1A	2.60	1.49	1.41
19	B	1214	CLA	C1B-CHB	2.60	1.47	1.39
19	A	1136	CLA	C1B-CHB	2.60	1.47	1.39
19	A	1119	CLA	C1B-CHB	2.60	1.47	1.39
19	A	1111	CLA	C1B-CHB	2.61	1.47	1.39
19	A	1109	CLA	C1B-CHB	2.61	1.47	1.39
19	1	1001	CLA	C4B-CHC	2.61	1.47	1.39
19	A	1139	CLA	C1B-CHB	2.61	1.47	1.39
19	B	1224	CLA	C1B-CHB	2.61	1.47	1.39
19	L	1130	CLA	C1B-CHB	2.62	1.47	1.39
22	H	7032	LMU	O1'-C1'	2.62	1.44	1.40
19	4	4003	CLA	C1B-CHB	2.62	1.47	1.39
19	A	1117	CLA	C1B-CHB	2.62	1.47	1.39
19	F	1305	CLA	C1B-CHB	2.62	1.47	1.39
21	B	6006	BCR	C23-C22	2.62	1.51	1.45
19	1	1015	CLA	CHA-C1A	2.62	1.49	1.41
19	A	1108	CLA	C1B-CHB	2.63	1.47	1.39
19	B	1209	CLA	C1B-CHB	2.63	1.47	1.39
19	B	9010	CLA	C1B-CHB	2.64	1.47	1.39
19	4	1004	CLA	C2-C3	2.64	1.38	1.33
19	G	1242	CLA	C1B-CHB	2.64	1.47	1.39
19	I	1204	CLA	C1B-CHB	2.64	1.47	1.39
19	A	9011	CLA	C1B-CHB	2.64	1.47	1.39
19	A	1112	CLA	C1B-CHB	2.64	1.47	1.39
19	A	1124	CLA	C1B-CHB	2.65	1.47	1.39
19	J	1311	CLA	C1B-CHB	2.65	1.47	1.39
19	L	1503	CLA	CMA-C3A	2.66	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1127	CLA	C1B-CHB	2.66	1.47	1.39
19	K	1143	CLA	C1B-CHB	2.66	1.47	1.39
19	A	1140	CLA	C1B-CHB	2.67	1.47	1.39
19	4	4013	CLA	CHA-C1A	2.68	1.49	1.41
19	B	1231	CLA	C1B-CHB	2.69	1.47	1.39
19	B	1223	CLA	C1B-CHB	2.70	1.47	1.39
19	A	1132	CLA	C1B-CHB	2.70	1.47	1.39
22	A	7044	LMU	O1'-C1'	2.71	1.45	1.40
19	B	1228	CLA	C1B-CHB	2.71	1.47	1.39
19	A	1137	CLA	C1B-CHB	2.71	1.47	1.39
22	4	7052	LMU	O1'-C1'	2.71	1.45	1.40
19	4	4014	CLA	C1B-CHB	2.72	1.47	1.39
19	3	3012	CLA	C4B-CHC	2.73	1.49	1.43
19	1	1005	CLA	C1B-CHB	2.73	1.47	1.39
21	B	6020	BCR	C11-C10	2.73	1.52	1.43
19	H	1241	CLA	C1B-CHB	2.74	1.47	1.39
19	A	1135	CLA	C1B-CHB	2.75	1.47	1.39
19	4	1306	CLA	C1B-CHB	2.75	1.47	1.39
19	A	1128	CLA	C1B-CHB	2.76	1.47	1.39
19	2	2004	CLA	C1B-CHB	2.76	1.47	1.39
19	B	1212	CLA	C1B-CHB	2.78	1.47	1.39
19	1	1014	CLA	C1B-CHB	2.79	1.47	1.39
19	B	1208	CLA	C1B-CHB	2.79	1.47	1.39
19	2	1307	CLA	C4B-CHC	2.79	1.49	1.43
19	B	1230	CLA	C1B-CHB	2.80	1.47	1.39
19	A	1138	CLA	C1B-CHB	2.81	1.47	1.39
19	A	1129	CLA	C1B-CHB	2.81	1.47	1.39
21	F	6014	BCR	C40-C30	2.82	1.59	1.53
19	2	2007	CLA	C1B-CHB	2.82	1.47	1.39
19	3	3005	CLA	CHA-C1A	2.82	1.49	1.41
19	B	1232	CLA	C1B-CHB	2.83	1.47	1.39
19	1	1003	CLA	C1B-CHB	2.83	1.47	1.39
19	A	1113	CLA	C1B-CHB	2.83	1.47	1.39
19	3	3012	CLA	CHA-C1A	2.83	1.49	1.41
19	B	1217	CLA	C1B-CHB	2.84	1.47	1.39
19	A	1125	CLA	C1B-CHB	2.85	1.47	1.39
19	3	3001	CLA	CHA-C1A	2.85	1.49	1.41
19	3	3003	CLA	C1B-CHB	2.85	1.47	1.39
19	B	1226	CLA	C1B-CHB	2.85	1.47	1.39
19	A	1103	CLA	C1B-CHB	2.86	1.47	1.39
19	3	1147	CLA	CHD-C4C	2.86	1.47	1.41
19	B	1236	CLA	C1B-CHB	2.89	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	G	7051	LMU	O1'-C1'	2.89	1.45	1.40
19	1	1008	CLA	C1B-CHB	2.89	1.47	1.39
19	I	1204	CLA	OBD-CAD	2.90	1.26	1.22
19	B	1239	CLA	C1B-CHB	2.90	1.47	1.39
19	1	1012	CLA	C1B-CHB	2.90	1.47	1.39
19	B	1213	CLA	C1B-CHB	2.91	1.47	1.39
19	B	1235	CLA	C1B-CHB	2.91	1.47	1.39
19	B	1222	CLA	C1B-CHB	2.92	1.47	1.39
19	3	3006	CLA	CHA-C1A	2.93	1.50	1.41
19	A	1116	CLA	C1B-CHB	2.93	1.47	1.39
19	R	1144	CLA	C1B-CHB	2.94	1.47	1.39
19	2	2008	CLA	CHA-C1A	2.94	1.50	1.41
19	2	2006	CLA	C1B-CHB	2.95	1.48	1.39
19	B	1301	CLA	C1B-CHB	2.95	1.48	1.39
19	3	3010	CLA	C4B-CHC	2.95	1.49	1.43
22	4	7009	LMU	O1'-C1'	2.96	1.45	1.40
19	B	1215	CLA	C1B-CHB	2.96	1.48	1.39
19	2	4009	CLA	C1B-CHB	2.97	1.48	1.39
19	A	1107	CLA	C1B-CHB	2.98	1.48	1.39
19	L	1148	CLA	CMA-C3A	2.98	1.60	1.53
19	2	2012	CLA	C1B-CHB	2.99	1.48	1.39
19	A	1105	CLA	C1B-CHB	3.00	1.48	1.39
19	1	1006	CLA	C1B-CHB	3.01	1.48	1.39
19	H	1505	CLA	C1B-CHB	3.01	1.48	1.39
19	B	1233	CLA	C1B-CHB	3.02	1.48	1.39
19	2	2008	CLA	C4B-CHC	3.02	1.50	1.43
19	4	4015	CLA	C1B-CHB	3.02	1.48	1.39
19	3	3013	CLA	C1B-CHB	3.03	1.48	1.39
19	3	1118	CLA	C1B-CHB	3.03	1.48	1.39
19	1	1310	CLA	C4B-CHC	3.03	1.50	1.43
19	K	3009	CLA	C1B-CHB	3.04	1.48	1.39
19	A	1101	CLA	C1B-CHB	3.04	1.48	1.39
21	L	6019	BCR	C24-C23	3.05	1.42	1.33
22	A	7010	LMU	O1'-C1'	3.05	1.45	1.40
19	A	1107	CLA	C4B-CHC	3.06	1.48	1.39
19	A	1309	CLA	C4B-CHC	3.07	1.50	1.43
22	4	7019	LMU	O1'-C1'	3.07	1.45	1.40
19	A	1149	CLA	C1B-CHB	3.09	1.48	1.39
19	1	1303	CLA	C4B-CHC	3.10	1.48	1.39
19	4	4006	CLA	C1B-CHB	3.11	1.48	1.39
19	2	2003	CLA	C4B-CHC	3.11	1.50	1.43
19	1	1010	CLA	C4B-CHC	3.12	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	3017	CLA	C4B-CHC	3.13	1.48	1.39
19	1	1015	CLA	C4B-CHC	3.13	1.50	1.43
19	4	4004	CLA	C4B-CHC	3.13	1.50	1.43
19	4	4007	CLA	C1B-CHB	3.14	1.48	1.39
19	4	4002	CLA	C4B-CHC	3.14	1.48	1.39
19	1	1007	CLA	C1B-CHB	3.14	1.48	1.39
21	B	6017	BCR	C32-C1	3.15	1.60	1.53
19	2	2005	CLA	C4B-CHC	3.17	1.50	1.43
19	B	1234	CLA	C1B-CHB	3.17	1.48	1.39
19	3	3007	CLA	C1B-CHB	3.18	1.48	1.39
19	3	3005	CLA	C4B-CHC	3.18	1.50	1.43
19	A	1237	CLA	C1B-CHB	3.18	1.48	1.39
19	2	2010	CLA	C4B-CHC	3.18	1.50	1.43
19	B	1216	CLA	C1B-CHB	3.19	1.48	1.39
19	B	1203	CLA	C4B-CHC	3.22	1.48	1.39
19	4	4001	CLA	C1B-CHB	3.22	1.48	1.39
19	4	1304	CLA	C4B-CHC	3.22	1.48	1.39
19	B	1235	CLA	OBD-CAD	3.23	1.27	1.22
19	1	1013	CLA	C1B-CHB	3.24	1.48	1.39
19	A	1121	CLA	C1B-CHB	3.25	1.48	1.39
21	A	6011	BCR	C8-C7	3.25	1.42	1.33
19	B	1235	CLA	C4B-CHC	3.25	1.48	1.39
19	4	4010	CLA	C4B-CHC	3.27	1.50	1.43
19	L	1501	CLA	C1B-CHB	3.27	1.48	1.39
22	2	7031	LMU	O1'-C1'	3.27	1.46	1.40
19	1	1013	CLA	C4B-CHC	3.27	1.48	1.39
19	L	1504	CLA	C1B-CHB	3.29	1.48	1.39
19	A	1103	CLA	OBD-CAD	3.30	1.27	1.22
19	B	1234	CLA	C4B-CHC	3.31	1.49	1.39
19	3	3006	CLA	C4B-CHC	3.32	1.50	1.43
19	3	3013	CLA	C4B-CHC	3.33	1.49	1.39
19	B	1225	CLA	C1B-CHB	3.34	1.49	1.39
19	R	1150	CLA	C1B-CHB	3.35	1.49	1.39
19	B	1203	CLA	OBD-CAD	3.36	1.27	1.22
19	4	4002	CLA	OBD-CAD	3.37	1.27	1.22
19	3	3015	CLA	C4B-CHC	3.37	1.50	1.43
19	4	4013	CLA	C4B-CHC	3.37	1.50	1.43
19	A	1103	CLA	C4B-CHC	3.37	1.49	1.39
19	4	1306	CLA	C4B-CHC	3.39	1.49	1.39
19	B	1226	CLA	C4B-CHC	3.40	1.49	1.39
19	1	1002	CLA	C4B-CHC	3.42	1.49	1.39
19	A	1132	CLA	C4B-CHC	3.44	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	1011	CLA	C4B-CHC	3.45	1.49	1.39
19	3	3014	CLA	C4B-CHC	3.46	1.50	1.43
19	B	1215	CLA	OBD-CAD	3.47	1.27	1.22
19	A	1125	CLA	OBD-CAD	3.49	1.27	1.22
19	B	1202	CLA	C4B-CHC	3.49	1.49	1.39
19	4	4011	CLA	C4B-CHC	3.50	1.51	1.43
19	4	4005	CLA	C4B-CHC	3.50	1.51	1.43
19	A	1121	CLA	C4B-CHC	3.51	1.49	1.39
19	4	4015	CLA	OBD-CAD	3.54	1.27	1.22
19	2	2007	CLA	C4B-CHC	3.55	1.49	1.39
19	B	1236	CLA	OBD-CAD	3.55	1.27	1.22
19	A	1149	CLA	C4B-CHC	3.55	1.49	1.39
19	B	1210	CLA	OBD-CAD	3.55	1.27	1.22
19	H	1145	CLA	C4B-CHC	3.55	1.49	1.39
19	A	1101	CLA	C4B-CHC	3.55	1.49	1.39
19	B	1239	CLA	C4B-CHC	3.57	1.49	1.39
19	B	1216	CLA	OBD-CAD	3.58	1.27	1.22
19	3	3001	CLA	C4B-CHC	3.58	1.51	1.43
19	A	9023	CLA	C4B-CHC	3.59	1.49	1.39
19	J	1308	CLA	C4B-CHC	3.60	1.49	1.39
19	3	3013	CLA	OBD-CAD	3.60	1.27	1.22
19	A	1117	CLA	C4B-CHC	3.61	1.49	1.39
19	A	1131	CLA	C4B-CHC	3.61	1.49	1.39
19	4	4015	CLA	C4B-CHC	3.63	1.49	1.39
19	B	1221	CLA	C4B-CHC	3.63	1.49	1.39
19	3	3007	CLA	C4B-CHC	3.64	1.49	1.39
19	3	3011	CLA	C4B-CHC	3.66	1.49	1.39
19	B	1215	CLA	C4B-CHC	3.67	1.50	1.39
19	A	1237	CLA	C4B-CHC	3.67	1.50	1.39
19	A	1111	CLA	C4B-CHC	3.67	1.50	1.39
19	B	1216	CLA	C4B-CHC	3.67	1.50	1.39
19	B	1205	CLA	C4B-CHC	3.68	1.50	1.39
19	K	1143	CLA	C4B-CHC	3.68	1.50	1.39
19	B	1209	CLA	C4B-CHC	3.68	1.50	1.39
19	B	1230	CLA	C4B-CHC	3.69	1.50	1.39
19	4	4003	CLA	C4B-CHC	3.69	1.50	1.39
19	A	1129	CLA	C4B-CHC	3.69	1.50	1.39
19	B	1239	CLA	OBD-CAD	3.69	1.28	1.22
19	A	1104	CLA	C4B-CHC	3.69	1.50	1.39
19	3	3002	CLA	C4B-CHC	3.70	1.51	1.43
19	A	1133	CLA	C4B-CHC	3.70	1.50	1.39
19	A	1127	CLA	C4B-CHC	3.71	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	7052	LMU	O6'-C6'	3.71	1.58	1.42
19	B	1201	CLA	C4B-CHC	3.71	1.50	1.39
19	B	1228	CLA	C4B-CHC	3.71	1.50	1.39
19	2	2011	CLA	C4B-CHC	3.72	1.51	1.43
19	A	1139	CLA	C4B-CHC	3.72	1.50	1.39
19	A	1123	CLA	C4B-CHC	3.72	1.50	1.39
19	B	1211	CLA	C4B-CHC	3.73	1.50	1.39
19	4	1004	CLA	C4B-CHC	3.73	1.50	1.39
19	2	4009	CLA	C4B-CHC	3.73	1.50	1.39
19	B	1206	CLA	O2A-CGA	3.73	1.44	1.33
19	A	1105	CLA	C4B-CHC	3.73	1.50	1.39
19	A	1128	CLA	C4B-CHC	3.74	1.50	1.39
19	A	1151	CLA	C4B-CHC	3.74	1.50	1.39
19	2	2014	CLA	C4B-CHC	3.74	1.50	1.39
19	B	1213	CLA	O2A-CGA	3.74	1.45	1.32
19	F	1305	CLA	O2A-CGA	3.75	1.44	1.33
19	A	1134	CLA	C4B-CHC	3.75	1.50	1.39
19	A	1136	CLA	C4B-CHC	3.75	1.50	1.39
19	2	2013	CLA	C4B-CHC	3.75	1.50	1.39
19	B	1219	CLA	C4B-CHC	3.75	1.50	1.39
19	K	1146	CLA	C4B-CHC	3.75	1.50	1.39
19	2	2012	CLA	C4B-CHC	3.76	1.50	1.39
19	A	1138	CLA	C4B-CHC	3.76	1.50	1.39
19	A	1109	CLA	C4B-CHC	3.76	1.50	1.39
19	H	1207	CLA	C4B-CHC	3.76	1.50	1.39
19	4	4007	CLA	C4B-CHC	3.76	1.50	1.39
19	2	2005	CLA	CHD-C4C	3.76	1.50	1.41
19	3	3008	CLA	C4B-CHC	3.76	1.50	1.39
19	B	1225	CLA	C4B-CHC	3.77	1.50	1.39
19	B	1220	CLA	O2D-CGD	3.77	1.42	1.33
19	A	1125	CLA	C4B-CHC	3.78	1.50	1.39
19	A	1129	CLA	OBD-CAD	3.78	1.28	1.22
19	1	1010	CLA	OBD-CAD	3.79	1.28	1.22
19	B	1217	CLA	OBD-CAD	3.79	1.28	1.22
19	L	1130	CLA	C4B-CHC	3.79	1.50	1.39
19	F	1305	CLA	C4B-CHC	3.79	1.50	1.39
19	4	1304	CLA	O2A-CGA	3.79	1.44	1.33
19	1	1014	CLA	C4B-CHC	3.79	1.50	1.39
19	A	1123	CLA	OBD-CAD	3.80	1.28	1.22
19	B	9010	CLA	C4B-CHC	3.80	1.50	1.39
19	B	1222	CLA	C4B-CHC	3.81	1.50	1.39
19	F	1240	CLA	C4B-CHC	3.81	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	J	1311	CLA	C4B-CHC	3.81	1.50	1.39
19	A	1137	CLA	C4B-CHC	3.81	1.50	1.39
19	3	3008	CLA	OBD-CAD	3.82	1.28	1.22
19	1	1013	CLA	CHD-C4C	3.83	1.50	1.41
19	3	2009	CLA	OBD-CAD	3.83	1.28	1.22
19	1	1005	CLA	C4B-CHC	3.83	1.50	1.39
19	4	4014	CLA	C4B-CHC	3.83	1.50	1.39
19	4	1009	CLA	C4B-CHC	3.83	1.50	1.39
19	1	1001	CLA	O2A-CGA	3.83	1.45	1.32
19	3	2009	CLA	C4B-CHC	3.83	1.50	1.39
19	3	1118	CLA	C4B-CHC	3.83	1.50	1.39
19	4	1004	CLA	O2D-CED	3.84	1.54	1.45
19	L	1504	CLA	C4B-CHC	3.84	1.50	1.39
19	B	1218	CLA	C4B-CHC	3.84	1.50	1.39
19	A	1141	CLA	C4B-CHC	3.85	1.50	1.39
19	4	4015	CLA	CHD-C4C	3.86	1.50	1.41
19	B	1220	CLA	C4B-CHC	3.86	1.50	1.39
19	1	1006	CLA	C4B-CHC	3.86	1.50	1.39
19	A	1106	CLA	C4B-CHC	3.86	1.50	1.39
19	B	1220	CLA	CHD-C4C	3.86	1.50	1.41
19	A	9012	CLA	C4B-CHC	3.86	1.50	1.39
19	B	9010	CLA	O2A-CGA	3.86	1.45	1.33
19	2	2001	CLA	C4B-CHC	3.86	1.50	1.39
19	3	3016	CLA	C4B-CHC	3.86	1.50	1.39
19	A	9013	CLA	O2A-CGA	3.87	1.45	1.33
19	A	1115	CLA	C4B-CHC	3.87	1.50	1.39
19	2	2014	CLA	O2A-CGA	3.87	1.45	1.33
19	B	1225	CLA	O2A-CGA	3.88	1.45	1.33
19	A	1126	CLA	O2A-CGA	3.88	1.45	1.33
19	A	1115	CLA	OBD-CAD	3.88	1.28	1.22
19	B	1223	CLA	C4B-CHC	3.89	1.50	1.39
19	A	9023	CLA	OBD-CAD	3.89	1.28	1.22
19	B	1206	CLA	C4B-CHC	3.89	1.50	1.39
19	K	1142	CLA	C4B-CHC	3.89	1.50	1.39
23	B	7101	LMG	O8-C28	3.90	1.45	1.33
19	3	3013	CLA	CHD-C4C	3.90	1.50	1.41
19	2	2006	CLA	C4B-CHC	3.91	1.50	1.39
19	H	1241	CLA	C4B-CHC	3.91	1.50	1.39
19	R	1144	CLA	C4B-CHC	3.91	1.50	1.39
19	A	9013	CLA	C4B-CHC	3.92	1.50	1.39
19	1	1007	CLA	C4B-CHC	3.92	1.50	1.39
19	B	1227	CLA	C4B-CHC	3.92	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1124	CLA	C4B-CHC	3.93	1.50	1.39
19	A	1135	CLA	C4B-CHC	3.93	1.50	1.39
19	A	1140	CLA	C4B-CHC	3.93	1.50	1.39
19	A	1106	CLA	OBD-CAD	3.94	1.28	1.22
19	A	9022	CLA	C4B-CHC	3.94	1.50	1.39
19	A	9011	CLA	OBD-CAD	3.94	1.28	1.22
19	A	1105	CLA	O2A-CGA	3.94	1.46	1.32
19	A	1111	CLA	OBD-CAD	3.95	1.28	1.22
19	A	1126	CLA	C4B-CHC	3.95	1.50	1.39
19	A	1132	CLA	OBD-CAD	3.95	1.28	1.22
19	A	1117	CLA	OBD-CAD	3.96	1.28	1.22
19	A	1122	CLA	C4B-CHC	3.96	1.50	1.39
21	B	6006	BCR	C24-C23	3.96	1.44	1.33
19	A	1113	CLA	C4B-CHC	3.96	1.50	1.39
19	B	1220	CLA	O2A-CGA	3.96	1.45	1.33
19	B	1231	CLA	C4B-CHC	3.97	1.50	1.39
19	B	1214	CLA	C4B-CHC	3.97	1.50	1.39
19	A	1124	CLA	O2A-CGA	3.97	1.45	1.33
19	H	1145	CLA	O2A-CGA	3.98	1.45	1.33
19	1	1010	CLA	O2A-CGA	3.98	1.46	1.32
19	B	1228	CLA	OBD-CAD	3.98	1.28	1.22
19	A	1115	CLA	O2A-CGA	3.99	1.45	1.33
19	B	1223	CLA	OBD-CAD	3.99	1.28	1.22
19	1	1008	CLA	C4B-CHC	3.99	1.50	1.39
19	J	1308	CLA	CHD-C4C	3.99	1.50	1.41
19	B	1238	CLA	C4B-CHC	3.99	1.50	1.39
19	A	1136	CLA	O2A-CGA	4.00	1.45	1.33
19	3	3003	CLA	C4B-CHC	4.00	1.50	1.39
19	2	2008	CLA	CHD-C4C	4.00	1.50	1.41
19	B	1232	CLA	C4B-CHC	4.01	1.50	1.39
19	2	2014	CLA	CHD-C4C	4.01	1.50	1.41
19	2	2011	CLA	CHD-C4C	4.01	1.50	1.41
19	A	1112	CLA	C4B-CHC	4.02	1.50	1.39
19	4	4013	CLA	CHD-C4C	4.02	1.50	1.41
19	B	1224	CLA	O2A-CGA	4.02	1.45	1.33
19	B	1203	CLA	O2A-CGA	4.02	1.45	1.33
19	3	3010	CLA	CHD-C4C	4.02	1.50	1.41
19	4	4001	CLA	C4B-CHC	4.02	1.50	1.39
19	J	1308	CLA	O2A-CGA	4.02	1.45	1.33
19	3	3017	CLA	O2A-CGA	4.02	1.45	1.33
19	1	1014	CLA	CHD-C4C	4.02	1.50	1.41
19	3	3013	CLA	O2A-CGA	4.03	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1234	CLA	OBD-CAD	4.03	1.28	1.22
19	B	1226	CLA	O2A-CGA	4.03	1.45	1.33
19	4	4006	CLA	C4B-CHC	4.03	1.51	1.39
19	1	1001	CLA	CHC-C1C	4.03	1.48	1.35
19	4	4002	CLA	O2A-CGA	4.04	1.45	1.33
19	B	1213	CLA	C4B-CHC	4.04	1.51	1.39
19	L	1148	CLA	OBD-CAD	4.05	1.28	1.22
19	2	2012	CLA	OBD-CAD	4.05	1.28	1.22
19	K	1146	CLA	O2A-CGA	4.05	1.45	1.33
19	L	1501	CLA	C4B-CHC	4.06	1.51	1.39
19	A	9011	CLA	O2A-CGA	4.06	1.45	1.33
19	B	1222	CLA	OBD-CAD	4.06	1.28	1.22
19	2	1307	CLA	CHD-C4C	4.06	1.50	1.41
19	A	1237	CLA	O2A-CGA	4.06	1.45	1.33
19	B	1226	CLA	CHD-C4C	4.06	1.50	1.41
19	1	1001	CLA	CHD-C4C	4.06	1.50	1.41
19	B	1301	CLA	C4B-CHC	4.07	1.51	1.39
19	A	1137	CLA	O2A-CGA	4.07	1.45	1.33
19	B	1236	CLA	C4B-CHC	4.07	1.51	1.39
19	B	1215	CLA	O2A-CGA	4.07	1.45	1.33
19	A	1108	CLA	C4B-CHC	4.07	1.51	1.39
19	4	4012	CLA	C4B-CHC	4.07	1.51	1.39
19	A	1116	CLA	C4B-CHC	4.07	1.51	1.39
19	2	2004	CLA	C4B-CHC	4.08	1.51	1.39
19	B	1202	CLA	OBD-CAD	4.09	1.28	1.22
19	L	1503	CLA	C4B-CHC	4.09	1.51	1.39
19	K	1143	CLA	O2A-CGA	4.09	1.45	1.33
19	L	1502	CLA	C4B-CHC	4.10	1.51	1.39
19	B	1227	CLA	OBD-CAD	4.10	1.28	1.22
19	3	3008	CLA	O2A-CGA	4.10	1.45	1.33
19	A	1140	CLA	OBD-CAD	4.10	1.28	1.22
19	B	1208	CLA	C4B-CHC	4.12	1.51	1.39
19	1	1011	CLA	CHD-C4C	4.12	1.50	1.41
19	B	1206	CLA	OBD-CAD	4.12	1.28	1.22
19	1	1010	CLA	CHD-C4C	4.12	1.50	1.41
19	J	1308	CLA	OBD-CAD	4.12	1.28	1.22
19	4	4011	CLA	CHD-C4C	4.12	1.50	1.41
19	B	1224	CLA	C4B-CHC	4.13	1.51	1.39
19	1	1012	CLA	OBD-CAD	4.13	1.28	1.22
19	H	1505	CLA	C4B-CHC	4.13	1.51	1.39
19	B	1238	CLA	OBD-CAD	4.13	1.28	1.22
19	A	1109	CLA	OBD-CAD	4.13	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	3013	CLA	CHC-C1C	4.13	1.48	1.35
19	A	1137	CLA	OBD-CAD	4.14	1.28	1.22
19	L	1501	CLA	CHD-C4C	4.14	1.50	1.41
19	A	1102	CLA	C4B-CHC	4.14	1.51	1.39
19	2	2004	CLA	OBD-CAD	4.14	1.28	1.22
19	A	1119	CLA	C4B-CHC	4.14	1.51	1.39
19	L	1148	CLA	O2D-CGD	4.14	1.43	1.33
19	F	1305	CLA	CHD-C4C	4.14	1.51	1.41
19	4	4002	CLA	CHD-C4C	4.14	1.51	1.41
19	K	1146	CLA	OBD-CAD	4.15	1.28	1.22
19	A	1124	CLA	OBD-CAD	4.15	1.28	1.22
19	A	1136	CLA	OBD-CAD	4.15	1.28	1.22
19	1	1011	CLA	OBD-CAD	4.15	1.28	1.22
19	L	1148	CLA	C4B-CHC	4.15	1.51	1.39
19	B	1239	CLA	CHD-C4C	4.15	1.51	1.41
19	A	1104	CLA	O2A-CGA	4.17	1.45	1.33
19	A	1110	CLA	C4B-CHC	4.17	1.51	1.39
19	B	1236	CLA	CHD-C4C	4.17	1.51	1.41
19	A	1133	CLA	OBD-CAD	4.18	1.28	1.22
19	A	1309	CLA	CHD-C4C	4.18	1.51	1.41
19	3	1147	CLA	O2D-CGD	4.18	1.43	1.33
19	A	1107	CLA	CHC-C1C	4.18	1.48	1.35
19	B	1212	CLA	OBD-CAD	4.18	1.28	1.22
19	2	2013	CLA	CHD-C4C	4.18	1.51	1.41
19	2	2006	CLA	O2A-CGA	4.19	1.45	1.33
19	R	1144	CLA	OBD-CAD	4.19	1.28	1.22
19	4	1004	CLA	O2A-CGA	4.19	1.45	1.33
19	A	1138	CLA	O2A-CGA	4.19	1.45	1.33
19	A	1125	CLA	CHD-C4C	4.19	1.51	1.41
19	L	1501	CLA	OBD-CAD	4.20	1.28	1.22
19	H	1145	CLA	OBD-CAD	4.20	1.28	1.22
19	2	2002	CLA	C4B-CHC	4.20	1.51	1.39
19	B	1205	CLA	OBD-CAD	4.21	1.28	1.22
19	2	2001	CLA	O2A-CGA	4.21	1.46	1.33
19	B	1217	CLA	C4B-CHC	4.22	1.51	1.39
19	A	1139	CLA	O2A-CGA	4.22	1.46	1.33
19	H	1145	CLA	CHD-C4C	4.22	1.51	1.41
19	4	4015	CLA	O2D-CGD	4.22	1.44	1.33
19	A	1135	CLA	O2A-CGA	4.23	1.46	1.33
19	B	1225	CLA	CHD-C4C	4.24	1.51	1.41
19	3	3015	CLA	CHD-C4C	4.24	1.51	1.41
19	I	1204	CLA	C4B-CHC	4.24	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1140	CLA	O2A-CGA	4.24	1.46	1.33
19	F	1302	CLA	C4B-CHC	4.24	1.51	1.39
19	B	1215	CLA	CHD-C4C	4.24	1.51	1.41
19	A	1149	CLA	OBD-CAD	4.24	1.28	1.22
19	A	1139	CLA	OBD-CAD	4.25	1.28	1.22
19	B	1226	CLA	OBD-CAD	4.25	1.28	1.22
19	B	1205	CLA	O2A-CGA	4.25	1.46	1.33
19	3	1147	CLA	CHC-C1C	4.25	1.48	1.35
19	4	4006	CLA	O2A-CGA	4.25	1.46	1.33
19	K	1142	CLA	OBD-CAD	4.26	1.28	1.22
19	R	1150	CLA	C4B-CHC	4.26	1.51	1.39
19	1	1303	CLA	CHC-C1C	4.26	1.48	1.35
19	B	1230	CLA	O2A-CGA	4.26	1.46	1.33
19	3	2009	CLA	CHD-C4C	4.27	1.51	1.41
19	A	1115	CLA	CHD-C4C	4.27	1.51	1.41
19	B	1235	CLA	O2A-CGA	4.27	1.46	1.33
19	A	1123	CLA	O2A-CGA	4.27	1.46	1.33
19	B	1212	CLA	C4B-CHC	4.28	1.51	1.39
19	1	1012	CLA	C4B-CHC	4.28	1.51	1.39
19	4	4014	CLA	CHD-C4C	4.28	1.51	1.41
19	4	4015	CLA	O2A-CGA	4.28	1.47	1.32
19	B	1224	CLA	OBD-CAD	4.28	1.28	1.22
19	B	1233	CLA	C4B-CHC	4.28	1.51	1.39
19	B	1301	CLA	CHD-C4C	4.29	1.51	1.41
19	B	1223	CLA	O2A-CGA	4.29	1.46	1.33
19	A	1134	CLA	OBD-CAD	4.29	1.28	1.22
19	3	3006	CLA	CHD-C4C	4.29	1.51	1.41
19	K	3009	CLA	C4B-CHC	4.30	1.51	1.39
19	3	3004	CLA	CHD-C4C	4.30	1.51	1.41
19	A	1128	CLA	O2A-CGA	4.30	1.46	1.33
19	A	1120	CLA	C4B-CHC	4.30	1.51	1.39
19	3	3014	CLA	CHD-C4C	4.30	1.51	1.41
19	1	1011	CLA	CHC-C1C	4.30	1.48	1.35
19	4	1004	CLA	OBD-CAD	4.30	1.28	1.22
19	G	1242	CLA	C4B-CHC	4.30	1.51	1.39
19	B	1229	CLA	CHD-C4C	4.30	1.51	1.41
19	A	1116	CLA	OBD-CAD	4.31	1.28	1.22
19	A	1106	CLA	O2A-CGA	4.31	1.46	1.33
19	1	1303	CLA	O2A-CGA	4.31	1.46	1.33
19	1	1003	CLA	C4B-CHC	4.31	1.51	1.39
19	B	1209	CLA	O2A-CGA	4.32	1.46	1.33
19	4	4012	CLA	CHD-C4C	4.32	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	9011	CLA	C4B-CHC	4.32	1.51	1.39
19	3	3017	CLA	CHC-C1C	4.33	1.48	1.35
19	B	1212	CLA	CHD-C4C	4.33	1.51	1.41
19	B	1209	CLA	OBD-CAD	4.33	1.29	1.22
19	4	1009	CLA	CHD-C4C	4.33	1.51	1.41
19	I	1204	CLA	CHD-C4C	4.34	1.51	1.41
19	A	1141	CLA	O2A-CGA	4.34	1.46	1.33
19	A	1126	CLA	O2D-CGD	4.34	1.44	1.33
19	B	1209	CLA	CHD-C4C	4.34	1.51	1.41
19	B	1216	CLA	CHD-C4C	4.34	1.51	1.41
19	2	2006	CLA	CHD-C4C	4.35	1.51	1.41
19	B	1210	CLA	C4B-CHC	4.36	1.51	1.39
19	A	1107	CLA	O2D-CGD	4.36	1.44	1.33
19	4	4014	CLA	OBD-CAD	4.36	1.29	1.22
19	B	1219	CLA	O2A-CGA	4.36	1.46	1.33
19	L	1148	CLA	CHD-C4C	4.36	1.51	1.41
19	A	9023	CLA	CHD-C4C	4.36	1.51	1.41
19	A	9011	CLA	CHD-C4C	4.37	1.51	1.41
19	K	1146	CLA	CHD-C4C	4.37	1.51	1.41
19	3	3002	CLA	CHD-C4C	4.37	1.51	1.41
19	A	1119	CLA	OBD-CAD	4.38	1.29	1.22
19	B	1229	CLA	C4B-CHC	4.38	1.51	1.39
19	B	1222	CLA	CHD-C4C	4.38	1.51	1.41
19	1	1007	CLA	CHD-C4C	4.38	1.51	1.41
19	A	1135	CLA	OBD-CAD	4.38	1.29	1.22
19	J	1311	CLA	CHD-C4C	4.38	1.51	1.41
19	B	1235	CLA	O2D-CGD	4.39	1.44	1.33
19	2	2014	CLA	OBD-CAD	4.39	1.29	1.22
19	A	1131	CLA	O2A-CGA	4.40	1.46	1.33
19	J	1311	CLA	OBD-CAD	4.40	1.29	1.22
19	1	1005	CLA	O2A-CGA	4.40	1.47	1.32
19	3	3005	CLA	CHD-C4C	4.40	1.51	1.41
19	4	1004	CLA	CHD-C4C	4.41	1.51	1.41
19	A	1151	CLA	O2A-CGA	4.41	1.46	1.33
19	A	9012	CLA	CHD-C4C	4.41	1.51	1.41
19	A	1127	CLA	OBD-CAD	4.41	1.29	1.22
19	1	1003	CLA	O2A-CGA	4.42	1.46	1.33
19	B	1231	CLA	CHD-C4C	4.42	1.51	1.41
19	B	1222	CLA	O2A-CGA	4.42	1.46	1.33
19	4	4010	CLA	CHD-C4C	4.43	1.51	1.41
19	A	1107	CLA	OBD-CAD	4.43	1.29	1.22
19	B	1230	CLA	CHC-C1C	4.43	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	G	1242	CLA	O2A-CGA	4.43	1.46	1.33
19	B	1229	CLA	OBD-CAD	4.43	1.29	1.22
19	B	1220	CLA	CHC-C1C	4.43	1.49	1.35
19	A	1138	CLA	OBD-CAD	4.44	1.29	1.22
19	B	1210	CLA	CHD-C4C	4.44	1.51	1.41
19	K	1142	CLA	CHD-C4C	4.44	1.51	1.41
19	2	4009	CLA	CHD-C4C	4.44	1.51	1.41
19	4	4001	CLA	O2A-CGA	4.44	1.46	1.33
19	1	1008	CLA	CHD-C4C	4.45	1.51	1.41
19	4	4004	CLA	CHD-C4C	4.45	1.51	1.41
19	A	1139	CLA	CHD-C4C	4.45	1.51	1.41
19	A	1137	CLA	CHD-C4C	4.46	1.51	1.41
19	B	1230	CLA	CHD-C4C	4.46	1.51	1.41
19	1	1013	CLA	OBD-CAD	4.46	1.29	1.22
19	2	2012	CLA	O2A-CGA	4.46	1.46	1.33
19	A	1126	CLA	OBD-CAD	4.47	1.29	1.22
19	B	1217	CLA	CHD-C4C	4.47	1.51	1.41
19	3	3017	CLA	OBD-CAD	4.48	1.29	1.22
19	A	9012	CLA	OBD-CAD	4.48	1.29	1.22
19	B	1229	CLA	O2D-CGD	4.48	1.44	1.33
19	2	2004	CLA	O2A-CGA	4.48	1.46	1.33
19	A	1131	CLA	O2D-CGD	4.48	1.44	1.33
19	A	1101	CLA	O2A-CGA	4.48	1.46	1.33
19	L	1502	CLA	OBD-CAD	4.48	1.29	1.22
19	K	3009	CLA	CHD-C4C	4.48	1.51	1.41
19	1	1015	CLA	CHD-C4C	4.48	1.51	1.41
19	A	1124	CLA	CHD-C4C	4.48	1.51	1.41
19	1	1014	CLA	OBD-CAD	4.49	1.29	1.22
19	1	1002	CLA	CHD-C4C	4.49	1.51	1.41
19	2	2010	CLA	CHD-C4C	4.49	1.51	1.41
19	F	1302	CLA	CHD-C4C	4.49	1.51	1.41
19	A	1237	CLA	CHD-C4C	4.50	1.51	1.41
19	R	1150	CLA	CHD-C4C	4.50	1.51	1.41
19	3	3016	CLA	CHD-C4C	4.51	1.51	1.41
19	3	3016	CLA	OBD-CAD	4.51	1.29	1.22
19	1	1007	CLA	O2A-CGA	4.51	1.46	1.33
19	A	1120	CLA	O2A-CGA	4.51	1.46	1.33
19	A	1136	CLA	CHD-C4C	4.51	1.51	1.41
19	A	1127	CLA	CHD-C4C	4.51	1.51	1.41
19	B	1223	CLA	CHD-C4C	4.52	1.51	1.41
19	A	1134	CLA	CHD-C4C	4.52	1.51	1.41
19	B	1213	CLA	CHD-C4C	4.52	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	J	1311	CLA	O2A-CGA	4.52	1.46	1.33
19	3	3016	CLA	O2A-CGA	4.52	1.46	1.33
19	4	4006	CLA	CHD-C4C	4.52	1.51	1.41
19	1	1303	CLA	CHD-C4C	4.52	1.51	1.41
19	4	1304	CLA	OBD-CAD	4.52	1.29	1.22
19	B	1233	CLA	CHD-C4C	4.52	1.51	1.41
19	3	3008	CLA	CHD-C4C	4.53	1.51	1.41
19	2	2003	CLA	CHD-C4C	4.53	1.51	1.41
19	B	1228	CLA	CHD-C4C	4.54	1.51	1.41
19	B	1225	CLA	O2D-CGD	4.54	1.44	1.33
19	B	1212	CLA	O2A-CGA	4.54	1.47	1.33
19	F	1302	CLA	OBD-CAD	4.54	1.29	1.22
19	A	1140	CLA	CHD-C4C	4.55	1.51	1.41
19	A	1135	CLA	CHD-C4C	4.55	1.51	1.41
19	B	1203	CLA	CHC-C1C	4.55	1.49	1.35
19	B	9010	CLA	CHD-C4C	4.55	1.51	1.41
19	3	3012	CLA	CHD-C4C	4.55	1.51	1.41
19	4	4007	CLA	CHD-C4C	4.56	1.51	1.41
19	4	4001	CLA	CHD-C4C	4.56	1.51	1.41
19	4	4007	CLA	O2A-CGA	4.56	1.47	1.33
19	K	1146	CLA	CHC-C1C	4.56	1.49	1.35
19	B	1232	CLA	OBD-CAD	4.56	1.29	1.22
19	A	1107	CLA	O2A-CGA	4.57	1.47	1.33
19	L	1148	CLA	O2A-CGA	4.57	1.47	1.33
19	A	1119	CLA	O2A-CGA	4.57	1.47	1.33
19	A	1117	CLA	CHD-C4C	4.57	1.52	1.41
19	B	1239	CLA	CHC-C1C	4.57	1.49	1.35
19	L	1504	CLA	CHD-C4C	4.57	1.52	1.41
19	1	1310	CLA	CHD-C4C	4.57	1.52	1.41
19	A	1237	CLA	OBD-CAD	4.57	1.29	1.22
19	H	1207	CLA	CHD-C4C	4.57	1.52	1.41
19	H	1505	CLA	O2A-CGA	4.58	1.47	1.33
19	A	1133	CLA	O2A-CGA	4.58	1.47	1.33
19	A	1141	CLA	CHD-C4C	4.58	1.52	1.41
19	2	2007	CLA	O2A-CGA	4.58	1.47	1.33
19	B	1221	CLA	CHC-C1C	4.58	1.49	1.35
19	2	2002	CLA	OBD-CAD	4.58	1.29	1.22
23	B	7101	LMG	O7-C10	4.58	1.48	1.34
19	K	1143	CLA	OBD-CAD	4.59	1.29	1.22
19	J	1308	CLA	CHC-C1C	4.59	1.49	1.35
19	B	1210	CLA	O2A-CGA	4.59	1.47	1.33
19	F	1240	CLA	OBD-CAD	4.59	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	3007	CLA	CHD-C4C	4.59	1.52	1.41
19	3	3011	CLA	O2A-CGA	4.59	1.47	1.33
19	1	1010	CLA	CHC-C1C	4.59	1.49	1.35
19	1	1013	CLA	CHC-C1C	4.60	1.49	1.35
19	2	2001	CLA	CHD-C4C	4.60	1.52	1.41
19	B	1228	CLA	CHC-C1C	4.60	1.49	1.35
19	H	1241	CLA	O2A-CGA	4.60	1.47	1.33
19	A	1125	CLA	O2A-CGA	4.60	1.47	1.33
19	1	1001	CLA	O2D-CED	4.60	1.56	1.45
19	B	1221	CLA	O2A-CGA	4.60	1.47	1.33
19	A	1128	CLA	OBD-CAD	4.61	1.29	1.22
19	2	2001	CLA	OBD-CAD	4.61	1.29	1.22
19	L	1503	CLA	CHD-C4C	4.61	1.52	1.41
19	L	1503	CLA	O2A-CGA	4.61	1.47	1.33
19	1	1013	CLA	O2A-CGA	4.61	1.47	1.33
19	3	3001	CLA	CHD-C4C	4.61	1.52	1.41
19	1	1005	CLA	CHD-C4C	4.62	1.52	1.41
19	A	1124	CLA	O2D-CGD	4.62	1.45	1.33
21	A	6007	BCR	C20-C21	4.62	1.58	1.43
19	A	9023	CLA	O2A-CGA	4.62	1.47	1.33
19	3	1147	CLA	OBD-CAD	4.63	1.29	1.22
19	A	1109	CLA	O2A-CGA	4.63	1.47	1.33
19	A	1123	CLA	O2D-CGD	4.63	1.45	1.33
19	3	3011	CLA	OBD-CAD	4.63	1.29	1.22
19	B	1217	CLA	O2A-CGA	4.63	1.47	1.33
19	H	1505	CLA	OBD-CAD	4.63	1.29	1.22
19	B	1218	CLA	O2A-CGA	4.63	1.48	1.32
19	B	1202	CLA	CHC-C1C	4.64	1.49	1.35
19	B	1218	CLA	CHD-C4C	4.64	1.52	1.41
19	B	1206	CLA	CHD-C4C	4.64	1.52	1.41
19	A	1141	CLA	OBD-CAD	4.64	1.29	1.22
19	B	1230	CLA	OBD-CAD	4.65	1.29	1.22
19	B	1203	CLA	CHD-C4C	4.65	1.52	1.41
19	A	1138	CLA	CHD-C4C	4.66	1.52	1.41
19	L	1130	CLA	O2A-CGA	4.66	1.47	1.33
19	1	1014	CLA	O2A-CGA	4.66	1.47	1.33
19	A	1110	CLA	OBD-CAD	4.66	1.29	1.22
19	A	1132	CLA	CHC-C1C	4.66	1.49	1.35
19	A	9013	CLA	CHC-C1C	4.66	1.50	1.35
19	B	1234	CLA	O2D-CGD	4.67	1.45	1.33
19	3	1118	CLA	CHD-C4C	4.67	1.52	1.41
19	A	1101	CLA	OBD-CAD	4.67	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1235	CLA	CHC-C1C	4.67	1.50	1.35
19	A	1106	CLA	O2D-CGD	4.67	1.45	1.33
19	B	9010	CLA	O2D-CGD	4.67	1.45	1.33
19	A	1106	CLA	CHD-C4C	4.67	1.52	1.41
19	A	1103	CLA	CHC-C1C	4.67	1.50	1.35
19	H	1505	CLA	CHD-C4C	4.67	1.52	1.41
19	B	9010	CLA	OBD-CAD	4.67	1.29	1.22
19	A	1121	CLA	CHC-C1C	4.67	1.50	1.35
19	A	1131	CLA	CHD-C4C	4.67	1.52	1.41
19	3	3011	CLA	CHD-C4C	4.68	1.52	1.41
19	A	1131	CLA	OBD-CAD	4.68	1.29	1.22
19	3	2009	CLA	O2A-CGA	4.68	1.47	1.33
19	A	1115	CLA	O2D-CGD	4.68	1.45	1.33
19	2	2004	CLA	CHD-C4C	4.68	1.52	1.41
19	L	1502	CLA	O2A-CGA	4.68	1.47	1.33
19	H	1207	CLA	O2A-CGA	4.68	1.47	1.33
19	K	1143	CLA	CHD-C4C	4.69	1.52	1.41
19	F	1305	CLA	CHC-C1C	4.69	1.50	1.35
19	B	1208	CLA	OBD-CAD	4.69	1.29	1.22
19	A	1120	CLA	OBD-CAD	4.69	1.29	1.22
19	4	4005	CLA	CHD-C4C	4.69	1.52	1.41
19	2	2012	CLA	O2D-CGD	4.70	1.45	1.33
19	A	1111	CLA	CHD-C4C	4.70	1.52	1.41
19	1	1008	CLA	O2A-CGA	4.70	1.47	1.33
19	B	1225	CLA	OBD-CAD	4.70	1.29	1.22
19	A	1132	CLA	O2A-CGA	4.70	1.47	1.33
19	1	1006	CLA	CHD-C4C	4.70	1.52	1.41
19	1	1012	CLA	CHD-C4C	4.70	1.52	1.41
19	B	1228	CLA	O2A-CGA	4.70	1.47	1.33
19	1	1003	CLA	CHD-C4C	4.71	1.52	1.41
19	1	1002	CLA	OBD-CAD	4.71	1.29	1.22
19	A	1128	CLA	CHD-C4C	4.71	1.52	1.41
19	B	1239	CLA	O2A-CGA	4.71	1.47	1.33
19	4	4003	CLA	O2A-CGA	4.71	1.47	1.33
19	A	1111	CLA	O2A-CGA	4.71	1.47	1.33
19	4	1304	CLA	CHC-C1C	4.72	1.50	1.35
19	B	1232	CLA	CHD-C4C	4.72	1.52	1.41
19	A	1122	CLA	CHD-C4C	4.72	1.52	1.41
19	A	1109	CLA	CHD-C4C	4.72	1.52	1.41
19	2	4009	CLA	O2A-CGA	4.73	1.47	1.33
19	B	1221	CLA	CHD-C4C	4.73	1.52	1.41
19	1	1014	CLA	CHC-C1C	4.73	1.50	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1116	CLA	CHD-C4C	4.73	1.52	1.41
19	A	1137	CLA	O2D-CGD	4.73	1.45	1.33
19	B	1225	CLA	CHC-C1C	4.73	1.50	1.35
19	A	1113	CLA	O2A-CGA	4.73	1.47	1.33
19	R	1144	CLA	CHD-C4C	4.74	1.52	1.41
19	F	1305	CLA	O2D-CGD	4.74	1.45	1.33
19	B	1234	CLA	O2A-CGA	4.74	1.47	1.33
19	A	9022	CLA	CHD-C4C	4.74	1.52	1.41
19	B	1216	CLA	O2A-CGA	4.74	1.47	1.33
19	4	4003	CLA	CHD-C4C	4.75	1.52	1.41
19	B	1236	CLA	O2A-CGA	4.75	1.47	1.33
19	A	1113	CLA	OBD-CAD	4.75	1.29	1.22
19	A	1105	CLA	CHC-C1C	4.76	1.50	1.35
19	A	1119	CLA	CHD-C4C	4.76	1.52	1.41
19	A	9012	CLA	O2A-CGA	4.76	1.47	1.33
19	4	1306	CLA	CHC-C1C	4.76	1.50	1.35
19	B	1234	CLA	CHC-C1C	4.76	1.50	1.35
19	A	1105	CLA	OBD-CAD	4.77	1.29	1.22
19	2	2013	CLA	OBD-CAD	4.77	1.29	1.22
19	A	1104	CLA	CHD-C4C	4.77	1.52	1.41
19	A	1136	CLA	O2D-CGD	4.77	1.45	1.33
19	A	1133	CLA	CHD-C4C	4.77	1.52	1.41
19	A	1131	CLA	CHC-C1C	4.78	1.50	1.35
19	B	1206	CLA	O2D-CGD	4.78	1.45	1.33
19	A	9022	CLA	OBD-CAD	4.78	1.29	1.22
19	B	1233	CLA	O2A-CGA	4.78	1.47	1.33
19	B	1238	CLA	O2A-CGA	4.78	1.47	1.33
19	3	3003	CLA	CHD-C4C	4.78	1.52	1.41
19	4	1306	CLA	CHD-C4C	4.78	1.52	1.41
19	B	1209	CLA	CHC-C1C	4.79	1.50	1.35
19	L	1504	CLA	O2A-CGA	4.79	1.47	1.33
19	2	2007	CLA	CHC-C1C	4.79	1.50	1.35
19	A	1129	CLA	CHD-C4C	4.79	1.52	1.41
19	A	1110	CLA	CHC-C1C	4.79	1.50	1.35
19	3	3011	CLA	CHC-C1C	4.80	1.50	1.35
19	4	4007	CLA	CHC-C1C	4.80	1.50	1.35
19	A	1101	CLA	CHD-C4C	4.80	1.52	1.41
19	A	1122	CLA	OBD-CAD	4.80	1.29	1.22
19	A	1151	CLA	CHC-C1C	4.80	1.50	1.35
19	G	1242	CLA	CHD-C4C	4.80	1.52	1.41
19	4	4003	CLA	CHC-C1C	4.80	1.50	1.35
19	L	1130	CLA	OBD-CAD	4.80	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1105	CLA	CHD-C4C	4.81	1.52	1.41
19	A	1122	CLA	CHC-C1C	4.81	1.50	1.35
19	B	1218	CLA	OBD-CAD	4.81	1.29	1.22
19	B	1222	CLA	O2D-CGD	4.81	1.45	1.33
19	B	1214	CLA	CHD-C4C	4.82	1.52	1.41
19	A	1117	CLA	O2D-CGD	4.82	1.45	1.33
19	A	1101	CLA	CHC-C1C	4.82	1.50	1.35
19	2	4009	CLA	OBD-CAD	4.82	1.29	1.22
19	4	4014	CLA	CHC-C1C	4.82	1.50	1.35
19	B	1208	CLA	O2D-CGD	4.82	1.45	1.33
19	3	3017	CLA	O2D-CGD	4.83	1.45	1.33
19	4	4002	CLA	CHC-C1C	4.83	1.50	1.35
19	A	1237	CLA	CHC-C1C	4.83	1.50	1.35
19	A	1102	CLA	O2D-CGD	4.83	1.45	1.33
19	4	4003	CLA	OBD-CAD	4.83	1.29	1.22
19	4	1306	CLA	O2A-CGA	4.83	1.47	1.33
19	A	1123	CLA	CHD-C4C	4.83	1.52	1.41
19	K	1143	CLA	CHC-C1C	4.83	1.50	1.35
19	1	1002	CLA	CHC-C1C	4.83	1.50	1.35
19	A	1129	CLA	O2D-CGD	4.84	1.45	1.33
19	4	4012	CLA	OBD-CAD	4.84	1.29	1.22
19	1	1007	CLA	CHC-C1C	4.84	1.50	1.35
19	K	3009	CLA	O2A-CGA	4.84	1.47	1.33
19	A	1102	CLA	CHD-C4C	4.84	1.52	1.41
19	B	1238	CLA	CHD-C4C	4.84	1.52	1.41
19	A	1125	CLA	O2D-CGD	4.85	1.45	1.33
19	H	1145	CLA	O2D-CGD	4.85	1.45	1.33
19	B	1218	CLA	CHC-C1C	4.85	1.50	1.35
19	L	1130	CLA	CHC-C1C	4.86	1.50	1.35
19	H	1145	CLA	CHC-C1C	4.86	1.50	1.35
19	B	1226	CLA	O2D-CGD	4.86	1.45	1.33
19	I	1204	CLA	O2D-CGD	4.86	1.45	1.33
19	A	1112	CLA	CHD-C4C	4.87	1.52	1.41
19	B	1201	CLA	O2D-CGD	4.87	1.45	1.33
19	B	1216	CLA	O2D-CGD	4.87	1.45	1.33
19	B	1211	CLA	CHC-C1C	4.87	1.50	1.35
19	1	1005	CLA	CHC-C1C	4.87	1.50	1.35
19	2	2006	CLA	CHC-C1C	4.87	1.50	1.35
19	A	1104	CLA	CHC-C1C	4.87	1.50	1.35
19	R	1150	CLA	O2A-CGA	4.87	1.48	1.33
19	B	1214	CLA	OBD-CAD	4.88	1.29	1.22
19	A	1139	CLA	CHC-C1C	4.88	1.50	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	9022	CLA	O2A-CGA	4.88	1.48	1.33
19	A	1136	CLA	CHC-C1C	4.88	1.50	1.35
19	1	1006	CLA	CHC-C1C	4.88	1.50	1.35
19	A	1108	CLA	OBD-CAD	4.88	1.29	1.22
19	4	4015	CLA	CHC-C1C	4.88	1.50	1.35
19	2	4009	CLA	CHC-C1C	4.88	1.50	1.35
19	A	1125	CLA	CHC-C1C	4.88	1.50	1.35
19	F	1302	CLA	CHC-C1C	4.89	1.50	1.35
19	A	1111	CLA	O2D-CGD	4.89	1.45	1.33
19	1	1010	CLA	O2D-CGD	4.89	1.45	1.33
19	A	1135	CLA	O2D-CGD	4.89	1.45	1.33
19	L	1501	CLA	O2A-CGA	4.89	1.48	1.33
19	4	4007	CLA	OBD-CAD	4.89	1.29	1.22
19	B	1206	CLA	CHC-C1C	4.89	1.50	1.35
19	3	1118	CLA	CHC-C1C	4.89	1.50	1.35
19	B	1210	CLA	O2D-CGD	4.89	1.45	1.33
19	1	1008	CLA	OBD-CAD	4.89	1.29	1.22
19	4	1304	CLA	CHD-C4C	4.90	1.52	1.41
19	A	1134	CLA	CHC-C1C	4.90	1.50	1.35
19	B	1226	CLA	CHC-C1C	4.90	1.50	1.35
19	B	1234	CLA	CHD-C4C	4.90	1.52	1.41
19	A	1115	CLA	CHC-C1C	4.90	1.50	1.35
19	A	1138	CLA	CHC-C1C	4.90	1.50	1.35
19	B	1216	CLA	CHC-C1C	4.90	1.50	1.35
19	A	1141	CLA	CHC-C1C	4.90	1.50	1.35
19	A	1103	CLA	CHD-C4C	4.90	1.52	1.41
19	H	1207	CLA	OBD-CAD	4.91	1.29	1.22
19	B	1301	CLA	CHC-C1C	4.91	1.50	1.35
19	A	1110	CLA	CHD-C4C	4.91	1.52	1.41
19	2	2001	CLA	CHC-C1C	4.91	1.50	1.35
19	B	1205	CLA	CHC-C1C	4.92	1.50	1.35
19	3	2009	CLA	CHC-C1C	4.92	1.50	1.35
19	A	1101	CLA	O2D-CGD	4.92	1.45	1.33
19	B	1203	CLA	O2D-CGD	4.92	1.45	1.33
19	B	1219	CLA	CHC-C1C	4.92	1.50	1.35
19	A	9022	CLA	CHC-C1C	4.92	1.50	1.35
19	B	1201	CLA	CHD-C4C	4.92	1.52	1.41
19	A	1109	CLA	CHC-C1C	4.92	1.50	1.35
19	F	1240	CLA	CHD-C4C	4.92	1.52	1.41
19	A	9012	CLA	CHC-C1C	4.92	1.50	1.35
19	A	1140	CLA	CHC-C1C	4.93	1.50	1.35
19	B	1229	CLA	O2A-CGA	4.93	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L	1503	CLA	CHC-C1C	4.94	1.50	1.35
19	A	1123	CLA	CHC-C1C	4.94	1.50	1.35
19	A	1116	CLA	O2A-CGA	4.94	1.48	1.33
19	2	2002	CLA	CHD-C4C	4.94	1.52	1.41
19	L	1502	CLA	CHD-C4C	4.94	1.52	1.41
19	A	1132	CLA	CHD-C4C	4.94	1.52	1.41
19	B	1213	CLA	CHC-C1C	4.95	1.50	1.35
19	B	1211	CLA	CHD-C4C	4.95	1.52	1.41
20	B	5002	PQN	C10-C5	4.95	1.48	1.40
19	B	1205	CLA	CHD-C4C	4.95	1.52	1.41
19	A	1149	CLA	CHD-C4C	4.95	1.52	1.41
19	K	1142	CLA	O2D-CGD	4.95	1.45	1.33
19	A	1127	CLA	O2A-CGA	4.96	1.48	1.33
19	4	1004	CLA	CHC-C1C	4.96	1.50	1.35
19	A	9013	CLA	O2D-CGD	4.96	1.45	1.33
19	3	3007	CLA	OBD-CAD	4.96	1.29	1.22
19	J	1311	CLA	CHC-C1C	4.96	1.50	1.35
19	A	1107	CLA	CHD-C4C	4.96	1.52	1.41
19	K	1142	CLA	CHC-C1C	4.97	1.50	1.35
19	3	3007	CLA	CHC-C1C	4.97	1.50	1.35
19	A	1134	CLA	O2D-CGD	4.97	1.45	1.33
19	A	9011	CLA	CHC-C1C	4.97	1.50	1.35
19	2	2012	CLA	CHC-C1C	4.97	1.50	1.35
19	2	2014	CLA	CHC-C1C	4.97	1.50	1.35
19	B	1223	CLA	CHC-C1C	4.98	1.50	1.35
19	A	1124	CLA	CHC-C1C	4.98	1.50	1.35
19	A	1120	CLA	CHD-C4C	4.98	1.52	1.41
19	B	1235	CLA	CHD-C4C	4.98	1.53	1.41
19	A	1110	CLA	O2A-CGA	4.98	1.48	1.33
19	4	1306	CLA	OBD-CAD	4.99	1.30	1.22
19	I	1204	CLA	O2A-CGA	4.99	1.48	1.33
19	A	1137	CLA	CHC-C1C	4.99	1.51	1.35
19	4	1304	CLA	O2D-CGD	5.00	1.46	1.33
19	A	1135	CLA	CHC-C1C	5.00	1.51	1.35
19	B	1227	CLA	O2A-CGA	5.00	1.48	1.33
19	B	1208	CLA	CHD-C4C	5.00	1.53	1.41
19	B	1239	CLA	O2D-CGD	5.00	1.46	1.33
19	3	3016	CLA	CHC-C1C	5.00	1.51	1.35
19	G	1242	CLA	OBD-CAD	5.00	1.30	1.22
19	4	4012	CLA	CHC-C1C	5.01	1.51	1.35
19	A	1117	CLA	O2A-CGA	5.01	1.48	1.33
19	H	1207	CLA	CHC-C1C	5.01	1.51	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1126	CLA	CHC-C1C	5.01	1.51	1.35
19	3	3003	CLA	CHC-C1C	5.01	1.51	1.35
19	A	1149	CLA	CHC-C1C	5.02	1.51	1.35
19	A	1117	CLA	CHC-C1C	5.02	1.51	1.35
19	B	9010	CLA	CHC-C1C	5.02	1.51	1.35
19	A	1121	CLA	CHD-C4C	5.02	1.53	1.41
19	R	1144	CLA	CHC-C1C	5.03	1.51	1.35
19	A	1128	CLA	CHC-C1C	5.03	1.51	1.35
19	L	1503	CLA	OBD-CAD	5.03	1.30	1.22
19	B	1227	CLA	CHD-C4C	5.03	1.53	1.41
19	K	3009	CLA	O2D-CGD	5.03	1.46	1.33
19	3	3008	CLA	CHC-C1C	5.04	1.51	1.35
19	A	1104	CLA	OBD-CAD	5.04	1.30	1.22
19	B	1202	CLA	O2D-CGD	5.04	1.46	1.33
19	B	1202	CLA	O2A-CGA	5.04	1.48	1.33
19	F	1240	CLA	CHC-C1C	5.05	1.51	1.35
19	3	3017	CLA	CHD-C4C	5.05	1.53	1.41
19	H	1505	CLA	CHC-C1C	5.05	1.51	1.35
19	A	1116	CLA	CHC-C1C	5.05	1.51	1.35
19	3	3003	CLA	OBD-CAD	5.05	1.30	1.22
19	B	1208	CLA	CHC-C1C	5.05	1.51	1.35
19	1	1003	CLA	O2D-CGD	5.05	1.46	1.33
19	B	1211	CLA	O2A-CGA	5.06	1.48	1.33
19	2	2014	CLA	O2D-CGD	5.06	1.46	1.33
19	B	1219	CLA	CHD-C4C	5.06	1.53	1.41
19	B	1214	CLA	O2A-CGA	5.06	1.48	1.33
19	1	1003	CLA	CHC-C1C	5.06	1.51	1.35
19	A	1138	CLA	O2D-CGD	5.06	1.46	1.33
19	A	1127	CLA	CHC-C1C	5.07	1.51	1.35
19	B	1215	CLA	CHC-C1C	5.08	1.51	1.35
19	B	1217	CLA	O2D-CGD	5.08	1.46	1.33
19	A	1133	CLA	CHC-C1C	5.08	1.51	1.35
19	R	1144	CLA	O2A-CGA	5.08	1.48	1.33
19	A	1113	CLA	CHC-C1C	5.08	1.51	1.35
19	A	9022	CLA	O2D-CGD	5.08	1.46	1.33
19	1	1003	CLA	OBD-CAD	5.09	1.30	1.22
19	B	1238	CLA	O2D-CGD	5.09	1.46	1.33
19	L	1502	CLA	CHC-C1C	5.09	1.51	1.35
19	B	1222	CLA	CHC-C1C	5.10	1.51	1.35
19	A	1139	CLA	O2D-CGD	5.10	1.46	1.33
19	A	1140	CLA	O2D-CGD	5.10	1.46	1.33
19	A	1111	CLA	CHC-C1C	5.10	1.51	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1211	CLA	OBD-CAD	5.10	1.30	1.22
19	B	1231	CLA	CHC-C1C	5.10	1.51	1.35
19	A	1112	CLA	CHC-C1C	5.10	1.51	1.35
19	2	2001	CLA	O2D-CGD	5.10	1.46	1.33
19	2	2013	CLA	CHC-C1C	5.10	1.51	1.35
19	H	1241	CLA	CHD-C4C	5.10	1.53	1.41
19	A	1109	CLA	O2D-CGD	5.11	1.46	1.33
19	J	1308	CLA	O2D-CGD	5.11	1.46	1.33
19	B	1202	CLA	CHD-C4C	5.12	1.53	1.41
19	B	1224	CLA	O2D-CGD	5.12	1.46	1.33
19	A	1127	CLA	O2D-CGD	5.12	1.46	1.33
19	A	1106	CLA	CHC-C1C	5.12	1.51	1.35
19	2	2002	CLA	CHC-C1C	5.13	1.51	1.35
19	B	1224	CLA	CHD-C4C	5.13	1.53	1.41
19	L	1130	CLA	CHD-C4C	5.13	1.53	1.41
19	L	1501	CLA	CHC-C1C	5.13	1.51	1.35
19	H	1241	CLA	CHC-C1C	5.14	1.51	1.35
19	B	1238	CLA	CHC-C1C	5.14	1.51	1.35
19	A	9023	CLA	CHC-C1C	5.14	1.51	1.35
19	A	1102	CLA	OBD-CAD	5.15	1.30	1.22
19	B	1201	CLA	CHC-C1C	5.16	1.51	1.35
19	3	3016	CLA	O2D-CGD	5.16	1.46	1.33
19	B	1219	CLA	OBD-CAD	5.17	1.30	1.22
19	A	9013	CLA	CHD-C4C	5.17	1.53	1.41
19	2	2012	CLA	CHD-C4C	5.17	1.53	1.41
19	A	1126	CLA	CHD-C4C	5.17	1.53	1.41
19	A	9023	CLA	O2D-CGD	5.17	1.46	1.33
19	B	1221	CLA	O2D-CGD	5.17	1.46	1.33
19	A	1102	CLA	O2A-CGA	5.17	1.48	1.33
19	B	1214	CLA	CHC-C1C	5.18	1.51	1.35
19	A	1151	CLA	CHD-C4C	5.18	1.53	1.41
19	B	1217	CLA	CHC-C1C	5.18	1.51	1.35
19	2	2013	CLA	O2A-CGA	5.19	1.49	1.33
19	A	9012	CLA	O2D-CGD	5.19	1.46	1.33
19	A	1129	CLA	CHC-C1C	5.19	1.51	1.35
19	2	2007	CLA	CHD-C4C	5.19	1.53	1.41
19	B	1236	CLA	CHC-C1C	5.20	1.51	1.35
19	K	1143	CLA	O2D-CGD	5.20	1.46	1.33
19	A	1129	CLA	O2A-CGA	5.20	1.49	1.33
19	1	1002	CLA	O2A-CGA	5.20	1.49	1.33
19	B	1227	CLA	CHC-C1C	5.20	1.51	1.35
19	4	1306	CLA	O2D-CGD	5.21	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	1303	CLA	O2D-CGD	5.21	1.46	1.33
19	B	1209	CLA	O2D-CGD	5.21	1.46	1.33
19	K	3009	CLA	OBD-CAD	5.21	1.30	1.22
19	2	2002	CLA	O2A-CGA	5.22	1.49	1.33
19	B	1215	CLA	O2D-CGD	5.23	1.46	1.33
19	3	3011	CLA	O2D-CGD	5.23	1.46	1.33
19	I	1204	CLA	CHC-C1C	5.23	1.51	1.35
19	2	2004	CLA	O2D-CGD	5.24	1.46	1.33
19	A	1120	CLA	CHC-C1C	5.24	1.51	1.35
19	R	1150	CLA	CHC-C1C	5.24	1.51	1.35
19	1	1012	CLA	CHC-C1C	5.24	1.51	1.35
19	4	1004	CLA	O2D-CGD	5.24	1.46	1.33
19	A	1141	CLA	O2D-CGD	5.24	1.46	1.33
19	A	1113	CLA	CHD-C4C	5.24	1.53	1.41
19	A	1108	CLA	CHD-C4C	5.25	1.53	1.41
19	3	2009	CLA	O2D-CGD	5.25	1.46	1.33
19	B	1232	CLA	CHC-C1C	5.25	1.51	1.35
19	B	1229	CLA	CHC-C1C	5.25	1.51	1.35
19	B	1224	CLA	CHC-C1C	5.25	1.51	1.35
19	4	4001	CLA	OBD-CAD	5.25	1.30	1.22
19	4	1009	CLA	CHC-C1C	5.25	1.51	1.35
19	A	1103	CLA	O2A-CGA	5.25	1.49	1.33
19	A	1128	CLA	O2D-CGD	5.25	1.46	1.33
19	1	1007	CLA	OBD-CAD	5.25	1.30	1.22
19	G	1242	CLA	CHC-C1C	5.26	1.51	1.35
19	4	4002	CLA	O2D-CGD	5.26	1.46	1.33
19	L	1504	CLA	CHC-C1C	5.26	1.51	1.35
19	A	1119	CLA	CHC-C1C	5.26	1.51	1.35
19	4	4003	CLA	O2D-CGD	5.27	1.46	1.33
19	A	1102	CLA	CHC-C1C	5.27	1.51	1.35
19	F	1302	CLA	O2D-CGD	5.28	1.46	1.33
19	B	1236	CLA	O2D-CGD	5.28	1.46	1.33
19	B	1301	CLA	OBD-CAD	5.29	1.30	1.22
19	B	1223	CLA	O2D-CGD	5.29	1.46	1.33
19	L	1148	CLA	CHC-C1C	5.30	1.51	1.35
19	B	1201	CLA	OBD-CAD	5.30	1.30	1.22
19	A	1122	CLA	O2A-CGA	5.31	1.49	1.33
19	A	1132	CLA	O2D-CGD	5.31	1.46	1.33
19	A	1105	CLA	O2D-CGD	5.32	1.46	1.33
19	L	1130	CLA	O2D-CGD	5.32	1.46	1.33
19	A	1237	CLA	O2D-CGD	5.32	1.46	1.33
19	4	4006	CLA	CHC-C1C	5.33	1.52	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	9011	CLA	O2D-CGD	5.33	1.46	1.33
19	1	1008	CLA	CHC-C1C	5.33	1.52	1.35
19	B	1233	CLA	CHC-C1C	5.34	1.52	1.35
19	1	1008	CLA	O2D-CGD	5.35	1.46	1.33
19	B	1211	CLA	O2D-CGD	5.35	1.46	1.33
19	B	1212	CLA	CHC-C1C	5.36	1.52	1.35
19	A	1151	CLA	O2D-CGD	5.36	1.46	1.33
19	B	1212	CLA	O2D-CGD	5.36	1.46	1.33
19	2	2007	CLA	OBD-CAD	5.37	1.30	1.22
19	4	4006	CLA	OBD-CAD	5.37	1.30	1.22
19	L	1504	CLA	O2D-CGD	5.38	1.46	1.33
19	A	9013	CLA	OBD-CAD	5.38	1.30	1.22
19	3	1118	CLA	OBD-CAD	5.38	1.30	1.22
19	4	4014	CLA	O2A-CGA	5.39	1.49	1.33
19	B	1232	CLA	O2D-CGD	5.39	1.47	1.33
19	B	1221	CLA	OBD-CAD	5.39	1.30	1.22
19	B	1233	CLA	OBD-CAD	5.39	1.30	1.22
19	B	1210	CLA	CHC-C1C	5.40	1.52	1.35
19	1	1006	CLA	OBD-CAD	5.40	1.30	1.22
19	F	1305	CLA	OBD-CAD	5.40	1.30	1.22
19	B	1227	CLA	O2D-CGD	5.40	1.47	1.33
19	B	1208	CLA	O2A-CGA	5.41	1.49	1.33
19	A	1151	CLA	OBD-CAD	5.42	1.30	1.22
19	K	3009	CLA	CHC-C1C	5.43	1.52	1.35
19	B	1205	CLA	O2D-CGD	5.44	1.47	1.33
20	A	5001	PQN	C10-C5	5.44	1.49	1.40
19	A	1108	CLA	CHC-C1C	5.45	1.52	1.35
19	4	4014	CLA	O2D-CGD	5.45	1.47	1.33
21	I	6021	BCR	C24-C23	5.46	1.49	1.33
19	B	1230	CLA	O2D-CGD	5.46	1.47	1.33
19	B	1213	CLA	OBD-CAD	5.46	1.30	1.22
19	2	4009	CLA	O2D-CGD	5.47	1.47	1.33
19	B	1231	CLA	O2D-CGD	5.47	1.47	1.33
19	A	1112	CLA	O2D-CGD	5.48	1.47	1.33
19	A	1104	CLA	O2D-CGD	5.48	1.47	1.33
19	H	1207	CLA	O2D-CGD	5.48	1.47	1.33
19	A	1119	CLA	O2D-CGD	5.49	1.47	1.33
19	2	2007	CLA	O2D-CGD	5.49	1.47	1.33
19	L	1502	CLA	O2D-CGD	5.50	1.47	1.33
19	H	1241	CLA	OBD-CAD	5.50	1.30	1.22
19	A	1122	CLA	O2D-CGD	5.50	1.47	1.33
19	4	4001	CLA	CHC-C1C	5.52	1.52	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1121	CLA	OBD-CAD	5.52	1.30	1.22
19	2	2004	CLA	CHC-C1C	5.54	1.52	1.35
19	2	2006	CLA	OBD-CAD	5.55	1.30	1.22
19	A	1103	CLA	O2D-CGD	5.55	1.47	1.33
19	1	1013	CLA	O2D-CGD	5.55	1.47	1.33
19	A	1110	CLA	O2D-CGD	5.56	1.47	1.33
19	2	2002	CLA	O2D-CGD	5.57	1.47	1.33
19	J	1311	CLA	O2D-CGD	5.57	1.47	1.33
19	1	1005	CLA	O2D-CGD	5.57	1.47	1.33
19	K	1146	CLA	O2D-CGD	5.57	1.47	1.33
19	B	1214	CLA	O2D-CGD	5.58	1.47	1.33
19	3	3007	CLA	O2D-CGD	5.58	1.47	1.33
19	B	1213	CLA	O2D-CGD	5.58	1.47	1.33
19	3	3008	CLA	O2D-CGD	5.59	1.47	1.33
19	4	1009	CLA	OBD-CAD	5.59	1.30	1.22
19	A	1120	CLA	O2D-CGD	5.59	1.47	1.33
19	R	1144	CLA	O2D-CGD	5.59	1.47	1.33
19	A	1133	CLA	O2D-CGD	5.61	1.47	1.33
19	2	2013	CLA	O2D-CGD	5.62	1.47	1.33
19	A	1112	CLA	OBD-CAD	5.62	1.30	1.22
19	A	1108	CLA	O2D-CGD	5.63	1.47	1.33
19	A	1149	CLA	O2A-CGA	5.63	1.50	1.33
19	A	1121	CLA	O2D-CGD	5.64	1.47	1.33
19	B	1228	CLA	O2D-CGD	5.65	1.47	1.33
19	1	1001	CLA	OBD-CAD	5.67	1.31	1.22
19	B	1233	CLA	O2D-CGD	5.67	1.47	1.33
19	4	4001	CLA	O2D-CGD	5.69	1.47	1.33
19	1	1303	CLA	OBD-CAD	5.70	1.31	1.22
19	A	1113	CLA	O2D-CGD	5.70	1.47	1.33
19	4	4007	CLA	O2D-CGD	5.71	1.47	1.33
19	4	4006	CLA	O2D-CGD	5.73	1.47	1.33
19	B	1231	CLA	OBD-CAD	5.73	1.31	1.22
19	L	1501	CLA	O2D-CGD	5.78	1.48	1.33
19	R	1150	CLA	O2D-CGD	5.79	1.48	1.33
20	B	5002	PQN	C3-C2	5.79	1.48	1.35
19	2	2006	CLA	O2D-CGD	5.80	1.48	1.33
19	B	1218	CLA	O2D-CGD	5.80	1.48	1.33
19	1	1007	CLA	O2D-CGD	5.83	1.48	1.33
21	A	6002	BCR	C11-C12	5.85	1.49	1.34
19	L	1503	CLA	O2D-CGD	5.87	1.48	1.33
19	A	1116	CLA	O2D-CGD	5.87	1.48	1.33
19	B	1219	CLA	O2D-CGD	5.87	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	G	1242	CLA	O2D-CGD	5.89	1.48	1.33
20	A	5001	PQN	C3-C2	5.90	1.49	1.35
19	H	1241	CLA	O2D-CGD	5.93	1.48	1.33
19	3	3013	CLA	O2D-CGD	5.93	1.48	1.33
19	1	1001	CLA	O2D-CGD	5.96	1.48	1.33
19	1	1002	CLA	O2D-CGD	5.98	1.48	1.33
19	A	1149	CLA	O2D-CGD	6.06	1.48	1.33
19	L	1504	CLA	OBD-CAD	6.11	1.31	1.22
21	A	6003	BCR	C24-C23	6.14	1.51	1.33
19	1	1014	CLA	O2D-CGD	6.18	1.49	1.33
19	H	1505	CLA	O2D-CGD	6.20	1.49	1.33
19	R	1150	CLA	OBD-CAD	6.32	1.32	1.22
21	A	6002	BCR	C11-C10	6.93	1.65	1.43
19	1	1005	CLA	OBD-CAD	9.61	1.37	1.22

All (3857) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1303	CLA	OBD-CAD-CBD	-20.54	94.95	125.94
21	1	6023	BCR	C2-C1-C6	-19.89	78.87	110.36
19	A	1105	CLA	OBD-CAD-CBD	-17.66	99.29	125.94
19	A	1126	CLA	OBD-CAD-CBD	-15.67	102.29	125.94
19	B	1215	CLA	OBD-CAD-CBD	-15.33	102.81	125.94
19	4	4002	CLA	OBD-CAD-CBD	-15.32	102.82	125.94
21	I	6021	BCR	C24-C23-C22	-15.31	102.88	126.22
19	4	4014	CLA	OBD-CAD-CBD	-15.22	102.97	125.94
19	A	1151	CLA	OBD-CAD-CBD	-15.17	103.05	125.94
19	A	1237	CLA	OBD-CAD-CBD	-15.13	103.10	125.94
19	I	1204	CLA	OBD-CAD-CBD	-14.78	103.64	125.94
19	2	4009	CLA	OBD-CAD-CBD	-14.67	103.80	125.94
19	2	4009	CLA	OBD-CAD-C3D	-14.53	98.70	128.35
19	A	9011	CLA	OBD-CAD-CBD	-14.45	104.14	125.94
19	2	2004	CLA	OBD-CAD-CBD	-14.43	104.16	125.94
19	2	2013	CLA	OBD-CAD-CBD	-14.42	104.18	125.94
19	1	1010	CLA	OBD-CAD-CBD	-14.40	104.21	125.94
21	1	6023	BCR	C29-C30-C25	-14.22	87.86	110.36
19	H	1241	CLA	OBD-CAD-CBD	-14.19	104.53	125.94
19	1	1013	CLA	OBD-CAD-C3D	-14.15	99.48	128.35
19	3	3013	CLA	OBD-CAD-CBD	-14.14	104.60	125.94
19	B	1210	CLA	OBD-CAD-CBD	-14.06	104.72	125.94
21	1	6023	BCR	C32-C1-C6	-14.03	88.31	110.30
19	A	1108	CLA	OBD-CAD-CBD	-14.03	104.78	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	2009	CLA	OBD-CAD-CBD	-14.02	104.79	125.94
19	4	4001	CLA	OBD-CAD-CBD	-14.00	104.81	125.94
19	1	1011	CLA	CAB-C3B-C4B	-13.95	105.28	128.36
19	3	3013	CLA	OBD-CAD-C3D	-13.86	100.06	128.35
19	3	3007	CLA	OBD-CAD-CBD	-13.86	105.02	125.94
19	R	1144	CLA	OBD-CAD-CBD	-13.86	105.03	125.94
19	B	1202	CLA	OBD-CAD-CBD	-13.76	105.17	125.94
19	A	1128	CLA	OBD-CAD-CBD	-13.65	105.34	125.94
19	B	1224	CLA	OBD-CAD-CBD	-13.60	105.42	125.94
19	A	1135	CLA	OBD-CAD-CBD	-13.57	105.46	125.94
19	A	1112	CLA	OBD-CAD-CBD	-13.49	105.58	125.94
19	B	1233	CLA	OBD-CAD-CBD	-13.41	105.70	125.94
19	B	1219	CLA	OBD-CAD-CBD	-13.40	105.72	125.94
19	B	1216	CLA	OBD-CAD-CBD	-13.02	106.29	125.94
19	A	1140	CLA	OBD-CAD-CBD	-12.86	106.53	125.94
19	4	4014	CLA	OBD-CAD-C3D	-12.79	102.24	128.35
19	2	2006	CLA	OBD-CAD-C3D	-12.73	102.38	128.35
19	4	1009	CLA	CAB-C3B-C4B	-12.65	107.43	128.36
19	B	1220	CLA	OBD-CAD-CBD	-12.62	106.89	125.94
19	A	1138	CLA	OBD-CAD-CBD	-12.60	106.92	125.94
19	B	1301	CLA	CAB-C3B-C4B	-12.55	107.59	128.36
19	B	1223	CLA	OBD-CAD-CBD	-12.50	107.08	125.94
19	L	1501	CLA	OBD-CAD-CBD	-12.46	107.13	125.94
19	L	1503	CLA	OBD-CAD-C3D	-12.44	102.97	128.35
19	4	4012	CLA	CAB-C3B-C4B	-12.37	107.89	128.36
19	1	1303	CLA	OBD-CAD-C3D	-12.33	103.20	128.35
19	L	1503	CLA	OBD-CAD-CBD	-12.28	107.41	125.94
19	H	1505	CLA	OBD-CAD-CBD	-12.23	107.48	125.94
19	A	1136	CLA	OBD-CAD-CBD	-12.22	107.50	125.94
19	1	1003	CLA	OBD-CAD-CBD	-12.21	107.52	125.94
19	A	1129	CLA	OBD-CAD-C3D	-12.20	103.45	128.35
19	A	9022	CLA	OBD-CAD-CBD	-12.16	107.58	125.94
19	H	1207	CLA	OBD-CAD-C3D	-12.15	103.56	128.35
19	B	1233	CLA	OBD-CAD-C3D	-12.14	103.57	128.35
19	B	1206	CLA	OBD-CAD-CBD	-12.13	107.64	125.94
19	B	1234	CLA	OBD-CAD-C3D	-12.12	103.61	128.35
19	B	1224	CLA	OBD-CAD-C3D	-12.11	103.64	128.35
19	A	1127	CLA	OBD-CAD-CBD	-12.10	107.68	125.94
19	3	3017	CLA	OBD-CAD-C3D	-12.03	103.80	128.35
19	A	1119	CLA	OBD-CAD-CBD	-12.03	107.78	125.94
19	A	1149	CLA	OBD-CAD-C3D	-12.03	103.81	128.35
19	I	1204	CLA	OBD-CAD-C3D	-12.01	103.84	128.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	K	1142	CLA	OBD-CAD-CBD	-11.97	107.87	125.94
19	A	1237	CLA	OBD-CAD-C3D	-11.96	103.95	128.35
19	A	1104	CLA	OBD-CAD-CBD	-11.95	107.90	125.94
21	1	6023	BCR	C31-C1-C6	-11.94	91.58	110.30
19	B	1218	CLA	OBD-CAD-C3D	-11.89	104.09	128.35
19	A	1149	CLA	CAB-C3B-C4B	-11.88	108.70	128.36
19	A	1128	CLA	OBD-CAD-C3D	-11.88	104.10	128.35
19	A	1129	CLA	OBD-CAD-CBD	-11.87	108.02	125.94
19	2	2006	CLA	OBD-CAD-CBD	-11.86	108.04	125.94
19	A	1116	CLA	OBD-CAD-CBD	-11.78	108.17	125.94
19	A	1119	CLA	OBD-CAD-C3D	-11.77	104.32	128.35
19	G	1242	CLA	OBD-CAD-CBD	-11.75	108.20	125.94
19	K	1146	CLA	OBD-CAD-CBD	-11.75	108.20	125.94
19	1	1012	CLA	CAB-C3B-C4B	-11.75	108.92	128.36
19	3	1118	CLA	CAB-C3B-C4B	-11.70	109.01	128.36
19	H	1145	CLA	OBD-CAD-C3D	-11.66	104.56	128.35
19	J	1311	CLA	OBD-CAD-CBD	-11.61	108.41	125.94
19	B	9010	CLA	OBD-CAD-CBD	-11.61	108.41	125.94
19	1	1001	CLA	OBD-CAD-C3D	-11.59	104.69	128.35
19	3	3016	CLA	OBD-CAD-CBD	-11.57	108.48	125.94
19	B	1236	CLA	OBD-CAD-CBD	-11.55	108.51	125.94
19	3	3008	CLA	OBD-CAD-CBD	-11.54	108.52	125.94
19	1	1006	CLA	OBD-CAD-C3D	-11.54	104.81	128.35
19	A	1139	CLA	OBD-CAD-CBD	-11.51	108.57	125.94
19	A	1113	CLA	OBD-CAD-CBD	-11.49	108.60	125.94
19	F	1305	CLA	OBD-CAD-CBD	-11.48	108.61	125.94
19	H	1207	CLA	OBD-CAD-CBD	-11.46	108.65	125.94
19	H	1145	CLA	OBD-CAD-CBD	-11.46	108.65	125.94
19	2	2013	CLA	OBD-CAD-C3D	-11.45	104.98	128.35
19	A	1121	CLA	OBD-CAD-CBD	-11.43	108.69	125.94
19	4	1004	CLA	OBD-CAD-CBD	-11.42	108.71	125.94
19	L	1148	CLA	OBD-CAD-C3D	-11.40	105.08	128.35
19	B	1206	CLA	OBD-CAD-C3D	-11.39	105.12	128.35
19	A	1126	CLA	OBD-CAD-C3D	-11.36	105.17	128.35
19	4	1004	CLA	OBD-CAD-C3D	-11.35	105.18	128.35
19	A	1133	CLA	OBD-CAD-CBD	-11.34	108.83	125.94
19	B	1220	CLA	OBD-CAD-C3D	-11.32	105.25	128.35
19	A	1106	CLA	OBD-CAD-C3D	-11.27	105.34	128.35
19	B	1230	CLA	OBD-CAD-C3D	-11.26	105.37	128.35
19	K	1143	CLA	OBD-CAD-CBD	-11.25	108.96	125.94
19	R	1150	CLA	OBD-CAD-CBD	-11.24	108.97	125.94
19	B	1222	CLA	OBD-CAD-CBD	-11.22	109.00	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1209	CLA	OBD-CAD-CBD	-11.21	109.02	125.94
19	B	1227	CLA	OBD-CAD-CBD	-11.18	109.07	125.94
19	A	1125	CLA	OBD-CAD-CBD	-11.14	109.13	125.94
19	3	3017	CLA	OBD-CAD-CBD	-11.13	109.15	125.94
19	A	1149	CLA	OBD-CAD-CBD	-11.07	109.23	125.94
21	B	6020	BCR	C15-C16-C17	-11.07	98.91	123.39
19	3	1118	CLA	OBD-CAD-C3D	-11.07	105.76	128.35
19	L	1148	CLA	OBD-CAD-CBD	-11.05	109.27	125.94
19	4	4002	CLA	OBD-CAD-C3D	-11.03	105.85	128.35
19	A	1134	CLA	OBD-CAD-C3D	-11.01	105.87	128.35
19	B	1232	CLA	OBD-CAD-C3D	-11.01	105.89	128.35
21	I	6018	BCR	C24-C23-C22	-10.96	109.51	126.22
19	A	1122	CLA	OBD-CAD-C3D	-10.94	106.03	128.35
19	4	4007	CLA	OBD-CAD-CBD	-10.92	109.45	125.94
19	A	1115	CLA	OBD-CAD-CBD	-10.90	109.50	125.94
19	A	1111	CLA	OBD-CAD-CBD	-10.88	109.52	125.94
19	4	4001	CLA	OBD-CAD-C3D	-10.86	106.19	128.35
19	B	1230	CLA	OBD-CAD-CBD	-10.85	109.56	125.94
19	A	1134	CLA	OBD-CAD-CBD	-10.84	109.58	125.94
19	A	1124	CLA	OBD-CAD-CBD	-10.80	109.64	125.94
19	A	1137	CLA	OBD-CAD-CBD	-10.80	109.65	125.94
19	B	1228	CLA	OBD-CAD-CBD	-10.76	109.70	125.94
19	B	1209	CLA	OBD-CAD-C3D	-10.75	106.41	128.35
19	A	9013	CLA	OBD-CAD-CBD	-10.74	109.73	125.94
19	A	9013	CLA	OBD-CAD-C3D	-10.74	106.43	128.35
19	3	3016	CLA	OBD-CAD-C3D	-10.73	106.45	128.35
19	A	1117	CLA	OBD-CAD-CBD	-10.70	109.78	125.94
19	B	1231	CLA	OBD-CAD-C3D	-10.70	106.52	128.35
19	A	1120	CLA	OBD-CAD-C3D	-10.68	106.56	128.35
19	F	1305	CLA	OBD-CAD-C3D	-10.67	106.57	128.35
19	A	1131	CLA	OBD-CAD-CBD	-10.64	109.88	125.94
19	L	1502	CLA	OBD-CAD-CBD	-10.63	109.90	125.94
19	2	2014	CLA	OBD-CAD-C3D	-10.63	106.67	128.35
19	A	1108	CLA	OBD-CAD-C3D	-10.62	106.68	128.35
19	3	3008	CLA	OBD-CAD-C3D	-10.58	106.77	128.35
19	A	9012	CLA	OBD-CAD-CBD	-10.55	110.01	125.94
19	1	1014	CLA	OBD-CAD-C3D	-10.54	106.83	128.35
19	4	1304	CLA	OBD-CAD-C3D	-10.54	106.84	128.35
19	A	1103	CLA	OBD-CAD-C3D	-10.51	106.90	128.35
19	A	1116	CLA	OBD-CAD-C3D	-10.50	106.92	128.35
19	K	3009	CLA	OBD-CAD-CBD	-10.50	110.10	125.94
19	A	1131	CLA	OBD-CAD-C3D	-10.46	107.02	128.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	1009	CLA	OBD-CAD-C3D	-10.45	107.03	128.35
19	4	4012	CLA	OBD-CAD-C3D	-10.44	107.04	128.35
19	A	1104	CLA	OBD-CAD-C3D	-10.44	107.06	128.35
19	A	1139	CLA	OBD-CAD-C3D	-10.40	107.13	128.35
19	1	1011	CLA	C3D-CAD-CBD	-10.38	100.81	107.75
19	1	1014	CLA	OBD-CAD-CBD	-10.38	110.28	125.94
19	2	2007	CLA	OBD-CAD-CBD	-10.38	110.28	125.94
19	R	1144	CLA	OBD-CAD-C3D	-10.38	107.18	128.35
19	A	1115	CLA	OBD-CAD-C3D	-10.38	107.18	128.35
19	A	1124	CLA	OBD-CAD-C3D	-10.36	107.20	128.35
19	1	1011	CLA	CAB-C3B-C2B	-10.36	103.95	125.14
19	A	1125	CLA	OBD-CAD-C3D	-10.36	107.22	128.35
21	B	6020	BCR	C7-C8-C9	-10.35	110.43	126.22
19	A	1132	CLA	OBD-CAD-CBD	-10.34	110.34	125.94
19	4	1304	CLA	OBD-CAD-CBD	-10.32	110.37	125.94
19	B	1217	CLA	OBD-CAD-CBD	-10.30	110.39	125.94
19	1	1010	CLA	OBD-CAD-C3D	-10.29	107.36	128.35
19	A	1110	CLA	OBD-CAD-CBD	-10.28	110.43	125.94
19	3	2009	CLA	OBD-CAD-C3D	-10.27	107.39	128.35
19	1	1011	CLA	OBD-CAD-C3D	-10.27	107.40	128.35
19	1	1003	CLA	OBD-CAD-C3D	-10.26	107.42	128.35
19	4	4012	CLA	C3D-CAD-CBD	-10.24	100.91	107.75
19	F	1302	CLA	OBD-CAD-C3D	-10.23	107.48	128.35
19	2	2001	CLA	OBD-CAD-CBD	-10.20	110.55	125.94
19	B	1208	CLA	CAB-C3B-C4B	-10.18	111.51	128.36
19	3	3003	CLA	CAB-C3B-C4B	-10.17	111.54	128.36
21	I	6018	BCR	C7-C8-C9	-10.16	110.72	126.22
19	B	1228	CLA	OBD-CAD-C3D	-10.10	107.75	128.35
19	A	1141	CLA	OBD-CAD-C3D	-10.08	107.79	128.35
19	J	1311	CLA	OBD-CAD-C3D	-10.06	107.82	128.35
19	4	1009	CLA	C3D-CAD-CBD	-10.05	101.04	107.75
19	B	9010	CLA	OBD-CAD-C3D	-10.04	107.87	128.35
19	B	1216	CLA	OBD-CAD-C3D	-10.00	107.95	128.35
19	K	1142	CLA	OBD-CAD-C3D	-9.99	107.97	128.35
19	3	3007	CLA	OBD-CAD-C3D	-9.98	107.98	128.35
19	K	1146	CLA	OBD-CAD-C3D	-9.97	108.00	128.35
19	B	1301	CLA	C3D-CAD-CBD	-9.96	101.09	107.75
19	F	1302	CLA	OBD-CAD-CBD	-9.96	110.92	125.94
19	B	1202	CLA	OBD-CAD-C3D	-9.95	108.04	128.35
19	A	9022	CLA	OBD-CAD-C3D	-9.94	108.06	128.35
19	K	1143	CLA	OBD-CAD-C3D	-9.94	108.08	128.35
19	A	1122	CLA	OBD-CAD-CBD	-9.92	110.96	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1222	CLA	OBD-CAD-C3D	-9.92	108.12	128.35
19	B	1213	CLA	OBD-CAD-CBD	-9.90	111.00	125.94
19	A	1141	CLA	OBD-CAD-CBD	-9.90	111.00	125.94
19	B	1205	CLA	OBD-CAD-CBD	-9.89	111.02	125.94
19	A	1101	CLA	OBD-CAD-C3D	-9.87	108.20	128.35
19	A	1113	CLA	OBD-CAD-C3D	-9.85	108.25	128.35
19	A	9012	CLA	OBD-CAD-C3D	-9.84	108.27	128.35
19	3	3003	CLA	OBD-CAD-C3D	-9.82	108.32	128.35
19	2	2012	CLA	OBD-CAD-C3D	-9.80	108.34	128.35
19	2	2014	CLA	OBD-CAD-CBD	-9.80	111.15	125.94
19	J	1308	CLA	OBD-CAD-CBD	-9.79	111.17	125.94
19	A	1136	CLA	OBD-CAD-C3D	-9.73	108.50	128.35
19	B	1218	CLA	OBD-CAD-CBD	-9.71	111.28	125.94
19	A	1120	CLA	OBD-CAD-CBD	-9.69	111.32	125.94
19	A	1107	CLA	OBD-CAD-CBD	-9.68	111.33	125.94
19	A	1137	CLA	OBD-CAD-C3D	-9.66	108.64	128.35
19	H	1241	CLA	OBD-CAD-C3D	-9.64	108.69	128.35
19	B	1229	CLA	OBD-CAD-C3D	-9.64	108.69	128.35
19	A	1149	CLA	C3D-CAD-CBD	-9.63	93.99	107.60
19	A	1105	CLA	OBD-CAD-C3D	-9.54	108.89	128.35
19	B	1227	CLA	OBD-CAD-C3D	-9.50	108.97	128.35
19	B	1203	CLA	OBD-CAD-CBD	-9.49	111.61	125.94
19	1	1006	CLA	C3D-CAD-CBD	-9.46	101.43	107.75
19	B	1217	CLA	OBD-CAD-C3D	-9.46	109.05	128.35
19	H	1505	CLA	OBD-CAD-C3D	-9.44	109.09	128.35
21	1	6023	BCR	C24-C23-C22	-9.43	111.85	126.22
19	B	1203	CLA	OBD-CAD-C3D	-9.38	109.21	128.35
19	B	1215	CLA	OBD-CAD-C3D	-9.37	109.22	128.35
19	A	1133	CLA	OBD-CAD-C3D	-9.37	109.24	128.35
19	2	2001	CLA	OBD-CAD-C3D	-9.31	109.36	128.35
19	J	1308	CLA	OBD-CAD-C3D	-9.30	109.38	128.35
19	F	1240	CLA	C3D-CAD-CBD	-9.28	101.55	107.75
19	A	1140	CLA	OBD-CAD-C3D	-9.28	109.42	128.35
19	B	1223	CLA	OBD-CAD-C3D	-9.28	109.42	128.35
19	1	1008	CLA	OBD-CAD-CBD	-9.25	111.99	125.94
19	L	1502	CLA	OBD-CAD-C3D	-9.24	109.50	128.35
19	B	1232	CLA	OBD-CAD-CBD	-9.24	112.00	125.94
19	A	1135	CLA	OBD-CAD-C3D	-9.23	109.52	128.35
19	4	4003	CLA	OBD-CAD-C3D	-9.20	109.57	128.35
19	A	1127	CLA	OBD-CAD-C3D	-9.20	109.58	128.35
19	B	1219	CLA	OBD-CAD-C3D	-9.18	109.61	128.35
19	B	1212	CLA	OBD-CAD-C3D	-9.18	109.63	128.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1103	CLA	OBD-CAD-CBD	-9.15	112.13	125.94
19	4	4007	CLA	OBD-CAD-C3D	-9.13	109.72	128.35
19	A	1138	CLA	OBD-CAD-C3D	-9.04	109.91	128.35
19	1	1012	CLA	C3D-CAD-CBD	-9.03	101.72	107.75
19	2	2007	CLA	OBD-CAD-C3D	-9.02	109.94	128.35
19	B	1213	CLA	OBD-CAD-C3D	-8.99	110.00	128.35
19	B	1236	CLA	OBD-CAD-C3D	-8.96	110.07	128.35
19	L	1501	CLA	OBD-CAD-C3D	-8.95	110.09	128.35
19	A	9023	CLA	OBD-CAD-CBD	-8.91	112.50	125.94
19	1	1012	CLA	CAB-C3B-C2B	-8.89	106.96	125.14
19	4	1306	CLA	OBD-CAD-C3D	-8.89	110.22	128.35
19	B	1201	CLA	OBD-CAD-C3D	-8.81	110.37	128.35
19	A	1132	CLA	OBD-CAD-C3D	-8.80	110.39	128.35
19	A	1101	CLA	OBD-CAD-CBD	-8.79	112.67	125.94
19	B	1231	CLA	OBD-CAD-CBD	-8.78	112.69	125.94
19	G	1242	CLA	OBD-CAD-C3D	-8.70	110.60	128.35
19	B	1212	CLA	OBD-CAD-CBD	-8.69	112.82	125.94
21	A	6003	BCR	C24-C23-C22	-8.68	112.99	126.22
21	B	6020	BCR	C15-C14-C13	-8.67	114.67	127.20
19	2	2002	CLA	OBD-CAD-C3D	-8.66	110.67	128.35
19	B	1238	CLA	OBD-CAD-CBD	-8.64	112.90	125.94
19	B	1229	CLA	CAA-C2A-C3A	-8.63	88.39	113.22
19	3	1147	CLA	OBD-CAD-CBD	-8.63	112.91	125.94
19	A	1149	CLA	CAB-C3B-C2B	-8.63	107.50	125.14
19	3	1118	CLA	C3D-CAD-CBD	-8.62	101.99	107.75
19	2	2012	CLA	OBD-CAD-CBD	-8.61	112.94	125.94
19	2	2004	CLA	OBD-CAD-C3D	-8.61	110.79	128.35
19	B	1301	CLA	CAB-C3B-C2B	-8.56	107.63	125.14
19	1	1006	CLA	CAB-C3B-C4B	-8.56	114.20	128.36
19	B	1226	CLA	OBD-CAD-C3D	-8.53	110.94	128.35
19	A	1109	CLA	OBD-CAD-CBD	-8.49	113.13	125.94
19	A	1121	CLA	OBD-CAD-C3D	-8.49	111.03	128.35
19	A	1110	CLA	OBD-CAD-C3D	-8.41	111.19	128.35
19	B	1301	CLA	OBD-CAD-C3D	-8.40	111.21	128.35
19	A	1102	CLA	OBD-CAD-CBD	-8.39	113.27	125.94
21	B	6020	BCR	C3-C4-C5	-8.36	100.61	113.87
19	B	1229	CLA	OBD-CAD-CBD	-8.36	113.33	125.94
19	1	1008	CLA	OBD-CAD-C3D	-8.35	111.31	128.35
19	A	1112	CLA	OBD-CAD-C3D	-8.34	111.33	128.35
19	A	1151	CLA	OBD-CAD-C3D	-8.33	111.35	128.35
19	1	1002	CLA	OBD-CAD-CBD	-8.33	113.37	125.94
19	4	1304	CLA	C3D-CAD-CBD	-8.26	95.93	107.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	4003	CLA	OBD-CAD-CBD	-8.23	113.52	125.94
19	B	1234	CLA	OBD-CAD-CBD	-8.18	113.60	125.94
19	3	3011	CLA	OBD-CAD-C3D	-8.17	111.68	128.35
19	A	1107	CLA	OBD-CAD-C3D	-8.17	111.69	128.35
19	B	1225	CLA	OBD-CAD-CBD	-8.14	113.66	125.94
21	I	6021	BCR	C16-C15-C14	-8.09	105.50	123.39
19	3	3003	CLA	C3D-CAD-CBD	-8.09	102.35	107.75
19	B	1238	CLA	OBD-CAD-C3D	-8.09	111.85	128.35
19	B	1210	CLA	OBD-CAD-C3D	-8.07	111.89	128.35
19	1	1007	CLA	OBD-CAD-C3D	-8.06	111.91	128.35
19	B	1225	CLA	OBD-CAD-C3D	-8.04	111.95	128.35
19	A	9023	CLA	OBD-CAD-C3D	-8.02	111.99	128.35
19	B	1201	CLA	OBD-CAD-CBD	-7.99	113.87	125.94
21	I	6021	BCR	C30-C25-C26	-7.96	110.98	122.66
19	A	9011	CLA	OBD-CAD-C3D	-7.95	112.12	128.35
19	B	1205	CLA	O1D-CGD-CBD	-7.94	113.24	124.62
19	A	1106	CLA	OBD-CAD-CBD	-7.93	113.97	125.94
19	1	1007	CLA	OBD-CAD-CBD	-7.91	114.00	125.94
19	B	1239	CLA	OBD-CAD-C3D	-7.91	112.21	128.35
22	H	7011	LMU	C1B-O1B-C4'	-7.86	97.46	118.01
19	K	3009	CLA	OBD-CAD-C3D	-7.86	112.31	128.35
19	A	1111	CLA	OBD-CAD-C3D	-7.85	112.33	128.35
19	B	1214	CLA	OBD-CAD-CBD	-7.82	114.14	125.94
19	4	4015	CLA	OBD-CAD-CBD	-7.81	114.15	125.94
19	4	4006	CLA	OBD-CAD-C3D	-7.78	112.48	128.35
19	A	1123	CLA	OBD-CAD-C3D	-7.73	112.58	128.35
21	I	6018	BCR	C3-C4-C5	-7.71	101.63	113.87
19	3	1118	CLA	CAB-C3B-C2B	-7.69	109.41	125.14
21	A	6007	BCR	C24-C23-C22	-7.69	114.49	126.22
19	B	1235	CLA	OBD-CAD-CBD	-7.69	114.33	125.94
19	B	1235	CLA	OBD-CAD-C3D	-7.60	112.84	128.35
19	B	1214	CLA	OBD-CAD-C3D	-7.53	112.98	128.35
19	1	1001	CLA	OBD-CAD-CBD	-7.52	114.58	125.94
19	B	1239	CLA	OBD-CAD-CBD	-7.51	114.61	125.94
21	3	6022	BCR	C16-C17-C18	-7.50	116.37	127.20
19	4	1009	CLA	C1D-CHD-C4C	-7.49	111.26	122.60
19	A	9011	CLA	C3D-CAD-CBD	-7.46	97.05	107.60
19	4	4015	CLA	OBD-CAD-C3D	-7.43	113.18	128.35
21	B	6006	BCR	C24-C23-C22	-7.43	114.89	126.22
19	L	1504	CLA	OBD-CAD-C3D	-7.43	113.20	128.35
19	L	1130	CLA	OBD-CAD-CBD	-7.40	114.77	125.94
19	L	1148	CLA	C1D-CHD-C4C	-7.37	111.45	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1117	CLA	OBD-CAD-C3D	-7.36	113.33	128.35
21	1	6023	BCR	C30-C25-C26	-7.32	111.91	122.66
19	L	1130	CLA	OBD-CAD-C3D	-7.30	113.46	128.35
19	4	1306	CLA	OBD-CAD-CBD	-7.27	114.96	125.94
19	4	1304	CLA	C1D-CHD-C4C	-7.27	111.60	122.60
19	4	4002	CLA	C1D-CHD-C4C	-7.26	111.62	122.60
19	3	3017	CLA	C4B-CHC-C1C	-7.26	113.67	129.26
19	A	1109	CLA	OBD-CAD-C3D	-7.22	113.62	128.35
19	B	1208	CLA	CAB-C3B-C2B	-7.19	110.43	125.14
19	1	1303	CLA	C1D-CHD-C4C	-7.19	111.72	122.60
22	E	7048	LMU	C1B-C2B-C3B	-7.16	95.86	109.97
19	H	1145	CLA	C3D-CAD-CBD	-7.14	97.50	107.60
19	4	4004	CLA	C3A-C4A-CHB	-7.10	116.90	124.06
19	1	1013	CLA	OBD-CAD-CBD	-7.06	115.28	125.94
19	3	3014	CLA	C3A-C4A-CHB	-7.05	116.94	124.06
19	1	1010	CLA	C4B-CHC-C1C	-7.03	114.16	129.26
19	1	1001	CLA	C4B-CHC-C1C	-7.01	114.19	129.26
19	4	1306	CLA	C4B-CHC-C1C	-6.98	114.27	129.26
19	3	1147	CLA	C1D-CHD-C4C	-6.96	112.06	122.60
19	A	1103	CLA	C4B-CHC-C1C	-6.95	114.34	129.26
19	B	1211	CLA	OBD-CAD-CBD	-6.94	115.47	125.94
19	1	1002	CLA	OBD-CAD-C3D	-6.93	114.22	128.35
19	3	3011	CLA	OBD-CAD-CBD	-6.92	115.49	125.94
19	2	2002	CLA	OBD-CAD-CBD	-6.91	115.51	125.94
22	3	7005	LMU	C2'-C3'-C4'	-6.89	94.48	109.60
19	B	1211	CLA	OBD-CAD-C3D	-6.84	114.40	128.35
19	3	3006	CLA	C3A-C4A-CHB	-6.84	117.16	124.06
19	4	4006	CLA	OBD-CAD-CBD	-6.83	115.63	125.94
19	B	9010	CLA	C4B-CHC-C1C	-6.82	114.61	129.26
19	4	4012	CLA	CAB-C3B-C2B	-6.81	111.21	125.14
19	L	1503	CLA	C3D-CAD-CBD	-6.75	98.05	107.60
19	B	1238	CLA	C4B-CHC-C1C	-6.74	114.78	129.26
19	3	3003	CLA	CAB-C3B-C2B	-6.73	111.38	125.14
19	A	9011	CLA	C4B-CHC-C1C	-6.70	114.86	129.26
19	1	1012	CLA	OBD-CAD-C3D	-6.70	114.68	128.35
21	F	6016	BCR	C15-C14-C13	-6.69	117.53	127.20
21	1	6023	BCR	C28-C27-C26	-6.69	103.26	113.87
19	1	1013	CLA	C1D-CHD-C4C	-6.68	112.50	122.60
19	2	2014	CLA	C1D-CHD-C4C	-6.67	112.50	122.60
19	R	1150	CLA	OBD-CAD-C3D	-6.66	114.75	128.35
19	4	1009	CLA	CAB-C3B-C2B	-6.64	111.56	125.14
19	A	1121	CLA	O1D-CGD-CBD	-6.63	115.12	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L	1503	CLA	C1D-CHD-C4C	-6.63	112.57	122.60
19	B	1208	CLA	OBD-CAD-C3D	-6.63	114.83	128.35
19	B	1239	CLA	C4B-CHC-C1C	-6.62	115.03	129.26
19	3	3013	CLA	O1D-CGD-CBD	-6.62	115.13	124.62
19	4	1304	CLA	C4B-CHC-C1C	-6.61	115.06	129.26
19	A	1107	CLA	C4B-CHC-C1C	-6.61	115.06	129.26
19	3	3013	CLA	C1D-CHD-C4C	-6.60	112.62	122.60
19	B	1208	CLA	OBD-CAD-CBD	-6.59	116.00	125.94
19	F	1240	CLA	OBD-CAD-C3D	-6.57	114.95	128.35
19	K	1146	CLA	C4B-CHC-C1C	-6.57	115.15	129.26
21	A	6003	BCR	C32-C1-C6	-6.57	100.01	110.30
19	2	2007	CLA	C4B-CHC-C1C	-6.55	115.19	129.26
19	3	3001	CLA	C3A-C4A-CHB	-6.54	117.46	124.06
19	1	1310	CLA	C3A-C4A-CHB	-6.54	117.46	124.06
19	B	1226	CLA	C4B-CHC-C1C	-6.51	115.28	129.26
19	3	3013	CLA	C4B-CHC-C1C	-6.50	115.30	129.26
19	1	1002	CLA	C4B-CHC-C1C	-6.49	115.31	129.26
19	1	1010	CLA	C1D-CHD-C4C	-6.48	112.79	122.60
19	B	1202	CLA	CAA-C2A-C3A	-6.48	94.58	113.22
19	4	4015	CLA	C1D-CHD-C4C	-6.47	112.81	122.60
19	B	1235	CLA	C4B-CHC-C1C	-6.47	115.36	129.26
19	1	1015	CLA	C3A-C4A-CHB	-6.47	117.53	124.06
19	3	3005	CLA	C3A-C4A-CHB	-6.46	117.53	124.06
19	A	1117	CLA	C4B-CHC-C1C	-6.44	115.42	129.26
19	A	1108	CLA	C4B-CHC-C1C	-6.43	115.44	129.26
21	1	6023	BCR	C40-C30-C29	-6.43	85.76	108.79
19	B	1202	CLA	C4B-CHC-C1C	-6.43	115.45	129.26
19	1	1014	CLA	C1D-CHD-C4C	-6.42	112.89	122.60
19	B	1205	CLA	OBD-CAD-C3D	-6.41	115.27	128.35
19	A	1102	CLA	C4B-CHC-C1C	-6.39	115.53	129.26
19	2	2006	CLA	C1D-CHD-C4C	-6.38	112.94	122.60
19	L	1503	CLA	O1D-CGD-CBD	-6.38	115.47	124.62
19	2	2011	CLA	C3A-C4A-CHB	-6.37	117.63	124.06
19	B	1220	CLA	C4B-CHC-C1C	-6.36	115.60	129.26
19	1	1303	CLA	C4B-CHC-C1C	-6.36	115.60	129.26
19	4	4002	CLA	C4B-CHC-C1C	-6.36	115.61	129.26
19	A	1121	CLA	C4B-CHC-C1C	-6.35	115.61	129.26
19	4	4007	CLA	C4B-CHC-C1C	-6.35	115.63	129.26
21	I	6021	BCR	C16-C17-C18	-6.34	118.04	127.20
19	1	1011	CLA	C4B-CHC-C1C	-6.33	115.66	129.26
19	B	1210	CLA	C1D-CHD-C4C	-6.29	113.08	122.60
19	B	1221	CLA	C1D-CHD-C4C	-6.29	113.08	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	6011	BCR	C15-C14-C13	-6.28	118.12	127.20
19	1	1013	CLA	C3D-CAD-CBD	-6.28	98.72	107.60
19	A	1131	CLA	C4B-CHC-C1C	-6.27	115.79	129.26
21	I	6021	BCR	C34-C9-C10	-6.26	113.66	122.90
19	1	1001	CLA	C1D-CHD-C4C	-6.25	113.14	122.60
19	1	1013	CLA	C4B-CHC-C1C	-6.25	115.83	129.26
19	4	4010	CLA	C3A-C4A-CHB	-6.25	117.75	124.06
19	I	1204	CLA	C1D-CHD-C4C	-6.24	113.16	122.60
21	I	6021	BCR	C38-C26-C25	-6.23	118.49	124.61
19	B	1211	CLA	C4B-CHC-C1C	-6.22	115.90	129.26
19	B	1218	CLA	C1D-CHD-C4C	-6.22	113.19	122.60
19	3	1147	CLA	C4B-CHC-C1C	-6.21	115.92	129.26
19	K	1142	CLA	C1D-CHD-C4C	-6.21	113.20	122.60
19	A	1139	CLA	C4B-CHC-C1C	-6.20	115.94	129.26
19	H	1145	CLA	C4B-CHC-C1C	-6.19	115.97	129.26
19	K	1143	CLA	C4B-CHC-C1C	-6.18	115.98	129.26
19	A	1101	CLA	C4B-CHC-C1C	-6.17	115.99	129.26
19	B	1226	CLA	C1D-CHD-C4C	-6.17	113.27	122.60
19	B	1232	CLA	C4B-CHC-C1C	-6.16	116.02	129.26
19	A	1109	CLA	C4B-CHC-C1C	-6.16	116.02	129.26
19	A	1127	CLA	C4B-CHC-C1C	-6.16	116.03	129.26
19	B	1219	CLA	C4B-CHC-C1C	-6.16	116.03	129.26
19	A	1134	CLA	C4B-CHC-C1C	-6.15	116.05	129.26
19	2	2013	CLA	C4B-CHC-C1C	-6.15	116.05	129.26
19	L	1502	CLA	CAA-C2A-C3A	-6.15	95.54	113.22
21	B	6006	BCR	C16-C17-C18	-6.14	118.33	127.20
19	F	1305	CLA	C1D-CHD-C4C	-6.13	113.32	122.60
19	3	2009	CLA	C4B-CHC-C1C	-6.13	116.09	129.26
21	B	6005	BCR	C31-C1-C6	-6.13	100.70	110.30
19	A	1132	CLA	C4B-CHC-C1C	-6.13	116.10	129.26
19	1	1006	CLA	C1D-CHD-C4C	-6.12	113.33	122.60
19	B	1230	CLA	C4B-CHC-C1C	-6.12	116.11	129.26
21	A	6007	BCR	C16-C17-C18	-6.12	118.36	127.20
19	B	1206	CLA	C4B-CHC-C1C	-6.11	116.14	129.26
19	B	1216	CLA	C4B-CHC-C1C	-6.10	116.15	129.26
19	B	1236	CLA	C4B-CHC-C1C	-6.10	116.16	129.26
19	B	1231	CLA	C1D-CHD-C4C	-6.10	113.38	122.60
22	R	7014	LMU	C4B-C3B-C2B	-6.10	99.42	110.79
19	4	4006	CLA	C1D-CHD-C4C	-6.09	113.38	122.60
19	J	1308	CLA	C1D-CHD-C4C	-6.09	113.38	122.60
19	A	1122	CLA	C4B-CHC-C1C	-6.09	116.18	129.26
19	3	2009	CLA	C1D-CHD-C4C	-6.09	113.39	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	R	1150	CLA	C4B-CHC-C1C	-6.08	116.21	129.26
19	B	1217	CLA	C4B-CHC-C1C	-6.07	116.22	129.26
19	1	1011	CLA	C1D-CHD-C4C	-6.06	113.43	122.60
21	1	6023	BCR	C38-C26-C25	-6.06	118.65	124.61
19	1	1014	CLA	C4B-CHC-C1C	-6.06	116.24	129.26
19	A	1125	CLA	C1D-CHD-C4C	-6.06	113.44	122.60
19	A	1129	CLA	C4B-CHC-C1C	-6.05	116.27	129.26
19	A	1104	CLA	C4B-CHC-C1C	-6.04	116.28	129.26
19	2	2006	CLA	C4B-CHC-C1C	-6.04	116.29	129.26
21	I	6021	BCR	C2-C1-C6	-6.04	100.81	110.36
19	4	4015	CLA	O1D-CGD-CBD	-6.04	115.97	124.62
19	B	1227	CLA	C4B-CHC-C1C	-6.03	116.30	129.26
19	B	1215	CLA	C4B-CHC-C1C	-6.03	116.30	129.26
19	L	1502	CLA	C4B-CHC-C1C	-6.02	116.32	129.26
19	A	1105	CLA	C4B-CHC-C1C	-6.02	116.32	129.26
19	B	1228	CLA	C4B-CHC-C1C	-6.02	116.32	129.26
19	B	1209	CLA	C4B-CHC-C1C	-6.02	116.33	129.26
19	A	1149	CLA	C4B-CHC-C1C	-6.02	116.34	129.26
19	H	1505	CLA	C4B-CHC-C1C	-6.02	116.34	129.26
19	2	2008	CLA	C3A-C4A-CHB	-6.01	117.99	124.06
19	A	1109	CLA	C1D-CHD-C4C	-6.01	113.50	122.60
19	A	1138	CLA	C4B-CHC-C1C	-6.01	116.34	129.26
19	B	1205	CLA	C4B-CHC-C1C	-6.01	116.35	129.26
19	3	3016	CLA	C1D-CHD-C4C	-6.01	113.51	122.60
19	A	1137	CLA	C1D-CHD-C4C	-6.00	113.51	122.60
19	B	1203	CLA	C1D-CHD-C4C	-6.00	113.52	122.60
19	4	4003	CLA	C4B-CHC-C1C	-6.00	116.38	129.26
19	3	3007	CLA	C4B-CHC-C1C	-5.99	116.39	129.26
19	L	1130	CLA	C4B-CHC-C1C	-5.99	116.39	129.26
19	1	1006	CLA	C4B-CHC-C1C	-5.99	116.39	129.26
19	A	1136	CLA	C4B-CHC-C1C	-5.99	116.39	129.26
21	F	6016	BCR	C3-C4-C5	-5.98	104.38	113.87
19	B	1218	CLA	C4B-CHC-C1C	-5.98	116.42	129.26
19	B	1223	CLA	C4B-CHC-C1C	-5.97	116.44	129.26
19	4	4001	CLA	C1D-CHD-C4C	-5.96	113.58	122.60
19	J	1311	CLA	C1D-CHD-C4C	-5.96	113.58	122.60
19	A	9012	CLA	C1D-CHD-C4C	-5.96	113.58	122.60
19	B	1236	CLA	C1D-CHD-C4C	-5.96	113.58	122.60
19	A	9012	CLA	C4B-CHC-C1C	-5.95	116.48	129.26
19	B	1225	CLA	C4B-CHC-C1C	-5.95	116.48	129.26
19	A	1141	CLA	C4B-CHC-C1C	-5.94	116.50	129.26
19	A	1106	CLA	C4B-CHC-C1C	-5.94	116.50	129.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1237	CLA	C4B-CHC-C1C	-5.94	116.50	129.26
19	3	3016	CLA	C4B-CHC-C1C	-5.93	116.52	129.26
21	B	6010	BCR	C24-C23-C22	-5.93	117.18	126.22
19	A	1140	CLA	C4B-CHC-C1C	-5.92	116.54	129.26
19	2	2012	CLA	C4B-CHC-C1C	-5.92	116.55	129.26
19	2	2013	CLA	C1D-CHD-C4C	-5.92	113.65	122.60
19	A	1123	CLA	C4B-CHC-C1C	-5.91	116.55	129.26
19	H	1207	CLA	C4B-CHC-C1C	-5.91	116.56	129.26
19	2	4009	CLA	C4B-CHC-C1C	-5.91	116.56	129.26
19	B	1214	CLA	C4B-CHC-C1C	-5.91	116.56	129.26
19	3	3010	CLA	C3A-C4A-CHB	-5.91	118.09	124.06
21	1	6023	BCR	C39-C30-C29	-5.90	87.65	108.79
21	A	6007	BCR	C31-C1-C6	-5.90	101.05	110.30
19	A	1115	CLA	C1D-CHD-C4C	-5.90	113.67	122.60
19	A	1135	CLA	C4B-CHC-C1C	-5.90	116.58	129.26
19	1	1007	CLA	C1D-CHD-C4C	-5.90	113.68	122.60
19	A	1128	CLA	C1D-CHD-C4C	-5.89	113.69	122.60
19	3	1118	CLA	C4B-CHC-C1C	-5.89	116.61	129.26
19	B	1222	CLA	C4B-CHC-C1C	-5.88	116.62	129.26
19	1	1007	CLA	C4B-CHC-C1C	-5.88	116.63	129.26
19	3	3011	CLA	C4B-CHC-C1C	-5.88	116.63	129.26
21	F	6014	BCR	C32-C1-C6	-5.87	101.09	110.30
19	J	1308	CLA	C4B-CHC-C1C	-5.87	116.65	129.26
19	B	1229	CLA	C4B-CHC-C1C	-5.87	116.65	129.26
19	R	1144	CLA	C4B-CHC-C1C	-5.87	116.66	129.26
19	1	1008	CLA	C4B-CHC-C1C	-5.86	116.67	129.26
19	B	1230	CLA	C1D-CHD-C4C	-5.86	113.73	122.60
19	4	1004	CLA	C4B-CHC-C1C	-5.86	116.68	129.26
19	J	1311	CLA	C4B-CHC-C1C	-5.86	116.68	129.26
19	2	2001	CLA	C1D-CHD-C4C	-5.86	113.74	122.60
19	A	1123	CLA	OBD-CAD-CBD	-5.85	117.11	125.94
19	A	1111	CLA	C4B-CHC-C1C	-5.85	116.70	129.26
19	K	1142	CLA	C4B-CHC-C1C	-5.85	116.70	129.26
19	B	1215	CLA	C1D-CHD-C4C	-5.84	113.76	122.60
19	A	1128	CLA	C4B-CHC-C1C	-5.84	116.71	129.26
19	H	1241	CLA	C4B-CHC-C1C	-5.84	116.71	129.26
19	2	2001	CLA	C4B-CHC-C1C	-5.84	116.71	129.26
19	2	2003	CLA	C3A-C4A-CHB	-5.84	118.16	124.06
19	A	1151	CLA	C4B-CHC-C1C	-5.84	116.72	129.26
19	2	1307	CLA	C3A-C4A-CHB	-5.83	118.18	124.06
19	K	1143	CLA	C1D-CHD-C4C	-5.83	113.78	122.60
19	3	1118	CLA	C1D-CHD-C4C	-5.82	113.80	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	2004	CLA	C4B-CHC-C1C	-5.80	116.79	129.26
19	A	1116	CLA	C4B-CHC-C1C	-5.80	116.79	129.26
21	B	6004	BCR	C32-C1-C6	-5.80	101.20	110.30
19	A	1124	CLA	C4B-CHC-C1C	-5.80	116.80	129.26
19	3	3003	CLA	C4B-CHC-C1C	-5.80	116.81	129.26
19	B	1234	CLA	C4B-CHC-C1C	-5.80	116.81	129.26
19	B	1206	CLA	C1D-CHD-C4C	-5.80	113.83	122.60
19	F	1240	CLA	C1D-CHD-C4C	-5.79	113.83	122.60
19	4	4012	CLA	C1D-CHD-C4C	-5.79	113.84	122.60
19	1	1006	CLA	CAB-C3B-C2B	-5.79	113.30	125.14
19	B	1201	CLA	C1D-CHD-C4C	-5.79	113.84	122.60
19	4	4014	CLA	C1D-CHD-C4C	-5.79	113.84	122.60
19	A	1137	CLA	C4B-CHC-C1C	-5.78	116.83	129.26
19	4	4014	CLA	C4B-CHC-C1C	-5.78	116.84	129.26
20	B	5002	PQN	C11-C12-C13	-5.78	116.91	126.70
19	3	3008	CLA	C4B-CHC-C1C	-5.78	116.85	129.26
22	3	7005	LMU	C1B-O5B-C5B	-5.77	102.55	113.75
19	3	3003	CLA	C1D-CHD-C4C	-5.76	113.88	122.60
19	A	1139	CLA	C1D-CHD-C4C	-5.76	113.88	122.60
21	A	6008	BCR	C31-C1-C6	-5.76	101.27	110.30
19	B	1223	CLA	C1D-CHD-C4C	-5.76	113.88	122.60
19	A	1111	CLA	C1D-CHD-C4C	-5.76	113.89	122.60
19	A	1136	CLA	C1D-CHD-C4C	-5.76	113.89	122.60
19	B	1210	CLA	C4B-CHC-C1C	-5.76	116.90	129.26
19	3	3013	CLA	CHD-C4C-C3C	-5.75	116.05	124.94
19	B	1234	CLA	C1D-CHD-C4C	-5.75	113.89	122.60
19	A	1132	CLA	C1D-CHD-C4C	-5.75	113.91	122.60
19	L	1501	CLA	C1D-CHD-C4C	-5.74	113.91	122.60
19	A	1117	CLA	C1D-CHD-C4C	-5.74	113.92	122.60
19	B	1229	CLA	C1D-CHD-C4C	-5.74	113.92	122.60
19	F	1240	CLA	C4B-CHC-C1C	-5.73	116.96	129.26
19	3	3008	CLA	C1D-CHD-C4C	-5.72	113.94	122.60
19	A	9013	CLA	C4B-CHC-C1C	-5.72	116.97	129.26
19	1	1013	CLA	CHD-C4C-C3C	-5.72	116.10	124.94
19	A	1125	CLA	C4B-CHC-C1C	-5.72	116.98	129.26
19	3	3012	CLA	C3A-C4A-CHB	-5.71	118.29	124.06
19	A	9022	CLA	C4B-CHC-C1C	-5.71	117.00	129.26
21	A	6008	BCR	C16-C17-C18	-5.70	118.96	127.20
19	B	1224	CLA	C1D-CHD-C4C	-5.70	113.98	122.60
22	H	7017	LMU	C1B-O1B-C4'	-5.69	103.13	118.01
19	4	4012	CLA	C4B-CHC-C1C	-5.69	117.03	129.26
19	B	1225	CLA	C1D-CHD-C4C	-5.69	114.00	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1008	CLA	CBA-CAA-C2A	-5.69	97.69	113.73
19	2	2002	CLA	C4B-CHC-C1C	-5.68	117.06	129.26
19	H	1505	CLA	C1D-CHD-C4C	-5.66	114.03	122.60
19	2	2010	CLA	C3A-C4A-CHB	-5.66	118.35	124.06
22	G	7051	LMU	C3'-C4'-C5'	-5.66	98.05	110.84
19	A	1140	CLA	C1D-CHD-C4C	-5.65	114.05	122.60
19	A	9023	CLA	C4B-CHC-C1C	-5.65	117.12	129.26
19	B	1221	CLA	C4B-CHC-C1C	-5.64	117.13	129.26
19	4	4011	CLA	C3A-C4A-CHB	-5.64	118.36	124.06
19	B	1224	CLA	O1D-CGD-CBD	-5.64	116.54	124.62
19	4	4015	CLA	C4B-CHC-C1C	-5.63	117.16	129.26
19	B	1203	CLA	C4B-CHC-C1C	-5.63	117.16	129.26
19	B	1217	CLA	C1D-CHD-C4C	-5.62	114.09	122.60
19	A	1113	CLA	C4B-CHC-C1C	-5.62	117.19	129.26
19	A	1126	CLA	C1D-CHD-C4C	-5.62	114.10	122.60
19	A	1134	CLA	C1D-CHD-C4C	-5.62	114.10	122.60
19	A	1116	CLA	C1D-CHD-C4C	-5.61	114.11	122.60
19	1	1010	CLA	CGD-CBD-CAD	-5.61	91.61	110.62
19	L	1501	CLA	C4B-CHC-C1C	-5.61	117.22	129.26
21	B	6010	BCR	C7-C8-C9	-5.60	117.68	126.22
19	1	1012	CLA	C1D-CHD-C4C	-5.60	114.13	122.60
19	A	1141	CLA	C1D-CHD-C4C	-5.60	114.13	122.60
19	1	1005	CLA	C4B-CHC-C1C	-5.59	117.24	129.26
19	B	1233	CLA	C4B-CHC-C1C	-5.59	117.25	129.26
19	B	1212	CLA	C1D-CHD-C4C	-5.59	114.14	122.60
19	A	1120	CLA	C4B-CHC-C1C	-5.59	117.25	129.26
19	B	1201	CLA	C4B-CHC-C1C	-5.59	117.25	129.26
19	G	1242	CLA	C1D-CHD-C4C	-5.59	114.15	122.60
19	A	9023	CLA	C1D-CHD-C4C	-5.58	114.15	122.60
19	B	1208	CLA	C4B-CHC-C1C	-5.58	117.27	129.26
19	A	1133	CLA	C4B-CHC-C1C	-5.58	117.27	129.26
19	A	1121	CLA	C3D-CAD-CBD	-5.58	99.71	107.60
19	L	1504	CLA	C1D-CHD-C4C	-5.58	114.16	122.60
19	B	1213	CLA	C4B-CHC-C1C	-5.57	117.28	129.26
19	1	1003	CLA	C4B-CHC-C1C	-5.57	117.30	129.26
19	F	1302	CLA	C1D-CHD-C4C	-5.56	114.18	122.60
19	1	1012	CLA	C4B-CHC-C1C	-5.56	117.31	129.26
19	B	1220	CLA	CHD-C4C-C3C	-5.55	116.36	124.94
19	B	1224	CLA	C4B-CHC-C1C	-5.55	117.34	129.26
19	A	1103	CLA	C1D-CHD-C4C	-5.55	114.21	122.60
19	2	2014	CLA	C4B-CHC-C1C	-5.54	117.35	129.26
19	A	1132	CLA	O1D-CGD-CBD	-5.54	116.68	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1230	CLA	O1D-CGD-CBD	-5.54	116.68	124.62
19	A	1135	CLA	C1D-CHD-C4C	-5.54	114.22	122.60
19	A	1112	CLA	C4B-CHC-C1C	-5.53	117.37	129.26
19	B	1212	CLA	C4B-CHC-C1C	-5.53	117.38	129.26
19	A	1124	CLA	C1D-CHD-C4C	-5.52	114.25	122.60
19	A	1131	CLA	C1D-CHD-C4C	-5.52	114.25	122.60
21	J	6012	BCR	C24-C23-C22	-5.51	117.82	126.22
19	B	1301	CLA	C4B-CHC-C1C	-5.51	117.43	129.26
19	4	4001	CLA	C4B-CHC-C1C	-5.51	117.43	129.26
19	4	4006	CLA	C4B-CHC-C1C	-5.49	117.46	129.26
19	H	1145	CLA	C1D-CHD-C4C	-5.49	114.29	122.60
21	A	6011	BCR	C7-C8-C9	-5.49	117.85	126.22
19	F	1302	CLA	C4B-CHC-C1C	-5.49	117.47	129.26
19	A	1110	CLA	C1D-CHD-C4C	-5.49	114.30	122.60
19	B	1216	CLA	C1D-CHD-C4C	-5.48	114.30	122.60
19	L	1504	CLA	C4B-CHC-C1C	-5.48	117.49	129.26
19	3	3004	CLA	C3A-C4A-CHB	-5.48	118.53	124.06
19	A	1110	CLA	C4B-CHC-C1C	-5.47	117.50	129.26
19	B	1231	CLA	C4B-CHC-C1C	-5.47	117.51	129.26
19	B	1222	CLA	C1D-CHD-C4C	-5.47	114.33	122.60
19	B	1208	CLA	C1D-CHD-C4C	-5.46	114.34	122.60
19	K	3009	CLA	C1D-CHD-C4C	-5.45	114.35	122.60
19	4	1004	CLA	C1D-CHD-C4C	-5.45	114.35	122.60
19	3	3015	CLA	C3A-C4A-CHB	-5.44	118.56	124.06
21	B	6017	BCR	C31-C1-C6	-5.44	101.77	110.30
19	1	1005	CLA	C1D-CHD-C4C	-5.44	114.37	122.60
19	A	1123	CLA	C1D-CHD-C4C	-5.43	114.38	122.60
19	A	1119	CLA	C4B-CHC-C1C	-5.43	117.60	129.26
19	1	1010	CLA	CHD-C4C-C3C	-5.42	116.56	124.94
19	B	1219	CLA	C1D-CHD-C4C	-5.42	114.40	122.60
19	A	1119	CLA	C1D-CHD-C4C	-5.41	114.41	122.60
19	B	1202	CLA	C1D-CHD-C4C	-5.41	114.41	122.60
21	F	6016	BCR	C32-C1-C6	-5.41	101.83	110.30
21	F	6014	BCR	C37-C22-C21	-5.41	114.92	122.90
21	L	6019	BCR	C31-C1-C6	-5.40	101.83	110.30
19	1	1008	CLA	C1D-CHD-C4C	-5.40	114.43	122.60
19	4	4005	CLA	C3A-C4A-CHB	-5.39	118.61	124.06
19	A	9022	CLA	C1D-CHD-C4C	-5.39	114.45	122.60
19	H	1241	CLA	C1D-CHD-C4C	-5.38	114.46	122.60
19	A	1138	CLA	C1D-CHD-C4C	-5.37	114.47	122.60
19	K	3009	CLA	C4B-CHC-C1C	-5.37	117.73	129.26
19	A	1309	CLA	C3A-C4A-CHB	-5.36	118.65	124.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	6003	BCR	C16-C17-C18	-5.35	119.47	127.20
19	4	4006	CLA	CHD-C4C-C3C	-5.35	116.67	124.94
19	B	1213	CLA	C1D-CHD-C4C	-5.34	114.52	122.60
21	I	6021	BCR	C1-C6-C5	-5.33	114.83	122.66
19	3	3002	CLA	C3A-C4A-CHB	-5.33	118.68	124.06
19	1	1010	CLA	C3D-CAD-CBD	-5.32	100.08	107.60
19	A	1102	CLA	OBD-CAD-C3D	-5.32	117.50	128.35
19	A	1151	CLA	C1D-CHD-C4C	-5.31	114.56	122.60
21	B	6004	BCR	C16-C17-C18	-5.31	119.53	127.20
21	A	6008	BCR	C32-C1-C6	-5.31	101.98	110.30
19	H	1207	CLA	C1D-CHD-C4C	-5.30	114.58	122.60
19	A	1122	CLA	C1D-CHD-C4C	-5.28	114.60	122.60
21	F	6016	BCR	C24-C23-C22	-5.28	118.16	126.22
19	B	1221	CLA	OBD-CAD-CBD	-5.27	117.98	125.94
19	B	1232	CLA	C1D-CHD-C4C	-5.27	114.63	122.60
19	2	4009	CLA	C1D-CHD-C4C	-5.26	114.64	122.60
19	A	1127	CLA	C1D-CHD-C4C	-5.26	114.64	122.60
19	B	1218	CLA	CHD-C4C-C3C	-5.25	116.82	124.94
21	A	6003	BCR	C23-C24-C25	-5.25	111.55	127.32
19	1	1003	CLA	C1D-CHD-C4C	-5.25	114.66	122.60
19	A	1107	CLA	C1D-CHD-C4C	-5.25	114.66	122.60
19	A	1102	CLA	C1D-CHD-C4C	-5.25	114.66	122.60
21	A	6003	BCR	C3-C4-C5	-5.24	105.55	113.87
19	I	1204	CLA	C4B-CHC-C1C	-5.24	118.00	129.26
19	2	2014	CLA	CAA-C2A-C3A	-5.23	98.17	113.22
19	B	1234	CLA	O2D-CGD-O1D	-5.23	113.00	123.79
19	A	1115	CLA	C4B-CHC-C1C	-5.22	118.04	129.26
21	3	6022	BCR	C7-C8-C9	-5.22	118.26	126.22
19	A	1129	CLA	C1D-CHD-C4C	-5.22	114.70	122.60
19	4	4003	CLA	C1D-CHD-C4C	-5.21	114.72	122.60
19	A	1133	CLA	C1D-CHD-C4C	-5.20	114.73	122.60
19	A	9011	CLA	CHD-C4C-C3C	-5.20	116.90	124.94
19	2	2005	CLA	C3A-C4A-CHB	-5.20	118.81	124.06
19	R	1144	CLA	C1D-CHD-C4C	-5.20	114.74	122.60
19	4	4013	CLA	C3A-C4A-CHB	-5.19	118.82	124.06
19	R	1150	CLA	C1D-CHD-C4C	-5.18	114.76	122.60
21	B	6004	BCR	C15-C14-C13	-5.18	119.72	127.20
19	4	1009	CLA	C4B-CHC-C1C	-5.17	118.15	129.26
19	B	1239	CLA	C1D-CHD-C4C	-5.17	114.78	122.60
19	3	3011	CLA	C1D-CHD-C4C	-5.16	114.79	122.60
19	A	1101	CLA	C1D-CHD-C4C	-5.16	114.79	122.60
19	3	3006	CLA	C1D-CHD-C4C	-5.16	113.06	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L	1502	CLA	C1D-CHD-C4C	-5.15	114.80	122.60
22	N	7049	LMU	C1B-O1B-C4'	-5.15	104.54	118.01
19	F	1305	CLA	C4B-CHC-C1C	-5.15	118.20	129.26
22	E	7037	LMU	C1B-O5B-C5B	-5.15	103.75	113.75
19	1	1002	CLA	C1D-CHD-C4C	-5.15	114.81	122.60
19	F	1240	CLA	CAB-C3B-C4B	-5.15	119.85	128.36
19	A	1237	CLA	C1D-CHD-C4C	-5.14	114.83	122.60
19	3	1147	CLA	OBD-CAD-C3D	-5.13	117.89	128.35
21	A	6011	BCR	C32-C1-C6	-5.11	102.29	110.30
19	B	1214	CLA	C1D-CHD-C4C	-5.09	114.89	122.60
19	B	1205	CLA	C1D-CHD-C4C	-5.09	114.89	122.60
19	4	1304	CLA	CAA-C2A-C3A	-5.09	98.59	113.22
19	1	1310	CLA	C3B-C2B-C1B	-5.08	101.84	106.29
19	A	1120	CLA	C1D-CHD-C4C	-5.07	114.92	122.60
19	B	1228	CLA	C1D-CHD-C4C	-5.07	114.93	122.60
19	4	4010	CLA	C1D-CHD-C4C	-5.06	113.30	126.32
19	B	1217	CLA	C3D-CAD-CBD	-5.06	100.44	107.60
19	A	1104	CLA	C1D-CHD-C4C	-5.06	114.94	122.60
19	L	1503	CLA	C4B-CHC-C1C	-5.05	118.40	129.26
21	1	6023	BCR	C15-C14-C13	-5.05	119.90	127.20
19	B	1210	CLA	CHD-C4C-C3C	-5.05	117.14	124.94
19	L	1503	CLA	CHD-C4C-C3C	-5.04	117.15	124.94
19	3	2009	CLA	C3D-CAD-CBD	-5.04	100.47	107.60
19	A	1121	CLA	C1D-CHD-C4C	-5.04	114.98	122.60
19	B	1228	CLA	CHD-C4C-C3C	-5.04	117.15	124.94
19	B	1209	CLA	C1D-CHD-C4C	-5.04	114.98	122.60
19	B	1233	CLA	C1D-CHD-C4C	-5.03	114.98	122.60
19	K	3009	CLA	CHD-C4C-C3C	-5.03	117.17	124.94
21	A	6002	BCR	C32-C1-C6	-5.02	102.44	110.30
19	A	1126	CLA	C4B-CHC-C1C	-5.01	118.49	129.26
21	F	6014	BCR	C7-C8-C9	-5.01	118.58	126.22
21	B	6010	BCR	C31-C1-C6	-5.01	102.45	110.30
19	1	1008	CLA	C3D-CAD-CBD	-5.00	100.52	107.60
21	B	6017	BCR	C15-C14-C13	-5.00	119.97	127.20
21	B	6004	BCR	C24-C23-C22	-5.00	118.60	126.22
19	A	1149	CLA	CMD-C2D-C3D	-4.99	115.33	125.09
21	B	6020	BCR	C4-C5-C6	-4.99	116.42	122.78
19	K	1146	CLA	C1D-CHD-C4C	-4.98	115.06	122.60
19	L	1504	CLA	OBD-CAD-CBD	-4.98	118.43	125.94
19	A	1112	CLA	C1D-CHD-C4C	-4.97	115.07	122.60
19	A	1149	CLA	C1D-CHD-C4C	-4.97	115.08	122.60
19	3	3017	CLA	C1D-CHD-C4C	-4.97	115.08	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1235	CLA	C1D-CHD-C4C	-4.96	115.09	122.60
19	4	4015	CLA	CHD-C4C-C3C	-4.96	117.28	124.94
21	1	6023	BCR	C3-C4-C5	-4.96	106.00	113.87
19	B	1218	CLA	C3D-CAD-CBD	-4.95	100.60	107.60
21	L	6019	BCR	C24-C23-C22	-4.94	118.68	126.22
21	A	6008	BCR	C15-C14-C13	-4.94	120.06	127.20
19	B	1220	CLA	C6-C5-C3	-4.94	101.65	112.48
19	A	9013	CLA	C1D-CHD-C4C	-4.94	115.13	122.60
19	3	3012	CLA	C3B-C2B-C1B	-4.93	101.98	106.29
19	3	3005	CLA	C1D-CHD-C4C	-4.93	113.65	126.32
19	2	2002	CLA	C1D-CHD-C4C	-4.93	115.15	122.60
21	A	6007	BCR	C33-C5-C6	-4.92	119.77	124.61
19	B	1225	CLA	CHD-C4C-C3C	-4.92	117.34	124.94
19	A	1113	CLA	C1D-CHD-C4C	-4.92	115.16	122.60
19	1	1310	CLA	C2A-C1A-CHA	-4.92	113.87	122.58
19	2	2004	CLA	C1D-CHD-C4C	-4.92	115.16	122.60
19	G	1242	CLA	C4B-CHC-C1C	-4.92	118.70	129.26
19	L	1130	CLA	C1D-CHD-C4C	-4.92	115.16	122.60
19	B	1206	CLA	C3D-CAD-CBD	-4.91	100.65	107.60
19	1	1014	CLA	CHD-C4C-C3C	-4.91	117.34	124.94
19	A	1106	CLA	C1D-CHD-C4C	-4.91	115.17	122.60
19	1	1008	CLA	CGD-CBD-CAD	-4.91	94.00	110.62
19	3	1147	CLA	C3D-CAD-CBD	-4.91	100.66	107.60
19	4	4005	CLA	C1D-CHD-C4C	-4.90	113.71	126.32
19	A	9011	CLA	C1D-CHD-C4C	-4.89	115.19	122.60
21	A	6008	BCR	C20-C19-C18	-4.89	111.91	126.32
19	A	9023	CLA	C3D-CAD-CBD	-4.89	100.69	107.60
21	3	6022	BCR	C33-C5-C6	-4.89	119.81	124.61
21	F	6016	BCR	C31-C1-C6	-4.88	102.65	110.30
19	3	1147	CLA	CHD-C4C-C3C	-4.87	117.41	124.94
19	3	3012	CLA	C2D-C3D-C4D	-4.87	102.01	106.30
19	R	1144	CLA	C3D-CAD-CBD	-4.87	100.71	107.60
21	A	6007	BCR	C15-C14-C13	-4.86	120.17	127.20
21	B	6005	BCR	C32-C1-C6	-4.85	102.69	110.30
21	A	6008	BCR	C7-C8-C9	-4.85	118.82	126.22
19	B	1230	CLA	C3D-CAD-CBD	-4.85	100.74	107.60
19	A	1122	CLA	C3D-CAD-CBD	-4.84	100.75	107.60
21	3	6022	BCR	C16-C15-C14	-4.84	112.69	123.39
19	4	4007	CLA	C1D-CHD-C4C	-4.84	115.28	122.60
19	4	4004	CLA	C3B-C2B-C1B	-4.83	102.06	106.29
21	A	6002	BCR	C15-C14-C13	-4.83	120.22	127.20
21	I	6018	BCR	C28-C27-C26	-4.83	106.20	113.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1003	CLA	C3D-CAD-CBD	-4.83	100.77	107.60
21	A	6008	BCR	C3-C4-C5	-4.82	106.21	113.87
19	2	2012	CLA	C1D-CHD-C4C	-4.82	115.30	122.60
22	4	7052	LMU	C1'-O5'-C5'	-4.81	104.41	113.75
19	4	4004	CLA	C1D-CHD-C4C	-4.80	113.96	126.32
19	B	1220	CLA	C1D-CHD-C4C	-4.80	115.34	122.60
19	B	9010	CLA	C3D-CAD-CBD	-4.80	100.82	107.60
22	3	7005	LMU	O1B-C1B-O5B	-4.80	98.54	110.68
21	I	6021	BCR	C29-C30-C25	-4.79	102.78	110.36
19	B	1213	CLA	O1D-CGD-CBD	-4.79	117.75	124.62
21	L	6019	BCR	C7-C8-C9	-4.79	118.91	126.22
19	1	1014	CLA	O1D-CGD-CBD	-4.79	117.76	124.62
19	3	3007	CLA	C1D-CHD-C4C	-4.78	115.37	122.60
19	B	1218	CLA	O1D-CGD-CBD	-4.78	117.77	124.62
21	A	6007	BCR	C32-C1-C6	-4.78	102.81	110.30
19	A	1105	CLA	C1D-CHD-C4C	-4.77	115.39	122.60
19	2	2010	CLA	C1D-CHD-C4C	-4.77	114.06	126.32
21	A	6007	BCR	C7-C8-C9	-4.76	118.95	126.22
19	2	2011	CLA	C3B-C2B-C1B	-4.76	102.12	106.29
19	B	1239	CLA	C3D-CAD-CBD	-4.76	100.87	107.60
19	3	3002	CLA	C1D-CHD-C4C	-4.75	114.10	126.32
19	2	2008	CLA	C1D-CHD-C4C	-4.75	114.10	126.32
19	1	1005	CLA	OBD-CAD-C3D	-4.75	118.66	128.35
21	B	6005	BCR	C38-C26-C25	-4.75	119.94	124.61
19	3	3014	CLA	C2D-C3D-C4D	-4.74	102.13	106.30
19	4	4011	CLA	C3B-C2B-C1B	-4.74	102.14	106.29
19	B	1221	CLA	OBD-CAD-C3D	-4.74	118.69	128.35
21	A	6003	BCR	C7-C8-C9	-4.73	119.00	126.22
19	3	3004	CLA	C2A-C1A-CHA	-4.73	114.20	122.58
19	4	4005	CLA	C2A-C1A-CHA	-4.73	114.21	122.58
19	B	1211	CLA	CMD-C2D-C3D	-4.72	115.85	125.09
19	B	1231	CLA	C3D-CAD-CBD	-4.72	100.92	107.60
19	A	1127	CLA	O1D-CGD-CBD	-4.72	117.86	124.62
19	2	2005	CLA	C2D-C3D-C4D	-4.72	102.15	106.30
19	L	1148	CLA	O2D-CGD-O1D	-4.72	114.05	123.79
19	B	1215	CLA	CHD-C4C-C3C	-4.72	117.65	124.94
21	A	6011	BCR	C33-C5-C6	-4.72	119.97	124.61
19	B	1213	CLA	C3D-CAD-CBD	-4.72	100.93	107.60
19	1	1007	CLA	C3D-CAD-CBD	-4.72	100.93	107.60
19	3	3001	CLA	C1D-CHD-C4C	-4.71	114.19	126.32
19	3	3014	CLA	C3B-C2B-C1B	-4.71	102.17	106.29
19	B	1205	CLA	C3D-CAD-CBD	-4.71	100.94	107.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	2005	CLA	C2A-C1A-CHA	-4.70	114.25	122.58
21	B	6017	BCR	C7-C8-C9	-4.70	119.05	126.22
19	1	1013	CLA	CMD-C2D-C3D	-4.70	115.90	125.09
19	2	2011	CLA	C1D-CHD-C4C	-4.70	114.24	126.32
21	B	6004	BCR	C31-C1-C6	-4.69	102.94	110.30
19	1	1013	CLA	O2A-CGA-O1A	-4.69	111.39	123.49
19	A	1101	CLA	O1D-CGD-CBD	-4.68	117.92	124.62
21	L	6019	BCR	C3-C4-C5	-4.68	106.45	113.87
19	B	1301	CLA	C1D-CHD-C4C	-4.67	115.53	122.60
19	L	1501	CLA	CHD-C4C-C3C	-4.67	117.72	124.94
21	F	6014	BCR	C15-C14-C13	-4.67	120.45	127.20
19	2	2003	CLA	C1D-CHD-C4C	-4.67	114.31	126.32
19	B	1227	CLA	C1D-CHD-C4C	-4.67	115.54	122.60
19	4	4011	CLA	C1D-CHD-C4C	-4.66	114.33	126.32
21	3	6022	BCR	C31-C1-C6	-4.66	103.00	110.30
19	B	1232	CLA	C3D-CAD-CBD	-4.65	101.02	107.60
19	A	9012	CLA	CHD-C4C-C3C	-4.65	117.75	124.94
19	B	1238	CLA	C1D-CHD-C4C	-4.65	115.56	122.60
19	A	1125	CLA	CHD-C4C-C3C	-4.65	117.76	124.94
21	I	6021	BCR	C31-C1-C6	-4.64	103.02	110.30
19	3	3017	CLA	C3D-CAD-CBD	-4.64	101.04	107.60
19	4	4006	CLA	C3D-CAD-CBD	-4.64	101.04	107.60
19	B	1217	CLA	CHD-C4C-C3C	-4.64	117.78	124.94
19	J	1308	CLA	CHD-C4C-C3C	-4.62	117.80	124.94
19	1	1007	CLA	CHD-C4C-C3C	-4.62	117.80	124.94
19	L	1148	CLA	C4B-CHC-C1C	-4.62	119.33	129.26
19	A	1131	CLA	C3D-CAD-CBD	-4.62	101.07	107.60
19	B	1216	CLA	CHD-C4C-C3C	-4.61	117.81	124.94
21	B	6010	BCR	C29-C30-C25	-4.61	103.07	110.36
21	F	6016	BCR	C16-C17-C18	-4.60	120.55	127.20
19	3	3008	CLA	CMD-C2D-C3D	-4.60	116.09	125.09
19	A	1112	CLA	O1D-CGD-CBD	-4.59	118.04	124.62
19	B	9010	CLA	C1D-CHD-C4C	-4.59	115.66	122.60
21	B	6005	BCR	C16-C17-C18	-4.58	120.58	127.20
19	A	1116	CLA	C3D-CAD-CBD	-4.58	101.12	107.60
19	B	1231	CLA	CHD-C4C-C3C	-4.58	117.87	124.94
19	4	4002	CLA	C3D-CAD-CBD	-4.58	101.13	107.60
19	A	1108	CLA	C1D-CHD-C4C	-4.58	115.68	122.60
21	B	6004	BCR	C7-C8-C9	-4.58	119.24	126.22
19	B	1229	CLA	CHD-C4C-C3C	-4.58	117.87	124.94
19	L	1504	CLA	CHD-C4C-C3C	-4.57	117.88	124.94
19	3	3010	CLA	C1D-CHD-C4C	-4.57	114.58	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	1307	CLA	C2D-C3D-C4D	-4.56	102.29	106.30
19	3	3015	CLA	C1D-CHD-C4C	-4.55	114.62	126.32
19	2	2008	CLA	C3C-C4C-CHD	-4.55	117.84	125.32
19	L	1148	CLA	C4-C3-C2	-4.55	114.58	123.50
19	4	1304	CLA	CHD-C4C-C3C	-4.54	117.92	124.94
21	A	6003	BCR	C31-C1-C6	-4.52	103.21	110.30
19	1	1310	CLA	C1D-CHD-C4C	-4.52	114.69	126.32
19	2	2007	CLA	C1D-CHD-C4C	-4.52	115.76	122.60
19	R	1150	CLA	C3D-CAD-CBD	-4.52	101.21	107.60
19	B	1239	CLA	CHD-C4C-C3C	-4.52	117.96	124.94
19	1	1002	CLA	C3D-CAD-CBD	-4.51	101.23	107.60
19	4	4002	CLA	CHD-C4C-C3C	-4.50	117.99	124.94
19	1	1015	CLA	C1D-CHD-C4C	-4.49	114.76	126.32
21	1	6023	BCR	C19-C18-C17	-4.49	111.75	118.98
21	A	6011	BCR	C31-C1-C6	-4.49	103.26	110.30
19	L	1148	CLA	CMD-C2D-C3D	-4.49	116.31	125.09
19	B	1236	CLA	O1D-CGD-CBD	-4.48	118.19	124.62
21	J	6012	BCR	C15-C14-C13	-4.48	120.73	127.20
19	A	1237	CLA	CHD-C4C-C3C	-4.48	118.02	124.94
21	A	6003	BCR	C38-C26-C25	-4.48	120.21	124.61
21	I	6018	BCR	C4-C5-C6	-4.47	117.08	122.78
21	3	6022	BCR	C2-C1-C6	-4.47	103.29	110.36
19	3	3017	CLA	O1D-CGD-CBD	-4.47	118.22	124.62
21	I	6018	BCR	C16-C15-C14	-4.46	113.53	123.39
22	R	7014	LMU	C1'-C2'-C3'	-4.46	101.19	109.97
22	4	7033	LMU	C1B-O1B-C4'	-4.45	106.37	118.01
19	4	4006	CLA	C4-C3-C2	-4.45	114.77	123.50
19	B	1234	CLA	C3D-CAD-CBD	-4.44	101.32	107.60
19	A	1151	CLA	C3D-CAD-CBD	-4.44	101.32	107.60
19	3	3002	CLA	C2A-C1A-CHA	-4.43	114.72	122.58
19	3	3008	CLA	C3D-CAD-CBD	-4.43	101.33	107.60
19	3	2009	CLA	CHD-C4C-C3C	-4.42	118.10	124.94
19	3	3006	CLA	C3C-C4C-CHD	-4.42	118.05	125.32
19	A	1111	CLA	C3D-CAD-CBD	-4.42	101.35	107.60
19	4	1306	CLA	C3D-CAD-CBD	-4.42	101.35	107.60
19	B	1232	CLA	CHD-C4C-C3C	-4.42	118.11	124.94
22	E	7037	LMU	C4B-C3B-C2B	-4.42	102.55	110.79
21	A	6002	BCR	C11-C10-C9	-4.41	120.82	127.20
19	B	1229	CLA	C3D-CAD-CBD	-4.41	101.37	107.60
19	1	1005	CLA	CHD-C4C-C3C	-4.41	118.13	124.94
19	4	4013	CLA	C1D-CHD-C4C	-4.40	115.00	126.32
19	B	1211	CLA	C3D-CAD-CBD	-4.40	101.38	107.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1211	CLA	C1D-CHD-C4C	-4.40	115.94	122.60
19	G	1242	CLA	CHD-C4C-C3C	-4.40	118.14	124.94
19	3	3014	CLA	C2A-C1A-CHA	-4.40	114.79	122.58
19	3	3001	CLA	C3B-C2B-C1B	-4.39	102.44	106.29
19	2	1307	CLA	C2A-C1A-CHA	-4.39	114.80	122.58
21	B	6017	BCR	C32-C1-C6	-4.39	103.42	110.30
19	H	1505	CLA	C3D-CAD-CBD	-4.39	101.39	107.60
19	2	2002	CLA	C3D-CAD-CBD	-4.39	101.39	107.60
19	1	1011	CLA	CMD-C2D-C3D	-4.39	116.51	125.09
19	3	3017	CLA	CBC-CAC-C3C	-4.38	99.00	112.39
19	4	4007	CLA	C3D-CAD-CBD	-4.38	101.40	107.60
21	B	6004	BCR	C20-C19-C18	-4.38	113.41	126.32
19	1	1003	CLA	CMD-C2D-C3D	-4.38	116.52	125.09
19	2	2006	CLA	CHD-C4C-C3C	-4.38	118.17	124.94
19	B	1222	CLA	CHD-C4C-C3C	-4.38	118.18	124.94
19	4	4011	CLA	C2A-C1A-CHA	-4.37	114.83	122.58
21	I	6021	BCR	C27-C26-C25	-4.37	117.21	122.78
19	B	1226	CLA	CMD-C2D-C3D	-4.37	116.54	125.09
19	B	1208	CLA	C3D-CAD-CBD	-4.37	101.42	107.60
19	1	1008	CLA	CHD-C4C-C3C	-4.36	118.20	124.94
19	F	1302	CLA	C3D-CAD-CBD	-4.36	101.43	107.60
19	B	1236	CLA	CHD-C4C-C3C	-4.36	118.20	124.94
21	A	6007	BCR	C2-C1-C6	-4.36	103.47	110.36
21	F	6014	BCR	C24-C23-C22	-4.36	119.57	126.22
19	B	1238	CLA	CMD-C2D-C3D	-4.36	116.57	125.09
19	A	1127	CLA	C3D-CAD-CBD	-4.35	101.44	107.60
19	A	1309	CLA	C1D-CHD-C4C	-4.35	115.12	126.32
19	3	3003	CLA	CHD-C4C-C3C	-4.35	117.54	124.83
19	H	1505	CLA	CHD-C4C-C3C	-4.34	118.24	124.94
21	1	6023	BCR	C16-C15-C14	-4.33	113.81	123.39
19	3	3007	CLA	C3D-CAD-CBD	-4.33	101.47	107.60
19	2	2012	CLA	C3D-CAD-CBD	-4.33	101.47	107.60
19	B	1230	CLA	CHD-C4C-C3C	-4.33	118.25	124.94
19	L	1148	CLA	CHD-C4C-C3C	-4.33	118.25	124.94
19	1	1001	CLA	C3D-CAD-CBD	-4.33	101.48	107.60
19	I	1204	CLA	CHD-C4C-C3C	-4.33	118.26	124.94
21	3	6022	BCR	C38-C26-C25	-4.32	120.36	124.61
21	L	6019	BCR	C29-C30-C25	-4.32	103.52	110.36
21	F	6014	BCR	C33-C5-C6	-4.32	120.36	124.61
21	A	6002	BCR	C38-C26-C25	-4.32	120.36	124.61
19	B	1226	CLA	CHD-C4C-C3C	-4.32	118.27	124.94
19	B	1238	CLA	CHD-C4C-C3C	-4.31	118.27	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1225	CLA	O2D-CGD-O1D	-4.31	114.88	123.79
19	3	3016	CLA	CHD-C4C-C3C	-4.31	118.28	124.94
19	A	1309	CLA	C2A-C1A-CHA	-4.31	114.95	122.58
19	3	1147	CLA	O1D-CGD-CBD	-4.31	118.45	124.62
19	A	1109	CLA	CMD-C2D-C3D	-4.30	116.67	125.09
19	B	1210	CLA	C3D-CAD-CBD	-4.30	101.52	107.60
19	A	1132	CLA	CMD-C2D-C3D	-4.30	116.68	125.09
19	K	1142	CLA	CHD-C4C-C3C	-4.30	118.30	124.94
21	A	6002	BCR	C31-C1-C6	-4.30	103.57	110.30
19	4	1009	CLA	CHD-C4C-C3C	-4.29	117.64	124.83
19	A	1117	CLA	CHD-C4C-C3C	-4.29	118.31	124.94
21	3	6022	BCR	C37-C22-C21	-4.29	116.57	122.90
19	4	4001	CLA	C3D-CAD-CBD	-4.28	101.54	107.60
19	A	1104	CLA	CHD-C4C-C3C	-4.28	118.33	124.94
19	A	1137	CLA	CHD-C4C-C3C	-4.28	118.33	124.94
19	2	2003	CLA	C2A-C1A-CHA	-4.27	115.01	122.58
19	1	1001	CLA	CMD-C2D-C3D	-4.27	116.73	125.09
19	A	1101	CLA	C3D-CAD-CBD	-4.27	101.56	107.60
19	A	1116	CLA	CHD-C4C-C3C	-4.27	118.34	124.94
21	L	6019	BCR	C27-C26-C25	-4.27	117.34	122.78
21	F	6014	BCR	C38-C26-C25	-4.27	120.41	124.61
19	3	3005	CLA	C3C-C4C-CHD	-4.27	118.30	125.32
19	F	1305	CLA	CHD-C4C-C3C	-4.26	118.36	124.94
21	A	6003	BCR	C33-C5-C6	-4.26	120.42	124.61
19	B	1209	CLA	C3D-CAD-CBD	-4.26	101.58	107.60
19	2	2013	CLA	CHD-C4C-C3C	-4.25	118.37	124.94
21	A	6008	BCR	C38-C26-C25	-4.25	120.43	124.61
19	2	2001	CLA	C3D-CAD-CBD	-4.25	101.59	107.60
19	1	1310	CLA	C2D-C3D-C4D	-4.25	102.56	106.30
19	A	1109	CLA	C3D-CAD-CBD	-4.24	101.60	107.60
19	B	1229	CLA	O2D-CGD-O1D	-4.24	115.03	123.79
19	1	1005	CLA	O2D-CGD-O1D	-4.24	115.03	123.79
19	3	3001	CLA	C2A-C1A-CHA	-4.24	115.07	122.58
19	1	1014	CLA	C3D-CAD-CBD	-4.24	101.60	107.60
19	2	1307	CLA	C3B-C2B-C1B	-4.24	102.58	106.29
19	R	1150	CLA	CHD-C4C-C3C	-4.23	118.40	124.94
19	2	2008	CLA	C2A-C1A-CHA	-4.23	115.09	122.58
19	J	1308	CLA	C3D-CAD-CBD	-4.23	101.62	107.60
19	A	1139	CLA	CHD-C4C-C3C	-4.23	118.41	124.94
19	B	1212	CLA	CHD-C4C-C3C	-4.23	118.41	124.94
19	B	1223	CLA	CHD-C4C-C3C	-4.23	118.41	124.94
19	B	1224	CLA	CHD-C4C-C3C	-4.23	118.41	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	J	1311	CLA	CHD-C4C-C3C	-4.23	118.41	124.94
19	3	3015	CLA	C2A-C1A-CHA	-4.22	115.10	122.58
19	2	1307	CLA	C1D-CHD-C4C	-4.22	115.46	126.32
19	2	2010	CLA	C3C-C4C-CHD	-4.22	118.38	125.32
19	4	4010	CLA	C3B-C2B-C1B	-4.22	102.60	106.29
19	3	3008	CLA	CHD-C4C-C3C	-4.22	118.42	124.94
19	A	1119	CLA	C3D-CAD-CBD	-4.22	101.64	107.60
19	1	1001	CLA	O1D-CGD-CBD	-4.21	118.58	124.62
21	B	6010	BCR	C38-C26-C25	-4.21	120.47	124.61
19	A	1139	CLA	C3D-CAD-CBD	-4.21	101.64	107.60
19	A	1126	CLA	C3D-CAD-CBD	-4.21	101.64	107.60
19	B	1201	CLA	CHD-C4C-C3C	-4.21	118.43	124.94
22	G	7039	LMU	C1B-O5B-C5B	-4.21	105.58	113.75
19	2	2005	CLA	C3C-C4C-CHD	-4.21	118.40	125.32
19	3	3010	CLA	C2A-C1A-CHA	-4.20	115.14	122.58
19	B	1201	CLA	O2D-CGD-O1D	-4.20	115.11	123.79
19	B	1226	CLA	C3D-CAD-CBD	-4.20	101.66	107.60
22	E	7048	LMU	C1B-O1B-C4'	-4.20	107.03	118.01
19	B	1222	CLA	C3D-CAD-CBD	-4.20	101.66	107.60
19	A	1136	CLA	C3D-CAD-CBD	-4.19	101.67	107.60
19	A	9013	CLA	CHD-C4C-C3C	-4.19	118.46	124.94
19	A	1101	CLA	CHD-C4C-C3C	-4.19	118.47	124.94
19	4	4001	CLA	CHD-C4C-C3C	-4.19	118.47	124.94
19	3	3004	CLA	C1D-CHD-C4C	-4.19	115.56	126.32
19	A	1141	CLA	C3D-CAD-CBD	-4.18	101.68	107.60
19	B	1232	CLA	O1D-CGD-CBD	-4.18	118.63	124.62
19	2	2007	CLA	O2D-CGD-O1D	-4.18	115.16	123.79
19	A	1112	CLA	C3D-CAD-CBD	-4.18	101.69	107.60
19	B	1225	CLA	C3D-CAD-CBD	-4.17	101.70	107.60
21	A	6003	BCR	C15-C14-C13	-4.17	121.17	127.20
19	3	3004	CLA	C2C-C1C-CHC	-4.17	117.74	125.15
19	B	1233	CLA	CHD-C4C-C3C	-4.17	118.49	124.94
21	L	6019	BCR	C33-C5-C6	-4.17	120.51	124.61
19	A	1128	CLA	CHD-C4C-C3C	-4.17	118.50	124.94
19	3	3006	CLA	C3B-C2B-C1B	-4.17	102.64	106.29
21	A	6002	BCR	C28-C27-C26	-4.17	107.26	113.87
19	1	1008	CLA	CMD-C2D-C3D	-4.17	116.94	125.09
19	2	2005	CLA	C1D-CHD-C4C	-4.16	115.61	126.32
19	B	1226	CLA	OBD-CAD-CBD	-4.16	119.66	125.94
21	B	6004	BCR	C33-C5-C6	-4.16	120.52	124.61
19	A	1117	CLA	C3D-CAD-CBD	-4.15	101.73	107.60
19	3	3014	CLA	C1D-CHD-C4C	-4.15	115.64	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L	1502	CLA	C3D-CAD-CBD	-4.15	101.73	107.60
21	B	6005	BCR	C33-C5-C6	-4.14	120.53	124.61
19	A	1141	CLA	CHD-C4C-C3C	-4.14	118.54	124.94
19	L	1148	CLA	C3D-CAD-CBD	-4.14	101.75	107.60
19	B	1203	CLA	C6-C5-C3	-4.14	103.40	112.48
19	2	2014	CLA	C3D-CAD-CBD	-4.14	101.75	107.60
19	2	2001	CLA	CHD-C4C-C3C	-4.13	118.56	124.94
19	3	3002	CLA	C3C-C4C-CHD	-4.13	118.52	125.32
19	J	1311	CLA	C3D-CAD-CBD	-4.13	101.76	107.60
19	A	9013	CLA	C3D-CAD-CBD	-4.13	101.76	107.60
19	4	4007	CLA	CHD-C4C-C3C	-4.13	118.56	124.94
19	L	1504	CLA	O2D-CGD-O1D	-4.13	115.27	123.79
19	B	1234	CLA	CMD-C2D-C3D	-4.12	117.02	125.09
19	4	4013	CLA	C3C-C4C-CHD	-4.12	118.54	125.32
19	A	1102	CLA	CHD-C4C-C3C	-4.12	118.57	124.94
21	A	6007	BCR	C38-C26-C25	-4.12	120.56	124.61
19	A	1134	CLA	C3D-CAD-CBD	-4.12	101.77	107.60
19	B	1219	CLA	C3D-CAD-CBD	-4.12	101.78	107.60
19	F	1302	CLA	CHD-C4C-C3C	-4.11	118.59	124.94
19	1	1013	CLA	CGD-CBD-CAD	-4.11	96.71	110.62
19	4	1004	CLA	C3D-CAD-CBD	-4.11	101.79	107.60
22	B	7040	LMU	O5B-C5B-C4B	-4.11	101.97	109.68
19	3	3015	CLA	C3C-C4C-CHD	-4.11	118.56	125.32
19	K	1142	CLA	C3D-CAD-CBD	-4.10	101.80	107.60
19	R	1144	CLA	CMD-C2D-C3D	-4.10	117.06	125.09
19	A	1149	CLA	O2D-CGD-O1D	-4.10	115.32	123.79
19	R	1150	CLA	CMD-C2D-C3D	-4.10	117.07	125.09
19	B	1201	CLA	C3D-CAD-CBD	-4.09	101.81	107.60
19	A	1140	CLA	CHD-C4C-C3C	-4.09	118.61	124.94
19	2	2013	CLA	O1D-CGD-CBD	-4.09	118.76	124.62
19	K	3009	CLA	C3D-CAD-CBD	-4.08	101.82	107.60
19	1	1015	CLA	C3B-C2B-C1B	-4.08	102.72	106.29
19	1	1006	CLA	CHD-C4C-C3C	-4.07	118.01	124.83
19	B	1202	CLA	CMD-C2D-C3D	-4.07	117.12	125.09
19	B	1223	CLA	C3D-CAD-CBD	-4.07	101.84	107.60
19	3	3012	CLA	C2A-C1A-CHA	-4.07	115.37	122.58
19	A	1124	CLA	C3D-CAD-CBD	-4.07	101.85	107.60
19	4	4010	CLA	C3C-C4C-CHD	-4.07	118.63	125.32
19	B	1213	CLA	CHD-C4C-C3C	-4.07	118.66	124.94
19	4	4003	CLA	C3D-CAD-CBD	-4.06	101.85	107.60
21	B	6006	BCR	C27-C26-C25	-4.06	117.61	122.78
19	1	1003	CLA	O2D-CGD-O1D	-4.06	115.41	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	F	1305	CLA	O2D-CGD-O1D	-4.05	115.43	123.79
19	H	1145	CLA	CHD-C4C-C3C	-4.05	118.68	124.94
19	H	1505	CLA	CMD-C2D-C3D	-4.05	117.17	125.09
21	A	6007	BCR	C20-C19-C18	-4.05	114.40	126.32
21	I	6018	BCR	C29-C30-C25	-4.05	103.96	110.36
19	3	1147	CLA	CBA-CAA-C2A	-4.04	102.34	113.73
21	A	6007	BCR	C3-C4-C5	-4.04	107.46	113.87
19	A	1107	CLA	CHC-C1C-C2C	-4.03	115.74	126.35
19	B	1227	CLA	C3D-CAD-CBD	-4.03	101.90	107.60
21	A	6002	BCR	C7-C8-C9	-4.03	120.08	126.22
19	A	1136	CLA	CHD-C4C-C3C	-4.03	118.72	124.94
19	B	1216	CLA	O1D-CGD-CBD	-4.03	118.85	124.62
19	B	1220	CLA	C3D-CAD-CBD	-4.02	101.91	107.60
21	A	6003	BCR	C2-C1-C6	-4.02	104.00	110.36
19	2	2011	CLA	C3C-C4C-CHD	-4.02	118.70	125.32
19	A	1133	CLA	C3D-CAD-CBD	-4.02	101.91	107.60
19	A	1138	CLA	C3D-CAD-CBD	-4.02	101.91	107.60
19	1	1003	CLA	CGD-CBD-CAD	-4.02	97.00	110.62
19	A	1237	CLA	C6-C5-C3	-4.02	103.67	112.48
19	1	1002	CLA	CHD-C4C-C3C	-4.02	118.73	124.94
19	B	1208	CLA	CMD-C2D-C3D	-4.02	117.23	125.09
19	3	3017	CLA	CMD-C2D-C3D	-4.02	117.23	125.09
19	B	1216	CLA	C3D-CAD-CBD	-4.01	101.92	107.60
19	A	1106	CLA	CHD-C4C-C3C	-4.01	118.74	124.94
19	F	1305	CLA	CBA-CAA-C2A	-4.01	102.42	113.73
19	A	1115	CLA	CHD-C4C-C3C	-4.01	118.75	124.94
19	A	1137	CLA	C3D-CAD-CBD	-4.01	101.93	107.60
19	A	1138	CLA	CHD-C4C-C3C	-4.00	118.75	124.94
19	A	9023	CLA	CHD-C4C-C3C	-4.00	118.75	124.94
19	2	2002	CLA	C4-C3-C2	-4.00	115.65	123.50
19	A	1135	CLA	CHD-C4C-C3C	-4.00	118.76	124.94
19	A	9012	CLA	O1D-CGD-CBD	-4.00	118.89	124.62
19	A	1101	CLA	O2D-CGD-O1D	-4.00	115.53	123.79
19	K	1143	CLA	C3D-CAD-CBD	-3.99	101.95	107.60
19	4	4010	CLA	C2A-C1A-CHA	-3.99	115.50	122.58
21	B	6004	BCR	C28-C27-C26	-3.99	107.53	113.87
19	A	1120	CLA	C3D-CAD-CBD	-3.99	101.95	107.60
19	1	1015	CLA	C2A-C1A-CHA	-3.99	115.51	122.58
22	B	7038	LMU	C3'-C4'-C5'	-3.99	101.82	110.84
19	1	1003	CLA	CHD-C4C-C3C	-3.98	118.79	124.94
19	H	1207	CLA	CHD-C4C-C3C	-3.98	118.79	124.94
19	R	1144	CLA	CHD-C4C-C3C	-3.97	118.80	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	L	6019	BCR	C23-C24-C25	-3.97	115.40	127.32
19	2	2007	CLA	C6-C5-C3	-3.97	103.78	112.48
21	B	6020	BCR	C7-C6-C5	-3.97	112.29	121.37
19	A	1107	CLA	C3D-CAD-CBD	-3.97	101.99	107.60
19	3	3010	CLA	C3B-C2B-C1B	-3.97	102.82	106.29
19	B	1209	CLA	C4-C3-C2	-3.96	115.72	123.50
19	2	2012	CLA	O2D-CGD-O1D	-3.96	115.62	123.79
19	2	2003	CLA	C3B-C2B-C1B	-3.96	102.83	106.29
19	A	1151	CLA	CMD-C2D-C3D	-3.95	117.36	125.09
19	2	2010	CLA	C2A-C1A-CHA	-3.95	115.58	122.58
21	B	6004	BCR	C38-C26-C25	-3.95	120.73	124.61
19	2	2002	CLA	CMD-C2D-C3D	-3.95	117.36	125.09
19	3	1118	CLA	CHD-C4C-C3C	-3.95	118.22	124.83
21	A	6011	BCR	C2-C1-C6	-3.94	104.12	110.36
19	B	1201	CLA	CMD-C2D-C3D	-3.94	117.37	125.09
19	A	1131	CLA	CHD-C4C-C3C	-3.94	118.85	124.94
19	3	3010	CLA	C3C-C4C-CHD	-3.94	118.84	125.32
21	B	6017	BCR	C15-C16-C17	-3.94	114.68	123.39
19	A	1140	CLA	C3D-CAD-CBD	-3.94	102.03	107.60
19	B	1238	CLA	C3D-CAD-CBD	-3.94	102.03	107.60
19	A	1108	CLA	O1D-CGD-CBD	-3.94	118.98	124.62
19	3	3004	CLA	C3C-C4C-CHD	-3.93	118.85	125.32
19	A	1134	CLA	CHD-C4C-C3C	-3.93	118.87	124.94
19	A	9012	CLA	C3D-CAD-CBD	-3.93	102.04	107.60
19	A	1105	CLA	C3D-CAD-CBD	-3.92	102.05	107.60
21	F	6014	BCR	C29-C30-C25	-3.92	104.15	110.36
21	A	6002	BCR	C10-C11-C12	-3.92	111.18	123.13
19	4	4002	CLA	CMB-C2B-C1B	-3.92	121.88	128.36
21	B	6010	BCR	C33-C5-C6	-3.92	120.76	124.61
21	B	6004	BCR	C3-C4-C5	-3.92	107.66	113.87
19	A	1112	CLA	CHD-C4C-C3C	-3.91	118.89	124.94
19	4	4005	CLA	C3B-C2B-C1B	-3.91	102.86	106.29
19	3	3005	CLA	C3B-C2B-C1B	-3.91	102.87	106.29
19	3	3016	CLA	C3D-CAD-CBD	-3.90	102.08	107.60
19	A	1309	CLA	C3C-C4C-CHD	-3.90	118.90	125.32
19	B	1206	CLA	CHD-C4C-C3C	-3.90	118.91	124.94
21	F	6014	BCR	C31-C1-C6	-3.90	104.19	110.30
19	3	3012	CLA	C2C-C1C-CHC	-3.90	118.22	125.15
22	B	7040	LMU	C1B-O1B-C4'	-3.90	107.82	118.01
19	A	1113	CLA	C3D-CAD-CBD	-3.90	102.09	107.60
19	1	1303	CLA	CHD-C4C-C3C	-3.89	118.93	124.94
19	B	1301	CLA	CAA-C2A-C3A	-3.89	106.89	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1119	CLA	CMD-C2D-C3D	-3.88	117.49	125.09
19	B	1226	CLA	O1D-CGD-CBD	-3.88	119.06	124.62
19	A	1120	CLA	CHD-C4C-C3C	-3.88	118.94	124.94
19	4	1304	CLA	CMD-C2D-C3D	-3.88	117.50	125.09
19	4	4015	CLA	C3D-CAD-CBD	-3.88	102.11	107.60
19	H	1241	CLA	O1D-CGD-CBD	-3.88	119.07	124.62
19	A	1105	CLA	O1D-CGD-CBD	-3.87	119.08	124.62
21	F	6016	BCR	C8-C7-C6	-3.87	115.70	127.32
22	G	7051	LMU	C1'-O5'-C5'	-3.87	106.24	113.75
19	1	1012	CLA	CHD-C4C-C3C	-3.86	118.36	124.83
21	A	6002	BCR	C33-C5-C6	-3.86	120.81	124.61
19	B	1214	CLA	CHD-C4C-C3C	-3.86	118.97	124.94
19	3	3001	CLA	C2D-C3D-C4D	-3.86	102.90	106.30
19	A	9022	CLA	CHD-C4C-C3C	-3.86	118.98	124.94
19	B	1234	CLA	CHD-C4C-C3C	-3.86	118.98	124.94
19	L	1504	CLA	C3D-CAD-CBD	-3.85	102.15	107.60
19	A	1129	CLA	O2D-CGD-O1D	-3.85	115.84	123.79
19	A	1125	CLA	C3D-CAD-CBD	-3.85	102.15	107.60
19	A	1116	CLA	O1D-CGD-CBD	-3.85	119.10	124.62
19	B	1202	CLA	C3D-CAD-CBD	-3.85	102.16	107.60
19	A	1103	CLA	C3D-CAD-CBD	-3.85	102.16	107.60
19	B	9010	CLA	CHD-C4C-C3C	-3.84	119.00	124.94
19	B	1235	CLA	O2D-CGD-O1D	-3.84	115.86	123.79
19	4	4014	CLA	CHD-C4C-C3C	-3.84	119.01	124.94
19	F	1305	CLA	C3D-CAD-CBD	-3.84	102.17	107.60
19	4	4013	CLA	C2A-C1A-CHA	-3.84	115.78	122.58
21	B	6005	BCR	C15-C14-C13	-3.84	121.66	127.20
19	L	1130	CLA	CHD-C4C-C3C	-3.83	119.02	124.94
19	F	1240	CLA	CMD-C2D-C3D	-3.82	117.61	125.09
21	A	6002	BCR	C11-C12-C13	-3.82	115.06	126.32
21	A	6002	BCR	C2-C1-C6	-3.82	104.31	110.36
19	B	1203	CLA	C3D-CAD-CBD	-3.82	102.19	107.60
19	A	1237	CLA	O1D-CGD-CBD	-3.82	119.15	124.62
22	H	7017	LMU	O5B-C5B-C4B	-3.82	102.51	109.68
19	A	1151	CLA	O1D-CGD-CBD	-3.82	119.15	124.62
19	A	1119	CLA	CHD-C4C-C3C	-3.82	119.04	124.94
19	A	1110	CLA	CHD-C4C-C3C	-3.82	119.04	124.94
19	B	1224	CLA	CMD-C2D-C3D	-3.82	117.62	125.09
21	B	6005	BCR	C24-C23-C22	-3.81	120.41	126.22
19	A	1120	CLA	CMD-C2D-C3D	-3.81	117.64	125.09
21	B	6004	BCR	C23-C24-C25	-3.80	115.90	127.32
21	A	6008	BCR	C33-C5-C6	-3.80	120.87	124.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1135	CLA	C3D-CAD-CBD	-3.80	102.23	107.60
21	J	6012	BCR	C28-C27-C26	-3.79	107.85	113.87
19	A	1237	CLA	C3D-CAD-CBD	-3.79	102.24	107.60
19	A	1124	CLA	CHD-C4C-C3C	-3.79	119.08	124.94
19	A	1108	CLA	CMD-C2D-C3D	-3.79	117.67	125.09
19	3	3005	CLA	C2A-C1A-CHA	-3.79	115.87	122.58
19	3	3001	CLA	C3C-C4C-CHD	-3.79	119.09	125.32
19	A	1109	CLA	CHD-C4C-C3C	-3.79	119.09	124.94
21	A	6008	BCR	C23-C24-C25	-3.79	115.95	127.32
21	A	6007	BCR	C28-C27-C26	-3.78	107.86	113.87
19	B	1215	CLA	C3D-CAD-CBD	-3.78	102.25	107.60
19	G	1242	CLA	C3D-CAD-CBD	-3.78	102.25	107.60
19	1	1015	CLA	C2D-C3D-C4D	-3.78	102.97	106.30
21	I	6021	BCR	C8-C7-C6	-3.78	115.96	127.32
21	A	6011	BCR	C23-C24-C25	-3.78	115.96	127.32
19	A	1123	CLA	CHD-C4C-C3C	-3.78	119.10	124.94
19	4	1004	CLA	CHD-C4C-C3C	-3.78	119.10	124.94
19	4	4011	CLA	C2D-C3D-C4D	-3.78	102.98	106.30
19	L	1501	CLA	O1D-CGD-CBD	-3.78	119.21	124.62
19	A	1133	CLA	CMD-C2D-C3D	-3.77	117.71	125.09
21	B	6005	BCR	C34-C9-C10	-3.77	117.34	122.90
19	2	2003	CLA	C3C-C4C-CHD	-3.76	119.13	125.32
19	B	1211	CLA	O1D-CGD-CBD	-3.76	119.23	124.62
19	2	2005	CLA	C2C-C1C-CHC	-3.76	118.47	125.15
19	A	1102	CLA	CMD-C2D-C3D	-3.76	117.74	125.09
19	B	1228	CLA	O1D-CGD-CBD	-3.76	119.24	124.62
21	I	6018	BCR	C12-C13-C14	-3.75	112.94	118.98
21	I	6018	BCR	C38-C26-C25	-3.75	120.92	124.61
19	A	9022	CLA	O2D-CGD-O1D	-3.75	116.05	123.79
19	A	1104	CLA	C3D-CAD-CBD	-3.74	102.30	107.60
19	H	1241	CLA	C3D-CAD-CBD	-3.74	102.31	107.60
19	B	1220	CLA	O2D-CGD-O1D	-3.74	116.07	123.79
19	A	1309	CLA	C3B-C2B-C1B	-3.74	103.02	106.29
19	3	3006	CLA	C2C-C1C-CHC	-3.74	118.51	125.15
22	H	7032	LMU	C1B-C2B-C3B	-3.74	102.61	109.97
19	B	1233	CLA	C3D-CAD-CBD	-3.73	102.32	107.60
19	4	4004	CLA	C2A-C1A-CHA	-3.73	115.97	122.58
19	L	1501	CLA	C3D-CAD-CBD	-3.73	102.32	107.60
19	B	1221	CLA	O2D-CGD-O1D	-3.73	116.08	123.79
19	2	2014	CLA	CHD-C4C-C3C	-3.73	119.17	124.94
21	A	6011	BCR	C28-C27-C26	-3.73	107.95	113.87
19	1	1015	CLA	C3C-C4C-CHD	-3.73	119.19	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	4009	CLA	CHD-C4C-C3C	-3.73	119.18	124.94
19	4	4011	CLA	C3C-C4C-CHD	-3.73	119.19	125.32
19	4	4004	CLA	C3C-C4C-CHD	-3.72	119.19	125.32
19	A	1115	CLA	C3D-CAD-CBD	-3.72	102.33	107.60
21	A	6011	BCR	C38-C26-C25	-3.72	120.95	124.61
19	K	3009	CLA	O2D-CGD-O1D	-3.72	116.10	123.79
19	1	1310	CLA	C3C-C4C-CHD	-3.72	119.20	125.32
21	B	6005	BCR	C3-C4-C5	-3.72	107.97	113.87
19	4	4005	CLA	C3C-C4C-CHD	-3.72	119.20	125.32
19	K	1146	CLA	CMD-C2D-C3D	-3.71	117.82	125.09
19	A	1127	CLA	CHD-C4C-C3C	-3.71	119.20	124.94
22	2	7027	LMU	C1B-O1B-C4'	-3.71	108.31	118.01
21	A	6002	BCR	C3-C4-C5	-3.71	107.98	113.87
19	B	1220	CLA	C2A-C1A-CHA	-3.71	117.06	123.89
19	3	3015	CLA	C3B-C2B-C1B	-3.70	103.05	106.29
19	A	1107	CLA	CMD-C2D-C3D	-3.70	117.85	125.09
22	3	7003	LMU	C1B-O1B-C4'	-3.70	108.34	118.01
21	B	6010	BCR	C15-C14-C13	-3.70	121.86	127.20
19	B	1212	CLA	C3D-CAD-CBD	-3.70	102.37	107.60
19	B	1218	CLA	CMD-C2D-C3D	-3.70	117.86	125.09
19	H	1145	CLA	CAA-C2A-C3A	-3.70	102.59	113.22
19	3	3007	CLA	CMD-C2D-C3D	-3.69	117.87	125.09
19	A	1110	CLA	C3D-CAD-CBD	-3.69	102.38	107.60
21	F	6016	BCR	C20-C19-C18	-3.69	115.47	126.32
19	3	3004	CLA	C3B-C2B-C1B	-3.69	103.06	106.29
19	2	2007	CLA	CHC-C1C-C2C	-3.68	116.66	126.35
19	1	1011	CLA	CHD-C4C-C3C	-3.68	118.67	124.83
19	1	1001	CLA	CHD-C4C-C3C	-3.68	119.26	124.94
21	B	6017	BCR	C24-C23-C22	-3.68	120.61	126.22
19	2	2004	CLA	CHD-C4C-C3C	-3.68	119.26	124.94
19	2	2011	CLA	C2A-C1A-CHA	-3.67	116.07	122.58
22	4	7052	LMU	O5'-C5'-C4'	-3.67	101.98	109.75
21	B	6017	BCR	C16-C17-C18	-3.67	121.90	127.20
19	2	2006	CLA	C3D-CAD-CBD	-3.67	102.42	107.60
19	A	1116	CLA	CMD-C2D-C3D	-3.67	117.92	125.09
21	A	6008	BCR	C24-C23-C22	-3.66	120.63	126.22
19	1	1012	CLA	CMD-C2D-C3D	-3.66	117.92	125.09
19	2	2007	CLA	C3D-CAD-CBD	-3.66	102.42	107.60
19	B	1221	CLA	C3D-CAD-CBD	-3.66	102.42	107.60
19	A	1138	CLA	CMD-C2D-C3D	-3.66	117.93	125.09
19	A	1105	CLA	CHD-C4C-C3C	-3.66	119.29	124.94
19	2	2004	CLA	C3D-CAD-CBD	-3.65	102.44	107.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	4009	CLA	O1D-CGD-CBD	-3.65	119.39	124.62
19	B	1219	CLA	CMD-C2D-C3D	-3.65	117.95	125.09
19	A	1109	CLA	CAA-C2A-C3A	-3.65	102.73	113.22
19	3	3006	CLA	C2A-C1A-CHA	-3.65	116.12	122.58
19	F	1302	CLA	CMD-C2D-C3D	-3.64	117.96	125.09
19	3	3015	CLA	C2C-C1C-CHC	-3.64	118.67	125.15
21	B	6010	BCR	C2-C1-C6	-3.64	104.60	110.36
19	2	2013	CLA	C3D-CAD-CBD	-3.64	102.45	107.60
19	L	1502	CLA	CHD-C4C-C3C	-3.64	119.32	124.94
19	4	4004	CLA	C2D-C3D-C4D	-3.63	103.10	106.30
19	2	2002	CLA	CHD-C4C-C3C	-3.63	119.33	124.94
19	F	1240	CLA	CHD-C4C-C3C	-3.63	118.76	124.83
19	A	1123	CLA	C3D-CAD-CBD	-3.62	102.47	107.60
22	E	7048	LMU	C1B-O5B-C5B	-3.62	106.71	113.75
21	L	6019	BCR	C28-C27-C26	-3.62	108.12	113.87
19	K	1146	CLA	CHD-C4C-C3C	-3.62	119.35	124.94
19	H	1207	CLA	C3D-CAD-CBD	-3.62	102.48	107.60
19	4	4010	CLA	C2C-C1C-CHC	-3.62	118.72	125.15
19	A	1126	CLA	CMD-C2D-C3D	-3.61	118.03	125.09
19	K	1143	CLA	CHD-C4C-C3C	-3.60	119.37	124.94
19	A	1139	CLA	CMD-C2D-C3D	-3.60	118.05	125.09
19	A	1132	CLA	C3D-CAD-CBD	-3.60	102.51	107.60
19	A	1309	CLA	C2C-C1C-CHC	-3.60	118.75	125.15
19	A	1103	CLA	CHD-C4C-C3C	-3.60	119.38	124.94
19	2	1307	CLA	C3C-C4C-CHD	-3.60	119.40	125.32
21	B	6010	BCR	C3-C4-C5	-3.59	108.16	113.87
19	3	3012	CLA	C1D-CHD-C4C	-3.59	117.09	126.32
19	B	1301	CLA	CHD-C4C-C3C	-3.59	118.82	124.83
19	4	1306	CLA	CHC-C1C-C2C	-3.59	116.91	126.35
19	3	3017	CLA	CHC-C1C-C2C	-3.58	116.92	126.35
19	B	1220	CLA	CAA-C2A-C1A	-3.58	99.83	112.47
19	B	1228	CLA	C1-C2-C3	-3.58	120.84	126.71
21	A	6003	BCR	C20-C19-C18	-3.58	115.78	126.32
19	2	2008	CLA	C2D-C3D-C4D	-3.58	103.15	106.30
19	K	1146	CLA	C3D-CAD-CBD	-3.58	102.54	107.60
19	4	1004	CLA	CMD-C2D-C3D	-3.57	118.10	125.09
19	A	1111	CLA	CHD-C4C-C3C	-3.57	119.42	124.94
19	A	1123	CLA	CMD-C2D-C3D	-3.57	118.10	125.09
21	B	6004	BCR	C2-C1-C6	-3.57	104.71	110.36
22	G	7039	LMU	C1B-C2B-C3B	-3.57	102.93	109.97
19	A	1132	CLA	CHC-C1C-C2C	-3.57	116.96	126.35
19	3	3017	CLA	CAA-C2A-C3A	-3.57	102.95	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1121	CLA	CHD-C4C-C3C	-3.57	119.42	124.94
21	F	6014	BCR	C3-C4-C5	-3.57	108.20	113.87
21	F	6014	BCR	C2-C1-C6	-3.57	104.72	110.36
19	2	2001	CLA	CMD-C2D-C3D	-3.56	118.12	125.09
19	3	3005	CLA	C2D-C3D-C4D	-3.56	103.17	106.30
19	3	2009	CLA	CMD-C2D-C3D	-3.56	118.12	125.09
21	B	6010	BCR	C27-C26-C25	-3.56	118.24	122.78
19	4	4003	CLA	CHD-C4C-C3C	-3.56	119.44	124.94
21	B	6010	BCR	C16-C17-C18	-3.55	122.06	127.20
19	B	1203	CLA	O2D-CGD-O1D	-3.55	116.45	123.79
19	J	1311	CLA	O1D-CGD-CBD	-3.55	119.53	124.62
19	3	3008	CLA	O1D-CGD-CBD	-3.55	119.53	124.62
19	A	1141	CLA	CMD-C2D-C3D	-3.55	118.15	125.09
19	A	1134	CLA	CMD-C2D-C3D	-3.54	118.16	125.09
21	A	6003	BCR	C15-C16-C17	-3.54	115.56	123.39
19	A	1106	CLA	C3D-CAD-CBD	-3.54	102.59	107.60
19	A	1128	CLA	C3D-CAD-CBD	-3.54	102.59	107.60
22	A	7035	LMU	C3'-C4'-C5'	-3.54	102.84	110.84
19	3	3014	CLA	C2C-C1C-CHC	-3.54	118.87	125.15
21	A	6011	BCR	C29-C30-C25	-3.53	104.77	110.36
19	I	1204	CLA	O1D-CGD-CBD	-3.53	119.56	124.62
19	4	4005	CLA	C2D-C3D-C4D	-3.53	103.19	106.30
22	B	7040	LMU	O3'-C3'-C2'	-3.53	102.39	110.34
19	B	1236	CLA	C3D-CAD-CBD	-3.53	102.61	107.60
19	A	1106	CLA	O2D-CGD-O1D	-3.53	116.50	123.79
21	B	6005	BCR	C28-C27-C26	-3.53	108.27	113.87
19	2	2010	CLA	C2C-C1C-CHC	-3.53	118.88	125.15
21	J	6012	BCR	C7-C8-C9	-3.53	120.84	126.22
21	F	6014	BCR	C20-C19-C18	-3.53	115.94	126.32
19	4	1306	CLA	CMD-C2D-C3D	-3.52	118.20	125.09
19	B	9010	CLA	CBA-CAA-C2A	-3.52	103.80	113.73
22	E	7037	LMU	C1B-O1B-C4'	-3.52	108.81	118.01
19	B	1221	CLA	CHD-C4C-C3C	-3.52	119.51	124.94
19	A	1107	CLA	O2D-CGD-O1D	-3.52	116.53	123.79
19	B	1224	CLA	C3D-CAD-CBD	-3.52	102.63	107.60
21	B	6006	BCR	C20-C19-C18	-3.51	115.97	126.32
21	J	6012	BCR	C2-C1-C6	-3.51	104.80	110.36
19	B	1209	CLA	CMD-C2D-C3D	-3.51	118.22	125.09
19	3	3011	CLA	C3D-CAD-CBD	-3.51	102.64	107.60
19	B	9010	CLA	CAA-C2A-C3A	-3.51	103.13	113.22
19	2	2011	CLA	C2D-C3D-C4D	-3.51	103.22	106.30
22	A	7045	LMU	C3B-C4B-C5B	-3.50	104.09	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	3005	CLA	C2C-C1C-CHC	-3.50	118.93	125.15
19	A	1126	CLA	CHD-C4C-C3C	-3.50	119.53	124.94
19	H	1145	CLA	CMD-C2D-C3D	-3.50	118.24	125.09
22	R	7024	LMU	C3B-C4B-C5B	-3.50	104.10	110.20
19	3	3002	CLA	C3B-C2B-C1B	-3.50	103.23	106.29
19	A	1133	CLA	CHD-C4C-C3C	-3.49	119.54	124.94
19	A	9013	CLA	O2D-CGD-O1D	-3.49	116.58	123.79
19	B	1214	CLA	C3D-CAD-CBD	-3.49	102.66	107.60
22	G	7051	LMU	O3'-C3'-C2'	-3.49	102.48	110.34
19	B	1222	CLA	CMD-C2D-C3D	-3.49	118.27	125.09
19	A	9022	CLA	C5-C3-C2	-3.49	114.44	121.05
19	L	1502	CLA	O2D-CGD-O1D	-3.49	116.59	123.79
21	J	6012	BCR	C31-C1-C6	-3.49	104.84	110.30
22	H	7030	LMU	C3B-C4B-C5B	-3.48	104.13	110.20
19	3	1118	CLA	CMD-C2D-C3D	-3.48	118.28	125.09
19	A	1121	CLA	CMD-C2D-C3D	-3.48	118.28	125.09
19	4	4005	CLA	C2C-C1C-CHC	-3.48	118.97	125.15
19	K	1143	CLA	CMD-C2D-C3D	-3.48	118.29	125.09
22	F	7036	LMU	C2'-C3'-C4'	-3.47	101.97	109.60
21	B	6005	BCR	C29-C30-C25	-3.47	104.87	110.36
19	B	1208	CLA	CHD-C4C-C3C	-3.47	119.58	124.94
19	2	4009	CLA	C3D-CAD-CBD	-3.47	102.70	107.60
19	B	1233	CLA	CMD-C2D-C3D	-3.47	118.31	125.09
21	J	6012	BCR	C15-C16-C17	-3.46	115.73	123.39
19	A	1127	CLA	O2D-CGD-O1D	-3.46	116.64	123.79
19	A	1113	CLA	CHD-C4C-C3C	-3.46	119.59	124.94
21	B	6017	BCR	C29-C30-C25	-3.46	104.88	110.36
21	A	6007	BCR	C29-C30-C25	-3.46	104.88	110.36
19	A	1136	CLA	CMD-C2D-C3D	-3.46	118.33	125.09
19	A	1128	CLA	O1D-CGD-CBD	-3.46	119.67	124.62
21	A	6007	BCR	C34-C9-C10	-3.45	117.80	122.90
19	B	1235	CLA	CHD-C4C-C3C	-3.45	119.61	124.94
19	L	1503	CLA	O2D-CGD-O1D	-3.45	116.66	123.79
19	2	2012	CLA	CMD-C2D-C3D	-3.45	118.34	125.09
21	F	6016	BCR	C30-C25-C26	-3.45	117.60	122.66
19	A	1135	CLA	CMD-C2D-C3D	-3.44	118.36	125.09
19	A	1122	CLA	CHD-C4C-C3C	-3.44	119.62	124.94
21	A	6007	BCR	C23-C24-C25	-3.44	116.98	127.32
19	A	1133	CLA	C1-C2-C3	-3.44	121.07	126.71
21	J	6012	BCR	C38-C26-C25	-3.43	121.23	124.61
19	A	1124	CLA	CMD-C2D-C3D	-3.43	118.38	125.09
19	A	1149	CLA	CHC-C1C-C2C	-3.42	117.34	126.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1108	CLA	C2A-C1A-CHA	-3.42	117.58	123.89
21	B	6004	BCR	C34-C9-C10	-3.42	117.85	122.90
21	B	6006	BCR	C16-C15-C14	-3.42	115.84	123.39
19	B	1235	CLA	C3D-CAD-CBD	-3.41	102.77	107.60
19	1	1001	CLA	CHC-C1C-C2C	-3.41	117.37	126.35
21	F	6016	BCR	C29-C30-C25	-3.41	104.96	110.36
21	F	6016	BCR	C27-C26-C25	-3.41	118.43	122.78
19	1	1010	CLA	O1D-CGD-CBD	-3.41	119.73	124.62
19	4	1306	CLA	O1D-CGD-CBD	-3.41	119.73	124.62
21	B	6017	BCR	C37-C22-C21	-3.41	117.86	122.90
19	2	2005	CLA	C3B-C2B-C1B	-3.41	103.30	106.29
19	4	4002	CLA	CBA-CAA-C2A	-3.41	104.12	113.73
19	A	1129	CLA	C3D-CAD-CBD	-3.41	102.78	107.60
21	L	6019	BCR	C15-C16-C17	-3.41	115.85	123.39
19	4	4015	CLA	CGD-CBD-CAD	-3.41	99.07	110.62
19	B	1217	CLA	CMD-C2D-C3D	-3.41	118.42	125.09
19	4	4002	CLA	O1D-CGD-CBD	-3.41	119.74	124.62
19	1	1010	CLA	CMD-C2D-C3D	-3.40	118.43	125.09
19	4	1009	CLA	CMD-C2D-C3D	-3.40	118.44	125.09
21	B	6020	BCR	C20-C19-C18	-3.40	116.31	126.32
19	3	3011	CLA	CHD-C4C-C3C	-3.40	119.69	124.94
19	4	4003	CLA	CMD-C2D-C3D	-3.40	118.44	125.09
22	B	7038	LMU	C2'-C3'-C4'	-3.40	102.14	109.60
19	B	1210	CLA	O1D-CGD-CBD	-3.40	119.75	124.62
21	A	6003	BCR	C16-C15-C14	-3.40	115.88	123.39
19	2	2003	CLA	C2D-C3D-C4D	-3.40	103.31	106.30
19	B	1202	CLA	O2D-CGD-O1D	-3.39	116.78	123.79
19	B	1212	CLA	C4-C3-C2	-3.38	116.86	123.50
19	1	1310	CLA	C2C-C1C-CHC	-3.38	119.15	125.15
19	4	4004	CLA	C2C-C1C-CHC	-3.37	119.16	125.15
19	2	2008	CLA	C2C-C1C-CHC	-3.37	119.16	125.15
21	B	6005	BCR	C4-C5-C6	-3.37	118.49	122.78
19	J	1311	CLA	CMD-C2D-C3D	-3.37	118.50	125.09
19	B	1226	CLA	O2D-CGD-O1D	-3.37	116.83	123.79
19	4	4012	CLA	CHD-C4C-C3C	-3.37	119.19	124.83
19	A	1113	CLA	O2D-CGD-O1D	-3.37	116.84	123.79
19	A	1104	CLA	O2D-CGD-O1D	-3.36	116.84	123.79
19	1	1007	CLA	O1D-CGD-CBD	-3.36	119.80	124.62
19	1	1002	CLA	CMD-C2D-C3D	-3.36	118.51	125.09
19	A	1103	CLA	CHC-C1C-C2C	-3.36	117.52	126.35
19	2	2002	CLA	O2D-CGD-O1D	-3.36	116.86	123.79
19	2	2010	CLA	C3B-C2B-C1B	-3.35	103.35	106.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	6006	BCR	C29-C30-C25	-3.35	105.06	110.36
21	A	6002	BCR	C24-C23-C22	-3.35	121.11	126.22
19	1	1303	CLA	O1D-CGD-CBD	-3.34	119.83	124.62
22	H	7011	LMU	O3'-C3'-C4'	-3.34	101.96	109.87
19	4	1306	CLA	O2D-CGD-O1D	-3.34	116.89	123.79
19	3	3010	CLA	C2C-C1C-CHC	-3.34	119.21	125.15
19	2	2013	CLA	CGD-CBD-CAD	-3.34	99.31	110.62
19	L	1130	CLA	C3D-CAD-CBD	-3.33	102.88	107.60
19	J	1308	CLA	O2D-CGD-O1D	-3.33	116.91	123.79
19	1	1303	CLA	CHC-C1C-C2C	-3.33	117.59	126.35
19	B	1203	CLA	CHC-C1C-C2C	-3.33	117.60	126.35
19	2	2004	CLA	CMD-C2D-C3D	-3.33	118.58	125.09
19	B	1228	CLA	C3D-CAD-CBD	-3.32	102.90	107.60
19	B	1209	CLA	CHD-C4C-C3C	-3.32	119.81	124.94
19	B	1202	CLA	CHD-C4C-C3C	-3.32	119.82	124.94
19	L	1502	CLA	CMD-C2D-C3D	-3.31	118.61	125.09
19	B	1231	CLA	CMD-C2D-C3D	-3.31	118.61	125.09
19	R	1150	CLA	C4-C3-C2	-3.31	117.00	123.50
19	K	1142	CLA	CMD-C2D-C3D	-3.31	118.62	125.09
19	B	1217	CLA	O1D-CGD-CBD	-3.30	119.89	124.62
19	A	1103	CLA	O1D-CGD-CBD	-3.30	119.89	124.62
19	B	1235	CLA	CMD-C2D-C3D	-3.30	118.63	125.09
19	4	4002	CLA	O2A-CGA-O1A	-3.30	114.98	123.49
19	4	1304	CLA	O2A-CGA-O1A	-3.30	114.98	123.49
19	1	1015	CLA	C2C-C1C-CHC	-3.29	119.30	125.15
21	B	6004	BCR	C29-C30-C25	-3.29	105.16	110.36
19	A	1108	CLA	CHD-C4C-C3C	-3.29	119.86	124.94
19	3	3014	CLA	C3C-C4C-CHD	-3.29	119.91	125.32
19	3	3001	CLA	C2C-C1C-CHC	-3.29	119.31	125.15
21	B	6017	BCR	C2-C1-C6	-3.28	105.16	110.36
19	2	2003	CLA	C2C-C1C-CHC	-3.28	119.32	125.15
19	1	1005	CLA	CMD-C2D-C3D	-3.28	118.67	125.09
19	B	1225	CLA	O1D-CGD-CBD	-3.28	119.92	124.62
21	J	6012	BCR	C23-C24-C25	-3.28	117.47	127.32
21	3	6022	BCR	C11-C12-C13	-3.27	116.68	126.32
19	A	1102	CLA	C3D-CAD-CBD	-3.27	102.97	107.60
21	J	6012	BCR	C8-C7-C6	-3.27	117.50	127.32
19	L	1504	CLA	C4-C3-C2	-3.27	117.09	123.50
19	3	3013	CLA	C4-C3-C2	-3.27	117.09	123.50
19	2	1307	CLA	C2C-C1C-CHC	-3.27	119.35	125.15
19	4	4006	CLA	O1D-CGD-CBD	-3.26	119.94	124.62
19	4	4002	CLA	CBC-CAC-C3C	-3.26	102.43	112.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	6010	BCR	C28-C27-C26	-3.26	108.70	113.87
21	B	6006	BCR	C31-C1-C6	-3.26	105.20	110.30
19	K	1146	CLA	C1-C2-C3	-3.25	121.38	126.71
19	4	4014	CLA	C3D-CAD-CBD	-3.25	103.00	107.60
19	J	1308	CLA	CMD-C2D-C3D	-3.25	118.73	125.09
19	A	1128	CLA	O2D-CGD-O1D	-3.25	117.08	123.79
22	R	7014	LMU	C1B-O1B-C4'	-3.24	109.53	118.01
19	A	1111	CLA	CHC-C1C-C2C	-3.24	117.82	126.35
19	2	4009	CLA	CMD-C2D-C3D	-3.24	118.75	125.09
19	A	1137	CLA	CMD-C2D-C3D	-3.24	118.75	125.09
21	B	6010	BCR	C34-C9-C10	-3.24	118.11	122.90
19	A	1106	CLA	C6-C5-C3	-3.24	105.37	112.48
21	B	6010	BCR	C37-C22-C21	-3.24	118.12	122.90
19	B	1210	CLA	CMD-C2D-C3D	-3.23	118.76	125.09
19	2	2008	CLA	C3B-C2B-C1B	-3.23	103.46	106.29
21	J	6012	BCR	C29-C30-C25	-3.23	105.25	110.36
19	4	4014	CLA	CMD-C2D-C3D	-3.23	118.77	125.09
19	2	2001	CLA	O1D-CGD-CBD	-3.23	119.99	124.62
21	B	6005	BCR	C7-C8-C9	-3.23	121.30	126.22
21	A	6011	BCR	C15-C16-C17	-3.23	116.26	123.39
22	G	7051	LMU	O5B-C1B-C2B	-3.22	103.66	110.28
21	1	6023	BCR	C7-C8-C9	-3.22	121.30	126.22
19	3	3002	CLA	C2C-C1C-CHC	-3.22	119.42	125.15
19	B	1219	CLA	CHD-C4C-C3C	-3.22	119.96	124.94
19	A	1113	CLA	CMD-C2D-C3D	-3.22	118.79	125.09
21	A	6002	BCR	C23-C24-C25	-3.22	117.65	127.32
19	A	1108	CLA	C3D-CAD-CBD	-3.22	103.05	107.60
19	A	1131	CLA	CMD-C2D-C3D	-3.22	118.80	125.09
19	B	1223	CLA	O1D-CGD-CBD	-3.22	120.01	124.62
21	3	6022	BCR	C20-C19-C18	-3.21	116.86	126.32
19	B	1214	CLA	CMD-C2D-C3D	-3.21	118.81	125.09
21	B	6017	BCR	C28-C27-C26	-3.21	108.78	113.87
19	3	3010	CLA	C2D-C3D-C4D	-3.21	103.48	106.30
22	G	7026	LMU	C1B-O1B-C4'	-3.20	109.65	118.01
19	I	1204	CLA	C3D-CAD-CBD	-3.20	103.08	107.60
21	I	6018	BCR	C27-C26-C25	-3.20	118.71	122.78
21	A	6003	BCR	C28-C27-C26	-3.20	108.80	113.87
19	A	1109	CLA	C11-C12-C13	-3.20	104.89	115.49
19	4	4012	CLA	CAA-C2A-C3A	-3.18	108.57	116.20
19	L	1148	CLA	CAA-CBA-CGA	-3.18	104.00	113.32
19	A	1106	CLA	CMD-C2D-C3D	-3.18	118.86	125.09
19	3	3016	CLA	CMD-C2D-C3D	-3.18	118.86	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1223	CLA	CMD-C2D-C3D	-3.18	118.86	125.09
19	1	1011	CLA	CAA-C2A-C3A	-3.18	108.58	116.20
21	F	6014	BCR	C16-C17-C18	-3.18	122.61	127.20
19	A	9013	CLA	CMD-C2D-C3D	-3.18	118.88	125.09
19	4	4006	CLA	CMD-C2D-C3D	-3.17	118.88	125.09
19	1	1006	CLA	CMD-C2D-C3D	-3.17	118.88	125.09
19	H	1241	CLA	C4-C3-C2	-3.17	117.28	123.50
22	4	7052	LMU	C3'-C4'-C5'	-3.17	103.68	110.84
19	A	1137	CLA	O2D-CGD-O1D	-3.17	117.25	123.79
19	B	1230	CLA	CMD-C2D-C3D	-3.16	118.90	125.09
19	A	1109	CLA	CHC-C1C-C2C	-3.16	118.03	126.35
19	A	1110	CLA	CMD-C2D-C3D	-3.16	118.90	125.09
19	1	1008	CLA	O2D-CGD-O1D	-3.16	117.26	123.79
21	A	6011	BCR	C3-C4-C5	-3.16	108.85	113.87
19	3	2009	CLA	O1D-CGD-CBD	-3.16	120.09	124.62
19	B	1221	CLA	CMD-C2D-C3D	-3.16	118.92	125.09
22	H	7017	LMU	O4'-C4B-C5B	-3.15	100.89	109.24
21	A	6011	BCR	C24-C23-C22	-3.15	121.42	126.22
19	4	1304	CLA	CHC-C1C-C2C	-3.15	118.07	126.35
19	L	1504	CLA	CMD-C2D-C3D	-3.14	118.94	125.09
19	2	2014	CLA	O1D-CGD-CBD	-3.14	120.12	124.62
19	1	1013	CLA	CAA-C2A-C1A	-3.14	101.41	112.47
19	2	2011	CLA	C2C-C1C-CHC	-3.13	119.58	125.15
19	B	1208	CLA	O1D-CGD-CBD	-3.13	120.13	124.62
21	F	6016	BCR	C15-C16-C17	-3.13	116.47	123.39
19	B	1227	CLA	O2D-CGD-O1D	-3.13	117.32	123.79
21	I	6018	BCR	C24-C25-C26	-3.13	114.20	121.37
19	3	3013	CLA	C3D-CAD-CBD	-3.13	103.18	107.60
21	B	6017	BCR	C27-C26-C25	-3.12	118.80	122.78
19	3	3012	CLA	C3C-C4C-CHD	-3.12	120.19	125.32
19	A	1112	CLA	CMD-C2D-C3D	-3.11	119.00	125.09
19	A	1103	CLA	CMD-C2D-C3D	-3.11	119.01	125.09
19	4	4013	CLA	C2C-C1C-CHC	-3.11	119.63	125.15
21	J	6012	BCR	C34-C9-C10	-3.11	118.31	122.90
19	B	1221	CLA	CGD-CBD-CAD	-3.11	100.09	110.62
19	L	1501	CLA	O2D-CGD-O1D	-3.11	117.38	123.79
19	1	1002	CLA	CHC-C1C-C2C	-3.10	118.19	126.35
19	A	1129	CLA	CHC-C1C-C2C	-3.10	118.19	126.35
22	H	7017	LMU	C1B-O5B-C5B	-3.10	107.73	113.75
19	A	1108	CLA	CMA-C3A-C2A	-3.10	100.64	114.35
21	3	6022	BCR	C15-C14-C13	-3.10	122.72	127.20
19	4	1306	CLA	C1D-CHD-C4C	-3.09	117.92	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1231	CLA	O1D-CGD-CBD	-3.09	120.19	124.62
21	3	6022	BCR	C32-C1-C6	-3.09	105.45	110.30
19	B	1211	CLA	CHD-C4C-C3C	-3.09	120.16	124.94
19	1	1001	CLA	CAC-C3C-C2C	-3.09	122.10	127.51
22	K	7001	LMU	C3B-C4B-C5B	-3.08	104.82	110.20
19	B	1221	CLA	CAA-CBA-CGA	-3.08	104.30	113.32
19	1	1303	CLA	O2D-CGD-O1D	-3.08	117.43	123.79
19	A	1309	CLA	C2D-C3D-C4D	-3.08	103.59	106.30
19	A	9022	CLA	C3D-CAD-CBD	-3.08	103.25	107.60
19	B	1209	CLA	CHC-C1C-C2C	-3.08	118.26	126.35
19	A	1122	CLA	CMD-C2D-C3D	-3.08	119.07	125.09
19	3	3006	CLA	C2D-C3D-C4D	-3.08	103.59	106.30
19	A	1140	CLA	CMD-C2D-C3D	-3.08	119.07	125.09
19	A	1111	CLA	CMD-C2D-C3D	-3.08	119.07	125.09
19	B	1301	CLA	CMA-C3A-C2A	-3.07	108.84	116.20
21	3	6022	BCR	C34-C9-C10	-3.07	118.36	122.90
19	A	1121	CLA	CHC-C1C-C2C	-3.07	118.27	126.35
19	3	2009	CLA	C4-C3-C2	-3.07	117.47	123.50
21	B	6020	BCR	C24-C23-C22	-3.07	121.54	126.22
19	B	1213	CLA	CMD-C2D-C3D	-3.07	119.09	125.09
19	A	1109	CLA	CAA-C2A-C1A	-3.07	101.65	112.47
19	A	1151	CLA	CHD-C4C-C3C	-3.07	120.20	124.94
19	B	1238	CLA	O1D-CGD-CBD	-3.07	120.23	124.62
21	A	6011	BCR	C27-C26-C25	-3.06	118.88	122.78
19	3	3007	CLA	CHD-C4C-C3C	-3.06	120.21	124.94
21	A	6011	BCR	C34-C9-C10	-3.06	118.38	122.90
19	B	1235	CLA	CHC-C1C-C2C	-3.06	118.30	126.35
21	A	6002	BCR	C37-C22-C21	-3.06	118.38	122.90
21	B	6020	BCR	C16-C17-C18	-3.06	122.78	127.20
21	B	6017	BCR	C34-C9-C10	-3.06	118.39	122.90
19	4	4001	CLA	CMD-C2D-C3D	-3.05	119.11	125.09
21	A	6011	BCR	C16-C17-C18	-3.05	122.79	127.20
19	4	4013	CLA	C3B-C2B-C1B	-3.05	103.62	106.29
19	3	3008	CLA	C1-C2-C3	-3.05	121.71	126.71
19	4	1306	CLA	CAC-C3C-C2C	-3.05	122.17	127.51
19	B	1203	CLA	CMD-C2D-C3D	-3.05	119.13	125.09
19	A	1120	CLA	O1D-CGD-CBD	-3.05	120.26	124.62
19	B	1205	CLA	CAA-C2A-C3A	-3.04	104.46	113.22
19	B	1214	CLA	O2D-CGD-O1D	-3.04	117.51	123.79
19	R	1144	CLA	C4-C3-C2	-3.03	117.55	123.50
19	3	3007	CLA	CHC-C1C-C2C	-3.03	118.38	126.35
19	3	3004	CLA	C2D-C3D-C4D	-3.02	103.64	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	6002	BCR	C16-C17-C18	-3.02	122.83	127.20
22	A	7044	LMU	O2'-C2'-C3'	-3.02	103.54	110.34
19	B	1219	CLA	C5-C3-C2	-3.02	115.33	121.05
19	A	1104	CLA	CMD-C2D-C3D	-3.02	119.18	125.09
21	I	6021	BCR	C20-C19-C18	-3.02	117.44	126.32
19	3	3011	CLA	CMD-C2D-C3D	-3.02	119.19	125.09
19	G	1242	CLA	O2D-CGD-O1D	-3.02	117.56	123.79
19	H	1145	CLA	CHC-C1C-C2C	-3.02	118.42	126.35
19	B	1227	CLA	CMD-C2D-C3D	-3.01	119.19	125.09
19	2	4009	CLA	CHC-C1C-C2C	-3.01	118.43	126.35
19	B	1226	CLA	CHC-C1C-C2C	-3.01	118.43	126.35
19	A	9012	CLA	O2A-CGA-O1A	-3.00	115.74	123.49
21	B	6006	BCR	C28-C27-C26	-3.00	109.11	113.87
19	A	1101	CLA	C1-C2-C3	-3.00	121.79	126.71
19	B	1202	CLA	CHC-C1C-C2C	-3.00	118.47	126.35
19	4	4002	CLA	C6-C5-C3	-2.99	109.44	114.43
19	B	1230	CLA	CHC-C1C-C2C	-2.99	118.49	126.35
22	4	7053	LMU	C4B-C3B-C2B	-2.99	105.22	110.79
19	4	4002	CLA	CHC-C1C-C2C	-2.98	118.50	126.35
19	B	1224	CLA	CAA-C2A-C3A	-2.98	104.64	113.22
19	2	4009	CLA	C4-C3-C2	-2.98	117.65	123.50
19	1	1303	CLA	CGD-CBD-CAD	-2.98	100.54	110.62
19	2	2012	CLA	CHD-C4C-C3C	-2.97	120.34	124.94
19	K	1142	CLA	O2D-CGD-O1D	-2.97	117.65	123.79
19	3	1147	CLA	CAC-C3C-C2C	-2.97	122.30	127.51
19	3	3017	CLA	O2D-CGD-O1D	-2.97	117.66	123.79
19	L	1502	CLA	CHC-C1C-C2C	-2.97	118.54	126.35
19	B	1203	CLA	CHD-C4C-C3C	-2.97	120.35	124.94
19	A	9023	CLA	CHC-C1C-C2C	-2.97	118.54	126.35
19	3	3017	CLA	CAC-C3C-C2C	-2.97	122.30	127.51
19	A	1101	CLA	CMD-C2D-C3D	-2.96	119.29	125.09
19	2	2013	CLA	CHC-C1C-C2C	-2.96	118.56	126.35
19	L	1130	CLA	CMD-C2D-C3D	-2.96	119.31	125.09
19	A	1115	CLA	CMD-C2D-C3D	-2.96	119.31	125.09
19	L	1130	CLA	O2D-CGD-O1D	-2.96	117.69	123.79
19	K	1143	CLA	CHC-C1C-C2C	-2.95	118.58	126.35
19	4	4007	CLA	CHC-C1C-C2C	-2.95	118.59	126.35
19	B	9010	CLA	CHC-C1C-C2C	-2.95	118.59	126.35
19	B	1208	CLA	CAA-C2A-C3A	-2.94	104.75	113.22
19	4	1009	CLA	CAA-C2A-C3A	-2.94	109.17	116.20
19	A	9011	CLA	CMD-C2D-C3D	-2.93	119.35	125.09
21	B	6010	BCR	C32-C1-C6	-2.93	105.70	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1205	CLA	CHD-C4C-C3C	-2.93	120.41	124.94
19	4	4007	CLA	CMD-C2D-C3D	-2.93	119.36	125.09
21	B	6017	BCR	C3-C4-C5	-2.93	109.22	113.87
21	1	6023	BCR	C8-C7-C6	-2.92	118.53	127.32
19	1	1011	CLA	CHC-C1C-C2C	-2.92	118.66	126.35
19	1	1013	CLA	CHC-C1C-C2C	-2.92	118.66	126.35
19	B	1226	CLA	C2A-C1A-CHA	-2.92	118.50	123.89
19	B	1211	CLA	CHC-C1C-C2C	-2.92	118.67	126.35
19	4	4002	CLA	C4-C3-C2	-2.92	117.77	123.50
19	B	1227	CLA	CHD-C4C-C3C	-2.92	120.43	124.94
19	A	1129	CLA	CHD-C4C-C3C	-2.92	120.44	124.94
19	B	1236	CLA	CMD-C2D-C3D	-2.91	119.39	125.09
19	A	1117	CLA	O2D-CGD-O1D	-2.91	117.77	123.79
21	B	6004	BCR	C4-C5-C6	-2.91	119.07	122.78
19	B	1221	CLA	CHC-C1C-C2C	-2.91	118.69	126.35
21	B	6020	BCR	C19-C18-C17	-2.91	114.30	118.98
21	J	6012	BCR	C33-C5-C6	-2.91	121.75	124.61
19	H	1505	CLA	O1D-CGD-CBD	-2.91	120.46	124.62
19	B	1205	CLA	CMD-C2D-C3D	-2.91	119.41	125.09
19	F	1305	CLA	C4-C3-C2	-2.90	117.80	123.50
22	R	7020	LMU	C3B-C4B-C5B	-2.90	105.13	110.20
19	K	1146	CLA	O2A-CGA-O1A	-2.90	116.01	123.49
19	H	1241	CLA	CHD-C4C-C3C	-2.90	120.47	124.94
21	3	6022	BCR	C23-C24-C25	-2.89	118.63	127.32
22	H	7028	LMU	C1B-O1B-C4'	-2.89	110.45	118.01
19	3	3007	CLA	O1D-CGD-CBD	-2.89	120.48	124.62
19	B	1224	CLA	O2A-CGA-O1A	-2.89	116.03	123.49
19	H	1207	CLA	CMD-C2D-C3D	-2.89	119.43	125.09
19	B	1219	CLA	CHC-C1C-C2C	-2.89	118.75	126.35
19	K	1143	CLA	O1D-CGD-CBD	-2.89	120.48	124.62
19	B	1205	CLA	O2A-CGA-O1A	-2.89	116.04	123.49
19	B	1239	CLA	CHC-C1C-C2C	-2.88	118.77	126.35
19	B	1205	CLA	CHC-C1C-C2C	-2.88	118.77	126.35
19	2	2006	CLA	CMD-C2D-C3D	-2.88	119.45	125.09
22	B	7040	LMU	O2'-C2'-C3'	-2.88	103.85	110.34
19	B	1229	CLA	CMD-C2D-C3D	-2.88	119.46	125.09
19	2	2012	CLA	CHC-C1C-C2C	-2.88	118.78	126.35
22	4	7052	LMU	O6'-C6'-C5'	-2.88	101.83	111.33
19	B	1234	CLA	CHC-C1C-C2C	-2.88	118.79	126.35
19	H	1241	CLA	CHC-C1C-C2C	-2.87	118.79	126.35
22	E	7048	LMU	C1'-C2'-C3'	-2.87	104.31	109.97
19	K	1146	CLA	CHC-C1C-C2C	-2.87	118.80	126.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	9023	CLA	CMD-C2D-C3D	-2.87	119.47	125.09
19	B	1208	CLA	O2D-CGD-O1D	-2.87	117.87	123.79
19	4	4013	CLA	C2D-C3D-C4D	-2.86	103.78	106.30
19	G	1242	CLA	CMD-C2D-C3D	-2.86	119.49	125.09
19	A	1115	CLA	O2D-CGD-O1D	-2.86	117.89	123.79
22	4	7052	LMU	O5'-C1'-O1'	-2.85	103.18	110.05
19	B	1215	CLA	CGD-CBD-CAD	-2.85	100.95	110.62
19	B	1232	CLA	CMD-C2D-C3D	-2.85	119.51	125.09
19	L	1503	CLA	C1-C2-C3	-2.85	122.03	126.71
19	4	4003	CLA	O1D-CGD-CBD	-2.85	120.54	124.62
22	3	7005	LMU	C1'-C2'-C3'	-2.85	104.36	109.97
19	B	1301	CLA	CMD-C2D-C3D	-2.84	119.53	125.09
19	B	1226	CLA	CMA-C3A-C2A	-2.84	101.78	114.35
19	2	2007	CLA	CMD-C2D-C3D	-2.84	119.53	125.09
21	I	6018	BCR	C31-C1-C6	-2.84	105.86	110.30
19	B	1220	CLA	CBC-CAC-C3C	-2.84	103.74	112.39
19	J	1311	CLA	O2D-CGD-O1D	-2.83	117.94	123.79
19	A	1119	CLA	CHC-C1C-C2C	-2.83	118.91	126.35
22	H	7032	LMU	C4B-C3B-C2B	-2.83	105.52	110.79
19	A	1116	CLA	CHC-C1C-C2C	-2.83	118.92	126.35
19	L	1130	CLA	O1D-CGD-CBD	-2.82	120.57	124.62
19	A	1131	CLA	CHC-C1C-C2C	-2.82	118.93	126.35
21	1	6023	BCR	C27-C26-C25	-2.82	119.19	122.78
21	B	6005	BCR	C2-C1-C6	-2.82	105.90	110.36
19	A	1113	CLA	CHC-C1C-C2C	-2.82	118.94	126.35
19	I	1204	CLA	CMD-C2D-C3D	-2.82	119.58	125.09
21	B	6017	BCR	C33-C5-C6	-2.82	121.84	124.61
19	A	1139	CLA	O1D-CGD-CBD	-2.82	120.59	124.62
19	F	1240	CLA	CAB-C3B-C2B	-2.81	119.39	125.14
19	A	9023	CLA	CAA-C2A-C3A	-2.81	105.13	113.22
19	4	1004	CLA	CHC-C1C-C2C	-2.81	118.95	126.35
19	A	1126	CLA	C4-C3-C2	-2.81	117.98	123.50
19	A	1135	CLA	O2D-CGD-O1D	-2.81	117.99	123.79
19	B	1216	CLA	O2D-CGD-O1D	-2.81	117.99	123.79
19	4	4011	CLA	C2C-C1C-CHC	-2.81	120.16	125.15
19	L	1502	CLA	CGD-CBD-CAD	-2.80	101.12	110.62
19	4	4003	CLA	CHC-C1C-C2C	-2.80	118.98	126.35
19	A	1134	CLA	CHC-C1C-C2C	-2.80	118.98	126.35
21	F	6016	BCR	C34-C9-C10	-2.80	118.76	122.90
19	A	1136	CLA	CHC-C1C-C2C	-2.80	118.99	126.35
19	A	1149	CLA	CHD-C4C-C3C	-2.80	120.62	124.94
19	A	1105	CLA	CMD-C2D-C3D	-2.80	119.62	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1151	CLA	CHC-C1C-C2C	-2.79	119.00	126.35
19	B	1227	CLA	CHC-C1C-C2C	-2.79	119.01	126.35
19	A	1125	CLA	CMD-C2D-C3D	-2.79	119.63	125.09
22	K	7041	LMU	C4B-C3B-C2B	-2.79	105.59	110.79
19	K	3009	CLA	CMD-C2D-C3D	-2.79	119.64	125.09
19	A	1129	CLA	CMD-C2D-C3D	-2.78	119.64	125.09
19	A	1132	CLA	CMA-C3A-C2A	-2.78	102.06	114.35
21	B	6006	BCR	C34-C9-C10	-2.78	118.80	122.90
19	A	1131	CLA	O2D-CGD-O1D	-2.77	118.06	123.79
19	A	1129	CLA	O1D-CGD-CBD	-2.77	120.65	124.62
19	4	1004	CLA	C4-C3-C2	-2.77	118.06	123.50
19	1	1001	CLA	CAA-C2A-C3A	-2.77	105.25	113.22
19	1	1006	CLA	CHC-C1C-C2C	-2.77	119.07	126.35
20	B	5002	PQN	C14-C13-C12	-2.77	118.07	123.50
19	A	1127	CLA	CHC-C1C-C2C	-2.77	119.07	126.35
21	I	6018	BCR	C39-C30-C29	-2.77	98.88	108.79
19	3	3013	CLA	CHC-C1C-C2C	-2.77	119.08	126.35
19	F	1302	CLA	CMA-C3A-C2A	-2.76	109.58	116.20
19	3	1147	CLA	CAA-C2A-C3A	-2.76	105.27	113.22
19	A	1104	CLA	C2A-C1A-CHA	-2.76	118.80	123.89
19	B	1206	CLA	O2A-CGA-O1A	-2.76	116.36	123.49
19	A	1101	CLA	CAA-C2A-C3A	-2.76	105.27	113.22
19	4	4010	CLA	C2D-C3D-C4D	-2.76	103.87	106.30
19	3	3003	CLA	CMD-C2D-C3D	-2.76	119.69	125.09
21	B	6005	BCR	C1-C6-C5	-2.76	118.61	122.66
19	1	1005	CLA	CAA-C2A-C3A	-2.76	105.29	113.22
19	A	1106	CLA	CAA-C2A-C1A	-2.75	102.76	112.47
19	1	1005	CLA	O1D-CGD-CBD	-2.75	120.68	124.62
19	B	1215	CLA	CHC-C1C-C2C	-2.75	119.11	126.35
19	2	2006	CLA	CHC-C1C-C2C	-2.75	119.12	126.35
19	A	1141	CLA	O1D-CGD-CBD	-2.75	120.68	124.62
19	B	1233	CLA	O1D-CGD-CBD	-2.75	120.69	124.62
19	B	1235	CLA	CBC-CAC-C3C	-2.75	104.01	112.39
19	4	4012	CLA	CHC-C1C-C2C	-2.75	119.13	126.35
22	3	7005	LMU	O5B-C5B-C4B	-2.74	104.54	109.68
21	A	6003	BCR	C29-C30-C25	-2.74	106.03	110.36
19	2	2001	CLA	CHC-C1C-C2C	-2.74	119.15	126.35
19	A	1102	CLA	O2A-CGA-O1A	-2.74	116.43	123.49
21	B	6017	BCR	C16-C15-C14	-2.74	117.34	123.39
19	L	1504	CLA	C2A-C1A-CHA	-2.73	118.85	123.89
19	1	1303	CLA	O2A-CGA-O1A	-2.73	116.44	123.49
19	2	2014	CLA	CHC-C1C-C2C	-2.73	119.17	126.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	E	7048	LMU	O4'-C4B-C5B	-2.73	102.01	109.24
22	K	7001	LMU	O5B-C5B-C4B	-2.73	104.56	109.68
19	B	1225	CLA	CHC-C1C-C2C	-2.73	119.18	126.35
22	N	7049	LMU	C1B-C2B-C3B	-2.72	104.60	109.97
19	K	1146	CLA	CMB-C2B-C1B	-2.72	123.86	128.36
19	A	1133	CLA	CHC-C1C-C2C	-2.72	119.19	126.35
19	1	1007	CLA	CMD-C2D-C3D	-2.72	119.77	125.09
19	R	1144	CLA	O2A-CGA-O1A	-2.72	116.47	123.49
19	A	1128	CLA	CHC-C1C-C2C	-2.72	119.20	126.35
21	I	6021	BCR	C23-C24-C25	-2.72	119.15	127.32
19	G	1242	CLA	C4-C3-C2	-2.72	118.16	123.50
19	3	3016	CLA	CHC-C1C-C2C	-2.72	119.21	126.35
21	A	6002	BCR	C29-C30-C25	-2.71	106.07	110.36
19	B	1219	CLA	O1D-CGD-CBD	-2.71	120.73	124.62
19	3	3016	CLA	O1D-CGD-CBD	-2.71	120.73	124.62
22	K	7042	LMU	C1B-O1B-C4'	-2.71	110.92	118.01
19	A	1101	CLA	CHC-C1C-C2C	-2.71	119.22	126.35
21	L	6019	BCR	C32-C1-C6	-2.71	106.05	110.30
19	F	1240	CLA	CAA-C2A-C3A	-2.71	109.71	116.20
21	A	6003	BCR	C34-C9-C10	-2.71	118.90	122.90
21	J	6012	BCR	C16-C17-C18	-2.71	123.28	127.20
19	3	3011	CLA	CHC-C1C-C2C	-2.71	119.22	126.35
19	B	1213	CLA	CHC-C1C-C2C	-2.71	119.22	126.35
19	3	3013	CLA	C2A-C1A-CHA	-2.71	118.90	123.89
19	B	1225	CLA	C16-C15-C13	-2.71	106.50	115.49
19	A	1138	CLA	CHC-C1C-C2C	-2.71	119.23	126.35
19	R	1150	CLA	CHC-C1C-C2C	-2.71	119.23	126.35
19	4	4014	CLA	CHC-C1C-C2C	-2.70	119.25	126.35
19	4	4001	CLA	O2D-CGD-O1D	-2.70	118.22	123.79
19	A	1138	CLA	O1D-CGD-CBD	-2.70	120.75	124.62
19	A	1140	CLA	O1D-CGD-CBD	-2.69	120.76	124.62
19	A	1104	CLA	CHC-C1C-C2C	-2.69	119.27	126.35
19	B	1227	CLA	C1-C2-C3	-2.69	122.30	126.71
19	1	1014	CLA	CMD-C2D-C3D	-2.69	119.83	125.09
19	A	1133	CLA	O2A-CGA-O1A	-2.69	116.56	123.49
20	B	5002	PQN	C16-C15-C13	-2.68	106.59	112.48
19	B	1239	CLA	O2A-CGA-O1A	-2.68	116.57	123.49
19	A	1124	CLA	O2D-CGD-O1D	-2.68	118.26	123.79
19	A	1111	CLA	O1D-CGD-CBD	-2.68	120.79	124.62
19	A	1117	CLA	CMD-C2D-C3D	-2.67	119.86	125.09
21	F	6016	BCR	C33-C5-C6	-2.67	121.99	124.61
19	4	1304	CLA	C11-C10-C8	-2.67	106.64	115.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	R	1144	CLA	O2D-CGD-O1D	-2.67	118.29	123.79
22	R	7020	LMU	C3'-C4'-C5'	-2.66	104.81	110.84
19	H	1241	CLA	O2D-CGD-O1D	-2.66	118.29	123.79
19	J	1308	CLA	CHC-C1C-C2C	-2.66	119.36	126.35
19	J	1308	CLA	CGD-CBD-CAD	-2.66	101.61	110.62
20	B	5002	PQN	C2M-C2-C3	-2.66	118.42	124.10
19	A	1112	CLA	CHC-C1C-C2C	-2.66	119.37	126.35
19	A	1110	CLA	CHC-C1C-C2C	-2.65	119.37	126.35
19	B	1209	CLA	O2D-CGD-O1D	-2.65	118.31	123.79
22	H	7002	LMU	O5B-C1B-C2B	-2.65	104.84	110.28
19	A	1137	CLA	CHC-C1C-C2C	-2.65	119.38	126.35
19	1	1014	CLA	CHC-C1C-C2C	-2.65	119.39	126.35
19	A	1105	CLA	CAA-C2A-C1A	-2.64	103.14	112.47
19	4	1004	CLA	O1D-CGD-CBD	-2.64	120.83	124.62
21	3	6022	BCR	C28-C27-C26	-2.64	109.67	113.87
19	A	1107	CLA	C5-C3-C2	-2.64	116.04	121.05
21	B	6020	BCR	C8-C7-C6	-2.64	119.39	127.32
19	3	1147	CLA	O2A-CGA-O1A	-2.64	114.32	123.02
19	F	1305	CLA	CBC-CAC-C3C	-2.64	104.34	112.39
19	4	4003	CLA	O2D-CGD-O1D	-2.64	118.35	123.79
19	F	1302	CLA	CAA-C2A-C3A	-2.64	109.89	116.20
22	A	7035	LMU	O5'-C5'-C4'	-2.64	104.18	109.75
19	A	1129	CLA	CAA-C2A-C3A	-2.63	105.65	113.22
19	A	1149	CLA	O2A-CGA-O1A	-2.63	116.70	123.49
19	3	1118	CLA	CHC-C1C-C2C	-2.63	119.43	126.35
19	A	1237	CLA	CMD-C2D-C3D	-2.63	119.94	125.09
21	A	6002	BCR	C20-C19-C18	-2.62	118.59	126.32
19	A	1111	CLA	CAA-C2A-C1A	-2.62	103.22	112.47
21	3	6022	BCR	C24-C23-C22	-2.62	122.22	126.22
19	A	1124	CLA	CHC-C1C-C2C	-2.62	119.46	126.35
19	A	1139	CLA	CHC-C1C-C2C	-2.62	119.46	126.35
19	3	3007	CLA	CAC-C3C-C2C	-2.62	122.91	127.51
19	K	1142	CLA	C2A-C1A-CHA	-2.62	119.06	123.89
19	3	3008	CLA	O2A-CGA-O1A	-2.62	116.74	123.49
19	K	1146	CLA	O2D-CGD-O1D	-2.62	118.39	123.79
19	A	1108	CLA	O2D-CGD-O1D	-2.62	118.39	123.79
19	R	1144	CLA	CHC-C1C-C2C	-2.62	119.47	126.35
19	F	1302	CLA	O1D-CGD-CBD	-2.61	120.88	124.62
19	R	1150	CLA	O1D-CGD-CBD	-2.61	120.88	124.62
19	A	9011	CLA	CAA-C2A-C3A	-2.61	105.71	113.22
19	B	1216	CLA	CHC-C1C-C2C	-2.60	119.50	126.35
19	B	1236	CLA	CHC-C1C-C2C	-2.60	119.52	126.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1119	CLA	O1D-CGD-CBD	-2.60	120.90	124.62
19	A	1117	CLA	CHC-C1C-C2C	-2.60	119.53	126.35
19	A	1141	CLA	CHC-C1C-C2C	-2.59	119.53	126.35
19	2	2007	CLA	O1D-CGD-CBD	-2.59	120.91	124.62
19	B	1203	CLA	CAA-C2A-C3A	-2.59	105.76	113.22
19	A	1140	CLA	CHC-C1C-C2C	-2.59	119.54	126.35
19	B	1230	CLA	CAA-CBA-CGA	-2.59	105.73	113.32
19	B	1214	CLA	CHC-C1C-C2C	-2.59	119.54	126.35
19	3	3008	CLA	CHC-C1C-C2C	-2.59	119.54	126.35
19	A	1124	CLA	O1D-CGD-CBD	-2.59	120.91	124.62
19	J	1311	CLA	CHC-C1C-C2C	-2.59	119.54	126.35
19	H	1505	CLA	CHC-C1C-C2C	-2.59	119.55	126.35
19	B	1206	CLA	CHC-C1C-C2C	-2.59	119.55	126.35
19	A	1123	CLA	CHC-C1C-C2C	-2.59	119.55	126.35
19	1	1010	CLA	CHC-C1C-C2C	-2.59	119.55	126.35
19	3	1147	CLA	CHC-C1C-C2C	-2.58	119.56	126.35
19	A	1120	CLA	O2D-CGD-O1D	-2.58	118.47	123.79
19	B	1225	CLA	CMA-C3A-C2A	-2.58	102.94	114.35
19	3	3002	CLA	C2D-C3D-C4D	-2.58	104.03	106.30
21	F	6014	BCR	C34-C9-C10	-2.58	119.10	122.90
19	F	1240	CLA	CHC-C1C-C2C	-2.58	119.58	126.35
19	B	1202	CLA	CAA-C2A-C1A	-2.57	103.39	112.47
19	A	1128	CLA	CMD-C2D-C3D	-2.57	120.05	125.09
19	A	1104	CLA	CAA-C2A-C1A	-2.57	103.39	112.47
19	B	1218	CLA	CHC-C1C-C2C	-2.57	119.58	126.35
21	I	6018	BCR	C34-C9-C10	-2.57	119.10	122.90
19	B	1223	CLA	CHC-C1C-C2C	-2.57	119.59	126.35
19	F	1302	CLA	CHC-C1C-C2C	-2.57	119.59	126.35
21	A	6003	BCR	C11-C12-C13	-2.57	118.75	126.32
19	A	1108	CLA	CHC-C1C-C2C	-2.57	119.60	126.35
19	2	2007	CLA	CHD-C4C-C3C	-2.57	120.98	124.94
19	A	1128	CLA	CAA-C2A-C1A	-2.57	103.42	112.47
19	A	1105	CLA	C2A-C1A-CHA	-2.56	119.16	123.89
19	1	1001	CLA	CBC-CAC-C3C	-2.56	104.57	112.39
19	B	1235	CLA	O1D-CGD-CBD	-2.56	120.95	124.62
19	A	1135	CLA	CHC-C1C-C2C	-2.56	119.62	126.35
19	H	1207	CLA	O2D-CGD-O1D	-2.56	118.50	123.79
22	H	7032	LMU	O5'-C1'-C2'	-2.56	105.02	110.28
19	B	1238	CLA	CAA-C2A-C3A	-2.56	105.86	113.22
19	R	1150	CLA	CGD-CBD-CAD	-2.56	101.96	110.62
21	B	6006	BCR	C3-C4-C5	-2.55	109.81	113.87
19	4	4014	CLA	O1D-CGD-CBD	-2.55	120.96	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1238	CLA	CHC-C1C-C2C	-2.55	119.64	126.35
21	B	6020	BCR	C34-C9-C10	-2.55	119.13	122.90
19	A	1123	CLA	O2A-CGA-O1A	-2.55	116.91	123.49
22	H	7002	LMU	O3'-C3'-C2'	-2.55	104.59	110.34
21	A	6007	BCR	C8-C7-C6	-2.55	119.66	127.32
21	B	6005	BCR	C20-C19-C18	-2.55	118.81	126.32
21	B	6010	BCR	C16-C15-C14	-2.55	117.75	123.39
22	H	7043	LMU	C6'-C5'-C4'	-2.55	105.83	113.25
19	B	1228	CLA	O2D-CGD-O1D	-2.55	118.53	123.79
19	B	1232	CLA	CHC-C1C-C2C	-2.55	119.65	126.35
19	A	1149	CLA	O1D-CGD-CBD	-2.55	120.97	124.62
19	B	1202	CLA	O1D-CGD-CBD	-2.55	120.97	124.62
20	A	5001	PQN	C21-C20-C18	-2.55	107.05	115.49
19	2	2002	CLA	CHC-C1C-C2C	-2.54	119.66	126.35
19	B	1208	CLA	CHC-C1C-C2C	-2.54	119.66	126.35
19	A	1113	CLA	C1-C2-C3	-2.54	122.54	126.71
19	1	1007	CLA	CHC-C1C-C2C	-2.54	119.67	126.35
22	A	7035	LMU	C2'-C3'-C4'	-2.54	104.02	109.60
21	A	6007	BCR	C15-C16-C17	-2.54	117.78	123.39
19	G	1242	CLA	CAA-CBA-CGA	-2.54	105.89	113.32
19	A	1106	CLA	O2A-CGA-O1A	-2.54	116.95	123.49
19	B	1201	CLA	CHC-C1C-C2C	-2.53	119.69	126.35
21	B	6006	BCR	C15-C14-C13	-2.53	123.54	127.20
19	B	1236	CLA	CAA-C2A-C3A	-2.53	105.93	113.22
19	3	3015	CLA	C2D-C3D-C4D	-2.53	104.08	106.30
21	A	6007	BCR	C4-C5-C6	-2.53	119.56	122.78
19	A	1113	CLA	CAA-C2A-C3A	-2.53	105.95	113.22
21	B	6006	BCR	C23-C24-C25	-2.52	119.74	127.32
22	A	7016	LMU	C1'-O5'-C5'	-2.52	108.85	113.75
19	L	1130	CLA	CHC-C1C-C2C	-2.52	119.72	126.35
22	H	7011	LMU	O3B-C3B-C4B	-2.52	104.66	110.34
19	2	2004	CLA	CAA-C2A-C3A	-2.52	105.97	113.22
21	A	6011	BCR	C8-C7-C6	-2.52	119.75	127.32
19	A	1122	CLA	CHC-C1C-C2C	-2.52	119.73	126.35
21	B	6020	BCR	C37-C22-C21	-2.52	119.18	122.90
19	A	1125	CLA	CHC-C1C-C2C	-2.52	119.74	126.35
19	A	1126	CLA	O2D-CGD-O1D	-2.51	118.60	123.79
19	A	1122	CLA	CAA-C2A-C3A	-2.51	105.99	113.22
19	2	4009	CLA	O2D-CGD-O1D	-2.51	118.60	123.79
19	H	1241	CLA	O2A-CGA-O1A	-2.51	117.00	123.49
19	4	4012	CLA	CMD-C2D-C3D	-2.51	120.17	125.09
19	1	1005	CLA	CHC-C1C-C2C	-2.51	119.75	126.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	H	1241	CLA	CMD-C2D-C3D	-2.51	120.18	125.09
19	A	1134	CLA	O2D-CGD-O1D	-2.51	118.61	123.79
19	A	1132	CLA	CHD-C4C-C3C	-2.51	121.07	124.94
19	3	3013	CLA	CMD-C2D-C3D	-2.50	120.19	125.09
19	L	1503	CLA	CMD-C2D-C3D	-2.50	120.19	125.09
21	B	6005	BCR	C23-C24-C25	-2.50	119.81	127.32
19	F	1305	CLA	CHC-C1C-C2C	-2.50	119.78	126.35
19	A	1115	CLA	O2A-CGA-O1A	-2.50	117.04	123.49
19	B	1231	CLA	CHC-C1C-C2C	-2.50	119.78	126.35
22	G	7051	LMU	O3B-C3B-C4B	-2.50	104.71	110.34
19	3	1118	CLA	CAA-C2A-C3A	-2.49	110.23	116.20
19	1	1303	CLA	CBA-CAA-C2A	-2.49	106.70	113.73
19	B	1217	CLA	CHC-C1C-C2C	-2.49	119.80	126.35
19	B	1222	CLA	CHC-C1C-C2C	-2.49	119.80	126.35
19	B	1210	CLA	CBA-CAA-C2A	-2.49	106.71	113.73
19	1	1008	CLA	O1D-CGD-CBD	-2.49	121.06	124.62
19	3	3003	CLA	CHC-C1C-C2C	-2.49	119.81	126.35
19	2	2014	CLA	C4-C3-C2	-2.49	118.62	123.50
19	2	2004	CLA	CHC-C1C-C2C	-2.49	119.81	126.35
19	1	1001	CLA	CBA-CAA-C2A	-2.48	106.74	113.73
21	A	6007	BCR	C27-C26-C25	-2.48	119.63	122.78
19	H	1505	CLA	CGD-CBD-CAD	-2.47	102.25	110.62
19	B	1210	CLA	CHC-C1C-C2C	-2.47	119.86	126.35
19	I	1204	CLA	CHC-C1C-C2C	-2.47	119.86	126.35
21	B	6005	BCR	C16-C15-C14	-2.47	117.94	123.39
19	1	1008	CLA	CHC-C1C-C2C	-2.46	119.87	126.35
19	4	4014	CLA	C2A-C1A-CHA	-2.46	119.35	123.89
19	B	1212	CLA	O2D-CGD-O1D	-2.46	118.71	123.79
19	A	1237	CLA	C6-C7-C8	-2.46	107.33	115.49
19	B	1229	CLA	CAA-CBA-CGA	-2.46	106.12	113.32
21	F	6016	BCR	C35-C13-C14	-2.46	119.27	122.90
22	E	7037	LMU	O2'-C2'-C1'	-2.46	104.63	110.02
19	2	2014	CLA	CMD-C2D-C3D	-2.45	120.29	125.09
19	B	1203	CLA	O1D-CGD-CBD	-2.45	121.11	124.62
21	A	6008	BCR	C29-C30-C25	-2.45	106.48	110.36
19	A	1110	CLA	O2D-CGD-O1D	-2.45	118.73	123.79
19	B	1301	CLA	CHC-C1C-C2C	-2.45	119.91	126.35
22	E	7037	LMU	C3B-C4B-C5B	-2.45	105.93	110.20
19	K	1142	CLA	CHC-C1C-C2C	-2.45	119.92	126.35
19	A	9012	CLA	CHC-C1C-C2C	-2.45	119.92	126.35
22	R	7025	LMU	C1B-O1B-C4'	-2.45	111.61	118.01
19	4	4014	CLA	O2D-CGD-O1D	-2.44	118.74	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1136	CLA	O2D-CGD-O1D	-2.44	118.75	123.79
19	B	1238	CLA	O2D-CGD-O1D	-2.44	118.75	123.79
19	A	1106	CLA	CHC-C1C-C2C	-2.44	119.94	126.35
19	B	1239	CLA	CMD-C2D-C3D	-2.44	120.32	125.09
19	A	1102	CLA	CHC-C1C-C2C	-2.44	119.94	126.35
19	A	1117	CLA	C4-C3-C2	-2.44	118.72	123.50
19	A	1136	CLA	O1D-CGD-CBD	-2.44	121.13	124.62
19	A	1132	CLA	O2A-CGA-O1A	-2.44	117.21	123.49
19	A	1123	CLA	C4-C3-C2	-2.43	118.72	123.50
19	A	1129	CLA	O2A-CGA-O1A	-2.43	117.22	123.49
19	A	9013	CLA	O2A-CGA-O1A	-2.43	117.23	123.49
19	A	1106	CLA	CAA-C2A-C3A	-2.42	106.24	113.22
22	H	7030	LMU	C4B-C3B-C2B	-2.42	106.27	110.79
19	4	4014	CLA	CAC-C3C-C2C	-2.42	123.27	127.51
19	A	1105	CLA	CHC-C1C-C2C	-2.42	119.99	126.35
19	A	1133	CLA	O1D-CGD-CBD	-2.42	121.16	124.62
19	A	1135	CLA	O1D-CGD-CBD	-2.42	121.16	124.62
19	B	1203	CLA	O2A-CGA-O1A	-2.42	117.26	123.49
19	B	1222	CLA	C4-C3-C2	-2.41	118.76	123.50
19	1	1012	CLA	CHC-C1C-C2C	-2.41	120.01	126.35
19	3	2009	CLA	CHC-C1C-C2C	-2.41	120.01	126.35
19	1	1005	CLA	C2A-C1A-CHA	-2.41	119.45	123.89
19	4	1304	CLA	C16-C15-C13	-2.41	107.50	115.49
19	4	4015	CLA	CBA-CAA-C2A	-2.41	106.94	113.73
19	3	3011	CLA	C5-C3-C2	-2.41	116.49	121.05
22	G	7051	LMU	O5'-C5'-C4'	-2.41	104.67	109.75
19	3	3017	CLA	CHD-C4C-C3C	-2.40	121.23	124.94
21	B	6020	BCR	C33-C5-C6	-2.40	122.25	124.61
19	B	9010	CLA	O2D-CGD-O1D	-2.40	118.83	123.79
19	B	1223	CLA	C2A-C1A-CHA	-2.40	119.47	123.89
19	3	3016	CLA	O2D-CGD-O1D	-2.40	118.84	123.79
19	B	1228	CLA	CHC-C1C-C2C	-2.40	120.04	126.35
19	A	1119	CLA	CAA-C2A-C3A	-2.40	106.32	113.22
21	A	6008	BCR	C28-C27-C26	-2.40	110.06	113.87
19	K	3009	CLA	C4-C3-C2	-2.39	118.80	123.50
21	A	6002	BCR	C34-C9-C10	-2.39	119.36	122.90
19	A	1149	CLA	CAA-CBA-CGA	-2.39	106.31	113.32
19	A	1134	CLA	O1D-CGD-CBD	-2.39	121.19	124.62
19	L	1501	CLA	CHC-C1C-C2C	-2.39	120.06	126.35
19	A	1115	CLA	CHC-C1C-C2C	-2.39	120.06	126.35
21	I	6021	BCR	C33-C5-C6	-2.39	122.26	124.61
21	B	6006	BCR	C8-C7-C6	-2.39	120.15	127.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	4007	CLA	C4-C3-C2	-2.39	118.82	123.50
19	B	1216	CLA	CMD-C2D-C3D	-2.39	120.42	125.09
19	A	9022	CLA	CHC-C1C-C2C	-2.38	120.08	126.35
19	K	1146	CLA	O1D-CGD-CBD	-2.38	121.20	124.62
19	B	1216	CLA	C4-C3-C2	-2.38	118.82	123.50
21	B	6005	BCR	C27-C26-C25	-2.38	119.75	122.78
21	F	6014	BCR	C23-C24-C25	-2.38	120.17	127.32
19	A	9013	CLA	CHC-C1C-C2C	-2.38	120.09	126.35
19	4	1304	CLA	C7-C6-C5	-2.38	106.03	113.06
19	3	3011	CLA	O2D-CGD-O1D	-2.38	118.88	123.79
19	A	1133	CLA	O2D-CGD-O1D	-2.38	118.88	123.79
19	1	1003	CLA	CHC-C1C-C2C	-2.38	120.10	126.35
21	F	6016	BCR	C4-C5-C6	-2.38	119.75	122.78
21	B	6020	BCR	C39-C30-C29	-2.38	100.28	108.79
21	B	6004	BCR	C16-C15-C14	-2.37	118.14	123.39
19	H	1145	CLA	O2A-CGA-O1A	-2.37	117.37	123.49
19	B	1203	CLA	C16-C15-C13	-2.37	107.62	115.49
21	B	6010	BCR	C15-C16-C17	-2.37	118.15	123.39
19	A	9013	CLA	C2A-C1A-CHA	-2.37	119.52	123.89
22	4	7053	LMU	O2B-C2B-C3B	-2.37	105.00	110.34
19	4	4007	CLA	CAA-C2A-C1A	-2.37	104.12	112.47
22	H	7002	LMU	C3'-C4'-C5'	-2.37	105.49	110.84
19	B	1229	CLA	CHC-C1C-C2C	-2.37	120.13	126.35
19	A	9011	CLA	C3B-C4B-NB	-2.37	106.15	109.21
19	F	1240	CLA	CAA-C2A-C1A	-2.36	105.62	112.17
21	B	6020	BCR	C31-C1-C6	-2.36	106.60	110.30
22	B	7038	LMU	C6B-C5B-C4B	-2.36	107.19	113.02
19	B	1215	CLA	O2A-CGA-O1A	-2.36	117.40	123.49
21	B	6006	BCR	C30-C25-C26	-2.36	119.19	122.66
20	A	5001	PQN	C2M-C2-C3	-2.36	119.05	124.10
19	A	9022	CLA	CMD-C2D-C3D	-2.36	120.47	125.09
21	I	6021	BCR	C28-C27-C26	-2.36	110.12	113.87
21	A	6007	BCR	C23-C22-C21	-2.36	115.18	118.98
19	L	1130	CLA	O2A-CGA-O1A	-2.36	117.40	123.49
19	H	1207	CLA	CHC-C1C-C2C	-2.36	120.15	126.35
19	A	1105	CLA	O2D-CGD-O1D	-2.36	118.92	123.79
19	A	1237	CLA	CHC-C1C-C2C	-2.36	120.15	126.35
19	A	1151	CLA	O2A-CGA-O1A	-2.36	117.41	123.49
19	A	1119	CLA	O2D-CGD-O1D	-2.35	118.93	123.79
19	A	1107	CLA	O2A-CGA-O1A	-2.35	117.42	123.49
19	B	1238	CLA	O2A-CGA-O1A	-2.35	117.42	123.49
19	4	1304	CLA	CBC-CAC-C3C	-2.35	105.22	112.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	6002	BCR	C7-C6-C5	-2.35	116.00	121.37
19	B	1225	CLA	O2A-CGA-O1A	-2.34	117.44	123.49
19	4	4001	CLA	CHC-C1C-C2C	-2.34	120.19	126.35
19	A	9011	CLA	C6-C7-C8	-2.34	107.73	115.49
19	2	2014	CLA	O2D-CGD-O1D	-2.34	118.96	123.79
19	A	1126	CLA	CHC-C1C-C2C	-2.34	120.20	126.35
21	B	6010	BCR	C40-C30-C25	-2.34	106.64	110.30
22	B	7040	LMU	O3B-C3B-C2B	-2.34	105.07	110.34
19	B	1224	CLA	CAA-C2A-C1A	-2.34	104.23	112.47
19	A	1127	CLA	CMD-C2D-C3D	-2.33	120.53	125.09
19	3	1147	CLA	CMD-C2D-C3D	-2.33	120.53	125.09
21	B	6004	BCR	C40-C30-C29	-2.33	100.44	108.79
21	A	6002	BCR	C4-C5-C6	-2.33	119.81	122.78
21	J	6012	BCR	C27-C26-C25	-2.33	119.81	122.78
19	B	1230	CLA	O2A-CGA-O1A	-2.33	117.49	123.49
19	1	1007	CLA	C4-C3-C2	-2.32	118.94	123.50
19	4	4007	CLA	O1D-CGD-CBD	-2.32	121.30	124.62
19	A	1126	CLA	O2A-CGA-O1A	-2.31	117.52	123.49
19	B	1210	CLA	C11-C10-C8	-2.31	107.82	115.49
19	A	1107	CLA	CAC-C3C-C2C	-2.31	123.45	127.51
19	3	3007	CLA	O2D-CGD-O1D	-2.31	119.02	123.79
19	L	1148	CLA	O2A-CGA-O1A	-2.31	117.53	123.49
19	A	1128	CLA	O2A-CGA-O1A	-2.31	117.54	123.49
19	A	1138	CLA	C2A-C1A-CHA	-2.31	119.64	123.89
19	B	1228	CLA	C2A-C1A-CHA	-2.31	119.64	123.89
19	3	2009	CLA	C6-C7-C8	-2.30	107.85	115.49
19	A	9012	CLA	C4-C3-C2	-2.30	118.98	123.50
19	2	2002	CLA	O1D-CGD-CBD	-2.30	121.32	124.62
19	2	4009	CLA	O2A-CGA-O1A	-2.30	117.55	123.49
21	I	6018	BCR	C40-C30-C29	-2.30	100.55	108.79
21	L	6019	BCR	C40-C30-C29	-2.30	100.55	108.79
19	B	1224	CLA	CHC-C1C-C2C	-2.30	120.30	126.35
19	J	1308	CLA	CAA-C2A-C3A	-2.30	106.60	113.22
19	4	4015	CLA	CHC-C1C-C2C	-2.30	120.31	126.35
19	A	1135	CLA	C2A-C1A-CHA	-2.30	119.65	123.89
21	A	6002	BCR	C15-C16-C17	-2.30	118.31	123.39
21	1	6023	BCR	C33-C5-C6	-2.29	122.35	124.61
21	A	6008	BCR	C16-C15-C14	-2.29	118.33	123.39
19	B	1239	CLA	CMA-C3A-C2A	-2.29	104.22	114.35
22	4	7019	LMU	O2'-C2'-C3'	-2.29	105.19	110.34
19	A	1111	CLA	O2D-CGD-O1D	-2.28	119.08	123.79
19	A	1125	CLA	O2D-CGD-O1D	-2.28	119.08	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	3017	CLA	O2A-CGA-O1A	-2.28	117.62	123.49
19	A	1138	CLA	O2D-CGD-O1D	-2.27	119.09	123.79
19	A	1117	CLA	CAA-CBA-CGA	-2.27	106.67	113.32
19	A	1125	CLA	C2A-C1A-CHA	-2.27	119.70	123.89
19	B	1203	CLA	CBC-CAC-C3C	-2.27	105.46	112.39
19	B	1221	CLA	O1D-CGD-CBD	-2.27	121.37	124.62
19	G	1242	CLA	C2A-C1A-CHA	-2.27	119.71	123.89
21	3	6022	BCR	C36-C18-C17	-2.26	119.56	122.90
19	4	4003	CLA	C4-C3-C2	-2.26	119.06	123.50
19	3	3011	CLA	O1D-CGD-CBD	-2.26	121.38	124.62
19	B	1201	CLA	O1D-CGD-CBD	-2.26	121.38	124.62
19	1	1010	CLA	CAC-C3C-C4C	-2.26	121.55	124.83
21	B	6017	BCR	C38-C26-C25	-2.26	122.39	124.61
19	B	1215	CLA	O2D-CGD-O1D	-2.26	119.13	123.79
19	B	1212	CLA	CHC-C1C-C2C	-2.26	120.42	126.35
19	3	3007	CLA	C2A-C1A-CHA	-2.25	119.73	123.89
19	1	1013	CLA	O1D-CGD-CBD	-2.25	121.39	124.62
21	A	6008	BCR	C8-C7-C6	-2.25	120.55	127.32
21	I	6018	BCR	C37-C22-C21	-2.25	119.58	122.90
19	A	1107	CLA	CHD-C4C-C3C	-2.25	121.47	124.94
19	2	2012	CLA	CAA-C2A-C3A	-2.25	106.75	113.22
19	3	3016	CLA	C4-C3-C2	-2.25	119.09	123.50
21	I	6018	BCR	C2-C1-C6	-2.25	106.80	110.36
19	A	1136	CLA	C2A-C1A-CHA	-2.25	119.75	123.89
21	A	6003	BCR	C4-C5-C6	-2.25	119.92	122.78
21	B	6006	BCR	C33-C5-C6	-2.25	122.40	124.61
19	A	1105	CLA	CGD-CBD-CAD	-2.24	103.02	110.62
19	A	1141	CLA	O2D-CGD-O1D	-2.24	119.16	123.79
21	B	6006	BCR	C40-C30-C29	-2.24	100.78	108.79
19	3	3008	CLA	C2A-C1A-CHA	-2.24	119.77	123.89
19	4	4001	CLA	O2A-CGA-O1A	-2.23	117.73	123.49
19	4	4006	CLA	C2A-C1A-CHA	-2.23	119.78	123.89
19	B	1233	CLA	CHC-C1C-C2C	-2.23	120.49	126.35
19	4	4007	CLA	O2D-CGD-O1D	-2.23	119.19	123.79
19	3	3016	CLA	O2A-CGA-O1A	-2.23	117.75	123.49
19	A	1115	CLA	C4-C3-C2	-2.23	119.13	123.50
19	A	1132	CLA	C5-C3-C2	-2.22	116.83	121.05
19	A	1122	CLA	CAC-C3C-C2C	-2.22	123.61	127.51
21	A	6002	BCR	C40-C30-C29	-2.22	100.83	108.79
19	K	3009	CLA	C2A-C1A-CHA	-2.22	119.80	123.89
19	L	1502	CLA	O1D-CGD-CBD	-2.22	121.44	124.62
19	2	2013	CLA	CMD-C2D-C3D	-2.22	120.75	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1007	CLA	O2A-CGA-O1A	-2.22	117.78	123.49
21	F	6014	BCR	C16-C15-C14	-2.21	118.50	123.39
19	A	9011	CLA	CHC-C1C-C2C	-2.21	120.54	126.35
19	L	1504	CLA	CHC-C1C-C2C	-2.20	120.56	126.35
19	B	1238	CLA	C2A-C1A-CHA	-2.20	119.83	123.89
19	A	1109	CLA	O2D-CGD-O1D	-2.20	119.25	123.79
21	A	6002	BCR	C8-C7-C6	-2.20	120.71	127.32
19	A	9011	CLA	CMA-C3A-C2A	-2.20	104.61	114.35
19	B	1203	CLA	CMA-C3A-C2A	-2.20	104.63	114.35
19	2	2002	CLA	CAA-C2A-C1A	-2.20	104.73	112.47
19	A	1139	CLA	C2A-C1A-CHA	-2.20	119.84	123.89
19	A	1122	CLA	O2D-CGD-O1D	-2.19	119.27	123.79
19	2	2007	CLA	C6-C7-C8	-2.19	108.23	115.49
19	A	1141	CLA	C6-C5-C3	-2.19	107.69	112.48
19	B	1212	CLA	O2A-CGA-O1A	-2.19	117.85	123.49
19	A	1115	CLA	O1D-CGD-CBD	-2.19	121.49	124.62
19	B	9010	CLA	CMD-C2D-C3D	-2.18	120.82	125.09
19	2	2013	CLA	O2A-CGA-O1A	-2.18	117.86	123.49
19	2	2012	CLA	CAC-C3C-C2C	-2.18	123.69	127.51
19	4	4002	CLA	CMD-C2D-C3D	-2.18	120.83	125.09
22	K	7042	LMU	C1'-O5'-C5'	-2.18	109.52	113.75
19	K	1143	CLA	C1-C2-C3	-2.18	123.14	126.71
21	A	6011	BCR	C19-C18-C17	-2.17	115.49	118.98
19	B	1222	CLA	O2D-CGD-O1D	-2.17	119.31	123.79
19	K	3009	CLA	CAA-CBA-CGA	-2.17	106.97	113.32
19	A	1128	CLA	C5-C3-C2	-2.16	116.95	121.05
19	A	1128	CLA	C2A-C1A-CHA	-2.16	119.91	123.89
21	F	6016	BCR	C28-C27-C26	-2.16	110.44	113.87
19	A	1102	CLA	O2D-CGD-O1D	-2.16	119.33	123.79
22	N	7049	LMU	O5B-C5B-C4B	-2.16	105.63	109.68
19	R	1150	CLA	O2A-CGA-O1A	-2.15	117.93	123.49
19	B	1206	CLA	CMD-C2D-C3D	-2.15	120.88	125.09
21	L	6019	BCR	C8-C7-C6	-2.15	120.86	127.32
19	B	1226	CLA	C7-C6-C5	-2.15	106.72	113.06
19	A	1120	CLA	CHC-C1C-C2C	-2.15	120.71	126.35
19	A	1140	CLA	C2A-C1A-CHA	-2.15	119.93	123.89
21	B	6004	BCR	C27-C26-C25	-2.15	120.05	122.78
19	4	1009	CLA	CHC-C1C-C2C	-2.15	120.71	126.35
19	2	2001	CLA	O2D-CGD-O1D	-2.14	119.36	123.79
19	B	1228	CLA	CMD-C2D-C3D	-2.14	120.89	125.09
19	B	1225	CLA	C11-C12-C13	-2.14	108.38	115.49
19	K	1143	CLA	O2A-CGA-O1A	-2.14	117.96	123.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1102	CLA	C3B-C4B-NB	-2.14	106.44	109.21
19	J	1308	CLA	CAA-CBA-CGA	-2.14	107.05	113.32
19	3	2009	CLA	CGD-CBD-CAD	-2.14	103.39	110.62
19	1	1003	CLA	CAA-CBA-CGA	-2.13	107.07	113.32
19	B	1235	CLA	C4-C3-C2	-2.13	119.31	123.50
19	1	1001	CLA	CGD-CBD-CAD	-2.13	103.40	110.62
19	4	4007	CLA	CAA-C2A-C3A	-2.13	107.09	113.22
21	I	6021	BCR	C32-C1-C6	-2.12	106.97	110.30
19	L	1503	CLA	CHC-C1C-C2C	-2.12	120.77	126.35
19	K	1143	CLA	CBC-CAC-C3C	-2.12	105.92	112.39
19	A	1125	CLA	O1D-CGD-CBD	-2.12	121.58	124.62
19	B	1215	CLA	CMD-C2D-C3D	-2.12	120.94	125.09
19	A	1129	CLA	C2A-C1A-CHA	-2.12	119.98	123.89
19	F	1305	CLA	CMD-C2D-C3D	-2.12	120.95	125.09
19	A	1104	CLA	O2A-CGA-O1A	-2.12	118.03	123.49
19	A	1134	CLA	C2A-C1A-CHA	-2.11	119.99	123.89
19	2	2004	CLA	O2D-CGD-O1D	-2.11	119.42	123.79
19	B	1233	CLA	O2D-CGD-O1D	-2.11	119.43	123.79
21	F	6016	BCR	C37-C22-C21	-2.11	119.79	122.90
19	B	9010	CLA	C16-C17-C18	-2.11	105.24	115.87
19	A	1109	CLA	C4-C3-C2	-2.11	119.36	123.50
19	A	1132	CLA	CAC-C3C-C2C	-2.11	123.81	127.51
19	A	9012	CLA	CMD-C2D-C3D	-2.11	120.97	125.09
22	C	7015	LMU	O5B-C5B-C4B	-2.10	105.73	109.68
22	G	7051	LMU	O2B-C2B-C3B	-2.10	105.60	110.34
19	A	1141	CLA	C4-C3-C2	-2.10	119.37	123.50
19	B	1236	CLA	O2D-CGD-O1D	-2.10	119.45	123.79
21	L	6019	BCR	C38-C26-C25	-2.10	122.54	124.61
21	L	6019	BCR	C19-C18-C17	-2.10	115.59	118.98
19	B	1219	CLA	C2A-C1A-CHA	-2.10	120.02	123.89
19	1	1303	CLA	CAA-C2A-C3A	-2.10	107.18	113.22
22	D	7050	LMU	C1'-O5'-C5'	-2.10	109.67	113.75
19	B	1209	CLA	C2A-C1A-CHA	-2.10	120.02	123.89
19	A	1139	CLA	CAA-CBA-CGA	-2.09	107.19	113.32
21	L	6019	BCR	C37-C22-C21	-2.09	119.81	122.90
19	B	1222	CLA	O1D-CGD-CBD	-2.09	121.62	124.62
19	B	1202	CLA	C5-C3-C2	-2.09	117.09	121.05
19	2	2001	CLA	O2A-CGA-O1A	-2.09	118.10	123.49
19	3	3017	CLA	CBA-CAA-C2A	-2.09	107.84	113.73
19	A	1137	CLA	O2A-CGA-O1A	-2.09	118.11	123.49
22	4	7008	LMU	O2'-C2'-C3'	-2.09	105.64	110.34
21	A	6008	BCR	C4-C5-C6	-2.09	120.12	122.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1131	CLA	O2A-CGA-O1A	-2.08	118.11	123.49
19	4	4002	CLA	C2C-C1C-NC	-2.08	108.69	110.24
19	B	1203	CLA	C11-C12-C13	-2.08	108.58	115.49
22	R	7021	LMU	C6B-C5B-C4B	-2.08	107.89	113.02
19	2	2002	CLA	CAA-C2A-C3A	-2.08	107.24	113.22
19	B	1211	CLA	CAC-C3C-C2C	-2.08	123.87	127.51
22	A	7045	LMU	O6'-C6'-C5'	-2.08	104.47	111.33
22	H	7011	LMU	O5'-C1'-C2'	-2.08	106.02	110.28
19	B	1202	CLA	C11-C12-C13	-2.07	108.61	115.49
21	B	6010	BCR	C7-C6-C5	-2.07	116.62	121.37
19	A	1110	CLA	C2A-C1A-CHA	-2.07	120.08	123.89
22	K	7042	LMU	C1'-C2'-C3'	-2.07	105.90	109.97
19	A	9023	CLA	CMA-C3A-C2A	-2.06	105.24	114.35
21	B	6006	BCR	C32-C1-C6	-2.06	107.08	110.30
19	H	1145	CLA	C4-C3-C2	-2.06	119.46	123.50
19	A	1124	CLA	C2A-C1A-CHA	-2.06	120.10	123.89
19	4	1304	CLA	O2D-CGD-O1D	-2.05	119.55	123.79
22	K	7042	LMU	C4B-C3B-C2B	-2.05	106.96	110.79
19	G	1242	CLA	O1D-CGD-CBD	-2.05	121.68	124.62
19	3	3017	CLA	C1-C2-C3	-2.05	123.34	126.71
19	1	1006	CLA	CMA-C3A-C2A	-2.05	111.29	116.20
19	B	1217	CLA	O2D-CGD-O1D	-2.05	119.56	123.79
21	F	6014	BCR	C15-C16-C17	-2.05	118.86	123.39
19	A	1139	CLA	O2D-CGD-O1D	-2.05	119.56	123.79
22	3	7005	LMU	O2B-C2B-C3B	-2.05	105.73	110.34
21	J	6012	BCR	C3-C4-C5	-2.05	110.62	113.87
20	A	5001	PQN	C15-C13-C12	-2.04	117.17	121.05
19	A	1136	CLA	O2A-CGA-O1A	-2.04	118.22	123.49
19	B	1217	CLA	CMA-C3A-C2A	-2.04	105.31	114.35
19	A	1140	CLA	O2A-CGA-O1A	-2.04	118.22	123.49
19	L	1503	CLA	CAA-CBA-CGA	-2.04	107.34	113.32
19	1	1003	CLA	C2A-C1A-CHA	-2.04	120.13	123.89
19	G	1242	CLA	CHC-C1C-C2C	-2.04	120.98	126.35
19	F	1302	CLA	C2A-C1A-CHA	-2.04	120.13	123.89
19	B	1210	CLA	C16-C15-C13	-2.04	108.74	115.49
19	4	1004	CLA	O2A-CGA-O1A	-2.03	118.24	123.49
21	3	6022	BCR	C3-C4-C5	-2.03	110.64	113.87
19	A	1117	CLA	C6-C5-C3	-2.03	108.03	112.48
19	A	1103	CLA	CAC-C3C-C2C	-2.03	123.95	127.51
19	A	1149	CLA	CAC-C3C-C2C	-2.03	123.95	127.51
19	A	1107	CLA	C2A-C1A-CHA	-2.03	120.15	123.89
19	A	1137	CLA	C2A-C1A-CHA	-2.03	120.15	123.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1135	CLA	CAA-C2A-C3A	-2.02	107.40	113.22
21	B	6004	BCR	C8-C7-C6	-2.02	121.24	127.32
19	B	1221	CLA	CAC-C3C-C2C	-2.02	123.96	127.51
19	B	1205	CLA	C4-C3-C2	-2.02	119.53	123.50
19	B	1216	CLA	CAA-C2A-C3A	-2.02	107.41	113.22
19	H	1505	CLA	O2A-CGA-O1A	-2.02	118.28	123.49
22	R	7020	LMU	C1'-O5'-C5'	-2.02	109.83	113.75
21	A	6002	BCR	C16-C15-C14	-2.02	118.93	123.39
19	A	1107	CLA	O1D-CGD-CBD	-2.02	121.73	124.62
19	3	3016	CLA	C2A-C1A-CHA	-2.01	120.17	123.89
19	B	1215	CLA	CAA-C2A-C3A	-2.01	107.42	113.22
19	4	1304	CLA	C2C-C1C-NC	-2.01	108.75	110.24
21	A	6008	BCR	C34-C9-C10	-2.01	119.93	122.90
19	A	1123	CLA	O1D-CGD-CBD	-2.01	121.74	124.62
21	A	6003	BCR	C40-C30-C29	-2.01	101.61	108.79
21	A	6011	BCR	C11-C12-C13	-2.00	120.42	126.32
19	B	1209	CLA	O2A-CGA-O1A	-2.00	118.32	123.49
22	H	7032	LMU	C3B-C4B-C5B	-2.00	106.70	110.20
21	A	6007	BCR	C16-C15-C14	-2.00	118.97	123.39
22	3	7003	LMU	C6B-C5B-C4B	-2.00	108.08	113.02
22	F	7036	LMU	O5B-C5B-C6B	2.00	111.42	106.36
19	K	1143	CLA	CAC-C3C-C4C	2.01	127.74	124.83
19	A	1127	CLA	C4-C3-C5	2.01	118.47	115.41
19	B	1203	CLA	C4-C3-C5	2.01	118.47	115.41
19	B	1206	CLA	CED-O2D-CGD	2.01	120.70	115.99
19	B	1217	CLA	C5-C3-C4	2.01	119.59	114.64
19	3	3016	CLA	CED-O2D-CGD	2.01	120.71	115.99
19	A	1141	CLA	CED-O2D-CGD	2.01	120.71	115.99
19	A	9022	CLA	CAA-C2A-C1A	2.01	119.57	112.47
19	A	1101	CLA	C5-C3-C4	2.01	119.59	114.64
22	A	7044	LMU	O5B-C5B-C4B	2.02	113.46	109.68
19	A	1109	CLA	O2A-CGA-CBA	2.02	118.04	111.90
19	B	1209	CLA	O2A-CGA-CBA	2.02	118.04	111.90
19	1	1002	CLA	CAA-CBA-CGA	2.02	119.22	113.32
19	1	1010	CLA	CAC-C3C-C2C	2.02	131.05	127.51
19	B	1214	CLA	C4-C3-C5	2.02	118.50	115.41
22	2	7046	LMU	O5'-C5'-C6'	2.02	111.47	106.36
19	B	1203	CLA	C4A-NA-C1A	2.03	108.98	106.36
19	A	1134	CLA	CED-O2D-CGD	2.03	120.74	115.99
19	A	1129	CLA	CAC-C3C-C4C	2.03	127.77	124.83
22	B	7012	LMU	O1B-C4'-C3'	2.03	112.40	107.17
22	R	7024	LMU	O5B-C5B-C6B	2.03	111.48	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	2009	CLA	CAC-C3C-C4C	2.03	127.78	124.83
19	B	1210	CLA	CHB-C4A-NA	2.03	127.32	124.51
19	A	1121	CLA	CAA-C2A-C3A	2.03	119.23	114.13
22	K	7001	LMU	C4B-C3B-C2B	2.03	114.58	110.79
22	E	7048	LMU	O5'-C5'-C6'	2.03	111.49	106.36
22	C	7015	LMU	O1B-C1B-C2B	2.03	113.05	108.10
19	A	1123	CLA	CED-O2D-CGD	2.03	120.76	115.99
19	A	1127	CLA	CGD-CBD-CAD	2.04	117.52	110.62
19	B	1225	CLA	C4-C3-C5	2.04	118.52	115.41
22	H	7002	LMU	C1B-O1B-C4'	2.04	123.33	118.01
21	B	6005	BCR	C36-C18-C19	2.04	121.49	118.10
21	B	6010	BCR	C39-C30-C25	2.04	113.50	110.30
21	B	6010	BCR	C1-C6-C7	2.04	121.54	115.82
19	K	1146	CLA	C5-C3-C4	2.04	119.66	114.64
22	K	7001	LMU	C2'-C3'-C4'	2.04	114.09	109.60
19	B	1232	CLA	CBA-CAA-C2A	2.04	119.50	113.55
21	J	6012	BCR	C40-C30-C39	2.05	114.93	108.37
22	A	7035	LMU	C1'-C2'-C3'	2.05	114.01	109.97
22	R	7022	LMU	O5B-C5B-C4B	2.05	113.53	109.68
21	A	6003	BCR	C31-C1-C2	2.05	116.13	108.79
22	R	7007	LMU	C1B-O5B-C5B	2.05	117.73	113.75
22	4	7019	LMU	O5'-C5'-C6'	2.05	111.55	106.36
19	A	1128	CLA	O2A-CGA-CBA	2.06	118.16	111.90
19	B	1301	CLA	CAC-C3C-C4C	2.06	128.20	125.02
19	3	3017	CLA	CMB-C2B-C3B	2.06	129.12	125.09
19	R	1150	CLA	CBA-CAA-C2A	2.06	119.55	113.73
19	1	1002	CLA	C4A-NA-C1A	2.06	109.03	106.36
19	B	1217	CLA	CMC-C2C-C1C	2.06	128.21	125.02
19	B	1229	CLA	C3A-C2A-C1A	2.06	105.00	101.50
22	L	7029	LMU	O1'-C1'-C2'	2.07	110.65	108.04
19	3	3015	CLA	C3D-C2D-C1D	2.07	108.12	106.30
21	A	6011	BCR	C1-C6-C7	2.07	121.61	115.82
22	H	7011	LMU	C1B-C2B-C3B	2.07	114.06	109.97
22	H	7011	LMU	C1'-C2'-C3'	2.07	114.06	109.97
19	B	1218	CLA	CMB-C2B-C3B	2.08	129.15	125.09
22	B	7040	LMU	C1B-C2B-C3B	2.08	114.07	109.97
19	B	1239	CLA	CMB-C2B-C1B	2.08	131.80	128.36
22	K	7047	LMU	C2'-C3'-C4'	2.08	114.16	109.60
19	3	3001	CLA	C2B-C3B-C4B	2.08	108.10	106.29
21	A	6008	BCR	C39-C30-C25	2.08	113.56	110.30
21	A	6007	BCR	C32-C1-C2	2.08	116.23	108.79
19	H	1207	CLA	CED-O2D-CGD	2.08	120.87	115.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	F	6014	BCR	C32-C1-C31	2.08	115.04	108.37
19	L	1502	CLA	CMB-C2B-C3B	2.08	129.16	125.09
19	A	1151	CLA	C5-C3-C4	2.09	119.77	114.64
22	2	7027	LMU	O5'-C1'-C2'	2.09	114.57	110.28
22	R	7025	LMU	O3B-C3B-C4B	2.09	115.05	110.34
19	J	1308	CLA	C4A-NA-C1A	2.09	109.06	106.36
21	B	6006	BCR	C1-C6-C7	2.09	121.68	115.82
22	A	7045	LMU	C1B-C2B-C3B	2.09	114.10	109.97
19	3	1147	CLA	CHB-C4A-NA	2.10	127.41	124.51
21	A	6011	BCR	C32-C1-C2	2.10	116.30	108.79
21	3	6022	BCR	C37-C22-C23	2.10	121.59	118.10
19	A	1110	CLA	CED-O2D-CGD	2.10	120.92	115.99
22	B	7038	LMU	O1B-C4'-C5'	2.10	114.85	109.32
19	B	9010	CLA	CMB-C2B-C3B	2.10	129.20	125.09
19	1	1014	CLA	CHB-C4A-NA	2.11	127.42	124.51
19	L	1504	CLA	CED-O2D-CGD	2.11	120.93	115.99
22	B	7040	LMU	O5B-C1B-C2B	2.11	114.60	110.28
19	4	4014	CLA	CED-O2D-CGD	2.11	120.94	115.99
19	A	9012	CLA	CMB-C2B-C3B	2.11	129.22	125.09
22	H	7030	LMU	C2'-C3'-C4'	2.11	114.24	109.60
19	A	1112	CLA	CMB-C2B-C1B	2.11	131.86	128.36
22	B	7012	LMU	O5'-C5'-C4'	2.12	114.22	109.75
22	F	7036	LMU	O5'-C5'-C6'	2.12	111.71	106.36
22	2	7031	LMU	O1B-C4'-C5'	2.12	114.89	109.32
19	B	1219	CLA	CAC-C3C-C4C	2.12	127.90	124.83
19	B	1205	CLA	C4A-NA-C1A	2.12	109.10	106.36
19	B	1215	CLA	CAC-C3C-C4C	2.12	127.91	124.83
19	A	1129	CLA	CBA-CAA-C2A	2.12	119.72	113.73
22	R	7022	LMU	O5'-C5'-C4'	2.12	114.23	109.75
22	K	7047	LMU	C1B-O5B-C5B	2.12	117.87	113.75
19	B	1220	CLA	O2A-CGA-CBA	2.13	118.38	111.90
22	2	7046	LMU	O1B-C4'-C5'	2.13	114.92	109.32
19	A	1126	CLA	CMB-C2B-C3B	2.13	129.25	125.09
19	B	1234	CLA	C4-C3-C5	2.13	118.66	115.41
19	A	9022	CLA	CMC-C2C-C1C	2.13	128.32	125.02
19	A	1120	CLA	CMB-C2B-C3B	2.13	129.26	125.09
22	R	7014	LMU	O2B-C2B-C1B	2.14	114.71	110.02
19	A	1123	CLA	CMB-C2B-C3B	2.14	129.27	125.09
19	2	2007	CLA	C2C-C1C-NC	2.14	111.84	110.24
19	B	1215	CLA	CED-O2D-CGD	2.15	121.03	115.99
22	G	7051	LMU	C1'-C2'-C3'	2.15	114.21	109.97
22	3	7003	LMU	O1B-C4'-C3'	2.15	112.72	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	5001	PQN	C30-C28-C29	2.15	121.37	110.55
22	B	7012	LMU	C3'-C4'-C5'	2.15	115.70	110.84
20	B	5002	PQN	C14-C13-C15	2.15	118.69	115.41
19	R	1150	CLA	C5-C3-C2	2.15	125.14	121.05
19	K	1142	CLA	CHB-C4A-NA	2.15	127.49	124.51
19	B	1221	CLA	CMC-C2C-C1C	2.15	128.35	125.02
19	3	3003	CLA	CMB-C2B-C3B	2.16	129.55	125.14
22	4	7033	LMU	O5'-C5'-C6'	2.16	111.80	106.36
19	B	1226	CLA	CHB-C4A-NA	2.16	127.49	124.51
22	A	7010	LMU	C3B-C4B-C5B	2.16	113.96	110.20
19	3	1147	CLA	CAA-CBA-CGA	2.16	119.63	113.32
19	A	1115	CLA	CMB-C2B-C3B	2.16	129.31	125.09
19	L	1501	CLA	O2A-CGA-CBA	2.16	118.48	111.90
19	4	4007	CLA	O2A-CGA-CBA	2.16	118.48	111.90
21	A	6002	BCR	C40-C30-C39	2.16	115.29	108.37
19	1	1003	CLA	CAC-C3C-C4C	2.16	127.97	124.83
19	3	3005	CLA	C2B-C3B-C4B	2.16	108.18	106.29
19	A	1128	CLA	CHB-C4A-NA	2.16	127.50	124.51
19	F	1305	CLA	C2C-C1C-NC	2.17	111.86	110.24
22	B	7012	LMU	C1'-C2'-C3'	2.17	114.25	109.97
21	A	6007	BCR	C40-C30-C39	2.17	115.32	108.37
21	B	6005	BCR	C34-C9-C8	2.17	121.71	118.10
19	A	1131	CLA	C4-C3-C5	2.17	118.72	115.41
19	A	1105	CLA	CMC-C2C-C1C	2.17	128.38	125.02
19	4	1004	CLA	CED-O2D-CGD	2.18	121.09	115.99
19	A	1149	CLA	CHB-C4A-NA	2.18	127.52	124.51
19	A	1237	CLA	CHB-C4A-NA	2.18	127.52	124.51
19	A	1113	CLA	CED-O2D-CGD	2.18	121.10	115.99
19	2	4009	CLA	CAC-C3C-C4C	2.18	127.99	124.83
19	L	1148	CLA	CAC-C3C-C4C	2.18	128.00	124.83
21	B	6004	BCR	C31-C1-C2	2.18	116.61	108.79
21	I	6021	BCR	C7-C6-C5	2.19	126.38	121.37
19	1	1013	CLA	CMB-C2B-C1B	2.19	131.98	128.36
19	B	1213	CLA	CED-O2D-CGD	2.19	121.12	115.99
19	L	1504	CLA	CHB-C4A-NA	2.19	127.54	124.51
19	A	1124	CLA	C4-C3-C5	2.19	118.75	115.41
22	4	7019	LMU	C3'-C4'-C5'	2.19	115.80	110.84
19	4	4006	CLA	CHB-C4A-NA	2.19	127.55	124.51
19	A	9011	CLA	CMB-C2B-C3B	2.19	129.38	125.09
19	3	3003	CLA	CHB-C4A-NA	2.20	127.56	124.51
22	3	7005	LMU	O5'-C1'-C2'	2.20	114.80	110.28
21	A	6007	BCR	C34-C9-C8	2.21	121.77	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L	1503	CLA	CHB-C4A-NA	2.21	127.56	124.51
19	3	2009	CLA	CHB-C4A-NA	2.21	127.57	124.51
19	B	1236	CLA	CED-O2D-CGD	2.21	121.17	115.99
19	A	1121	CLA	CHB-C4A-NA	2.21	127.57	124.51
19	1	1001	CLA	CMC-C2C-C1C	2.21	128.44	125.02
19	A	1105	CLA	CAC-C3C-C4C	2.21	128.04	124.83
19	A	1237	CLA	O2A-CGA-CBA	2.21	118.64	111.90
19	B	1232	CLA	CED-O2D-CGD	2.21	121.18	115.99
19	B	1208	CLA	C4-C3-C5	2.21	118.79	115.41
22	H	7011	LMU	O5B-C1B-C2B	2.22	114.82	110.28
19	A	1109	CLA	C3A-C2A-C1A	2.22	105.26	101.50
19	B	1210	CLA	CMB-C2B-C3B	2.22	129.43	125.09
19	4	4007	CLA	CED-O2D-CGD	2.22	121.20	115.99
19	1	1310	CLA	C2B-C3B-C4B	2.22	108.23	106.29
22	E	7048	LMU	O1B-C1B-O5B	2.23	116.33	110.68
22	2	7031	LMU	C1-O1'-C1'	2.23	117.84	113.94
19	H	1207	CLA	CAC-C3C-C4C	2.23	128.07	124.83
19	A	1107	CLA	C2C-C1C-NC	2.23	111.91	110.24
21	F	6014	BCR	C40-C30-C39	2.23	115.53	108.37
22	R	7025	LMU	O1B-C1B-C2B	2.23	113.54	108.10
19	A	1111	CLA	C4-C3-C5	2.24	118.83	115.41
19	B	1230	CLA	CAC-C3C-C4C	2.24	128.08	124.83
19	2	2013	CLA	C4A-NA-C1A	2.24	109.26	106.36
19	3	1147	CLA	O2A-CGA-CBA	2.25	121.72	112.36
19	A	9013	CLA	CGD-CBD-CAD	2.25	118.23	110.62
19	B	1223	CLA	CHB-C4A-NA	2.25	127.62	124.51
19	B	1201	CLA	CMB-C2B-C3B	2.25	129.49	125.09
19	B	1216	CLA	CMC-C2C-C1C	2.25	128.50	125.02
19	4	4004	CLA	C2B-C3B-C4B	2.25	108.26	106.29
19	L	1503	CLA	CAA-C2A-C1A	2.25	120.42	112.47
19	2	4009	CLA	CED-O2D-CGD	2.26	121.28	115.99
19	A	1117	CLA	CHB-C4A-NA	2.26	127.63	124.51
22	G	7026	LMU	O4'-C4B-C5B	2.26	115.23	109.24
19	A	1140	CLA	C4-C3-C5	2.26	118.86	115.41
22	2	7031	LMU	O5'-C1'-O1'	2.26	115.50	110.05
19	B	1227	CLA	CAC-C3C-C4C	2.26	128.12	124.83
21	B	6004	BCR	C35-C13-C12	2.26	121.86	118.10
19	A	1237	CLA	CAC-C3C-C4C	2.26	128.12	124.83
19	A	1102	CLA	CHB-C4A-NA	2.27	127.64	124.51
22	H	7043	LMU	O5'-C5'-C6'	2.27	112.09	106.36
19	B	1232	CLA	CHB-C4A-NA	2.27	127.65	124.51
22	2	7027	LMU	C3'-C4'-C5'	2.27	115.98	110.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	2012	CLA	C4A-NA-C1A	2.27	109.30	106.36
19	A	1119	CLA	O2A-CGA-CBA	2.28	118.86	111.90
19	1	1005	CLA	CGD-CBD-CAD	2.29	118.37	110.62
19	4	4001	CLA	CED-O2D-CGD	2.29	121.35	115.99
22	C	7015	LMU	O2'-C2'-C3'	2.29	115.48	110.34
19	1	1002	CLA	C3A-C2A-C1A	2.29	105.38	101.50
19	1	1010	CLA	CMB-C2B-C3B	2.29	129.56	125.09
22	A	7035	LMU	O5'-C5'-C6'	2.29	112.14	106.36
19	B	1222	CLA	CAC-C3C-C4C	2.29	128.16	124.83
19	A	1112	CLA	CHB-C4A-NA	2.29	127.68	124.51
19	B	1211	CLA	O2A-CGA-CBA	2.29	118.88	111.90
19	A	1112	CLA	CED-O2D-CGD	2.29	121.37	115.99
19	B	1226	CLA	O2A-CGA-CBA	2.29	118.89	111.90
19	K	3009	CLA	CHB-C4A-NA	2.29	127.68	124.51
19	A	1116	CLA	C4-C3-C5	2.29	118.91	115.41
21	A	6011	BCR	C37-C22-C23	2.30	121.92	118.10
19	H	1145	CLA	O2D-CGD-CBD	2.30	114.46	111.30
19	A	1132	CLA	C2C-C1C-NC	2.30	111.96	110.24
19	A	1151	CLA	O2A-CGA-CBA	2.31	118.93	111.90
19	3	3017	CLA	O2A-CGA-CBA	2.31	118.94	111.90
19	A	1124	CLA	CAC-C3C-C4C	2.31	128.19	124.83
22	E	7037	LMU	C1'-C2'-C3'	2.31	114.53	109.97
22	4	7033	LMU	O1B-C1B-C2B	2.32	113.75	108.10
19	2	2014	CLA	C3A-C2A-C1A	2.32	105.43	101.50
22	B	7038	LMU	O5'-C5'-C6'	2.32	112.22	106.36
19	3	2009	CLA	O2A-CGA-CBA	2.32	118.97	111.90
19	4	4003	CLA	CHB-C4A-NA	2.32	127.72	124.51
19	2	2012	CLA	O2A-CGA-CBA	2.32	118.98	111.90
19	A	1131	CLA	CMB-C2B-C3B	2.32	129.63	125.09
19	1	1013	CLA	C4A-NA-C1A	2.33	109.37	106.36
21	1	6023	BCR	C23-C24-C25	2.33	134.31	127.32
19	B	1208	CLA	CHB-C4A-NA	2.33	127.73	124.51
19	R	1150	CLA	CAA-CBA-CGA	2.33	120.15	113.32
19	1	1012	CLA	CHB-C4A-NA	2.34	127.74	124.51
19	A	1138	CLA	CHB-C4A-NA	2.34	127.75	124.51
19	2	2006	CLA	O2A-CGA-CBA	2.34	119.04	111.90
19	B	1236	CLA	O2A-CGA-CBA	2.35	119.05	111.90
19	A	1113	CLA	CHB-C4A-NA	2.35	127.76	124.51
19	A	1139	CLA	O2A-CGA-CBA	2.35	119.06	111.90
19	B	1221	CLA	CAC-C3C-C4C	2.35	128.24	124.83
19	3	3008	CLA	CHB-C4A-NA	2.35	127.77	124.51
22	G	7026	LMU	O5'-C5'-C4'	2.36	114.73	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1230	CLA	CMB-C2B-C3B	2.36	129.71	125.09
19	3	3014	CLA	C2B-C3B-C4B	2.36	108.35	106.29
22	H	7043	LMU	O5'-C1'-C2'	2.36	115.12	110.28
19	L	1130	CLA	CBA-CAA-C2A	2.36	120.40	113.73
19	B	1211	CLA	CED-O2D-CGD	2.36	121.54	115.99
22	A	7035	LMU	O1'-C1'-C2'	2.37	111.03	108.04
19	2	2006	CLA	CHB-C4A-NA	2.37	127.78	124.51
21	I	6021	BCR	C31-C1-C2	2.37	117.26	108.79
19	B	1301	CLA	CMC-C2C-C1C	2.37	128.69	125.02
22	4	7033	LMU	C2'-C3'-C4'	2.37	114.81	109.60
19	3	3012	CLA	C2B-C3B-C4B	2.37	108.36	106.29
22	4	7019	LMU	O5'-C5'-C4'	2.37	114.76	109.75
19	A	1129	CLA	CHB-C4A-NA	2.37	127.79	124.51
19	4	4006	CLA	O2A-CGA-CBA	2.37	119.13	111.90
19	F	1305	CLA	CHB-C4A-NA	2.37	127.80	124.51
19	A	1117	CLA	CMB-C2B-C3B	2.37	129.73	125.09
19	1	1010	CLA	O2A-CGA-CBA	2.38	122.27	112.36
22	A	7023	LMU	O5B-C5B-C6B	2.38	112.36	106.36
19	A	1120	CLA	CED-O2D-CGD	2.38	121.56	115.99
21	B	6005	BCR	C37-C22-C23	2.38	122.05	118.10
21	B	6017	BCR	C34-C9-C8	2.38	122.05	118.10
22	G	7026	LMU	O1B-C1B-C2B	2.39	113.91	108.10
19	1	1005	CLA	CHB-C4A-NA	2.39	127.81	124.51
19	B	1217	CLA	CHB-C4A-NA	2.39	127.82	124.51
19	B	1203	CLA	CAC-C3C-C4C	2.39	128.30	124.83
19	A	1127	CLA	O2A-CGA-CBA	2.39	119.19	111.90
22	A	7044	LMU	C2'-C3'-C4'	2.39	114.86	109.60
19	B	1214	CLA	CMB-C2B-C3B	2.39	129.77	125.09
19	A	1135	CLA	CHB-C4A-NA	2.40	127.83	124.51
19	B	1224	CLA	CMB-C2B-C3B	2.40	129.78	125.09
19	A	1139	CLA	CHB-C4A-NA	2.40	127.83	124.51
19	A	1106	CLA	O2A-CGA-CBA	2.40	119.22	111.90
19	4	4013	CLA	C3D-C4D-ND	2.40	112.26	110.13
22	K	7047	LMU	O1'-C1'-C2'	2.40	111.07	108.04
22	H	7017	LMU	C1'-C2'-C3'	2.40	114.71	109.97
21	A	6008	BCR	C40-C30-C25	2.40	114.07	110.30
19	F	1302	CLA	CHB-C4A-NA	2.40	127.84	124.51
22	2	7031	LMU	O5B-C5B-C4B	2.40	114.19	109.68
22	A	7023	LMU	C3'-C4'-C5'	2.41	116.28	110.84
19	G	1242	CLA	O2A-CGA-CBA	2.41	119.23	111.90
22	A	7016	LMU	C3'-C4'-C5'	2.41	116.28	110.84
19	4	4010	CLA	C3D-C4D-ND	2.41	112.27	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	4013	CLA	C3D-C2D-C1D	2.41	108.42	106.30
21	B	6017	BCR	C32-C1-C2	2.41	117.41	108.79
19	L	1504	CLA	CMC-C2C-C1C	2.41	128.75	125.02
19	A	9012	CLA	CED-O2D-CGD	2.41	121.64	115.99
19	2	4009	CLA	CMB-C2B-C3B	2.41	129.80	125.09
19	B	1212	CLA	CHB-C4A-NA	2.41	127.85	124.51
19	B	1209	CLA	CAC-C3C-C4C	2.41	128.33	124.83
19	1	1003	CLA	CMC-C2C-C1C	2.41	128.75	125.02
19	A	1129	CLA	CGD-CBD-CAD	2.41	118.81	110.62
19	A	1102	CLA	C4-C3-C5	2.42	119.10	115.41
19	1	1014	CLA	O2A-CGA-CBA	2.42	119.28	111.90
19	3	3011	CLA	CMB-C2B-C3B	2.42	129.82	125.09
19	2	2002	CLA	CHB-C4A-NA	2.42	127.86	124.51
22	4	7033	LMU	C1'-C2'-C3'	2.42	114.75	109.97
22	A	7035	LMU	O1B-C4'-C5'	2.43	115.70	109.32
19	2	4009	CLA	C4-C3-C5	2.43	119.11	115.41
22	K	7042	LMU	O5B-C1B-C2B	2.43	115.26	110.28
21	L	6019	BCR	C33-C5-C4	2.43	118.03	113.43
19	3	3007	CLA	CHB-C4A-NA	2.43	127.88	124.51
22	4	7018	LMU	O5'-C5'-C6'	2.44	112.51	106.36
21	B	6020	BCR	C10-C11-C12	2.44	130.56	123.13
19	I	1204	CLA	CHB-C4A-NA	2.44	127.88	124.51
19	2	2004	CLA	CED-O2D-CGD	2.45	121.72	115.99
19	K	3009	CLA	CHC-C1C-NC	2.45	128.29	123.67
19	2	2004	CLA	O2A-CGA-CBA	2.45	119.37	111.90
22	2	7027	LMU	O5'-C5'-C6'	2.46	112.56	106.36
19	G	1242	CLA	CED-O2D-CGD	2.46	121.76	115.99
19	1	1008	CLA	CMB-C2B-C3B	2.46	129.90	125.09
19	L	1130	CLA	CHB-C4A-NA	2.46	127.91	124.51
22	G	7039	LMU	O1'-C1'-C2'	2.46	111.15	108.04
19	B	1214	CLA	CED-O2D-CGD	2.46	121.76	115.99
19	A	1135	CLA	C4-C3-C5	2.46	118.47	115.68
21	A	6002	BCR	C8-C9-C10	2.46	122.95	118.98
21	I	6018	BCR	C35-C13-C12	2.47	122.20	118.10
19	B	1239	CLA	CAA-CBA-CGA	2.47	120.54	113.32
19	4	4011	CLA	C2B-C3B-C4B	2.47	108.45	106.29
19	B	1238	CLA	CHB-C4A-NA	2.47	127.93	124.51
19	B	1206	CLA	CHB-C4A-NA	2.47	127.93	124.51
19	H	1207	CLA	CMC-C2C-C1C	2.48	128.86	125.02
19	2	2007	CLA	CGD-CBD-CAD	2.48	119.03	110.62
22	E	7037	LMU	O1B-C1B-C2B	2.48	114.14	108.10
19	4	4012	CLA	CMC-C2C-C1C	2.48	128.86	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1122	CLA	CMC-C2C-C1C	2.48	128.86	125.02
19	A	1138	CLA	CED-O2D-CGD	2.48	121.81	115.99
19	1	1011	CLA	CHB-C4A-NA	2.48	127.94	124.51
19	A	1101	CLA	CHB-C4A-NA	2.48	127.95	124.51
22	4	7008	LMU	O1'-C1'-C2'	2.48	111.18	108.04
19	B	1227	CLA	CHB-C4A-NA	2.49	127.95	124.51
19	B	1234	CLA	O2A-CGA-CBA	2.49	119.48	111.90
19	J	1308	CLA	O2A-CGA-CBA	2.49	119.48	111.90
19	A	1125	CLA	CHB-C4A-NA	2.49	127.96	124.51
19	B	1211	CLA	CAC-C3C-C4C	2.49	128.45	124.83
19	B	1228	CLA	CHB-C4A-NA	2.49	127.96	124.51
19	B	1236	CLA	CHB-C4A-NA	2.49	127.96	124.51
22	K	7041	LMU	C1'-O5'-C5'	2.49	118.58	113.75
19	B	1222	CLA	CHB-C4A-NA	2.50	127.96	124.51
19	F	1305	CLA	CHC-C1C-NC	2.50	128.37	123.67
19	A	1140	CLA	CHB-C4A-NA	2.50	127.97	124.51
21	B	6020	BCR	C30-C25-C26	2.50	126.33	122.66
19	A	1116	CLA	CED-O2D-CGD	2.50	121.85	115.99
19	A	1108	CLA	CED-O2D-CGD	2.50	121.85	115.99
22	4	7019	LMU	O5B-C5B-C6B	2.50	112.68	106.36
22	G	7026	LMU	O3'-C3'-C4'	2.50	115.79	109.87
19	B	1216	CLA	O2A-CGA-CBA	2.50	119.53	111.90
19	1	1014	CLA	C4-C3-C5	2.51	119.23	115.41
19	4	4003	CLA	CED-O2D-CGD	2.51	121.87	115.99
19	B	1233	CLA	CHB-C4A-NA	2.51	127.98	124.51
22	K	7042	LMU	O5'-C5'-C6'	2.51	112.69	106.36
21	A	6011	BCR	C39-C30-C25	2.51	114.23	110.30
21	A	6007	BCR	C32-C1-C31	2.51	116.41	108.37
19	A	1137	CLA	CHB-C4A-NA	2.51	127.99	124.51
19	A	1135	CLA	O2A-CGA-CBA	2.52	119.56	111.90
19	B	1216	CLA	CAA-C2A-C1A	2.52	121.35	112.47
19	A	1151	CLA	CHB-C4A-NA	2.52	127.99	124.51
19	B	1210	CLA	O2A-CGA-CBA	2.52	119.57	111.90
19	3	3006	CLA	C2B-C3B-C4B	2.52	108.49	106.29
19	A	1116	CLA	CHB-C4A-NA	2.52	128.00	124.51
19	A	1119	CLA	CED-O2D-CGD	2.52	121.90	115.99
22	H	7032	LMU	O1'-C1'-C2'	2.52	111.23	108.04
22	H	7017	LMU	O1B-C1B-C2B	2.52	114.25	108.10
19	B	1225	CLA	C4A-NA-C1A	2.53	109.62	106.36
19	3	3010	CLA	C3D-C4D-ND	2.53	112.37	110.13
19	A	1106	CLA	CMB-C2B-C3B	2.53	130.03	125.09
19	A	1119	CLA	CHB-C4A-NA	2.53	128.01	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	H	7011	LMU	O5B-C5B-C6B	2.53	112.75	106.36
19	A	1113	CLA	CGD-CBD-CAD	2.54	119.22	110.62
19	2	2002	CLA	CAC-C3C-C4C	2.54	128.51	124.83
19	2	2001	CLA	CHB-C4A-NA	2.54	128.03	124.51
22	2	7027	LMU	O1B-C1B-C2B	2.54	114.29	108.10
22	3	7005	LMU	O5'-C5'-C6'	2.54	112.78	106.36
21	3	6022	BCR	C40-C30-C39	2.54	116.52	108.37
19	2	2007	CLA	CHB-C4A-NA	2.54	128.03	124.51
22	K	7047	LMU	C1'-O5'-C5'	2.55	118.69	113.75
21	B	6005	BCR	C40-C30-C39	2.55	116.53	108.37
19	4	4010	CLA	C3D-C2D-C1D	2.55	108.55	106.30
21	F	6016	BCR	C33-C5-C4	2.55	118.26	113.43
19	B	1233	CLA	O2A-CGA-CBA	2.55	119.67	111.90
21	A	6002	BCR	C1-C6-C7	2.55	122.96	115.82
19	A	9022	CLA	O2A-CGA-CBA	2.55	119.68	111.90
19	4	4007	CLA	CMB-C2B-C3B	2.55	130.08	125.09
21	I	6018	BCR	C8-C9-C10	2.56	123.11	118.98
19	1	1003	CLA	CHB-C4A-NA	2.56	128.05	124.51
19	3	3002	CLA	C3D-C2D-C1D	2.56	108.56	106.30
19	A	1109	CLA	C4-C3-C5	2.57	119.33	115.41
21	I	6021	BCR	C39-C30-C25	2.57	114.33	110.30
23	B	7101	LMG	O8-C28-C29	2.57	119.72	111.90
22	4	7033	LMU	O5B-C5B-C6B	2.57	112.84	106.36
19	2	2011	CLA	C2B-C3B-C4B	2.57	108.53	106.29
19	A	1125	CLA	O2A-CGA-CBA	2.57	119.73	111.90
19	3	1118	CLA	CHB-C4A-NA	2.57	128.07	124.51
19	2	2004	CLA	CHB-C4A-NA	2.57	128.07	124.51
21	L	6019	BCR	C40-C30-C39	2.57	116.61	108.37
22	H	7030	LMU	O5B-C5B-C6B	2.57	112.86	106.36
19	J	1311	CLA	CHB-C4A-NA	2.58	128.07	124.51
19	A	1128	CLA	CED-O2D-CGD	2.58	122.04	115.99
19	A	1111	CLA	CAC-C3C-C4C	2.58	128.58	124.83
19	A	1136	CLA	C4-C3-C5	2.58	119.35	115.41
22	R	7014	LMU	O5'-C1'-O1'	2.58	116.28	110.05
19	A	1136	CLA	CHB-C4A-NA	2.59	128.09	124.51
19	L	1148	CLA	CMA-C3A-C2A	2.59	125.81	114.35
19	K	1143	CLA	CHB-C4A-NA	2.60	128.10	124.51
19	B	1301	CLA	CHB-C4A-NA	2.60	128.10	124.51
19	4	4003	CLA	O2A-CGA-CBA	2.60	119.81	111.90
21	F	6014	BCR	C38-C26-C27	2.60	118.35	113.43
19	B	1214	CLA	CHB-C4A-NA	2.60	128.11	124.51
19	3	1147	CLA	C3B-C4B-NB	2.61	112.58	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1101	CLA	CMB-C2B-C3B	2.61	130.19	125.09
19	B	1224	CLA	C4-C3-C5	2.61	119.39	115.41
19	A	9023	CLA	CED-O2D-CGD	2.61	122.11	115.99
21	3	6022	BCR	C32-C1-C31	2.61	116.74	108.37
19	H	1207	CLA	CHB-C4A-NA	2.61	128.12	124.51
19	L	1148	CLA	CHC-C1C-NC	2.62	128.60	123.67
19	A	1104	CLA	CHB-C4A-NA	2.62	128.13	124.51
19	B	1223	CLA	O2A-CGA-CBA	2.62	119.89	111.90
19	3	3016	CLA	CHB-C4A-NA	2.62	128.14	124.51
19	K	3009	CLA	C4-C3-C5	2.62	119.41	115.41
21	J	6012	BCR	C39-C30-C25	2.63	114.42	110.30
22	C	7015	LMU	C4B-C3B-C2B	2.63	115.70	110.79
19	4	4006	CLA	CED-O2D-CGD	2.63	122.16	115.99
19	1	1010	CLA	CHB-C4A-NA	2.63	128.15	124.51
19	A	1136	CLA	O2A-CGA-CBA	2.63	119.92	111.90
22	K	7001	LMU	O1B-C4'-C5'	2.64	116.25	109.32
19	B	1238	CLA	C4-C3-C5	2.64	119.43	115.41
19	A	1124	CLA	CHB-C4A-NA	2.64	128.16	124.51
19	2	2001	CLA	O2A-CGA-CBA	2.64	119.93	111.90
19	A	1103	CLA	CHB-C4A-NA	2.64	128.16	124.51
19	A	1149	CLA	CAA-C2A-C1A	2.64	121.77	112.47
19	3	3011	CLA	CED-O2D-CGD	2.64	122.18	115.99
19	A	1132	CLA	CAC-C3C-C4C	2.64	128.67	124.83
19	F	1305	CLA	CED-O2D-CGD	2.64	122.19	115.99
19	4	4003	CLA	C4-C3-C5	2.64	119.45	115.41
19	4	1009	CLA	CHB-C4A-NA	2.64	128.17	124.51
21	B	6010	BCR	C33-C5-C4	2.65	118.44	113.43
19	A	1102	CLA	CMB-C2B-C3B	2.65	130.27	125.09
19	B	1220	CLA	CHC-C1C-NC	2.65	128.65	123.67
19	3	3011	CLA	CAC-C3C-C4C	2.65	128.68	124.83
22	A	7035	LMU	O5'-C1'-C2'	2.66	115.72	110.28
19	B	1206	CLA	CGD-CBD-CAD	2.66	119.62	110.62
19	B	1213	CLA	CAC-C3C-C4C	2.66	128.69	124.83
19	L	1502	CLA	CED-O2D-CGD	2.66	122.22	115.99
19	B	1233	CLA	CED-O2D-CGD	2.66	122.23	115.99
19	4	1304	CLA	CED-O2D-CGD	2.66	122.23	115.99
19	K	1146	CLA	CED-O2D-CGD	2.66	122.24	115.99
19	A	1141	CLA	O2A-CGA-CBA	2.67	120.02	111.90
22	2	7027	LMU	C3B-C4B-C5B	2.67	114.85	110.20
21	B	6010	BCR	C32-C1-C31	2.67	116.92	108.37
22	A	7045	LMU	C1'-C2'-C3'	2.67	115.23	109.97
19	A	1123	CLA	CHB-C4A-NA	2.67	128.20	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	9012	CLA	C4-C3-C5	2.67	119.48	115.41
22	B	7040	LMU	C2'-C3'-C4'	2.67	115.47	109.60
19	4	1004	CLA	CAC-C3C-C4C	2.67	128.71	124.83
21	A	6008	BCR	C37-C22-C23	2.67	122.54	118.10
22	4	7009	LMU	O1B-C1B-C2B	2.67	114.61	108.10
19	B	1210	CLA	C4-C3-C5	2.68	119.49	115.41
21	F	6016	BCR	C38-C26-C27	2.68	118.50	113.43
19	A	1120	CLA	CHB-C4A-NA	2.68	128.21	124.51
19	4	4002	CLA	CHB-C4A-NA	2.68	128.22	124.51
19	3	3015	CLA	C3D-C4D-ND	2.68	112.51	110.13
20	A	5001	PQN	C2M-C2-C1	2.68	120.62	116.27
19	B	1206	CLA	O2A-CGA-CBA	2.69	120.08	111.90
19	4	1009	CLA	CMB-C2B-C3B	2.69	130.63	125.14
19	B	1209	CLA	CHB-C4A-NA	2.69	128.23	124.51
22	A	7010	LMU	C4B-C3B-C2B	2.69	115.81	110.79
19	B	1206	CLA	CMB-C2B-C3B	2.69	130.35	125.09
21	A	6008	BCR	C32-C1-C2	2.69	118.42	108.79
19	A	1131	CLA	CHB-C4A-NA	2.69	128.23	124.51
22	2	7027	LMU	C6B-C5B-C4B	2.69	119.66	113.02
22	R	7024	LMU	O5'-C5'-C6'	2.69	113.16	106.36
19	A	1132	CLA	CED-O2D-CGD	2.70	122.31	115.99
19	4	4007	CLA	CHB-C4A-NA	2.70	128.24	124.51
19	A	1134	CLA	CHB-C4A-NA	2.70	128.25	124.51
19	L	1503	CLA	O2A-CGA-CBA	2.70	120.13	111.90
19	A	1138	CLA	O2A-CGA-CBA	2.70	120.13	111.90
19	A	1103	CLA	CED-O2D-CGD	2.70	122.33	115.99
19	4	4002	CLA	CED-O2D-CGD	2.71	122.34	115.99
19	A	9022	CLA	C6-C5-C3	2.71	118.43	112.48
19	A	9022	CLA	CAC-C3C-C4C	2.71	128.77	124.83
22	H	7032	LMU	C3'-C4'-C5'	2.71	116.98	110.84
19	1	1011	CLA	CAC-C3C-C4C	2.72	129.22	125.02
22	B	7012	LMU	C2'-C3'-C4'	2.72	115.57	109.60
19	B	1228	CLA	CED-O2D-CGD	2.72	122.37	115.99
19	4	1004	CLA	C4-C3-C5	2.73	119.57	115.41
21	B	6006	BCR	C40-C30-C39	2.73	117.11	108.37
19	L	1148	CLA	CMB-C2B-C3B	2.73	130.42	125.09
19	A	1309	CLA	C3D-C4D-ND	2.73	112.55	110.13
19	A	1104	CLA	CMB-C2B-C3B	2.73	130.43	125.09
19	A	1108	CLA	CMB-C2B-C3B	2.73	130.43	125.09
19	1	1003	CLA	CHC-C1C-NC	2.74	128.82	123.67
22	4	7019	LMU	O1'-C1'-C2'	2.74	111.50	108.04
19	B	1212	CLA	CMB-C2B-C3B	2.74	130.45	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	6003	BCR	C40-C30-C25	2.74	114.61	110.30
19	3	3008	CLA	CED-O2D-CGD	2.74	122.43	115.99
19	3	3006	CLA	C3D-C4D-ND	2.75	112.57	110.13
19	B	1230	CLA	O2A-CGA-CBA	2.75	120.28	111.90
19	A	1137	CLA	O2A-CGA-CBA	2.75	120.28	111.90
22	R	7022	LMU	O1'-C1'-C2'	2.75	111.52	108.04
19	A	1115	CLA	O2A-CGA-CBA	2.75	120.29	111.90
19	B	1227	CLA	CGD-CBD-CAD	2.76	119.96	110.62
19	A	1102	CLA	CBA-CAA-C2A	2.76	121.51	113.73
19	H	1145	CLA	CGD-CBD-CAD	2.76	119.98	110.62
22	A	7035	LMU	O3'-C3'-C4'	2.76	116.41	109.87
19	1	1001	CLA	CED-O2D-CGD	2.76	122.46	115.99
19	2	2003	CLA	C3D-C2D-C1D	2.76	108.74	106.30
19	1	1008	CLA	O2A-CGA-CBA	2.77	120.33	111.90
19	L	1503	CLA	CHC-C1C-NC	2.77	128.88	123.67
19	3	3002	CLA	C3D-C4D-ND	2.77	112.59	110.13
22	3	7003	LMU	O2B-C2B-C3B	2.77	116.57	110.34
22	2	7046	LMU	O1B-C4'-C3'	2.77	114.32	107.17
19	L	1502	CLA	O2A-CGA-CBA	2.77	120.35	111.90
21	J	6012	BCR	C40-C30-C25	2.77	114.65	110.30
22	A	7044	LMU	C1B-O5B-C5B	2.78	119.13	113.75
19	A	9013	CLA	O2A-CGA-CBA	2.78	120.36	111.90
19	3	3004	CLA	C3D-C2D-C1D	2.78	108.75	106.30
19	4	4002	CLA	CGD-CBD-CAD	2.78	120.04	110.62
19	J	1311	CLA	CED-O2D-CGD	2.78	122.51	115.99
19	B	1217	CLA	O2A-CGA-CBA	2.78	120.38	111.90
19	B	1215	CLA	CHB-C4A-NA	2.78	128.36	124.51
19	A	1132	CLA	CHB-C4A-NA	2.78	128.36	124.51
21	A	6011	BCR	C33-C5-C4	2.79	118.71	113.43
19	B	1213	CLA	CHB-C4A-NA	2.79	128.37	124.51
19	A	1104	CLA	CED-O2D-CGD	2.79	122.53	115.99
19	A	1119	CLA	C4-C3-C5	2.79	119.67	115.41
19	H	1207	CLA	O2A-CGA-CBA	2.79	120.40	111.90
19	3	3004	CLA	C3D-C4D-ND	2.79	112.61	110.13
22	R	7025	LMU	O5'-C5'-C4'	2.79	115.64	109.75
19	A	1132	CLA	O2A-CGA-CBA	2.79	120.41	111.90
21	F	6014	BCR	C33-C5-C4	2.79	118.73	113.43
22	4	7019	LMU	C1B-C2B-C3B	2.80	115.48	109.97
19	1	1013	CLA	CHB-C4A-NA	2.80	128.38	124.51
19	2	2007	CLA	O2A-CGA-CBA	2.80	120.42	111.90
19	2	2014	CLA	CAC-C3C-C4C	2.80	128.89	124.83
19	1	1003	CLA	O2A-CGA-CBA	2.80	120.44	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1110	CLA	O2A-CGA-CBA	2.80	120.44	111.90
21	B	6010	BCR	C40-C30-C39	2.80	117.36	108.37
19	R	1150	CLA	CED-O2D-CGD	2.80	122.57	115.99
19	B	1228	CLA	O2A-CGA-CBA	2.81	120.46	111.90
19	A	1103	CLA	CAC-C3C-C4C	2.81	128.91	124.83
21	A	6003	BCR	C38-C26-C27	2.81	118.76	113.43
22	R	7020	LMU	O5B-C1B-C2B	2.82	116.05	110.28
22	E	7037	LMU	O5'-C5'-C6'	2.82	113.48	106.36
21	B	6005	BCR	C32-C1-C2	2.82	118.89	108.79
19	A	1101	CLA	O2A-CGA-CBA	2.83	120.51	111.90
22	3	7005	LMU	O5B-C5B-C6B	2.83	113.50	106.36
19	A	1124	CLA	O2A-CGA-CBA	2.83	120.52	111.90
19	A	1109	CLA	CHB-C4A-NA	2.83	128.43	124.51
19	A	9011	CLA	O2A-CGA-CBA	2.83	120.53	111.90
22	H	7011	LMU	O1'-C1'-C2'	2.83	111.62	108.04
19	A	9011	CLA	CMC-C2C-C1C	2.84	129.41	125.02
21	B	6017	BCR	C38-C26-C27	2.84	118.81	113.43
19	B	1209	CLA	C5-C3-C2	2.84	126.43	121.05
19	A	1122	CLA	CHB-C4A-NA	2.84	128.44	124.51
19	A	1127	CLA	CHB-C4A-NA	2.84	128.44	124.51
19	A	9011	CLA	CHC-C1C-NC	2.84	129.02	123.67
19	B	1222	CLA	O2A-CGA-CBA	2.84	120.57	111.90
19	4	1306	CLA	O2A-CGA-CBA	2.85	120.57	111.90
19	3	3013	CLA	O2A-CGA-CBA	2.85	120.57	111.90
21	I	6018	BCR	C31-C1-C2	2.85	118.98	108.79
21	I	6021	BCR	C32-C1-C31	2.85	117.50	108.37
21	B	6017	BCR	C36-C18-C19	2.85	122.84	118.10
19	2	2014	CLA	CMB-C2B-C3B	2.85	130.66	125.09
22	4	7053	LMU	C1'-C2'-C3'	2.85	115.59	109.97
19	3	3016	CLA	O2A-CGA-CBA	2.85	120.60	111.90
22	3	7003	LMU	O1'-C1'-C2'	2.86	111.65	108.04
22	R	7020	LMU	C1B-C2B-C3B	2.86	115.60	109.97
19	2	2011	CLA	C3D-C2D-C1D	2.86	108.82	106.30
22	H	7043	LMU	C1'-O5'-C5'	2.86	119.30	113.75
19	F	1305	CLA	O2A-CGA-CBA	2.87	120.64	111.90
19	2	2008	CLA	C3D-C2D-C1D	2.87	108.83	106.30
22	R	7022	LMU	O1B-C1B-C2B	2.87	115.08	108.10
19	A	1109	CLA	CMB-C2B-C1B	2.87	133.11	128.36
22	E	7037	LMU	O4'-C4B-C5B	2.87	116.84	109.24
19	3	3005	CLA	C3D-C4D-ND	2.87	112.68	110.13
19	4	1004	CLA	O2A-CGA-CBA	2.88	120.66	111.90
21	A	6008	BCR	C38-C26-C27	2.88	118.88	113.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1122	CLA	CAC-C3C-C4C	2.88	129.01	124.83
19	B	1231	CLA	CHC-C1C-NC	2.88	129.09	123.67
19	1	1006	CLA	CHB-C4A-NA	2.88	128.50	124.51
19	B	1224	CLA	CHB-C4A-NA	2.88	128.50	124.51
19	4	1004	CLA	CHB-C4A-NA	2.89	128.50	124.51
22	H	7043	LMU	C1'-C2'-C3'	2.89	115.66	109.97
19	A	1133	CLA	CHB-C4A-NA	2.89	128.51	124.51
19	A	1103	CLA	C4-C3-C5	2.89	119.82	115.41
19	L	1504	CLA	O2A-CGA-CBA	2.89	120.70	111.90
19	A	1120	CLA	O2A-CGA-CBA	2.89	120.71	111.90
19	3	3011	CLA	C4-C3-C5	2.89	119.83	115.41
19	G	1242	CLA	CHB-C4A-NA	2.89	128.51	124.51
19	L	1504	CLA	CHC-C1C-NC	2.90	129.12	123.67
22	H	7017	LMU	O5'-C1'-C2'	2.90	116.22	110.28
19	K	1143	CLA	O2A-CGA-CBA	2.90	120.73	111.90
21	A	6002	BCR	C32-C1-C31	2.90	117.66	108.37
21	F	6016	BCR	C31-C1-C2	2.91	119.19	108.79
22	4	7053	LMU	O1'-C1'-C2'	2.91	111.71	108.04
19	3	3006	CLA	C3D-C2D-C1D	2.91	108.87	106.30
21	J	6012	BCR	C38-C26-C27	2.91	118.95	113.43
19	B	1211	CLA	CHB-C4A-NA	2.92	128.54	124.51
19	1	1002	CLA	CHB-C4A-NA	2.92	128.54	124.51
19	3	3017	CLA	CAC-C3C-C4C	2.92	129.07	124.83
19	A	9023	CLA	O2A-CGA-CBA	2.92	120.80	111.90
19	B	1202	CLA	C4-C3-C5	2.92	119.87	115.41
19	B	1231	CLA	CED-O2D-CGD	2.93	122.86	115.99
19	4	4006	CLA	CHC-C1C-NC	2.93	129.18	123.67
22	B	7038	LMU	O1B-C1B-C2B	2.93	115.23	108.10
19	B	1301	CLA	CHC-C1C-NC	2.93	129.19	123.67
22	F	7036	LMU	O2'-C2'-C1'	2.93	116.45	110.02
19	B	1239	CLA	CHB-C4A-NA	2.93	128.57	124.51
19	A	1140	CLA	O2A-CGA-CBA	2.93	120.84	111.90
19	A	1149	CLA	CGD-CBD-CAD	2.94	120.57	110.62
19	A	9013	CLA	CHC-C1C-NC	2.94	129.20	123.67
21	A	6008	BCR	C33-C5-C4	2.94	119.00	113.43
19	B	1229	CLA	CHB-C4A-NA	2.94	128.57	124.51
19	A	1103	CLA	O2A-CGA-CBA	2.94	120.85	111.90
19	B	1219	CLA	CED-O2D-CGD	2.94	122.89	115.99
19	A	1141	CLA	CHB-C4A-NA	2.94	128.58	124.51
21	B	6004	BCR	C39-C30-C25	2.95	114.93	110.30
19	B	1238	CLA	CMB-C2B-C3B	2.95	130.86	125.09
19	K	3009	CLA	O2A-CGA-CBA	2.95	120.89	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1151	CLA	CAC-C3C-C4C	2.95	129.12	124.83
22	4	7019	LMU	C1'-C2'-C3'	2.96	115.80	109.97
19	R	1144	CLA	CED-O2D-CGD	2.96	122.92	115.99
22	B	7040	LMU	C1'-C2'-C3'	2.96	115.81	109.97
21	B	6020	BCR	C39-C30-C25	2.96	114.94	110.30
21	3	6022	BCR	C38-C26-C27	2.97	119.06	113.43
22	R	7007	LMU	O1'-C1'-C2'	2.97	111.79	108.04
21	F	6014	BCR	C39-C30-C25	2.98	114.97	110.30
19	B	1201	CLA	CHB-C4A-NA	2.98	128.63	124.51
21	I	6018	BCR	C33-C5-C4	2.98	119.08	113.43
19	J	1311	CLA	O2A-CGA-CBA	2.98	120.98	111.90
19	B	1206	CLA	C4-C3-C5	2.98	119.96	115.41
19	4	4005	CLA	C3D-C4D-ND	2.99	112.78	110.13
21	1	6023	BCR	C31-C1-C2	2.99	119.49	108.79
22	B	7012	LMU	O5B-C5B-C4B	2.99	115.29	109.68
21	A	6011	BCR	C40-C30-C39	2.99	117.95	108.37
19	G	1242	CLA	CHC-C1C-NC	2.99	129.30	123.67
19	B	1235	CLA	O2A-CGA-CBA	2.99	121.02	111.90
21	A	6002	BCR	C38-C26-C27	2.99	119.10	113.43
20	B	5002	PQN	C2M-C2-C1	3.00	121.14	116.27
22	4	7033	LMU	C4B-C3B-C2B	3.01	116.41	110.79
19	A	1104	CLA	O2A-CGA-CBA	3.01	121.07	111.90
19	J	1311	CLA	C4-C3-C5	3.01	120.00	115.41
21	1	6023	BCR	C30-C25-C24	3.01	124.25	115.82
22	3	7005	LMU	O1B-C1B-C2B	3.01	115.43	108.10
19	4	4015	CLA	CHB-C4A-NA	3.01	128.68	124.51
19	A	1149	CLA	CAC-C3C-C4C	3.02	129.21	124.83
19	A	1309	CLA	C3D-C2D-C1D	3.02	108.96	106.30
22	R	7014	LMU	O5B-C5B-C6B	3.02	113.99	106.36
22	B	7040	LMU	O1'-C1'-C2'	3.02	111.86	108.04
19	B	1216	CLA	CHC-C1C-NC	3.02	129.36	123.67
19	2	2011	CLA	C3D-C4D-ND	3.02	112.81	110.13
19	A	1133	CLA	O2A-CGA-CBA	3.03	121.12	111.90
19	L	1148	CLA	CHB-C4A-NA	3.03	128.70	124.51
19	B	1214	CLA	O2A-CGA-CBA	3.03	121.13	111.90
19	H	1241	CLA	O2A-CGA-CBA	3.03	121.13	111.90
21	A	6011	BCR	C36-C18-C19	3.03	123.14	118.10
19	B	1233	CLA	CHC-C1C-NC	3.03	129.37	123.67
19	2	2014	CLA	O2A-CGA-CBA	3.04	121.15	111.90
19	H	1207	CLA	CMB-C2B-C3B	3.04	131.03	125.09
19	B	1212	CLA	CED-O2D-CGD	3.04	123.12	115.99
19	H	1241	CLA	CED-O2D-CGD	3.04	123.12	115.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	R	7022	LMU	O1B-C4'-C3'	3.04	115.02	107.17
19	2	4009	CLA	O2A-CGA-CBA	3.04	121.17	111.90
21	I	6021	BCR	C30-C25-C24	3.05	124.35	115.82
19	2	2013	CLA	CAA-C2A-C1A	3.05	123.22	112.47
19	L	1130	CLA	O2A-CGA-CBA	3.05	121.19	111.90
19	4	4015	CLA	CHC-C1C-NC	3.05	129.41	123.67
19	B	1239	CLA	C4-C3-C5	3.05	120.07	115.41
19	B	1212	CLA	CHC-C1C-NC	3.06	129.42	123.67
21	B	6004	BCR	C38-C26-C27	3.06	119.22	113.43
19	1	1007	CLA	O2A-CGA-CBA	3.06	121.22	111.90
19	A	1120	CLA	CHC-C1C-NC	3.06	129.43	123.67
19	A	1110	CLA	CHB-C4A-NA	3.06	128.74	124.51
19	A	1105	CLA	CHC-C1C-NC	3.06	129.44	123.67
22	R	7022	LMU	C1-O1'-C1'	3.07	119.31	113.94
21	B	6005	BCR	C39-C30-C25	3.08	115.13	110.30
19	B	1227	CLA	CED-O2D-CGD	3.09	123.23	115.99
22	K	7047	LMU	O1B-C4'-C5'	3.09	117.44	109.32
22	A	7044	LMU	O5'-C5'-C4'	3.09	116.27	109.75
22	B	7038	LMU	O5'-C1'-C2'	3.09	116.62	110.28
22	E	7037	LMU	O1B-C1B-O5B	3.10	118.52	110.68
19	B	1239	CLA	O2D-CGD-CBD	3.10	115.55	111.30
19	1	1002	CLA	CMB-C2B-C3B	3.10	131.15	125.09
22	E	7048	LMU	O1B-C1B-C2B	3.10	115.66	108.10
22	H	7017	LMU	C3B-C4B-C5B	3.11	115.62	110.20
22	R	7024	LMU	C1'-C2'-C3'	3.11	116.10	109.97
19	4	4004	CLA	C3D-C2D-C1D	3.11	109.04	106.30
22	K	7041	LMU	O1B-C1B-C2B	3.11	115.68	108.10
22	4	7053	LMU	O1B-C4'-C5'	3.12	117.52	109.32
19	A	9011	CLA	CHB-C4A-NA	3.12	128.82	124.51
19	A	1237	CLA	CHC-C1C-NC	3.12	129.54	123.67
19	A	9013	CLA	CHB-C4A-NA	3.13	128.84	124.51
19	B	1222	CLA	C4-C3-C5	3.13	120.18	115.41
22	3	7005	LMU	O3'-C3'-C4'	3.13	117.28	109.87
19	A	1126	CLA	CHB-C4A-NA	3.13	128.85	124.51
21	A	6002	BCR	C33-C5-C4	3.14	119.37	113.43
19	A	1122	CLA	C4-C3-C5	3.14	120.20	115.41
22	E	7037	LMU	O5B-C5B-C6B	3.14	114.29	106.36
19	B	9010	CLA	CHB-C4A-NA	3.14	128.86	124.51
22	A	7044	LMU	C3B-C4B-C5B	3.15	115.68	110.20
19	I	1204	CLA	CHC-C1C-NC	3.15	129.59	123.67
19	B	9010	CLA	O2A-CGA-CBA	3.15	121.49	111.90
19	3	3010	CLA	C3D-C2D-C1D	3.15	109.07	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	J	1308	CLA	CED-O2D-CGD	3.15	123.38	115.99
19	B	1212	CLA	O2A-CGA-CBA	3.15	121.50	111.90
19	H	1207	CLA	CHC-C1C-NC	3.15	129.60	123.67
19	H	1145	CLA	C4-C3-C5	3.15	120.22	115.41
21	B	6010	BCR	C36-C18-C19	3.16	123.35	118.10
19	A	1126	CLA	CHC-C1C-NC	3.16	129.61	123.67
19	B	1229	CLA	C4-C3-C5	3.16	120.23	115.41
19	H	1505	CLA	O2A-CGA-CBA	3.16	121.53	111.90
19	1	1005	CLA	CHC-C1C-NC	3.16	129.62	123.67
19	2	2013	CLA	O2A-CGA-CBA	3.16	121.54	111.90
19	3	1118	CLA	CHC-C1C-NC	3.17	129.63	123.67
22	H	7011	LMU	O1B-C4'-C3'	3.17	115.35	107.17
19	A	1115	CLA	CHC-C1C-NC	3.17	129.64	123.67
19	H	1145	CLA	CAA-C2A-C1A	3.17	123.66	112.47
19	A	1131	CLA	O2A-CGA-CBA	3.17	121.56	111.90
22	N	7049	LMU	O1'-C1'-C2'	3.17	112.05	108.04
19	1	1310	CLA	C3D-C2D-C1D	3.17	109.10	106.30
19	B	1221	CLA	CHC-C1C-NC	3.18	129.65	123.67
19	A	1123	CLA	O2A-CGA-CBA	3.18	121.58	111.90
19	B	1206	CLA	O2D-CGD-CBD	3.18	115.66	111.30
22	H	7017	LMU	O5B-C5B-C6B	3.18	114.39	106.36
22	3	7005	LMU	O1B-C4'-C3'	3.18	115.38	107.17
22	4	7018	LMU	C1B-O5B-C5B	3.18	119.92	113.75
19	4	1306	CLA	C4-C3-C5	3.18	120.27	115.41
19	F	1302	CLA	CHC-C1C-NC	3.18	129.66	123.67
19	B	1228	CLA	CHC-C1C-NC	3.19	129.66	123.67
22	H	7002	LMU	O5'-C5'-C6'	3.19	114.41	106.36
19	4	4001	CLA	CHC-C1C-NC	3.19	129.67	123.67
22	3	7003	LMU	O4'-C4B-C3B	3.19	117.53	110.34
22	3	7005	LMU	O2'-C2'-C1'	3.20	117.03	110.02
19	A	1138	CLA	C4-C3-C5	3.20	120.30	115.41
19	2	2012	CLA	CHB-C4A-NA	3.20	128.94	124.51
22	A	7016	LMU	C1B-C2B-C3B	3.20	116.29	109.97
19	H	1505	CLA	CED-O2D-CGD	3.20	123.51	115.99
19	J	1308	CLA	C4-C3-C5	3.21	120.30	115.41
19	A	1141	CLA	C4-C3-C5	3.21	120.30	115.41
19	2	1307	CLA	CHC-C1C-NC	3.21	129.51	123.78
19	B	1231	CLA	CHB-C4A-NA	3.21	128.95	124.51
22	K	7001	LMU	O5B-C5B-C6B	3.21	114.47	106.36
19	A	1122	CLA	CHC-C1C-NC	3.21	129.72	123.67
19	B	1224	CLA	CHC-C1C-NC	3.22	129.73	123.67
19	A	1117	CLA	O2A-CGA-CBA	3.22	121.71	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1106	CLA	CHC-C1C-NC	3.22	129.73	123.67
19	4	4012	CLA	CAC-C3C-C4C	3.22	130.00	125.02
19	A	1106	CLA	CHB-C4A-NA	3.22	128.97	124.51
19	H	1145	CLA	O2A-CGA-CBA	3.22	121.72	111.90
19	1	1303	CLA	O2A-CGA-CBA	3.22	121.72	111.90
19	A	1149	CLA	CED-O2D-CGD	3.23	123.55	115.99
22	2	7027	LMU	C1'-C2'-C3'	3.23	116.33	109.97
21	B	6006	BCR	C38-C26-C27	3.23	119.55	113.43
19	R	1150	CLA	CHC-C1C-NC	3.23	129.75	123.67
19	2	2013	CLA	CHC-C1C-NC	3.23	129.75	123.67
19	4	1306	CLA	CHB-C4A-NA	3.24	128.99	124.51
21	I	6021	BCR	C10-C11-C12	3.24	133.01	123.13
22	A	7010	LMU	C2'-C3'-C4'	3.24	116.72	109.60
19	1	1007	CLA	C4-C3-C5	3.24	120.36	115.41
19	4	4014	CLA	O2A-CGA-CBA	3.24	121.78	111.90
19	4	1009	CLA	CHC-C1C-NC	3.25	129.78	123.67
19	A	1110	CLA	CHC-C1C-NC	3.25	129.78	123.67
19	2	2002	CLA	C4-C3-C5	3.25	120.37	115.41
19	B	1208	CLA	O2A-CGA-CBA	3.25	121.80	111.90
19	B	1239	CLA	CHC-C1C-NC	3.25	129.79	123.67
19	1	1008	CLA	CAA-CBA-CGA	3.25	122.84	113.32
19	L	1501	CLA	CHC-C1C-NC	3.26	129.80	123.67
22	2	7027	LMU	C1'-O5'-C5'	3.26	120.07	113.75
22	A	7010	LMU	O5'-C5'-C6'	3.26	114.59	106.36
22	3	7005	LMU	C1'-O5'-C5'	3.26	120.07	113.75
22	1	7004	LMU	O1'-C1'-C2'	3.26	112.16	108.04
19	3	3001	CLA	C3D-C4D-ND	3.26	113.03	110.13
19	R	1144	CLA	CHC-C1C-NC	3.27	129.82	123.67
19	B	1217	CLA	CHC-C1C-NC	3.27	129.82	123.67
22	R	7021	LMU	O1'-C1'-C2'	3.27	112.17	108.04
19	B	1229	CLA	CHC-C1C-NC	3.27	129.82	123.67
22	4	7033	LMU	O5'-C1'-C2'	3.27	116.98	110.28
19	B	1216	CLA	C4-C3-C5	3.27	120.40	115.41
19	1	1015	CLA	C3D-C2D-C1D	3.27	109.18	106.30
19	B	1220	CLA	CBA-CAA-C2A	3.28	122.98	113.73
19	4	4012	CLA	CHB-C4A-NA	3.28	129.05	124.51
19	B	1223	CLA	C4-C3-C5	3.28	120.42	115.41
19	A	1133	CLA	CHC-C1C-NC	3.28	129.85	123.67
22	A	7045	LMU	C2'-C3'-C4'	3.28	116.81	109.60
19	A	1107	CLA	CAC-C3C-C4C	3.28	129.60	124.83
21	I	6018	BCR	C39-C30-C25	3.29	115.45	110.30
21	A	6003	BCR	C33-C5-C4	3.29	119.66	113.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1010	CLA	C3A-C2A-C1A	3.29	107.07	101.50
19	2	2013	CLA	CHB-C4A-NA	3.29	129.07	124.51
19	B	1221	CLA	CHB-C4A-NA	3.30	129.07	124.51
22	R	7024	LMU	C2'-C3'-C4'	3.31	116.86	109.60
22	B	7038	LMU	O1B-C4'-C3'	3.31	115.71	107.17
19	F	1240	CLA	CHB-C4A-NA	3.31	129.09	124.51
19	1	1001	CLA	C4A-NA-C1A	3.31	110.64	106.36
19	B	1230	CLA	CED-O2D-CGD	3.31	123.76	115.99
22	A	7023	LMU	O1'-C1'-C2'	3.31	112.22	108.04
19	B	1218	CLA	CHC-C1C-NC	3.32	129.91	123.67
19	B	1225	CLA	CHC-C1C-NC	3.32	129.91	123.67
19	B	1234	CLA	CHC-C1C-NC	3.32	129.91	123.67
19	4	4014	CLA	CHC-C1C-NC	3.32	129.92	123.67
19	B	1232	CLA	CHC-C1C-NC	3.32	129.93	123.67
19	A	9012	CLA	CAA-C2A-C1A	3.33	124.20	112.47
19	4	1304	CLA	O2A-CGA-CBA	3.33	122.04	111.90
21	I	6018	BCR	C15-C14-C13	3.33	132.01	127.20
19	1	1014	CLA	CHC-C1C-NC	3.33	129.94	123.67
19	A	1123	CLA	CHC-C1C-NC	3.34	129.95	123.67
19	A	1149	CLA	CBA-CAA-C2A	3.34	123.15	113.73
19	A	1139	CLA	C4-C3-C5	3.34	119.46	115.68
19	A	9012	CLA	CHB-C4A-NA	3.34	129.13	124.51
21	L	6019	BCR	C36-C18-C19	3.34	123.66	118.10
19	2	2014	CLA	CHB-C4A-NA	3.34	129.13	124.51
21	A	6003	BCR	C39-C30-C25	3.34	115.54	110.30
22	B	7012	LMU	C3B-C4B-C5B	3.35	116.03	110.20
19	1	1007	CLA	CHC-C1C-NC	3.35	129.97	123.67
19	B	1206	CLA	CHC-C1C-NC	3.35	129.97	123.67
19	A	1101	CLA	CHC-C1C-NC	3.35	129.98	123.67
22	2	7027	LMU	C2'-C3'-C4'	3.35	116.96	109.60
19	K	1142	CLA	CHC-C1C-NC	3.36	129.99	123.67
19	2	2002	CLA	O2A-CGA-CBA	3.36	122.13	111.90
19	4	4011	CLA	C3D-C4D-ND	3.36	113.11	110.13
19	2	2012	CLA	CAC-C3C-C4C	3.36	129.71	124.83
19	I	1204	CLA	O2A-CGA-CBA	3.36	122.15	111.90
19	4	4012	CLA	CHC-C1C-NC	3.37	130.01	123.67
21	A	6007	BCR	C38-C26-C27	3.37	119.81	113.43
19	1	1001	CLA	CAC-C3C-C4C	3.37	129.73	124.83
19	A	1115	CLA	CHB-C4A-NA	3.37	129.18	124.51
19	L	1130	CLA	CHC-C1C-NC	3.38	130.02	123.67
22	G	7051	LMU	C1B-O1B-C4'	3.38	126.83	118.01
19	2	2004	CLA	CHC-C1C-NC	3.38	130.02	123.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1208	CLA	CHC-C1C-NC	3.38	130.03	123.67
19	4	4004	CLA	C3D-C4D-ND	3.38	113.13	110.13
19	1	1008	CLA	CHC-C1C-NC	3.39	130.04	123.67
19	2	4009	CLA	CHC-C1C-NC	3.39	130.05	123.67
19	B	1202	CLA	O2A-CGA-CBA	3.39	122.23	111.90
22	A	7045	LMU	C1B-O5B-C5B	3.39	120.33	113.75
22	R	7024	LMU	C1B-O5B-C5B	3.39	120.33	113.75
19	A	1111	CLA	CHB-C4A-NA	3.39	129.21	124.51
19	4	4014	CLA	CHB-C4A-NA	3.39	129.21	124.51
19	A	1125	CLA	CHC-C1C-NC	3.39	130.06	123.67
19	H	1241	CLA	CHB-C4A-NA	3.40	129.21	124.51
22	B	7038	LMU	O5B-C5B-C4B	3.40	116.06	109.68
19	A	1113	CLA	O2A-CGA-CBA	3.40	122.25	111.90
19	1	1012	CLA	CHC-C1C-NC	3.40	130.07	123.67
19	B	1227	CLA	CHC-C1C-NC	3.40	130.07	123.67
19	K	3009	CLA	CMC-C2C-C1C	3.40	130.29	125.02
19	A	1126	CLA	O2A-CGA-CBA	3.41	122.29	111.90
19	B	1203	CLA	O2A-CGA-CBA	3.41	122.29	111.90
19	A	9011	CLA	CED-O2D-CGD	3.41	123.99	115.99
22	4	7009	LMU	C2'-C3'-C4'	3.41	117.09	109.60
21	A	6007	BCR	C40-C30-C25	3.41	115.65	110.30
22	A	7044	LMU	C3'-C4'-C5'	3.41	118.56	110.84
19	3	1147	CLA	CHC-C1C-NC	3.41	130.10	123.67
19	3	2009	CLA	C4-C3-C5	3.42	120.62	115.41
19	4	4011	CLA	CHC-C1C-NC	3.42	129.89	123.78
19	B	1205	CLA	CHB-C4A-NA	3.42	129.24	124.51
21	F	6014	BCR	C23-C22-C21	3.42	124.49	118.98
19	H	1505	CLA	CHC-C1C-NC	3.42	130.11	123.67
19	1	1007	CLA	CAC-C3C-C4C	3.43	129.81	124.83
22	H	7043	LMU	O1B-C4'-C3'	3.43	116.02	107.17
21	F	6016	BCR	C34-C9-C8	3.43	123.81	118.10
19	J	1311	CLA	CHC-C1C-NC	3.44	130.14	123.67
19	A	1107	CLA	O2A-CGA-CBA	3.44	122.39	111.90
19	1	1015	CLA	C3D-C4D-ND	3.44	113.19	110.13
19	2	2014	CLA	CHC-C1C-NC	3.45	130.16	123.67
19	A	9012	CLA	CHC-C1C-NC	3.46	130.18	123.67
19	A	1135	CLA	CHC-C1C-NC	3.46	130.18	123.67
19	B	1223	CLA	CHC-C1C-NC	3.46	130.18	123.67
19	A	1104	CLA	CHC-C1C-NC	3.46	130.18	123.67
19	A	1117	CLA	C4-C3-C5	3.46	120.69	115.41
21	B	6020	BCR	C37-C22-C23	3.46	123.86	118.10
19	2	2006	CLA	CED-O2D-CGD	3.47	124.12	115.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1221	CLA	O2A-CGA-CBA	3.47	122.46	111.90
19	L	1130	CLA	CMB-C2B-C3B	3.47	131.87	125.09
19	A	1112	CLA	CHC-C1C-NC	3.47	130.20	123.67
19	3	3016	CLA	C4-C3-C5	3.47	120.70	115.41
19	H	1241	CLA	C4-C3-C5	3.47	120.71	115.41
19	4	4013	CLA	CHC-C1C-NC	3.47	129.99	123.78
19	A	1140	CLA	CHC-C1C-NC	3.47	130.21	123.67
19	B	1205	CLA	O2A-CGA-CBA	3.48	122.50	111.90
19	3	3001	CLA	CHC-C1C-NC	3.48	130.00	123.78
22	H	7002	LMU	O1'-C1'-C2'	3.48	112.44	108.04
19	F	1240	CLA	CMB-C2B-C3B	3.48	132.26	125.14
19	R	1144	CLA	C4-C3-C5	3.49	120.73	115.41
19	A	1131	CLA	CHC-C1C-NC	3.49	130.23	123.67
19	B	1215	CLA	O2A-CGA-CBA	3.49	122.53	111.90
19	J	1308	CLA	CHB-C4A-NA	3.49	129.34	124.51
19	2	2011	CLA	CHC-C1C-NC	3.49	130.02	123.78
19	K	1146	CLA	CHB-C4A-NA	3.49	129.34	124.51
19	F	1305	CLA	C4-C3-C5	3.49	120.74	115.41
19	2	2014	CLA	C4-C3-C5	3.50	120.75	115.41
19	2	2012	CLA	CHC-C1C-NC	3.50	130.25	123.67
19	L	1148	CLA	CBA-CAA-C2A	3.50	123.60	113.73
19	A	1116	CLA	CHC-C1C-NC	3.50	130.25	123.67
19	3	3003	CLA	CHC-C1C-NC	3.50	130.26	123.67
19	2	2006	CLA	C4-C3-C5	3.50	120.76	115.41
19	B	1230	CLA	CHC-C1C-NC	3.50	130.26	123.67
19	A	9022	CLA	CHC-C1C-NC	3.50	130.26	123.67
19	A	1107	CLA	C4-C3-C5	3.50	120.76	115.41
19	3	3005	CLA	C3D-C2D-C1D	3.51	109.39	106.30
19	2	2002	CLA	CHC-C1C-NC	3.51	130.27	123.67
22	4	7053	LMU	O1B-C1B-C2B	3.51	116.64	108.10
19	3	3008	CLA	CHC-C1C-NC	3.51	130.27	123.67
19	B	1213	CLA	CHC-C1C-NC	3.51	130.27	123.67
19	A	1141	CLA	CHC-C1C-NC	3.51	130.28	123.67
22	R	7024	LMU	O1'-C1'-C2'	3.51	112.48	108.04
21	B	6004	BCR	C40-C30-C25	3.52	115.81	110.30
19	B	1225	CLA	CHB-C4A-NA	3.52	129.37	124.51
21	B	6020	BCR	C1-C6-C7	3.52	125.67	115.82
19	1	1013	CLA	O2D-CGD-CBD	3.52	116.13	111.30
22	G	7051	LMU	O5'-C5'-C6'	3.52	115.26	106.36
22	4	7052	LMU	C6'-C5'-C4'	3.52	123.50	113.25
22	H	7043	LMU	O5B-C1B-C2B	3.53	117.51	110.28
22	H	7011	LMU	C3'-C4'-C5'	3.53	118.81	110.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	L	6019	BCR	C38-C26-C27	3.53	120.12	113.43
19	1	1005	CLA	CED-O2D-CGD	3.54	124.29	115.99
19	1	1010	CLA	CHC-C1C-NC	3.54	130.33	123.67
22	H	7043	LMU	C1B-C2B-C3B	3.54	116.95	109.97
22	R	7025	LMU	C1'-O5'-C5'	3.54	120.62	113.75
19	B	1219	CLA	CHC-C1C-NC	3.54	130.34	123.67
19	4	4003	CLA	CHC-C1C-NC	3.54	130.34	123.67
19	B	1222	CLA	CHC-C1C-NC	3.55	130.34	123.67
22	H	7032	LMU	C2'-C3'-C4'	3.55	117.39	109.60
19	J	1308	CLA	CHC-C1C-NC	3.55	130.35	123.67
19	B	1212	CLA	C4-C3-C5	3.55	120.83	115.41
19	A	1128	CLA	CHC-C1C-NC	3.55	130.35	123.67
19	A	1137	CLA	CHC-C1C-NC	3.55	130.36	123.67
21	A	6011	BCR	C38-C26-C27	3.56	120.17	113.43
19	2	2003	CLA	C3D-C4D-ND	3.56	113.29	110.13
19	B	1211	CLA	CHC-C1C-NC	3.56	130.37	123.67
19	3	3013	CLA	CHC-C1C-NC	3.57	130.39	123.67
19	A	1121	CLA	CHC-C1C-NC	3.57	130.39	123.67
19	H	1241	CLA	CHC-C1C-NC	3.58	130.40	123.67
19	3	3011	CLA	CHC-C1C-NC	3.58	130.41	123.67
19	L	1501	CLA	CED-O2D-CGD	3.58	124.39	115.99
19	3	2009	CLA	CHC-C1C-NC	3.59	130.42	123.67
19	A	1124	CLA	CHC-C1C-NC	3.59	130.43	123.67
19	B	1225	CLA	O2A-CGA-CBA	3.59	122.85	111.90
19	A	9012	CLA	O2A-CGA-CBA	3.59	122.85	111.90
22	A	7016	LMU	C2'-C3'-C4'	3.59	117.49	109.60
19	3	3011	CLA	CHB-C4A-NA	3.60	129.49	124.51
19	2	2006	CLA	CHC-C1C-NC	3.61	130.46	123.67
19	A	1117	CLA	CHC-C1C-NC	3.61	130.47	123.67
22	H	7030	LMU	O1'-C1'-C2'	3.61	112.60	108.04
19	3	3007	CLA	CAC-C3C-C4C	3.61	130.08	124.83
19	A	1113	CLA	CHC-C1C-NC	3.62	130.47	123.67
19	A	1121	CLA	CAA-C2A-C1A	3.62	120.14	112.14
19	3	3016	CLA	CHC-C1C-NC	3.62	130.48	123.67
22	B	7040	LMU	O1B-C1B-C2B	3.62	116.91	108.10
19	3	3013	CLA	C4-C3-C5	3.63	120.94	115.41
19	4	4001	CLA	O2A-CGA-CBA	3.63	122.95	111.90
21	I	6018	BCR	C30-C25-C24	3.63	125.97	115.82
21	B	6005	BCR	C38-C26-C27	3.63	120.31	113.43
19	B	1205	CLA	CHC-C1C-NC	3.63	130.50	123.67
22	H	7017	LMU	C4B-C3B-C2B	3.63	117.57	110.79
22	4	7018	LMU	O1'-C1'-C2'	3.63	112.63	108.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	4004	CLA	CHC-C1C-NC	3.63	130.28	123.78
19	A	1139	CLA	CHC-C1C-NC	3.64	130.51	123.67
22	H	7011	LMU	O1B-C1B-O5B	3.64	119.89	110.68
19	B	1238	CLA	O2A-CGA-CBA	3.64	122.98	111.90
22	A	7010	LMU	O1'-C1'-C2'	3.64	112.63	108.04
19	R	1144	CLA	O2A-CGA-CBA	3.65	123.02	111.90
19	1	1013	CLA	CBA-CAA-C2A	3.65	124.03	113.73
19	A	1102	CLA	CHC-C1C-NC	3.65	130.54	123.67
22	A	7016	LMU	C4B-C3B-C2B	3.65	117.61	110.79
21	I	6018	BCR	C38-C26-C27	3.66	120.37	113.43
19	3	3010	CLA	CHC-C1C-NC	3.66	130.33	123.78
19	3	3014	CLA	CHC-C1C-NC	3.66	130.33	123.78
19	L	1502	CLA	CHC-C1C-NC	3.67	130.57	123.67
19	A	1138	CLA	CHC-C1C-NC	3.67	130.58	123.67
19	2	2001	CLA	CHC-C1C-NC	3.67	130.58	123.67
19	B	1226	CLA	CHC-C1C-NC	3.68	130.59	123.67
19	B	1214	CLA	CHC-C1C-NC	3.68	130.59	123.67
21	B	6004	BCR	C33-C5-C4	3.68	120.41	113.43
19	A	9023	CLA	CGD-CBD-CAD	3.68	123.11	110.62
19	3	3007	CLA	CHC-C1C-NC	3.68	130.60	123.67
19	1	1002	CLA	O2D-CGD-CBD	3.69	116.36	111.30
19	A	1127	CLA	CHC-C1C-NC	3.69	130.62	123.67
19	B	1209	CLA	CHC-C1C-NC	3.69	130.62	123.67
19	A	1151	CLA	CHC-C1C-NC	3.69	130.62	123.67
19	K	1146	CLA	CMB-C2B-C3B	3.70	132.32	125.09
22	A	7045	LMU	O5B-C1B-C2B	3.70	117.86	110.28
19	A	1128	CLA	C4-C3-C5	3.70	121.05	115.41
19	A	1119	CLA	CHC-C1C-NC	3.70	130.63	123.67
19	2	2008	CLA	C3D-C4D-ND	3.70	113.41	110.13
19	3	3002	CLA	CHC-C1C-NC	3.70	130.40	123.78
19	B	1218	CLA	CHB-C4A-NA	3.71	129.64	124.51
19	4	4014	CLA	CAC-C3C-C4C	3.71	130.22	124.83
19	L	1148	CLA	O2A-CGA-CBA	3.72	123.23	111.90
19	A	9022	CLA	CHB-C4A-NA	3.72	129.66	124.51
19	4	1004	CLA	CHC-C1C-NC	3.73	130.68	123.67
19	1	1002	CLA	CHC-C1C-NC	3.73	130.69	123.67
19	A	1136	CLA	CHC-C1C-NC	3.73	130.69	123.67
19	A	1108	CLA	CHC-C1C-NC	3.73	130.69	123.67
19	1	1002	CLA	O2A-CGA-CBA	3.74	123.29	111.90
19	3	3008	CLA	O2A-CGA-CBA	3.74	123.30	111.90
19	4	4010	CLA	CHC-C1C-NC	3.74	130.47	123.78
19	3	1147	CLA	CMC-C2C-C1C	3.75	130.82	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	2001	CLA	C4-C3-C5	3.75	119.93	115.68
19	1	1002	CLA	CED-O2D-CGD	3.75	124.80	115.99
19	1	1002	CLA	CAA-C2A-C1A	3.76	125.72	112.47
19	4	4005	CLA	CHC-C1C-NC	3.76	130.50	123.78
19	A	1129	CLA	O2A-CGA-CBA	3.76	123.35	111.90
21	B	6020	BCR	C8-C9-C10	3.76	125.05	118.98
19	1	1015	CLA	CHC-C1C-NC	3.76	130.51	123.78
19	A	1149	CLA	C3A-C2A-C1A	3.76	107.88	101.50
19	1	1006	CLA	CHC-C1C-NC	3.77	130.76	123.67
19	3	3017	CLA	CHB-C4A-NA	3.77	129.72	124.51
21	I	6021	BCR	C7-C8-C9	3.77	131.96	126.22
19	H	1145	CLA	CHC-C1C-NC	3.77	130.76	123.67
19	B	1235	CLA	CHC-C1C-NC	3.77	130.76	123.67
19	4	4005	CLA	C3D-C2D-C1D	3.77	109.62	106.30
19	A	1129	CLA	CHC-C1C-NC	3.78	130.78	123.67
19	B	1219	CLA	O2D-CGD-CBD	3.78	116.48	111.30
19	B	1202	CLA	CHB-C4A-NA	3.78	129.74	124.51
21	B	6020	BCR	C36-C18-C19	3.79	124.40	118.10
19	A	1123	CLA	C4-C3-C5	3.79	121.19	115.41
19	B	9010	CLA	CHC-C1C-NC	3.79	130.81	123.67
19	B	1210	CLA	CHC-C1C-NC	3.80	130.82	123.67
22	R	7020	LMU	C1B-O5B-C5B	3.80	121.12	113.75
19	A	1109	CLA	O2D-CGD-CBD	3.81	116.52	111.30
19	2	2010	CLA	CHC-C1C-NC	3.81	130.59	123.78
21	I	6021	BCR	C15-C16-C17	3.81	131.82	123.39
22	R	7021	LMU	C1B-O5B-C5B	3.81	121.15	113.75
22	C	7015	LMU	C1B-C2B-C3B	3.82	117.49	109.97
21	A	6007	BCR	C33-C5-C4	3.82	120.67	113.43
22	K	7001	LMU	O1'-C1'-C2'	3.82	112.87	108.04
19	B	1201	CLA	CHC-C1C-NC	3.83	130.87	123.67
19	F	1240	CLA	CHC-C1C-NC	3.84	130.89	123.67
21	B	6017	BCR	C39-C30-C25	3.84	116.32	110.30
19	3	1147	CLA	CAA-C2A-C1A	3.84	126.00	112.47
22	G	7039	LMU	O1B-C1B-C2B	3.84	117.45	108.10
22	F	7036	LMU	O1B-C1B-C2B	3.85	117.46	108.10
19	2	2005	CLA	C3D-C2D-C1D	3.85	109.69	106.30
21	I	6021	BCR	C15-C14-C13	3.85	132.76	127.20
19	1	1310	CLA	CHC-C1C-NC	3.86	130.68	123.78
22	B	7038	LMU	C1B-O5B-C5B	3.86	121.23	113.75
19	4	4007	CLA	CHC-C1C-NC	3.86	130.93	123.67
19	4	4011	CLA	C3D-C2D-C1D	3.86	109.70	106.30
19	K	1146	CLA	O2A-CGA-CBA	3.87	123.69	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	7038	LMU	C1'-O5'-C5'	3.87	121.27	113.75
19	2	1307	CLA	C3D-C2D-C1D	3.88	109.72	106.30
19	1	1013	CLA	CHC-C1C-NC	3.88	130.98	123.67
19	3	3015	CLA	CHC-C1C-NC	3.89	130.73	123.78
19	K	1143	CLA	CHC-C1C-NC	3.90	131.01	123.67
19	4	4006	CLA	C4-C3-C5	3.90	121.37	115.41
19	A	1134	CLA	CHC-C1C-NC	3.91	131.03	123.67
19	4	1306	CLA	CAC-C3C-C4C	3.91	130.51	124.83
22	E	7048	LMU	O5B-C5B-C6B	3.92	116.25	106.36
19	1	1001	CLA	CHC-C1C-NC	3.92	131.05	123.67
21	I	6018	BCR	C23-C22-C21	3.93	125.31	118.98
19	B	1215	CLA	CHC-C1C-NC	3.93	131.07	123.67
19	B	1236	CLA	CHC-C1C-NC	3.94	131.07	123.67
19	A	1132	CLA	CHC-C1C-NC	3.94	131.08	123.67
22	B	7012	LMU	O1'-C1'-C2'	3.94	113.02	108.04
19	L	1504	CLA	C4-C3-C5	3.94	121.43	115.41
22	H	7043	LMU	O5B-C5B-C4B	3.95	117.09	109.68
19	3	3012	CLA	CHC-C1C-NC	3.95	130.84	123.78
21	A	6002	BCR	C39-C30-C25	3.96	116.52	110.30
21	B	6005	BCR	C33-C5-C4	3.97	120.96	113.43
19	1	1011	CLA	CHC-C1C-NC	3.98	131.15	123.67
19	3	3013	CLA	CED-O2D-CGD	3.98	125.33	115.99
19	A	1309	CLA	CHC-C1C-NC	4.01	130.94	123.78
19	2	2003	CLA	CHC-C1C-NC	4.01	130.95	123.78
22	A	7044	LMU	O2'-C2'-C1'	4.02	118.83	110.02
19	3	3001	CLA	C3D-C2D-C1D	4.02	109.84	106.30
22	A	7023	LMU	C2'-C3'-C4'	4.04	118.47	109.60
19	L	1502	CLA	CHB-C4A-NA	4.04	130.10	124.51
19	4	4002	CLA	O2A-CGA-CBA	4.05	124.23	111.90
19	4	4002	CLA	CMB-C2B-C3B	4.05	133.01	125.09
19	B	1238	CLA	CHC-C1C-NC	4.05	131.29	123.67
19	B	1239	CLA	O2A-CGA-CBA	4.06	124.26	111.90
21	F	6016	BCR	C39-C30-C25	4.06	116.67	110.30
22	R	7024	LMU	O5B-C1B-C2B	4.06	118.61	110.28
19	A	1149	CLA	CHC-C1C-NC	4.06	131.32	123.67
19	B	1203	CLA	CHB-C4A-NA	4.07	130.15	124.51
19	3	3005	CLA	CHC-C1C-NC	4.08	131.07	123.78
23	B	7101	LMG	O7-C10-C11	4.09	120.42	111.53
22	H	7043	LMU	C1B-O5B-C5B	4.09	121.68	113.75
21	B	6006	BCR	C40-C30-C25	4.09	116.72	110.30
19	A	1116	CLA	O2A-CGA-CBA	4.09	124.37	111.90
19	3	3014	CLA	C3D-C4D-ND	4.10	113.77	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	K	1146	CLA	CHC-C1C-NC	4.11	131.41	123.67
19	2	2008	CLA	CHC-C1C-NC	4.11	131.13	123.78
19	B	1224	CLA	O2A-CGA-CBA	4.12	124.46	111.90
19	2	2006	CLA	O2D-CGD-CBD	4.13	116.96	111.30
19	B	1202	CLA	CHC-C1C-NC	4.13	131.45	123.67
22	A	7016	LMU	O1'-C1'-C2'	4.14	113.26	108.04
21	B	6010	BCR	C38-C26-C27	4.15	121.29	113.43
21	1	6023	BCR	C40-C30-C39	4.15	121.66	108.37
19	3	3017	CLA	CHC-C1C-NC	4.15	131.47	123.67
19	4	1304	CLA	O2D-CGD-CBD	4.15	117.00	111.30
19	2	2007	CLA	CHC-C1C-NC	4.16	131.50	123.67
22	H	7028	LMU	O1'-C1'-C2'	4.16	113.30	108.04
21	B	6020	BCR	C33-C5-C4	4.17	121.33	113.43
19	4	4002	CLA	O2D-CGD-CBD	4.17	117.02	111.30
19	A	1120	CLA	C4-C3-C5	4.19	120.43	115.68
19	B	1203	CLA	CHC-C1C-NC	4.21	131.59	123.67
19	3	1147	CLA	CAC-C3C-C4C	4.21	130.95	124.83
22	H	7017	LMU	C1'-O5'-C5'	4.22	121.93	113.75
19	1	1310	CLA	C3D-C4D-ND	4.22	113.87	110.13
19	2	2005	CLA	C3D-C4D-ND	4.23	113.89	110.13
19	A	9023	CLA	CHC-C1C-NC	4.23	131.64	123.67
19	4	1306	CLA	CHC-C1C-NC	4.24	131.65	123.67
19	A	1109	CLA	CHC-C1C-NC	4.25	131.66	123.67
22	1	7013	LMU	O1B-C4'-C3'	4.25	118.14	107.17
19	A	9023	CLA	CHB-C4A-NA	4.26	130.40	124.51
19	A	1122	CLA	O2D-CGD-CBD	4.26	117.15	111.30
19	2	2005	CLA	CHC-C1C-NC	4.27	131.41	123.78
22	C	7015	LMU	O1'-C1'-C2'	4.27	113.44	108.04
19	B	1219	CLA	C4-C3-C5	4.28	121.94	115.41
19	A	1117	CLA	O2D-CGD-CBD	4.28	117.17	111.30
19	1	1303	CLA	CHC-C1C-NC	4.28	131.72	123.67
19	3	3006	CLA	CHC-C1C-NC	4.28	131.44	123.78
22	K	7001	LMU	C1B-C2B-C3B	4.29	118.43	109.97
19	R	1150	CLA	O2A-CGA-CBA	4.29	124.98	111.90
19	3	3014	CLA	C3D-C2D-C1D	4.31	110.10	106.30
22	A	7045	LMU	O1'-C1'-C2'	4.32	113.50	108.04
19	A	1103	CLA	CHC-C1C-NC	4.32	131.80	123.67
19	1	1008	CLA	CAA-C2A-C3A	4.34	125.69	113.22
19	H	1145	CLA	CHB-C4A-NA	4.37	130.55	124.51
19	4	4013	CLA	C2B-C1B-NB	4.37	114.02	110.09
19	2	1307	CLA	C3D-C4D-ND	4.38	114.02	110.13
19	3	2009	CLA	O2D-CGD-CBD	4.39	117.32	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1235	CLA	C4-C3-C5	4.40	122.12	115.41
21	I	6018	BCR	C10-C11-C12	4.41	136.57	123.13
22	4	7052	LMU	C1'-C2'-C3'	4.45	118.73	109.97
21	1	6023	BCR	C32-C1-C2	4.46	124.75	108.79
20	A	5001	PQN	C14-C13-C15	4.46	122.22	115.41
19	3	3012	CLA	C3D-C2D-C1D	4.47	110.24	106.30
19	3	3004	CLA	CHC-C1C-NC	4.48	131.80	123.78
22	4	7019	LMU	C2'-C3'-C4'	4.50	119.48	109.60
21	1	6023	BCR	C38-C26-C27	4.50	121.97	113.43
19	A	9023	CLA	O2D-CGD-CBD	4.51	117.49	111.30
19	A	1115	CLA	C4-C3-C5	4.51	122.30	115.41
19	4	4002	CLA	C3A-C2A-C1A	4.52	109.16	101.50
22	2	7031	LMU	O1B-C1B-C2B	4.52	119.10	108.10
21	L	6019	BCR	C39-C30-C25	4.53	117.40	110.30
19	A	1149	CLA	O2A-CGA-CBA	4.53	125.70	111.90
19	R	1150	CLA	O2D-CGD-CBD	4.56	117.56	111.30
19	3	3012	CLA	C3D-C4D-ND	4.57	114.19	110.13
21	1	6023	BCR	C36-C18-C19	4.59	125.74	118.10
19	A	1102	CLA	O2A-CGA-CBA	4.59	125.90	111.90
19	A	1107	CLA	CHC-C1C-NC	4.61	132.35	123.67
22	R	7020	LMU	O1'-C1'-C2'	4.61	113.87	108.04
19	H	1505	CLA	C4-C3-C5	4.62	122.46	115.41
19	A	1111	CLA	CHC-C1C-NC	4.63	132.38	123.67
22	H	7032	LMU	C1B-O5B-C5B	4.63	122.73	113.75
19	A	1102	CLA	O2D-CGD-CBD	4.64	117.67	111.30
19	1	1001	CLA	CHB-C4A-NA	4.64	130.94	124.51
19	A	1132	CLA	C4-C3-C5	4.66	122.52	115.41
22	4	7009	LMU	O1'-C1'-C2'	4.67	113.94	108.04
19	1	1013	CLA	O2A-CGA-CBA	4.72	126.27	111.90
19	1	1010	CLA	CAA-C2A-C1A	4.75	129.22	112.47
19	L	1130	CLA	C4-C3-C5	4.80	122.74	115.41
19	B	9010	CLA	O2D-CGD-CBD	4.81	117.89	111.30
22	R	7021	LMU	O1B-C4'-C3'	4.84	119.67	107.17
19	4	1009	CLA	CBD-CHA-C1A	4.85	130.81	128.59
19	4	4002	CLA	CHC-C1C-NC	4.85	132.80	123.67
19	A	1151	CLA	O2D-CGD-CBD	4.87	117.98	111.30
19	A	1123	CLA	O2D-CGD-CBD	4.87	117.98	111.30
22	2	7031	LMU	O1'-C1'-C2'	4.89	114.22	108.04
22	2	7027	LMU	O1'-C1'-C2'	4.91	114.24	108.04
22	R	7014	LMU	O2B-C2B-C3B	4.92	121.41	110.34
19	4	4006	CLA	O2D-CGD-CBD	4.95	118.09	111.30
22	R	7014	LMU	O1B-C1B-C2B	4.97	120.19	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	1304	CLA	CHC-C1C-NC	5.06	133.18	123.67
19	B	1231	CLA	O2D-CGD-CBD	5.07	118.26	111.30
19	2	2005	CLA	C2B-C1B-NB	5.09	114.65	110.09
19	4	1004	CLA	O2D-CGD-CBD	5.09	118.28	111.30
19	H	1505	CLA	O2D-CGD-CBD	5.10	118.30	111.30
22	G	7051	LMU	O1'-C1'-C2'	5.15	114.55	108.04
19	B	1211	CLA	O2D-CGD-CBD	5.15	118.37	111.30
22	G	7026	LMU	C1'-O5'-C5'	5.18	123.79	113.75
22	4	7033	LMU	C3B-C4B-C5B	5.18	119.23	110.20
22	3	7003	LMU	C4B-C3B-C2B	5.18	120.47	110.79
19	A	1103	CLA	O2D-CGD-CBD	5.21	118.45	111.30
19	A	1113	CLA	O2D-CGD-CBD	5.21	118.45	111.30
19	2	2004	CLA	O2D-CGD-CBD	5.25	118.50	111.30
21	1	6023	BCR	C20-C19-C18	5.26	141.79	126.32
21	I	6021	BCR	C8-C9-C10	5.26	127.46	118.98
19	3	3015	CLA	C2B-C1B-NB	5.26	114.81	110.09
19	4	4002	CLA	CAA-C2A-C1A	5.28	131.09	112.47
21	1	6023	BCR	C40-C30-C25	5.28	118.58	110.30
19	B	1233	CLA	C4-C3-C5	5.29	121.67	115.68
22	R	7014	LMU	O1'-C1'-C2'	5.29	114.72	108.04
19	L	1148	CLA	C4-C3-C5	5.30	123.50	115.41
19	A	1309	CLA	C2B-C1B-NB	5.33	114.87	110.09
19	3	3005	CLA	C2B-C1B-NB	5.34	114.88	110.09
21	F	6016	BCR	C10-C11-C12	5.34	139.42	123.13
19	1	1015	CLA	C2B-C1B-NB	5.34	114.89	110.09
19	3	3006	CLA	C2B-C1B-NB	5.35	114.89	110.09
21	A	6007	BCR	C21-C20-C19	5.37	139.49	123.13
19	B	1210	CLA	O2D-CGD-CBD	5.40	118.70	111.30
19	A	1126	CLA	O2D-CGD-CBD	5.41	118.72	111.30
19	B	1215	CLA	O2D-CGD-CBD	5.43	118.75	111.30
19	1	1303	CLA	C4-C3-C5	5.45	121.85	115.68
19	A	9012	CLA	O2D-CGD-CBD	5.46	118.79	111.30
19	2	2010	CLA	C2B-C1B-NB	5.46	114.99	110.09
19	2	2008	CLA	C2B-C1B-NB	5.47	115.00	110.09
19	3	3002	CLA	C2B-C1B-NB	5.49	115.02	110.09
19	4	4005	CLA	C2B-C1B-NB	5.53	115.05	110.09
21	1	6023	BCR	C39-C30-C25	5.54	118.98	110.30
19	1	1303	CLA	CAA-C2A-C1A	5.58	132.14	112.47
19	A	1131	CLA	O2D-CGD-CBD	5.59	118.97	111.30
19	A	1110	CLA	O2D-CGD-CBD	5.62	119.01	111.30
19	B	1212	CLA	O2D-CGD-CBD	5.66	119.06	111.30
19	B	1222	CLA	O2D-CGD-CBD	5.66	119.06	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	I	6021	BCR	C38-C26-C27	5.68	124.19	113.43
19	B	1220	CLA	O2D-CGD-CBD	5.68	119.10	111.30
19	B	1227	CLA	O2D-CGD-CBD	5.69	119.10	111.30
19	B	1218	CLA	O2D-CGD-CBD	5.69	119.10	111.30
19	4	4010	CLA	C2B-C1B-NB	5.71	115.22	110.09
19	F	1302	CLA	O2D-CGD-CBD	5.74	119.17	111.30
19	A	1149	CLA	CAA-C2A-C3A	5.74	129.71	113.22
19	3	3010	CLA	C2B-C1B-NB	5.75	115.25	110.09
19	A	9022	CLA	C4-C3-C5	5.76	124.20	115.41
19	4	4011	CLA	C2B-C1B-NB	5.82	115.31	110.09
19	A	1125	CLA	O2D-CGD-CBD	5.85	119.33	111.30
19	B	1209	CLA	O2D-CGD-CBD	5.86	119.33	111.30
19	R	1144	CLA	O2D-CGD-CBD	5.89	119.38	111.30
19	A	1140	CLA	O2D-CGD-CBD	5.90	119.39	111.30
19	2	1307	CLA	C2B-C1B-NB	5.92	115.40	110.09
19	3	3001	CLA	C2B-C1B-NB	5.92	115.40	110.09
19	2	2003	CLA	C2B-C1B-NB	5.94	115.42	110.09
19	4	4007	CLA	O2D-CGD-CBD	5.99	119.51	111.30
19	3	3004	CLA	C2B-C1B-NB	6.00	115.47	110.09
22	F	7036	LMU	O1'-C1'-C2'	6.05	115.68	108.04
22	A	7035	LMU	O1B-C4'-C3'	6.05	122.79	107.17
19	3	3008	CLA	O2D-CGD-CBD	6.06	119.62	111.30
19	H	1207	CLA	O2D-CGD-CBD	6.07	119.62	111.30
19	G	1242	CLA	C4-C3-C5	6.09	122.58	115.68
19	4	4004	CLA	C2B-C1B-NB	6.15	115.61	110.09
19	3	3011	CLA	O2D-CGD-CBD	6.15	119.74	111.30
19	4	4001	CLA	O2D-CGD-CBD	6.16	119.75	111.30
19	2	2011	CLA	C2B-C1B-NB	6.17	115.63	110.09
19	K	1143	CLA	O2D-CGD-CBD	6.17	119.77	111.30
19	A	1139	CLA	O2D-CGD-CBD	6.24	119.85	111.30
19	B	1233	CLA	O2D-CGD-CBD	6.25	119.88	111.30
19	3	1147	CLA	O2D-CGD-CBD	6.27	119.90	111.30
19	A	1104	CLA	O2D-CGD-CBD	6.30	119.94	111.30
19	A	1133	CLA	O2D-CGD-CBD	6.32	119.96	111.30
19	3	3014	CLA	C2B-C1B-NB	6.34	115.78	110.09
19	A	1136	CLA	O2D-CGD-CBD	6.42	120.11	111.30
19	A	1111	CLA	O2D-CGD-CBD	6.44	120.13	111.30
19	A	1138	CLA	O2D-CGD-CBD	6.45	120.15	111.30
19	A	1141	CLA	O2D-CGD-CBD	6.45	120.15	111.30
19	A	1119	CLA	O2D-CGD-CBD	6.46	120.16	111.30
22	A	7044	LMU	O1'-C1'-C2'	6.47	116.22	108.04
19	A	1116	CLA	O2D-CGD-CBD	6.48	120.19	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1134	CLA	O2D-CGD-CBD	6.48	120.19	111.30
19	K	1142	CLA	O2D-CGD-CBD	6.48	120.19	111.30
22	H	7002	LMU	O1B-C4'-C3'	6.48	123.90	107.17
19	B	1223	CLA	O2D-CGD-CBD	6.52	120.24	111.30
19	4	4014	CLA	O2D-CGD-CBD	6.54	120.27	111.30
19	3	3012	CLA	C2B-C1B-NB	6.57	115.98	110.09
19	1	1007	CLA	O2D-CGD-CBD	6.62	120.38	111.30
19	K	1146	CLA	O2D-CGD-CBD	6.63	120.40	111.30
19	3	3016	CLA	O2D-CGD-CBD	6.65	120.43	111.30
19	1	1010	CLA	O2D-CGD-CBD	6.67	120.45	111.30
21	B	6017	BCR	C10-C11-C12	6.68	143.50	123.13
19	3	3007	CLA	O2D-CGD-CBD	6.70	120.50	111.30
19	1	1001	CLA	O2D-CGD-CBD	6.71	120.50	111.30
19	B	1214	CLA	O2D-CGD-CBD	6.71	120.50	111.30
19	B	1217	CLA	O2D-CGD-CBD	6.73	120.53	111.30
19	B	1232	CLA	O2D-CGD-CBD	6.73	120.54	111.30
22	4	7052	LMU	O1'-C1'-C2'	6.76	116.58	108.04
19	1	1310	CLA	C2B-C1B-NB	6.76	116.16	110.09
19	A	1115	CLA	O2D-CGD-CBD	6.79	120.61	111.30
22	E	7048	LMU	C3B-C4B-C5B	6.79	122.03	110.20
19	2	2001	CLA	O2D-CGD-CBD	6.81	120.65	111.30
19	A	1137	CLA	O2D-CGD-CBD	6.83	120.67	111.30
21	B	6004	BCR	C10-C11-C12	6.83	143.95	123.13
19	I	1204	CLA	O2D-CGD-CBD	6.84	120.68	111.30
21	A	6007	BCR	C20-C21-C22	6.85	137.09	127.20
19	A	1237	CLA	O2D-CGD-CBD	6.86	120.71	111.30
19	F	1240	CLA	CBD-CHA-C1A	6.86	131.74	128.59
19	A	1106	CLA	O2D-CGD-CBD	6.87	120.73	111.30
19	G	1242	CLA	O2D-CGD-CBD	6.89	120.76	111.30
19	A	1124	CLA	O2D-CGD-CBD	6.95	120.83	111.30
19	F	1305	CLA	O2D-CGD-CBD	6.96	120.84	111.30
19	2	2014	CLA	O2D-CGD-CBD	6.96	120.86	111.30
19	A	1135	CLA	O2D-CGD-CBD	6.97	120.86	111.30
21	I	6018	BCR	C40-C30-C25	7.05	121.35	110.30
19	1	1008	CLA	C3A-C2A-C1A	7.07	113.48	101.50
19	4	1304	CLA	CGD-CBD-CAD	7.07	134.60	110.62
19	B	1238	CLA	O2D-CGD-CBD	7.08	121.01	111.30
21	1	6023	BCR	C21-C20-C19	7.10	144.78	123.13
22	G	7051	LMU	O1B-C4'-C3'	7.11	125.51	107.17
19	2	2013	CLA	O2D-CGD-CBD	7.12	121.07	111.30
19	3	3003	CLA	CBD-CHA-C1A	7.15	131.87	128.59
19	4	4003	CLA	O2D-CGD-CBD	7.15	121.12	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	2012	CLA	O2D-CGD-CBD	7.24	121.23	111.30
19	J	1308	CLA	O2D-CGD-CBD	7.24	121.23	111.30
19	A	1120	CLA	O2D-CGD-CBD	7.27	121.27	111.30
21	B	6010	BCR	C10-C11-C12	7.32	145.43	123.13
21	A	6008	BCR	C10-C11-C12	7.40	145.68	123.13
19	1	1012	CLA	CBD-CHA-C1A	7.41	131.99	128.59
21	F	6016	BCR	C11-C10-C9	7.45	137.96	127.20
19	B	1213	CLA	O2D-CGD-CBD	7.47	121.54	111.30
21	B	6006	BCR	C10-C11-C12	7.47	145.91	123.13
19	1	1008	CLA	O2D-CGD-CBD	7.48	121.56	111.30
19	A	9013	CLA	O2D-CGD-CBD	7.48	121.56	111.30
19	A	1107	CLA	O2D-CGD-CBD	7.53	121.63	111.30
19	L	1130	CLA	O2D-CGD-CBD	7.58	121.70	111.30
19	K	3009	CLA	O2D-CGD-CBD	7.60	121.72	111.30
19	1	1014	CLA	O2D-CGD-CBD	7.63	121.77	111.30
21	I	6021	BCR	C21-C20-C19	7.66	146.49	123.13
19	2	2002	CLA	O2D-CGD-CBD	7.67	121.82	111.30
19	A	1112	CLA	O2D-CGD-CBD	7.70	121.86	111.30
19	L	1502	CLA	O2D-CGD-CBD	7.76	121.95	111.30
19	A	9022	CLA	O2D-CGD-CBD	7.76	121.95	111.30
19	A	1105	CLA	O2D-CGD-CBD	7.78	121.97	111.30
19	B	1208	CLA	O2D-CGD-CBD	7.80	122.00	111.30
19	2	4009	CLA	O2D-CGD-CBD	7.81	122.01	111.30
21	A	6007	BCR	C10-C11-C12	7.84	147.02	123.13
19	B	1228	CLA	O2D-CGD-CBD	7.95	122.21	111.30
19	B	1202	CLA	O2D-CGD-CBD	7.97	122.24	111.30
21	B	6005	BCR	C10-C11-C12	7.98	147.44	123.13
21	J	6012	BCR	C10-C11-C12	7.98	147.45	123.13
19	B	1229	CLA	O2D-CGD-CBD	7.99	122.26	111.30
19	B	1236	CLA	O2D-CGD-CBD	8.02	122.31	111.30
19	B	1230	CLA	O2D-CGD-CBD	8.03	122.31	111.30
21	L	6019	BCR	C10-C11-C12	8.03	147.60	123.13
19	1	1003	CLA	O2D-CGD-CBD	8.03	122.32	111.30
19	B	1203	CLA	O2D-CGD-CBD	8.11	122.42	111.30
19	B	1221	CLA	O2D-CGD-CBD	8.11	122.43	111.30
19	J	1311	CLA	O2D-CGD-CBD	8.19	122.53	111.30
19	A	1108	CLA	O2D-CGD-CBD	8.25	122.62	111.30
19	H	1241	CLA	O2D-CGD-CBD	8.26	122.64	111.30
19	1	1303	CLA	O2D-CGD-CBD	8.33	122.73	111.30
19	B	1224	CLA	O2D-CGD-CBD	8.35	122.75	111.30
19	L	1504	CLA	O2D-CGD-CBD	8.44	122.88	111.30
21	F	6014	BCR	C10-C11-C12	8.54	149.16	123.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1121	CLA	O2D-CGD-CBD	8.56	123.04	111.30
19	A	1149	CLA	O2D-CGD-CBD	8.59	123.09	111.30
19	A	1132	CLA	O2D-CGD-CBD	8.60	123.10	111.30
19	4	4015	CLA	O2D-CGD-CBD	8.64	123.15	111.30
19	B	1216	CLA	O2D-CGD-CBD	8.65	123.16	111.30
19	B	1235	CLA	O2D-CGD-CBD	8.66	123.18	111.30
19	A	1128	CLA	O2D-CGD-CBD	8.71	123.25	111.30
21	I	6018	BCR	C21-C20-C19	8.76	149.84	123.13
19	4	1306	CLA	O2D-CGD-CBD	8.80	123.37	111.30
19	L	1501	CLA	O2D-CGD-CBD	8.82	123.40	111.30
21	B	6017	BCR	C21-C20-C19	8.82	150.03	123.13
19	A	1129	CLA	O2D-CGD-CBD	8.89	123.49	111.30
19	B	1201	CLA	O2D-CGD-CBD	8.89	123.50	111.30
21	A	6011	BCR	C10-C11-C12	8.90	150.25	123.13
19	B	1234	CLA	O2D-CGD-CBD	8.90	123.51	111.30
19	3	1118	CLA	CBD-CHA-C1A	9.01	132.72	128.59
19	L	1148	CLA	O2D-CGD-CBD	9.01	123.67	111.30
19	3	3013	CLA	O2D-CGD-CBD	9.06	123.74	111.30
21	A	6008	BCR	C21-C20-C19	9.12	150.92	123.13
19	2	2007	CLA	O2D-CGD-CBD	9.15	123.86	111.30
21	A	6003	BCR	C10-C11-C12	9.22	151.22	123.13
21	3	6022	BCR	C10-C11-C12	9.29	151.45	123.13
21	F	6016	BCR	C21-C20-C19	9.30	151.49	123.13
19	B	1226	CLA	O2D-CGD-CBD	9.33	124.10	111.30
19	3	3017	CLA	O2D-CGD-CBD	9.34	124.12	111.30
19	1	1005	CLA	O2D-CGD-CBD	9.40	124.20	111.30
21	B	6020	BCR	C21-C20-C19	9.53	152.19	123.13
19	1	1011	CLA	CBD-CHA-C1A	9.66	133.02	128.59
21	L	6019	BCR	C21-C20-C19	9.70	152.70	123.13
21	B	6010	BCR	C21-C20-C19	9.80	153.00	123.13
21	B	6004	BCR	C21-C20-C19	9.98	153.54	123.13
21	A	6003	BCR	C21-C20-C19	10.02	153.69	123.13
19	B	1225	CLA	O2D-CGD-CBD	10.07	125.12	111.30
21	3	6022	BCR	C11-C10-C9	10.12	141.81	127.20
19	B	1205	CLA	O2D-CGD-CBD	10.13	125.20	111.30
21	A	6011	BCR	C21-C20-C19	10.18	154.16	123.13
21	L	6019	BCR	C11-C10-C9	10.30	142.08	127.20
19	A	1127	CLA	O2D-CGD-CBD	10.34	125.48	111.30
21	A	6003	BCR	C11-C10-C9	10.35	142.15	127.20
21	B	6006	BCR	C21-C20-C19	10.41	154.87	123.13
19	B	1301	CLA	CBD-CHA-C1A	10.52	133.41	128.59
21	B	6010	BCR	C11-C10-C9	10.58	142.48	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1006	CLA	CBD-CHA-C1A	10.89	133.58	128.59
19	A	1128	CLA	C3B-CAB-CBB	10.91	148.65	126.32
19	A	1101	CLA	O2D-CGD-CBD	11.11	126.55	111.30
21	B	6004	BCR	C11-C10-C9	11.39	143.65	127.20
19	4	4012	CLA	CBD-CHA-C1A	11.49	133.85	128.59
19	L	1503	CLA	O2D-CGD-CBD	11.83	127.53	111.30
21	F	6014	BCR	C11-C10-C9	12.36	145.04	127.20
21	A	6008	BCR	C11-C10-C9	12.40	145.11	127.20
19	A	1108	CLA	C3B-CAB-CBB	12.41	151.70	126.32
21	I	6021	BCR	C11-C10-C9	12.44	145.17	127.20
21	1	6023	BCR	C10-C11-C12	12.73	161.95	123.13
21	B	6017	BCR	C11-C10-C9	12.80	145.68	127.20
21	B	6005	BCR	C21-C20-C19	12.80	162.16	123.13
21	J	6012	BCR	C21-C20-C19	13.09	163.04	123.13
21	A	6003	BCR	C20-C21-C22	13.13	146.16	127.20
21	B	6005	BCR	C11-C10-C9	13.54	146.76	127.20
19	B	1230	CLA	C3B-CAB-CBB	13.92	154.80	126.32
21	3	6022	BCR	C21-C20-C19	14.11	166.13	123.13
21	F	6016	BCR	C20-C21-C22	14.12	147.59	127.20
21	A	6002	BCR	C21-C20-C19	14.44	167.16	123.13
21	A	6011	BCR	C11-C10-C9	14.52	148.17	127.20
21	I	6021	BCR	C20-C21-C22	14.53	148.18	127.20
21	A	6011	BCR	C20-C21-C22	14.57	148.24	127.20
21	A	6007	BCR	C11-C10-C9	14.76	148.52	127.20
19	A	1106	CLA	C3B-CAB-CBB	14.86	156.72	126.32
21	F	6014	BCR	C21-C20-C19	14.98	168.81	123.13
21	I	6018	BCR	C20-C21-C22	15.02	148.89	127.20
21	J	6012	BCR	C11-C10-C9	15.49	149.57	127.20
21	B	6006	BCR	C11-C10-C9	15.71	149.89	127.20
19	B	1226	CLA	C3B-CAB-CBB	16.46	159.99	126.32
21	B	6017	BCR	C20-C21-C22	16.56	151.11	127.20
19	F	1305	CLA	C3B-CAB-CBB	16.60	160.28	126.32
21	A	6008	BCR	C20-C21-C22	16.73	151.36	127.20
19	B	1235	CLA	C3B-CAB-CBB	17.09	161.28	126.32
19	B	9010	CLA	C3B-CAB-CBB	17.15	161.42	126.32
19	A	1107	CLA	C3B-CAB-CBB	17.36	161.84	126.32
21	I	6018	BCR	C11-C10-C9	17.44	152.38	127.20
19	1	1002	CLA	C3B-CAB-CBB	17.47	162.06	126.32
19	2	2012	CLA	C3B-CAB-CBB	17.80	162.75	126.32
19	4	4007	CLA	C3B-CAB-CBB	17.83	162.79	126.32
19	2	2007	CLA	C3B-CAB-CBB	18.10	163.35	126.32
19	B	1209	CLA	C3B-CAB-CBB	18.19	163.54	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1127	CLA	C3B-CAB-CBB	18.20	163.56	126.32
19	A	1112	CLA	C3B-CAB-CBB	18.26	163.68	126.32
19	B	1236	CLA	C3B-CAB-CBB	18.29	163.73	126.32
21	B	6004	BCR	C20-C21-C22	18.49	153.91	127.20
19	A	1126	CLA	C3B-CAB-CBB	18.50	164.18	126.32
19	A	1101	CLA	C3B-CAB-CBB	18.51	164.19	126.32
19	3	3017	CLA	C3B-CAB-CBB	18.75	164.69	126.32
19	A	1102	CLA	C3B-CAB-CBB	18.89	164.97	126.32
19	B	1213	CLA	C3B-CAB-CBB	19.14	165.48	126.32
19	A	1125	CLA	C3B-CAB-CBB	19.25	165.71	126.32
19	A	1117	CLA	C3B-CAB-CBB	19.57	166.35	126.32
21	B	6020	BCR	C20-C21-C22	19.80	155.79	127.20
21	B	6010	BCR	C20-C21-C22	20.00	156.09	127.20
19	B	1201	CLA	C3B-CAB-CBB	20.03	167.31	126.32
19	B	1238	CLA	C3B-CAB-CBB	20.24	167.73	126.32
19	B	1224	CLA	C3B-CAB-CBB	20.27	167.80	126.32
19	B	1223	CLA	C3B-CAB-CBB	20.27	167.80	126.32
19	4	1306	CLA	C3B-CAB-CBB	20.33	167.91	126.32
19	A	1109	CLA	C3B-CAB-CBB	20.39	168.04	126.32
19	A	1110	CLA	C3B-CAB-CBB	20.40	168.05	126.32
21	1	6023	BCR	C11-C10-C9	20.44	156.72	127.20
19	B	1225	CLA	C3B-CAB-CBB	20.46	168.18	126.32
19	A	1135	CLA	C3B-CAB-CBB	20.48	168.21	126.32
19	1	1014	CLA	C3B-CAB-CBB	20.52	168.30	126.32
19	H	1241	CLA	C3B-CAB-CBB	20.53	168.32	126.32
19	K	1143	CLA	C3B-CAB-CBB	20.54	168.35	126.32
21	B	6006	BCR	C20-C21-C22	20.56	156.90	127.20
19	B	1231	CLA	C3B-CAB-CBB	20.65	168.56	126.32
19	A	1123	CLA	C3B-CAB-CBB	20.67	168.62	126.32
19	1	1007	CLA	C3B-CAB-CBB	20.69	168.64	126.32
19	B	1206	CLA	C3B-CAB-CBB	20.83	168.93	126.32
19	A	1121	CLA	C3B-CAB-CBB	20.88	169.03	126.32
19	L	1504	CLA	C3B-CAB-CBB	20.93	169.15	126.32
19	B	1227	CLA	C3B-CAB-CBB	20.93	169.15	126.32
19	A	1103	CLA	C3B-CAB-CBB	20.97	169.22	126.32
19	A	9011	CLA	C3B-CAB-CBB	20.97	169.23	126.32
21	L	6019	BCR	C20-C21-C22	20.98	157.50	127.20
19	L	1148	CLA	C3B-CAB-CBB	21.02	169.33	126.32
19	2	2013	CLA	C3B-CAB-CBB	21.17	169.62	126.32
19	B	1210	CLA	C3B-CAB-CBB	21.17	169.64	126.32
19	1	1013	CLA	C3B-CAB-CBB	21.21	169.71	126.32
19	A	1111	CLA	C3B-CAB-CBB	21.26	169.82	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1211	CLA	C3B-CAB-CBB	21.32	169.94	126.32
19	B	1212	CLA	C3B-CAB-CBB	21.36	170.02	126.32
19	1	1010	CLA	C3B-CAB-CBB	21.42	170.14	126.32
19	A	1151	CLA	C3B-CAB-CBB	21.58	170.48	126.32
19	2	2004	CLA	C3B-CAB-CBB	21.60	170.51	126.32
19	A	1113	CLA	C3B-CAB-CBB	21.69	170.69	126.32
19	A	1124	CLA	C3B-CAB-CBB	21.76	170.83	126.32
19	4	4001	CLA	C3B-CAB-CBB	21.78	170.88	126.32
19	A	9022	CLA	C3B-CAB-CBB	21.92	171.17	126.32
21	B	6005	BCR	C20-C21-C22	22.06	159.05	127.20
19	B	1218	CLA	C3B-CAB-CBB	22.09	171.52	126.32
19	B	1214	CLA	C3B-CAB-CBB	22.15	171.63	126.32
19	4	4002	CLA	C3B-CAB-CBB	22.23	171.81	126.32
19	A	1120	CLA	C3B-CAB-CBB	22.30	171.94	126.32
19	2	2002	CLA	C3B-CAB-CBB	22.36	172.06	126.32
19	B	1233	CLA	C3B-CAB-CBB	22.43	172.21	126.32
19	R	1144	CLA	C3B-CAB-CBB	22.44	172.22	126.32
19	A	1119	CLA	C3B-CAB-CBB	22.46	172.28	126.32
19	2	2001	CLA	C3B-CAB-CBB	22.48	172.31	126.32
21	F	6014	BCR	C20-C21-C22	22.48	159.67	127.20
19	A	1129	CLA	C3B-CAB-CBB	22.50	172.36	126.32
19	4	1304	CLA	C3B-CAB-CBB	22.58	172.52	126.32
19	2	4009	CLA	C3B-CAB-CBB	22.67	172.69	126.32
19	3	2009	CLA	C3B-CAB-CBB	22.68	172.73	126.32
19	1	1001	CLA	C3B-CAB-CBB	22.74	172.85	126.32
19	B	1202	CLA	C3B-CAB-CBB	22.77	172.91	126.32
19	G	1242	CLA	C3B-CAB-CBB	22.78	172.92	126.32
19	3	3016	CLA	C3B-CAB-CBB	22.96	173.29	126.32
19	K	1142	CLA	C3B-CAB-CBB	22.97	173.32	126.32
19	B	1215	CLA	C3B-CAB-CBB	23.01	173.41	126.32
19	4	4006	CLA	C3B-CAB-CBB	23.04	173.45	126.32
19	A	1115	CLA	C3B-CAB-CBB	23.06	173.51	126.32
19	A	1139	CLA	C3B-CAB-CBB	23.08	173.55	126.32
19	1	1008	CLA	C3B-CAB-CBB	23.12	173.63	126.32
19	1	1303	CLA	C3B-CAB-CBB	23.21	173.81	126.32
19	2	2014	CLA	C3B-CAB-CBB	23.23	173.84	126.32
19	A	1132	CLA	C3B-CAB-CBB	23.25	173.88	126.32
19	B	1217	CLA	C3B-CAB-CBB	23.25	173.90	126.32
19	4	4003	CLA	C3B-CAB-CBB	23.27	173.93	126.32
19	A	1133	CLA	C3B-CAB-CBB	23.32	174.03	126.32
19	A	1237	CLA	C3B-CAB-CBB	23.33	174.05	126.32
19	B	1239	CLA	C3B-CAB-CBB	23.39	174.18	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1104	CLA	C3B-CAB-CBB	23.43	174.25	126.32
19	H	1207	CLA	C3B-CAB-CBB	23.44	174.27	126.32
19	A	9023	CLA	C3B-CAB-CBB	23.68	174.76	126.32
19	H	1505	CLA	C3B-CAB-CBB	23.68	174.77	126.32
19	K	1146	CLA	C3B-CAB-CBB	23.69	174.78	126.32
19	R	1150	CLA	C3B-CAB-CBB	23.74	174.88	126.32
19	A	1138	CLA	C3B-CAB-CBB	23.74	174.90	126.32
19	3	3013	CLA	C3B-CAB-CBB	23.88	175.18	126.32
19	3	3007	CLA	C3B-CAB-CBB	23.88	175.19	126.32
19	A	1122	CLA	C3B-CAB-CBB	23.92	175.27	126.32
19	A	1140	CLA	C3B-CAB-CBB	23.93	175.28	126.32
19	A	9012	CLA	C3B-CAB-CBB	23.94	175.30	126.32
19	1	1005	CLA	C3B-CAB-CBB	23.98	175.38	126.32
19	B	1221	CLA	C3B-CAB-CBB	24.08	175.59	126.32
19	B	1205	CLA	C3B-CAB-CBB	24.12	175.66	126.32
19	A	1131	CLA	C3B-CAB-CBB	24.22	175.87	126.32
19	B	1216	CLA	C3B-CAB-CBB	24.22	175.88	126.32
21	3	6022	BCR	C20-C21-C22	24.30	162.30	127.20
19	L	1502	CLA	C3B-CAB-CBB	24.32	176.08	126.32
19	2	2006	CLA	C3B-CAB-CBB	24.32	176.08	126.32
19	A	1116	CLA	C3B-CAB-CBB	24.32	176.08	126.32
19	B	1203	CLA	C3B-CAB-CBB	24.40	176.25	126.32
19	F	1302	CLA	C3B-CAB-CBB	24.41	176.27	126.32
21	A	6002	BCR	C20-C21-C22	24.50	162.58	127.20
19	1	1003	CLA	C3B-CAB-CBB	24.52	176.50	126.32
19	3	3011	CLA	C3B-CAB-CBB	24.54	176.52	126.32
19	B	1234	CLA	C3B-CAB-CBB	24.57	176.58	126.32
19	3	1147	CLA	C3B-CAB-CBB	24.59	176.63	126.32
19	A	1136	CLA	C3B-CAB-CBB	24.59	176.63	126.32
19	B	1229	CLA	C3B-CAB-CBB	24.66	176.78	126.32
19	B	1232	CLA	C3B-CAB-CBB	24.68	176.81	126.32
19	J	1311	CLA	C3B-CAB-CBB	24.71	176.87	126.32
19	B	1220	CLA	C3B-CAB-CBB	24.71	176.87	126.32
19	A	1105	CLA	C3B-CAB-CBB	24.78	177.02	126.32
19	B	1219	CLA	C3B-CAB-CBB	24.78	177.03	126.32
19	4	4015	CLA	C3B-CAB-CBB	24.93	177.33	126.32
19	H	1145	CLA	C3B-CAB-CBB	24.93	177.33	126.32
19	B	1222	CLA	C3B-CAB-CBB	25.05	177.56	126.32
19	B	1228	CLA	C3B-CAB-CBB	25.06	177.59	126.32
19	A	1141	CLA	C3B-CAB-CBB	25.07	177.61	126.32
19	4	4014	CLA	C3B-CAB-CBB	25.07	177.61	126.32
19	L	1130	CLA	C3B-CAB-CBB	25.19	177.86	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L	1501	CLA	C3B-CAB-CBB	25.21	177.89	126.32
19	A	9013	CLA	C3B-CAB-CBB	25.26	178.00	126.32
19	4	1004	CLA	C3B-CAB-CBB	25.41	178.31	126.32
19	L	1503	CLA	C3B-CAB-CBB	25.46	178.41	126.32
19	K	3009	CLA	C3B-CAB-CBB	25.63	178.75	126.32
19	A	1137	CLA	C3B-CAB-CBB	25.66	178.82	126.32
19	J	1308	CLA	C3B-CAB-CBB	25.71	178.91	126.32
19	A	1134	CLA	C3B-CAB-CBB	25.85	179.20	126.32
19	I	1204	CLA	C3B-CAB-CBB	25.87	179.24	126.32
19	3	3008	CLA	C3B-CAB-CBB	26.01	179.53	126.32
21	J	6012	BCR	C20-C21-C22	29.78	170.21	127.20

All (619) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	A	1105	CLA	NC
19	A	1105	CLA	ND
19	A	1105	CLA	NA
19	A	9012	CLA	C8
19	A	9012	CLA	NC
19	A	9012	CLA	ND
19	A	9012	CLA	NA
19	1	1014	CLA	C8
19	1	1014	CLA	NC
19	1	1014	CLA	ND
19	1	1014	CLA	NA
19	B	1235	CLA	C8
19	B	1235	CLA	NC
19	B	1235	CLA	ND
19	B	1235	CLA	NA
19	1	1003	CLA	NC
19	1	1003	CLA	ND
19	1	1003	CLA	NA
19	3	3007	CLA	NC
19	3	3007	CLA	ND
19	3	3007	CLA	NA
19	B	1230	CLA	NC
19	B	1230	CLA	ND
19	B	1230	CLA	NA
19	3	3011	CLA	C8
19	3	3011	CLA	NC
19	3	3011	CLA	ND

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Mol	Chain	Res	Type	Atom
19	3	3011	CLA	NA
19	2	2006	CLA	C8
19	2	2006	CLA	NC
19	2	2006	CLA	ND
19	2	2006	CLA	NA
19	2	2008	CLA	NC
19	2	2008	CLA	ND
19	2	2008	CLA	NA
19	A	9011	CLA	C8
19	A	9011	CLA	NC
19	A	9011	CLA	ND
19	A	9011	CLA	NA
19	L	1504	CLA	C8
19	L	1504	CLA	NC
19	L	1504	CLA	ND
19	L	1504	CLA	NA
19	A	1101	CLA	NC
19	A	1101	CLA	ND
19	A	1101	CLA	NA
19	F	1305	CLA	C2A
19	F	1305	CLA	NA
19	F	1305	CLA	CBD
19	F	1305	CLA	NC
19	F	1305	CLA	ND
19	F	1305	CLA	C3A
19	4	4012	CLA	NC
19	4	4012	CLA	ND
19	4	4012	CLA	NA
19	A	1139	CLA	NC
19	A	1139	CLA	ND
19	A	1139	CLA	NA
19	A	1136	CLA	C8
19	A	1136	CLA	NC
19	A	1136	CLA	ND
19	A	1136	CLA	NA
19	B	1224	CLA	C8
19	B	1224	CLA	NC
19	B	1224	CLA	ND
19	B	1224	CLA	NA
19	L	1130	CLA	C8
19	L	1130	CLA	NC
19	L	1130	CLA	ND

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Mol	Chain	Res	Type	Atom
19	L	1130	CLA	NA
19	A	1151	CLA	NC
19	A	1151	CLA	ND
19	A	1151	CLA	NA
19	B	1236	CLA	NC
19	B	1236	CLA	ND
19	B	1236	CLA	NA
19	A	1112	CLA	NC
19	A	1112	CLA	ND
19	A	1112	CLA	NA
19	1	1007	CLA	C8
19	1	1007	CLA	NC
19	1	1007	CLA	ND
19	1	1007	CLA	NA
19	A	1108	CLA	NC
19	A	1108	CLA	ND
19	A	1108	CLA	NA
19	B	1206	CLA	C8
19	B	1206	CLA	NC
19	B	1206	CLA	ND
19	B	1206	CLA	NA
19	B	1209	CLA	C8
19	B	1209	CLA	NC
19	B	1209	CLA	ND
19	B	1209	CLA	NA
19	2	2001	CLA	NC
19	2	2001	CLA	ND
19	2	2001	CLA	NA
19	3	3012	CLA	NC
19	3	3012	CLA	ND
19	3	3012	CLA	NA
19	B	1239	CLA	C8
19	B	1239	CLA	NC
19	B	1239	CLA	ND
19	B	1239	CLA	NA
19	A	1128	CLA	C8
19	A	1128	CLA	NC
19	A	1128	CLA	ND
19	A	1128	CLA	NA
19	A	1127	CLA	C8
19	A	1127	CLA	NC
19	A	1127	CLA	ND

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Mol	Chain	Res	Type	Atom
19	A	1127	CLA	NA
19	A	1117	CLA	C8
19	A	1117	CLA	NC
19	A	1117	CLA	ND
19	A	1117	CLA	NA
19	B	1232	CLA	NC
19	B	1232	CLA	ND
19	B	1232	CLA	NA
19	1	1303	CLA	C2A
19	1	1303	CLA	NC
19	1	1303	CLA	ND
19	1	1303	CLA	NA
19	1	1303	CLA	C3A
19	B	1238	CLA	C8
19	B	1238	CLA	NC
19	B	1238	CLA	ND
19	B	1238	CLA	NA
19	2	2007	CLA	C8
19	2	2007	CLA	NC
19	2	2007	CLA	ND
19	2	2007	CLA	NA
19	J	1311	CLA	C8
19	J	1311	CLA	NC
19	J	1311	CLA	ND
19	J	1311	CLA	NA
19	A	1140	CLA	C8
19	A	1140	CLA	NC
19	A	1140	CLA	ND
19	A	1140	CLA	NA
19	B	1228	CLA	NC
19	B	1228	CLA	ND
19	B	1228	CLA	NA
19	R	1144	CLA	C8
19	R	1144	CLA	NC
19	R	1144	CLA	ND
19	R	1144	CLA	NA
19	B	1218	CLA	NC
19	B	1218	CLA	ND
19	B	1218	CLA	NA
19	4	1009	CLA	NC
19	4	1009	CLA	ND
19	4	1009	CLA	NA

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Mol	Chain	Res	Type	Atom
19	L	1148	CLA	C2A
19	L	1148	CLA	NC
19	L	1148	CLA	ND
19	L	1148	CLA	NA
19	L	1148	CLA	C3A
19	B	1205	CLA	C8
19	B	1205	CLA	NC
19	B	1205	CLA	ND
19	B	1205	CLA	NA
19	2	2011	CLA	NC
19	2	2011	CLA	ND
19	2	2011	CLA	NA
19	B	1212	CLA	C8
19	B	1212	CLA	NC
19	B	1212	CLA	ND
19	B	1212	CLA	NA
19	B	1219	CLA	C8
19	B	1219	CLA	NC
19	B	1219	CLA	ND
19	B	1219	CLA	NA
19	J	1308	CLA	C8
19	J	1308	CLA	NC
19	J	1308	CLA	ND
19	J	1308	CLA	NA
19	A	1132	CLA	C8
19	A	1132	CLA	NC
19	A	1132	CLA	ND
19	A	1132	CLA	NA
19	L	1503	CLA	CBD
19	L	1503	CLA	NC
19	L	1503	CLA	ND
19	L	1503	CLA	NA
19	A	1123	CLA	C8
19	A	1123	CLA	NC
19	A	1123	CLA	ND
19	A	1123	CLA	NA
19	3	3016	CLA	C8
19	3	3016	CLA	NC
19	3	3016	CLA	ND
19	3	3016	CLA	NA
19	4	4004	CLA	NC
19	4	4004	CLA	ND

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Mol	Chain	Res	Type	Atom
19	4	4004	CLA	NA
19	A	1113	CLA	NC
19	A	1113	CLA	ND
19	A	1113	CLA	NA
19	4	4003	CLA	C8
19	4	4003	CLA	NC
19	4	4003	CLA	ND
19	4	4003	CLA	NA
19	B	1201	CLA	NC
19	B	1201	CLA	ND
19	B	1201	CLA	NA
19	3	3003	CLA	NC
19	3	3003	CLA	ND
19	3	3003	CLA	NA
19	1	1002	CLA	NC
19	1	1002	CLA	ND
19	1	1002	CLA	NA
19	1	1008	CLA	C2A
19	1	1008	CLA	NC
19	1	1008	CLA	ND
19	1	1008	CLA	NA
19	A	1103	CLA	C8
19	A	1103	CLA	NC
19	A	1103	CLA	ND
19	A	1103	CLA	NA
19	1	1011	CLA	NC
19	1	1011	CLA	ND
19	1	1011	CLA	NA
19	4	4010	CLA	NC
19	4	4010	CLA	ND
19	4	4010	CLA	NA
19	K	3009	CLA	C8
19	K	3009	CLA	NC
19	K	3009	CLA	ND
19	K	3009	CLA	NA
19	L	1501	CLA	NC
19	L	1501	CLA	ND
19	L	1501	CLA	NA
19	2	2004	CLA	NC
19	2	2004	CLA	ND
19	2	2004	CLA	NA
19	B	1226	CLA	C8

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Mol	Chain	Res	Type	Atom
19	B	1226	CLA	NC
19	B	1226	CLA	ND
19	B	1226	CLA	NA
19	B	1208	CLA	C8
19	B	1208	CLA	NC
19	B	1208	CLA	ND
19	B	1208	CLA	NA
19	B	1223	CLA	C8
19	B	1223	CLA	NC
19	B	1223	CLA	ND
19	B	1223	CLA	NA
19	4	4015	CLA	NC
19	4	4015	CLA	ND
19	4	4015	CLA	NA
19	4	1004	CLA	C8
19	4	1004	CLA	NC
19	4	1004	CLA	ND
19	4	1004	CLA	NA
19	A	1131	CLA	C8
19	A	1131	CLA	NC
19	A	1131	CLA	ND
19	A	1131	CLA	NA
19	2	2005	CLA	NC
19	2	2005	CLA	ND
19	2	2005	CLA	NA
19	H	1207	CLA	C8
19	H	1207	CLA	NC
19	H	1207	CLA	ND
19	H	1207	CLA	NA
19	A	1126	CLA	C8
19	A	1126	CLA	NC
19	A	1126	CLA	ND
19	A	1126	CLA	NA
19	L	1502	CLA	NC
19	L	1502	CLA	ND
19	L	1502	CLA	NA
19	1	1013	CLA	CBD
19	1	1013	CLA	NC
19	1	1013	CLA	ND
19	1	1013	CLA	NA
19	4	4007	CLA	NC
19	4	4007	CLA	ND

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Mol	Chain	Res	Type	Atom
19	4	4007	CLA	NA
19	G	1242	CLA	NC
19	G	1242	CLA	ND
19	G	1242	CLA	NA
19	A	9022	CLA	C8
19	A	9022	CLA	NC
19	A	9022	CLA	ND
19	A	9022	CLA	NA
19	4	4001	CLA	NC
19	4	4001	CLA	ND
19	4	4001	CLA	NA
19	B	1211	CLA	C8
19	B	1211	CLA	NC
19	B	1211	CLA	ND
19	B	1211	CLA	NA
19	A	1110	CLA	NC
19	A	1110	CLA	ND
19	A	1110	CLA	NA
19	3	3002	CLA	NC
19	3	3002	CLA	ND
19	3	3002	CLA	NA
19	B	9010	CLA	C8
19	B	9010	CLA	NC
19	B	9010	CLA	ND
19	B	9010	CLA	NA
19	B	1225	CLA	C8
19	B	1225	CLA	NC
19	B	1225	CLA	ND
19	B	1225	CLA	NA
19	2	2002	CLA	C8
19	2	2002	CLA	NC
19	2	2002	CLA	ND
19	2	2002	CLA	NA
19	A	9013	CLA	C8
19	A	9013	CLA	NC
19	A	9013	CLA	ND
19	A	9013	CLA	NA
19	3	3014	CLA	NC
19	3	3014	CLA	ND
19	3	3014	CLA	NA
19	B	1234	CLA	C8
19	B	1234	CLA	NC

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Mol	Chain	Res	Type	Atom
19	B	1234	CLA	ND
19	B	1234	CLA	NA
19	B	1217	CLA	NC
19	B	1217	CLA	ND
19	B	1217	CLA	NA
19	A	1111	CLA	NC
19	A	1111	CLA	ND
19	A	1111	CLA	NA
19	3	3008	CLA	NC
19	3	3008	CLA	ND
19	3	3008	CLA	NA
19	1	1006	CLA	NC
19	1	1006	CLA	ND
19	1	1006	CLA	NA
19	A	1149	CLA	NC
19	A	1149	CLA	C2A
19	A	1149	CLA	ND
19	A	1149	CLA	NA
19	A	1149	CLA	CBD
19	A	1135	CLA	NC
19	A	1135	CLA	ND
19	A	1135	CLA	NA
19	3	3017	CLA	NC
19	3	3017	CLA	ND
19	3	3017	CLA	NA
19	H	1505	CLA	C8
19	H	1505	CLA	NC
19	H	1505	CLA	ND
19	H	1505	CLA	NA
19	B	1221	CLA	NC
19	B	1221	CLA	ND
19	B	1221	CLA	NA
19	H	1145	CLA	C8
19	H	1145	CLA	CBD
19	H	1145	CLA	NC
19	H	1145	CLA	ND
19	H	1145	CLA	NA
19	R	1150	CLA	C8
19	R	1150	CLA	NC
19	R	1150	CLA	ND
19	R	1150	CLA	NA
19	K	1146	CLA	NC

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Mol	Chain	Res	Type	Atom
19	K	1146	CLA	ND
19	K	1146	CLA	NA
19	B	1203	CLA	C8
19	B	1203	CLA	NC
19	B	1203	CLA	ND
19	B	1203	CLA	NA
19	2	2014	CLA	C8
19	2	2014	CLA	NC
19	2	2014	CLA	ND
19	2	2014	CLA	NA
19	3	3004	CLA	NC
19	3	3004	CLA	ND
19	3	3004	CLA	NA
19	4	1304	CLA	C8
19	4	1304	CLA	CBD
19	4	1304	CLA	NC
19	4	1304	CLA	ND
19	4	1304	CLA	NA
19	3	3010	CLA	NC
19	3	3010	CLA	ND
19	3	3010	CLA	NA
19	A	1124	CLA	C8
19	A	1124	CLA	NC
19	A	1124	CLA	ND
19	A	1124	CLA	NA
19	B	1222	CLA	C8
19	B	1222	CLA	NC
19	B	1222	CLA	ND
19	B	1222	CLA	NA
19	4	4005	CLA	NC
19	4	4005	CLA	ND
19	4	4005	CLA	NA
19	A	1121	CLA	NC
19	A	1121	CLA	ND
19	A	1121	CLA	NA
19	2	2012	CLA	NC
19	2	2012	CLA	ND
19	2	2012	CLA	NA
19	A	1138	CLA	C8
19	A	1138	CLA	NC
19	A	1138	CLA	ND
19	A	1138	CLA	NA

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Mol	Chain	Res	Type	Atom
19	3	1147	CLA	NC
19	3	1147	CLA	ND
19	3	1147	CLA	NA
19	1	1005	CLA	NC
19	1	1005	CLA	ND
19	1	1005	CLA	NA
19	3	3013	CLA	C8
19	3	3013	CLA	NC
19	3	3013	CLA	ND
19	3	3013	CLA	NA
19	1	1012	CLA	NC
19	1	1012	CLA	ND
19	1	1012	CLA	NA
19	A	1104	CLA	C8
19	A	1104	CLA	NC
19	A	1104	CLA	ND
19	A	1104	CLA	NA
19	3	3001	CLA	NC
19	3	3001	CLA	ND
19	3	3001	CLA	NA
19	2	1307	CLA	NC
19	2	1307	CLA	ND
19	2	1307	CLA	NA
19	A	1116	CLA	NC
19	A	1116	CLA	ND
19	A	1116	CLA	NA
19	A	1309	CLA	NC
19	A	1309	CLA	ND
19	A	1309	CLA	NA
19	A	1102	CLA	C8
19	A	1102	CLA	NC
19	A	1102	CLA	ND
19	A	1102	CLA	NA
19	4	4011	CLA	NC
19	4	4011	CLA	ND
19	4	4011	CLA	NA
19	A	1119	CLA	C8
19	A	1119	CLA	NC
19	A	1119	CLA	ND
19	A	1119	CLA	NA
19	K	1142	CLA	NC
19	K	1142	CLA	ND

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Mol	Chain	Res	Type	Atom
19	K	1142	CLA	NA
19	I	1204	CLA	C8
19	I	1204	CLA	NC
19	I	1204	CLA	ND
19	I	1204	CLA	NA
19	B	1215	CLA	C8
19	B	1215	CLA	NC
19	B	1215	CLA	ND
19	B	1215	CLA	NA
19	K	1143	CLA	NC
19	K	1143	CLA	ND
19	K	1143	CLA	NA
19	4	4006	CLA	C8
19	4	4006	CLA	NC
19	4	4006	CLA	ND
19	4	4006	CLA	NA
19	2	2010	CLA	NC
19	2	2010	CLA	ND
19	2	2010	CLA	NA
19	A	1120	CLA	NC
19	A	1120	CLA	ND
19	A	1120	CLA	NA
19	B	1213	CLA	NC
19	B	1213	CLA	ND
19	B	1213	CLA	NA
19	A	1129	CLA	NC
19	A	1129	CLA	ND
19	A	1129	CLA	NA
19	A	1137	CLA	NC
19	A	1137	CLA	ND
19	A	1137	CLA	NA
19	B	1231	CLA	NC
19	B	1231	CLA	ND
19	B	1231	CLA	NA
19	B	1216	CLA	C8
19	B	1216	CLA	NC
19	B	1216	CLA	ND
19	B	1216	CLA	NA
19	2	4009	CLA	C8
19	2	4009	CLA	NC
19	2	4009	CLA	ND
19	2	4009	CLA	NA

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Mol	Chain	Res	Type	Atom
19	A	1141	CLA	C8
19	A	1141	CLA	NC
19	A	1141	CLA	ND
19	A	1141	CLA	NA
19	A	1122	CLA	C8
19	A	1122	CLA	NC
19	A	1122	CLA	ND
19	A	1122	CLA	NA
19	1	1001	CLA	NC
19	1	1001	CLA	ND
19	1	1001	CLA	NA
19	2	2013	CLA	NC
19	2	2013	CLA	ND
19	2	2013	CLA	NA
19	A	1134	CLA	NC
19	A	1134	CLA	ND
19	A	1134	CLA	NA
19	3	3005	CLA	NC
19	3	3005	CLA	ND
19	3	3005	CLA	NA
19	3	2009	CLA	C8
19	3	2009	CLA	NC
19	3	2009	CLA	ND
19	3	2009	CLA	NA
19	4	4002	CLA	NC
19	4	4002	CLA	C2A
19	4	4002	CLA	ND
19	4	4002	CLA	NA
19	3	1118	CLA	NC
19	3	1118	CLA	ND
19	3	1118	CLA	NA
19	A	1115	CLA	C8
19	A	1115	CLA	NC
19	A	1115	CLA	ND
19	A	1115	CLA	NA
19	3	3015	CLA	NC
19	3	3015	CLA	ND
19	3	3015	CLA	NA
19	A	1107	CLA	C8
19	A	1107	CLA	NC
19	A	1107	CLA	ND
19	A	1107	CLA	NA

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Mol	Chain	Res	Type	Atom
19	B	1220	CLA	NC
19	B	1220	CLA	ND
19	B	1220	CLA	NA
19	4	4014	CLA	NC
19	4	4014	CLA	ND
19	4	4014	CLA	NA
19	B	1229	CLA	C8
19	B	1229	CLA	NC
19	B	1229	CLA	ND
19	B	1229	CLA	NA
19	B	1210	CLA	C8
19	B	1210	CLA	NC
19	B	1210	CLA	ND
19	B	1210	CLA	NA
19	A	1133	CLA	NC
19	A	1133	CLA	ND
19	A	1133	CLA	NA
19	B	1301	CLA	NC
19	B	1301	CLA	ND
19	B	1301	CLA	NA
19	1	1010	CLA	NC
19	1	1010	CLA	ND
19	1	1010	CLA	NA
19	B	1227	CLA	NC
19	B	1227	CLA	ND
19	B	1227	CLA	NA
19	A	1106	CLA	C8
19	A	1106	CLA	NC
19	A	1106	CLA	ND
19	A	1106	CLA	NA
19	A	1109	CLA	C8
19	A	1109	CLA	NC
19	A	1109	CLA	ND
19	A	1109	CLA	NA
19	1	1015	CLA	NC
19	1	1015	CLA	ND
19	1	1015	CLA	NA
19	3	3006	CLA	NC
19	3	3006	CLA	ND
19	3	3006	CLA	NA
19	F	1302	CLA	NC
19	F	1302	CLA	ND

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Mol	Chain	Res	Type	Atom
19	F	1302	CLA	NA
19	B	1214	CLA	C8
19	B	1214	CLA	NC
19	B	1214	CLA	ND
19	B	1214	CLA	NA
20	A	5001	PQN	C23
19	2	2003	CLA	NC
19	2	2003	CLA	ND
19	2	2003	CLA	NA
19	1	1310	CLA	NC
19	1	1310	CLA	ND
19	1	1310	CLA	NA
19	A	9023	CLA	C8
19	A	9023	CLA	NC
19	A	9023	CLA	ND
19	A	9023	CLA	NA
19	4	1306	CLA	C8
19	4	1306	CLA	NC
19	4	1306	CLA	ND
19	4	1306	CLA	NA
19	B	1202	CLA	C8
19	B	1202	CLA	NC
19	B	1202	CLA	ND
19	B	1202	CLA	NA
19	A	1237	CLA	C8
19	A	1237	CLA	NC
19	A	1237	CLA	ND
19	A	1237	CLA	NA
19	A	1125	CLA	C8
19	A	1125	CLA	NC
19	A	1125	CLA	ND
19	A	1125	CLA	NA
19	H	1241	CLA	C8
19	H	1241	CLA	NC
19	H	1241	CLA	ND
19	H	1241	CLA	NA
19	B	1233	CLA	NC
19	B	1233	CLA	ND
19	B	1233	CLA	NA
19	F	1240	CLA	NC
19	F	1240	CLA	ND
19	F	1240	CLA	NA

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Mol	Chain	Res	Type	Atom
19	4	4013	CLA	NC
19	4	4013	CLA	ND
19	4	4013	CLA	NA
20	B	5002	PQN	C23

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	F	6014	BCR	C21-C20-C19-C18
21	1	6023	BCR	C11-C10-C9-C34
21	1	6023	BCR	C11-C10-C9-C8
22	L	7029	LMU	C1-O1'-C1'-O5'
21	3	6022	BCR	C21-C20-C19-C18
22	F	7036	LMU	C1-O1'-C1'-O5'
19	L	1501	CLA	CED-O2D-CGD-CBD
19	J	1308	CLA	CED-O2D-CGD-CBD
19	B	1222	CLA	CED-O2D-CGD-CBD
19	J	1311	CLA	CED-O2D-CGD-CBD
19	L	1504	CLA	CED-O2D-CGD-CBD
19	1	1013	CLA	CED-O2D-CGD-CBD
19	A	1124	CLA	CED-O2D-CGD-CBD
19	B	1227	CLA	CED-O2D-CGD-CBD
19	A	9012	CLA	CED-O2D-CGD-CBD
19	1	1005	CLA	CED-O2D-CGD-CBD
19	F	1305	CLA	CED-O2D-CGD-CBD

There are no ring outliers.

234 monomers are involved in 3097 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	1	1001	CLA	11	0
19	1	1002	CLA	10	0
19	1	1003	CLA	5	0
19	1	1005	CLA	5	0
19	1	1006	CLA	15	0
19	1	1007	CLA	19	0
19	1	1008	CLA	8	1
19	1	1010	CLA	8	0
19	1	1011	CLA	6	0
19	1	1012	CLA	2	0
19	1	1013	CLA	13	0
19	1	1014	CLA	17	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	1	1015	CLA	3	0
19	1	1303	CLA	10	0
21	1	6023	BCR	6	0
22	1	7004	LMU	6	0
22	1	7013	LMU	4	0
19	2	2001	CLA	13	0
19	2	2002	CLA	19	0
19	2	2003	CLA	1	0
19	2	2004	CLA	18	0
19	2	2006	CLA	7	0
19	2	2007	CLA	18	0
19	2	2011	CLA	1	0
19	2	2012	CLA	20	0
19	2	2013	CLA	5	0
19	2	2014	CLA	35	0
19	2	4009	CLA	6	0
22	2	7006	LMU	8	0
22	2	7027	LMU	3	0
22	2	7031	LMU	2	0
22	2	7046	LMU	1	0
19	3	1147	CLA	15	0
19	3	2009	CLA	37	0
19	3	3003	CLA	7	0
19	3	3004	CLA	7	0
19	3	3005	CLA	9	0
19	3	3006	CLA	9	0
19	3	3007	CLA	2	0
19	3	3008	CLA	15	0
19	3	3010	CLA	5	0
19	3	3011	CLA	12	0
19	3	3012	CLA	11	0
19	3	3013	CLA	18	0
19	3	3016	CLA	14	0
19	3	3017	CLA	4	0
21	3	6022	BCR	6	0
22	3	7003	LMU	20	0
22	3	7005	LMU	38	0
19	4	1004	CLA	33	0
19	4	1009	CLA	3	0
19	4	1304	CLA	23	0
19	4	1306	CLA	19	0
19	4	4001	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	4	4002	CLA	23	0
19	4	4003	CLA	2	0
19	4	4004	CLA	2	0
19	4	4006	CLA	11	0
19	4	4010	CLA	2	0
19	4	4011	CLA	2	0
19	4	4012	CLA	7	0
19	4	4013	CLA	11	0
19	4	4014	CLA	8	0
19	4	4015	CLA	4	0
22	4	7008	LMU	3	0
22	4	7009	LMU	3	0
22	4	7019	LMU	1	0
22	4	7033	LMU	7	0
22	4	7034	LMU	36	0
22	4	7052	LMU	36	0
22	4	7053	LMU	13	0
19	A	1101	CLA	15	0
19	A	1102	CLA	19	0
19	A	1103	CLA	19	0
19	A	1104	CLA	15	0
19	A	1105	CLA	26	0
19	A	1106	CLA	27	0
19	A	1107	CLA	40	0
19	A	1108	CLA	7	0
19	A	1109	CLA	18	0
19	A	1110	CLA	3	0
19	A	1111	CLA	21	0
19	A	1112	CLA	31	0
19	A	1113	CLA	9	0
19	A	1115	CLA	76	0
19	A	1116	CLA	9	0
19	A	1117	CLA	27	0
19	A	1119	CLA	43	0
19	A	1120	CLA	10	0
19	A	1121	CLA	8	0
19	A	1122	CLA	24	0
19	A	1123	CLA	29	0
19	A	1124	CLA	59	0
19	A	1125	CLA	65	0
19	A	1126	CLA	43	0
19	A	1127	CLA	16	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	1128	CLA	21	0
19	A	1129	CLA	8	0
19	A	1131	CLA	36	0
19	A	1132	CLA	18	0
19	A	1133	CLA	31	0
19	A	1134	CLA	20	0
19	A	1135	CLA	23	0
19	A	1136	CLA	24	0
19	A	1137	CLA	8	0
19	A	1138	CLA	29	0
19	A	1139	CLA	31	0
19	A	1140	CLA	47	0
19	A	1141	CLA	29	0
19	A	1149	CLA	7	0
19	A	1151	CLA	18	0
19	A	1237	CLA	31	0
20	A	5001	PQN	9	0
21	A	6002	BCR	43	0
21	A	6003	BCR	14	0
21	A	6007	BCR	32	0
21	A	6008	BCR	27	0
21	A	6011	BCR	46	0
22	A	7010	LMU	6	0
22	A	7016	LMU	12	0
22	A	7023	LMU	6	0
22	A	7044	LMU	1	0
22	A	7045	LMU	2	0
24	A	8001	SF4	2	0
19	A	9011	CLA	13	0
19	A	9012	CLA	39	0
19	A	9013	CLA	29	0
19	A	9022	CLA	39	0
19	A	9023	CLA	53	0
19	B	1201	CLA	11	0
19	B	1202	CLA	31	0
19	B	1203	CLA	19	0
19	B	1205	CLA	25	0
19	B	1206	CLA	20	0
19	B	1208	CLA	6	0
19	B	1209	CLA	14	0
19	B	1210	CLA	21	0
19	B	1211	CLA	19	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	1212	CLA	14	0
19	B	1213	CLA	19	0
19	B	1214	CLA	23	0
19	B	1215	CLA	10	0
19	B	1216	CLA	15	0
19	B	1217	CLA	9	0
19	B	1218	CLA	20	0
19	B	1219	CLA	13	0
19	B	1220	CLA	44	0
19	B	1221	CLA	21	0
19	B	1222	CLA	43	0
19	B	1223	CLA	38	0
19	B	1224	CLA	19	0
19	B	1225	CLA	28	0
19	B	1226	CLA	21	0
19	B	1227	CLA	11	0
19	B	1228	CLA	14	0
19	B	1229	CLA	20	0
19	B	1230	CLA	21	0
19	B	1231	CLA	16	0
19	B	1232	CLA	18	0
19	B	1233	CLA	6	0
19	B	1234	CLA	11	0
19	B	1235	CLA	62	0
19	B	1236	CLA	24	0
19	B	1238	CLA	24	0
19	B	1239	CLA	22	0
19	B	1301	CLA	6	0
20	B	5002	PQN	22	0
21	B	6004	BCR	6	0
21	B	6005	BCR	7	0
21	B	6006	BCR	14	0
21	B	6010	BCR	23	0
21	B	6017	BCR	42	0
21	B	6020	BCR	24	0
22	B	7012	LMU	1	0
22	B	7038	LMU	7	0
22	B	7040	LMU	3	0
23	B	7101	LMG	19	0
19	B	9010	CLA	17	0
24	C	8002	SF4	6	0
24	C	8003	SF4	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	D	7050	LMU	21	0
22	E	7037	LMU	7	0
22	E	7048	LMU	17	0
19	F	1302	CLA	10	0
19	F	1305	CLA	13	0
21	F	6014	BCR	24	0
21	F	6016	BCR	37	0
22	F	7036	LMU	12	0
19	G	1242	CLA	9	0
22	G	7026	LMU	9	0
22	G	7039	LMU	4	0
22	G	7051	LMU	1	0
19	H	1145	CLA	22	0
19	H	1207	CLA	25	0
19	H	1241	CLA	11	0
19	H	1505	CLA	3	0
22	H	7002	LMU	3	0
22	H	7011	LMU	15	0
22	H	7017	LMU	2	0
22	H	7028	LMU	2	0
22	H	7030	LMU	4	0
22	H	7032	LMU	11	0
22	H	7043	LMU	3	0
19	I	1204	CLA	7	0
21	I	6018	BCR	15	0
21	I	6021	BCR	32	0
19	J	1308	CLA	31	0
19	J	1311	CLA	20	0
21	J	6012	BCR	32	0
19	K	1142	CLA	15	1
19	K	1143	CLA	29	0
19	K	1146	CLA	7	0
19	K	3009	CLA	3	7
22	K	7001	LMU	11	0
22	K	7041	LMU	6	0
22	K	7042	LMU	16	0
22	K	7047	LMU	5	2
19	L	1130	CLA	29	0
19	L	1148	CLA	21	0
19	L	1501	CLA	17	0
19	L	1502	CLA	27	0
19	L	1503	CLA	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	L	1504	CLA	21	0
21	L	6019	BCR	34	0
22	L	7029	LMU	11	0
22	N	7049	LMU	9	0
19	R	1144	CLA	10	0
19	R	1150	CLA	3	0
22	R	7007	LMU	5	0
22	R	7014	LMU	4	0
22	R	7020	LMU	10	0
22	R	7021	LMU	9	0
22	R	7022	LMU	5	0
22	R	7025	LMU	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	730/738 (98%)	0.18	22 (3%) 54 47	12, 19, 25, 27	0
2	B	733/733 (100%)	0.11	15 (2%) 68 62	8, 18, 26, 28	0
3	C	81/81 (100%)	0.73	10 (12%) 5 4	17, 21, 23, 24	0
4	D	138/138 (100%)	0.27	9 (6%) 22 18	18, 22, 25, 27	0
5	E	64/64 (100%)	0.18	4 (6%) 23 19	17, 21, 24, 25	0
6	F	154/154 (100%)	0.14	8 (5%) 31 25	17, 22, 25, 26	0
7	G	95/95 (100%)	0.44	5 (5%) 30 24	20, 25, 28, 29	0
8	H	69/69 (100%)	0.27	3 (4%) 39 32	22, 24, 29, 30	0
9	I	30/30 (100%)	0.05	2 (6%) 21 17	17, 19, 22, 22	0
10	J	42/42 (100%)	0.28	3 (7%) 19 15	17, 21, 25, 26	0
11	K	84/84 (100%)	1.06	16 (19%) 2 1	24, 27, 29, 30	0
12	L	161/161 (100%)	0.22	9 (5%) 28 22	16, 20, 26, 27	0
13	N	85/85 (100%)	0.15	3 (3%) 48 40	22, 25, 28, 29	0
14	R	0/53	-	-	-	-
15	1	165/170 (97%)	0.40	14 (8%) 13 10	32, 59, 69, 70	0
16	2	176/176 (100%)	0.23	10 (5%) 27 22	32, 52, 63, 66	0
17	3	156/172 (90%)	0.30	9 (5%) 26 21	25, 28, 32, 33	0
18	4	166/166 (100%)	0.30	13 (7%) 16 13	20, 44, 56, 57	0
All	All	3129/3211 (97%)	0.24	155 (4%) 32 26	8, 22, 57, 70	0

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	K	62	SER	9.1
16	2	181	PRO	8.7
15	1	132	GLY	8.5

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Mol	Chain	Res	Type	RSRZ
2	B	491	ASN	6.8
18	4	118	ILE	5.3
6	F	229	ASN	5.2
12	L	126	ALA	5.1
12	L	127	GLY	5.0
1	A	251	ASN	4.8
12	L	163	SER	4.6
1	A	505	PRO	4.6
12	L	162	PRO	4.5
4	D	170	ASP	4.5
15	1	174	SER	4.5
15	1	153	SER	4.4
7	G	130	TRP	4.3
11	K	109	CYS	4.3
11	K	90	ASP	4.2
13	N	141	LYS	4.1
3	C	17	CYS	4.0
15	1	127	ASN	3.9
4	D	195	VAL	3.9
16	2	197	GLY	3.8
17	3	86	PRO	3.7
11	K	68	GLY	3.6
1	A	249	ILE	3.6
15	1	212	GLY	3.6
1	A	635	THR	3.6
11	K	72	LEU	3.5
12	L	130	GLY	3.5
18	4	230	ASP	3.5
2	B	562	PRO	3.4
18	4	187	GLY	3.3
4	D	205	LYS	3.3
18	4	182	VAL	3.2
4	D	78	THR	3.2
11	K	105	ASP	3.2
1	A	391	THR	3.2
7	G	142	LEU	3.1
18	4	119	GLY	3.1
2	B	502	ASN	3.1
17	3	167	PHE	3.1
4	D	169	LYS	3.1
7	G	143	ALA	3.0
1	A	752	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	66	SER	3.0
15	1	217	LEU	3.0
13	N	162	CYS	3.0
6	F	115	PRO	3.0
16	2	180	ASP	3.0
16	2	168	TRP	2.9
1	A	124	TRP	2.9
18	4	196	PRO	2.9
10	J	7	TYR	2.9
15	1	218	ALA	2.9
18	4	130	GLY	2.9
11	K	71	GLY	2.9
16	2	268	PRO	2.8
3	C	34	CYS	2.8
17	3	166	GLY	2.8
10	J	41	PHE	2.8
3	C	15	THR	2.8
16	2	198	GLY	2.8
15	1	164	PRO	2.8
5	E	66	ILE	2.7
1	A	494	ASN	2.7
3	C	37	LYS	2.7
8	H	60	ASN	2.7
15	1	154	MET	2.7
17	3	130	GLN	2.7
11	K	67	ALA	2.6
5	E	102	PRO	2.6
4	D	86	SER	2.6
1	A	245	PRO	2.6
10	J	4	LEU	2.6
15	1	215	GLU	2.6
18	4	185	PRO	2.5
1	A	181	ALA	2.5
11	K	47	ASP	2.5
2	B	263	PRO	2.5
2	B	484	PRO	2.5
1	A	487	VAL	2.5
6	F	114	ALA	2.5
1	A	486	PRO	2.5
16	2	199	LEU	2.5
17	3	84	SER	2.5
2	B	492	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
3	C	67	VAL	2.4
3	C	56	SER	2.4
5	E	68	PRO	2.4
6	F	214	PRO	2.4
11	K	80	ALA	2.4
2	B	212	PHE	2.4
15	1	116	ALA	2.4
6	F	215	VAL	2.4
17	3	135	ALA	2.4
18	4	186	GLY	2.4
11	K	128	GLY	2.3
16	2	196	PRO	2.3
9	I	30	LYS	2.3
18	4	242	ASN	2.3
15	1	87	CYS	2.3
12	L	157	ALA	2.3
2	B	479	SER	2.3
4	D	203	THR	2.3
3	C	50	GLY	2.2
8	H	54	ASP	2.2
5	E	103	VAL	2.2
1	A	32	GLU	2.2
13	N	164	SER	2.2
6	F	187	ASP	2.2
11	K	51	SER	2.2
17	3	102	GLU	2.2
2	B	210	ASN	2.2
11	K	73	ALA	2.2
11	K	54	ASN	2.2
17	3	194	PHE	2.2
16	2	231	ALA	2.2
15	1	120	GLY	2.2
3	C	16	GLN	2.1
3	C	60	THR	2.1
11	K	110	GLY	2.1
12	L	161	ALA	2.1
1	A	69	SER	2.1
9	I	29	GLU	2.1
1	A	101	ALA	2.1
7	G	132	SER	2.1
4	D	210	LEU	2.1
2	B	260	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
17	3	106	GLY	2.1
18	4	129	ALA	2.1
18	4	193	ASN	2.1
1	A	34	TRP	2.1
16	2	171	ILE	2.1
1	A	344	LYS	2.1
4	D	204	GLY	2.1
6	F	228	ASP	2.1
2	B	319	HIS	2.1
3	C	80	ALA	2.1
8	H	74	SER	2.1
11	K	101	PHE	2.1
7	G	109	GLU	2.1
2	B	69	ALA	2.1
1	A	220	ARG	2.0
2	B	124	TRP	2.0
2	B	208	ARG	2.0
12	L	160	THR	2.0
1	A	100	GLY	2.0
1	A	33	GLN	2.0
6	F	212	SER	2.0
12	L	186	THR	2.0
15	1	192	ARG	2.0
2	B	487	ASN	2.0
1	A	484	LEU	2.0
18	4	85	PRO	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
19	CLA	L	1504	55/65	0.57	0.42	5.65	18,25,27,27	0
21	BCR	A	6002	40/40	0.65	0.40	4.95	23,27,32,33	0
19	CLA	1	1006	36/65	0.63	0.43	3.88	29,30,30,31	0
21	BCR	A	6007	40/40	0.74	0.38	3.26	19,23,28,28	0
19	CLA	4	4004	25/65	0.68	0.35	3.06	29,30,30,30	0
21	BCR	B	6017	40/40	0.81	0.34	2.91	15,18,20,20	0
19	CLA	B	1213	46/65	0.69	0.37	2.73	19,21,24,25	0
21	BCR	A	6008	40/40	0.81	0.35	2.72	21,24,27,27	0
19	CLA	B	1201	45/65	0.80	0.28	2.64	19,21,22,22	0
19	CLA	A	1119	65/65	0.81	0.35	2.30	13,18,19,20	0
23	LMG	B	7101	49/55	0.75	0.36	1.91	14,18,26,27	0
19	CLA	B	1301	36/65	0.77	0.30	1.87	27,28,29,29	0
21	BCR	B	6010	40/40	0.82	0.34	1.68	13,15,16,16	0
19	CLA	B	1216	61/65	0.84	0.28	1.64	12,18,19,20	0
21	BCR	J	6012	40/40	0.76	0.33	1.64	19,24,26,26	0
19	CLA	L	1130	65/65	0.81	0.28	1.60	13,18,19,20	0
19	CLA	A	1136	65/65	0.89	0.27	1.57	14,15,16,17	0
21	BCR	A	6003	40/40	0.76	0.35	1.56	21,24,26,26	0
21	BCR	F	6016	40/40	0.84	0.28	1.56	13,16,17,17	0
19	CLA	4	4001	50/65	0.68	0.43	1.55	21,23,25,25	0
21	BCR	I	6018	40/40	0.81	0.31	1.52	14,15,18,18	0
19	CLA	A	1120	51/65	0.85	0.37	1.49	22,24,24,26	0
19	CLA	4	4003	55/65	0.63	0.29	1.46	15,34,47,50	0
19	CLA	L	1502	47/65	0.83	0.25	1.45	17,19,20,20	0
21	BCR	F	6014	40/40	0.83	0.31	1.44	9,11,15,15	0
21	BCR	I	6021	40/40	0.76	0.30	1.42	16,20,22,22	0
19	CLA	A	1102	55/65	0.79	0.30	1.40	13,19,20,20	0
19	CLA	B	1231	45/65	0.81	0.28	1.35	19,20,21,21	0
22	LMU	K	7047	35/35	0.71	0.27	1.30	14,33,46,49	0
19	CLA	A	1124	65/65	0.84	0.28	1.25	18,21,23,24	0
19	CLA	B	1226	65/65	0.88	0.31	1.21	11,12,19,19	0
19	CLA	A	1112	45/65	0.69	0.41	1.19	23,26,26,27	0
19	CLA	A	1138	65/65	0.85	0.29	1.16	15,18,19,20	0
19	CLA	B	1239	65/65	0.87	0.30	1.15	8,11,13,14	0
21	BCR	L	6019	40/40	0.79	0.34	1.11	15,17,19,19	0
19	CLA	K	3009	65/65	0.70	0.37	1.03	22,25,27,28	0
19	CLA	H	1207	65/65	0.81	0.28	1.02	15,17,19,20	0
21	BCR	B	6006	40/40	0.80	0.38	1.01	15,19,20,21	0
21	BCR	B	6005	40/40	0.87	0.29	0.99	14,16,17,17	0
19	CLA	A	1237	65/65	0.86	0.28	0.91	8,17,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
19	CLA	1	1015	25/65	0.71	0.24	0.89	27,28,28,28	0
19	CLA	B	1211	65/65	0.82	0.31	0.88	17,20,21,21	0
19	CLA	B	1232	45/65	0.69	0.42	0.85	23,26,27,27	0
19	CLA	B	1230	50/65	0.83	0.28	0.84	17,18,19,20	0
20	PQN	A	5001	33/33	0.88	0.29	0.82	12,13,14,15	0
21	BCR	B	6020	40/40	0.89	0.25	0.82	8,11,12,13	0
19	CLA	A	1126	65/65	0.88	0.29	0.78	12,14,15,15	0
19	CLA	3	3003	36/65	0.74	0.34	0.77	29,30,31,31	0
19	CLA	A	1117	65/65	0.84	0.31	0.76	10,20,21,22	0
19	CLA	A	1104	57/65	0.89	0.27	0.75	13,15,18,18	0
19	CLA	B	1205	65/65	0.89	0.26	0.74	9,13,14,14	0
19	CLA	A	1106	65/65	0.91	0.29	0.73	10,12,13,14	0
19	CLA	G	1242	51/65	0.68	0.34	0.72	26,28,29,29	0
21	BCR	B	6004	40/40	0.80	0.33	0.71	18,20,22,22	0
19	CLA	A	1103	65/65	0.85	0.28	0.70	13,14,21,22	0
19	CLA	F	1240	36/65	0.87	0.23	0.70	15,16,17,17	0
19	CLA	B	1202	65/65	0.89	0.25	0.69	7,16,16,18	0
19	CLA	A	1105	46/65	0.77	0.37	0.68	22,23,24,24	0
19	CLA	A	1128	65/65	0.86	0.27	0.67	14,16,17,18	0
19	CLA	A	1123	65/65	0.83	0.30	0.64	12,18,19,20	0
19	CLA	B	1223	65/65	0.82	0.32	0.61	13,18,19,20	0
19	CLA	A	1139	51/65	0.88	0.23	0.59	16,16,17,18	0
19	CLA	A	9022	65/65	0.90	0.28	0.57	2,12,26,31	0
19	CLA	B	1225	65/65	0.88	0.29	0.57	9,12,13,14	0
19	CLA	B	1224	65/65	0.88	0.27	0.57	9,13,14,15	0
19	CLA	4	4006	55/65	0.78	0.23	0.56	16,23,24,24	0
19	CLA	A	1116	52/65	0.78	0.28	0.55	24,25,26,26	0
19	CLA	B	1212	60/65	0.74	0.32	0.53	20,23,25,26	0
19	CLA	B	1222	58/65	0.79	0.34	0.53	18,21,23,24	0
19	CLA	L	1501	50/65	0.86	0.24	0.51	20,20,21,21	0
19	CLA	A	1135	51/65	0.84	0.27	0.51	16,19,19,21	0
19	CLA	A	1125	65/65	0.86	0.24	0.46	15,17,19,20	0
21	BCR	A	6011	40/40	0.86	0.30	0.45	10,15,16,16	0
19	CLA	A	1132	65/65	0.86	0.27	0.44	13,17,18,19	0
19	CLA	B	1229	65/65	0.82	0.27	0.42	8,12,14,15	0
22	LMU	L	7029	35/35	0.63	0.31	0.40	30,44,53,55	0
19	CLA	B	1215	60/65	0.88	0.27	0.39	11,13,15,16	0
19	CLA	B	1218	46/65	0.78	0.30	0.38	20,20,22,23	0
19	CLA	A	9023	65/65	0.89	0.27	0.37	2,14,29,38	0
19	CLA	I	1204	60/65	0.84	0.24	0.37	13,17,18,18	0
19	CLA	3	3005	25/65	0.59	0.28	0.36	31,31,31,31	0
19	CLA	L	1503	50/65	0.81	0.25	0.36	19,21,23,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
19	CLA	A	1111	54/65	0.84	0.26	0.29	20,24,24,24	0
19	CLA	B	1206	65/65	0.87	0.27	0.25	10,12,17,18	0
19	CLA	B	1234	60/65	0.85	0.28	0.24	13,14,21,21	0
19	CLA	4	1306	55/65	0.71	0.32	0.23	20,26,27,27	0
19	CLA	3	3002	25/65	0.75	0.27	0.21	28,28,28,28	0
19	CLA	B	1219	55/65	0.85	0.24	0.21	18,18,21,21	0
19	CLA	A	1131	65/65	0.88	0.25	0.18	12,14,16,16	0
19	CLA	B	1217	50/65	0.84	0.26	0.17	19,21,22,23	0
19	CLA	2	2012	50/65	0.81	0.26	0.15	20,22,23,23	0
19	CLA	B	1208	54/65	0.85	0.26	0.13	18,18,21,22	0
19	CLA	B	1236	47/65	0.88	0.28	0.12	14,15,17,17	0
19	CLA	B	1209	55/65	0.83	0.26	0.12	18,19,20,21	0
19	CLA	B	1238	65/65	0.86	0.27	0.11	10,14,15,16	0
19	CLA	B	1235	65/65	0.88	0.26	0.08	14,15,16,17	0
19	CLA	4	4012	36/65	0.86	0.21	0.08	14,15,16,16	0
19	CLA	A	1122	55/65	0.88	0.22	0.01	13,14,18,18	0
19	CLA	A	1101	50/65	0.87	0.23	-0.01	17,18,18,19	0
19	CLA	A	1109	65/65	0.84	0.28	-0.02	13,20,22,23	0
20	PQN	B	5002	33/33	0.90	0.26	-0.05	7,8,14,14	0
19	CLA	1	1003	47/65	0.74	0.24	-0.08	17,19,19,20	0
19	CLA	B	1214	59/65	0.87	0.24	-0.09	18,20,22,23	0
19	CLA	4	1004	55/65	0.73	0.26	-0.10	22,25,26,27	0
19	CLA	B	1220	65/65	0.87	0.24	-0.11	13,15,20,21	0
19	CLA	B	1228	50/65	0.86	0.23	-0.12	12,14,14,15	0
19	CLA	B	1203	65/65	0.91	0.24	-0.15	10,13,14,15	0
19	CLA	A	1115	65/65	0.81	0.24	-0.16	10,28,41,42	0
19	CLA	A	1127	55/65	0.89	0.25	-0.17	13,16,17,18	0
19	CLA	A	1140	65/65	0.85	0.28	-0.17	15,18,19,21	0
19	CLA	3	1147	46/65	0.73	0.29	-0.19	25,27,28,28	0
19	CLA	A	1108	45/65	0.78	0.29	-0.21	19,22,23,24	0
19	CLA	A	1107	55/65	0.87	0.26	-0.23	15,16,24,24	0
19	CLA	A	1133	50/65	0.85	0.23	-0.24	17,19,19,20	0
19	CLA	B	1221	54/65	0.91	0.22	-0.24	13,13,16,16	0
19	CLA	B	9010	65/65	0.89	0.25	-0.26	2,12,34,40	0
19	CLA	F	1302	41/65	0.73	0.25	-0.26	24,26,26,26	0
19	CLA	3	3013	65/65	0.77	0.26	-0.27	20,21,24,25	0
19	CLA	A	9011	65/65	0.91	0.26	-0.28	2,11,30,40	0
19	CLA	B	1210	65/65	0.90	0.23	-0.30	16,20,21,22	0
19	CLA	A	1113	50/65	0.75	0.31	-0.31	19,22,23,24	0
22	LMU	A	7044	35/35	0.78	0.18	-0.35	8,20,39,40	0
19	CLA	2	2004	50/65	0.74	0.26	-0.36	23,25,25,25	0
19	CLA	A	1129	50/65	0.88	0.20	-0.38	17,19,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
19	CLA	1	1012	36/65	0.86	0.22	-0.40	23,24,25,25	0
19	CLA	A	9012	65/65	0.89	0.25	-0.43	2,14,28,36	0
19	CLA	A	1137	47/65	0.90	0.24	-0.43	13,14,15,17	0
19	CLA	B	1227	50/65	0.89	0.23	-0.46	13,15,16,17	0
19	CLA	A	9013	65/65	0.89	0.25	-0.46	2,10,29,32	0
22	LMU	A	7045	35/35	0.77	0.19	-0.65	11,23,41,43	0
19	CLA	1	1011	36/65	0.82	0.22	-0.66	27,27,28,28	0
19	CLA	A	1121	42/65	0.75	0.24	-0.88	26,28,28,28	0
19	CLA	3	3010	25/65	0.70	0.23	-0.89	32,32,33,33	0
19	CLA	4	4011	25/65	0.86	0.18	-1.55	10,11,12,12	0
24	SF4	A	8001	8/8	0.99	0.09	-1.75	12,17,19,21	0
24	SF4	C	8002	8/8	0.97	0.08	-2.11	14,16,24,28	0
24	SF4	C	8003	8/8	0.98	0.07	-3.24	14,19,21,22	0
19	CLA	3	3017	50/65	0.76	0.23	-	26,37,49,52	0
21	BCR	3	6022	40/40	0.71	0.25	-	21,22,23,23	0
19	CLA	H	1505	55/65	0.64	0.39	-	18,27,28,29	0
22	LMU	B	7012	25/35	0.82	0.18	-	22,32,44,49	0
22	LMU	H	7043	35/35	0.68	0.19	-	12,31,46,47	0
22	LMU	A	7035	35/35	0.85	0.27	-	6,18,32,40	0
22	LMU	2	7027	35/35	0.76	0.22	-	6,17,40,40	0
22	LMU	R	7022	35/35	0.79	0.18	-	5,21,33,35	0
19	CLA	H	1145	65/65	0.76	0.24	-	12,24,33,39	0
22	LMU	1	7004	35/35	0.61	0.49	-	17,44,50,52	0
22	LMU	A	7016	35/35	0.76	0.26	-	10,30,46,46	0
19	CLA	R	1150	65/65	0.75	0.29	-	22,24,25,25	0
22	LMU	4	7018	35/35	0.73	0.30	-	9,23,41,42	0
19	CLA	K	1146	50/65	0.77	0.27	-	25,28,30,30	0
19	CLA	3	3007	42/65	0.73	0.32	-	27,30,30,30	0
22	LMU	G	7039	35/35	0.87	0.15	-	15,30,47,47	0
19	CLA	2	2014	61/65	0.64	0.33	-	24,26,28,28	0
22	LMU	R	7021	35/35	0.75	0.25	-	17,28,45,46	0
22	LMU	H	7002	35/35	0.76	0.17	-	16,29,41,43	0
19	CLA	3	3004	25/65	0.77	0.20	-	27,28,28,28	0
19	CLA	4	1304	65/65	0.72	0.26	-	21,23,25,25	0
19	CLA	A	1151	50/65	0.72	0.37	-	24,27,29,29	0
19	CLA	1	1002	47/65	0.81	0.23	-	22,23,24,24	0
22	LMU	H	7028	35/35	0.77	0.17	-	7,21,40,40	0
19	CLA	1	1008	51/65	0.75	0.35	-	24,26,27,27	0
22	LMU	4	7033	35/35	0.80	0.19	-	12,26,40,41	0
19	CLA	4	4005	25/65	0.77	0.28	-	20,21,22,22	0
19	CLA	1	1303	51/65	0.77	0.32	-	23,28,28,29	0
22	LMU	2	7031	35/35	0.74	0.23	-	17,37,45,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
19	CLA	4	4010	25/65	0.78	0.23	-	26,27,27,27	0
22	LMU	A	7023	35/35	0.78	0.25	-	6,20,39,41	0
22	LMU	4	7008	35/35	0.70	0.34	-	11,29,41,42	0
22	LMU	3	7005	35/35	0.74	0.25	-	20,32,42,43	0
19	CLA	1	1005	46/65	0.82	0.23	-	19,21,22,22	0
19	CLA	2	2007	65/65	0.66	0.30	-	17,25,26,26	0
19	CLA	J	1311	61/65	0.73	0.27	-	19,26,27,28	0
22	LMU	R	7014	35/35	0.77	0.36	-	9,26,40,44	0
19	CLA	3	3011	65/65	0.74	0.29	-	23,25,26,26	0
22	LMU	H	7030	35/35	0.68	0.36	-	16,29,46,50	0
19	CLA	3	3001	25/65	0.79	0.28	-	24,25,25,25	0
19	CLA	2	1307	25/65	0.72	0.50	-	29,30,31,31	0
22	LMU	K	7001	35/35	0.75	0.20	-	17,34,48,50	0
22	LMU	H	7032	35/35	0.81	0.31	-	8,25,36,45	0
19	CLA	A	1309	25/65	0.57	0.56	-	25,46,54,54	0
19	CLA	R	1144	57/65	0.76	0.25	-	24,27,28,28	0
19	CLA	4	4015	46/65	0.72	0.37	-	24,25,26,27	0
22	LMU	R	7007	35/35	0.85	0.24	-	8,21,40,41	0
19	CLA	K	1142	45/65	0.67	0.25	-	27,29,30,31	0
19	CLA	F	1305	53/65	0.68	0.36	-	22,23,25,25	0
19	CLA	4	1009	36/65	0.85	0.20	-	20,22,22,23	0
19	CLA	K	1143	50/65	0.77	0.26	-	24,27,28,28	0
19	CLA	2	2005	25/65	0.66	0.25	-	30,31,32,32	0
19	CLA	L	1148	55/65	0.74	0.31	-	21,25,26,27	0
19	CLA	2	2010	25/65	0.77	0.28	-	23,23,24,24	0
22	LMU	K	7042	35/35	0.73	0.24	-	13,23,42,43	0
19	CLA	1	1007	61/65	0.78	0.26	-	14,20,21,22	0
19	CLA	2	2006	65/65	0.77	0.38	-	18,23,24,25	0
19	CLA	1	1013	51/65	0.75	0.42	-	26,27,29,29	0
19	CLA	4	4007	52/65	0.70	0.29	-	22,26,27,28	0
22	LMU	E	7048	35/35	0.58	0.31	-	19,30,44,46	0
22	LMU	E	7037	35/35	0.69	0.22	-	8,21,40,40	0
19	CLA	2	4009	65/65	0.80	0.23	-	18,23,24,24	0
19	CLA	A	1141	65/65	0.71	0.27	-	28,30,31,32	0
22	LMU	C	7015	35/35	0.72	0.34	-	9,22,37,39	0
22	LMU	2	7046	35/35	0.66	0.29	-	4,27,42,42	0
22	LMU	R	7025	35/35	0.77	0.25	-	5,22,39,42	0
22	LMU	3	7003	35/35	0.75	0.20	-	8,25,41,41	0
19	CLA	1	1001	46/65	0.72	0.27	-	28,29,30,30	0
19	CLA	2	2013	50/65	0.74	0.27	-	20,22,24,26	0
19	CLA	A	1134	45/65	0.73	0.26	-	22,26,27,28	0
19	CLA	2	2011	25/65	0.71	0.31	-	24,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
19	CLA	3	2009	56/65	0.78	0.23	-	13,35,50,50	0
19	CLA	4	4002	52/65	0.82	0.21	-	21,22,24,25	0
22	LMU	4	7034	35/35	0.73	0.28	-	14,30,42,47	0
19	CLA	3	1118	36/65	0.62	0.33	-	28,29,30,30	0
22	LMU	K	7041	35/35	0.72	0.24	-	15,31,45,45	0
22	LMU	4	7052	35/35	0.65	0.26	-	18,30,48,75	0
19	CLA	1	1014	61/65	0.72	0.27	-	3,31,46,46	0
19	CLA	3	3015	25/65	0.72	0.42	-	28,28,29,29	0
22	LMU	1	7013	35/35	0.56	0.33	-	15,34,47,48	0
19	CLA	2	2008	25/65	0.72	0.22	-	24,24,25,25	0
19	CLA	4	4014	47/65	0.65	0.28	-	21,35,46,48	0
19	CLA	A	1110	54/65	0.81	0.25	-	19,22,23,23	0
22	LMU	R	7024	35/35	0.77	0.20	-	6,19,32,40	0
19	CLA	J	1308	55/65	0.80	0.23	-	12,30,44,45	0
22	LMU	D	7050	35/35	0.76	0.23	-	14,31,46,46	0
19	CLA	1	1010	46/65	0.69	0.26	-	24,25,26,27	0
22	LMU	B	7038	35/35	0.66	0.42	-	13,35,48,48	0
22	LMU	A	7010	35/35	0.64	0.32	-	16,38,45,48	0
22	LMU	F	7036	34/35	0.76	0.30	-	19,32,42,45	0
19	CLA	2	2002	56/65	0.78	0.23	-	21,22,25,25	0
22	LMU	4	7053	34/35	0.58	0.30	-	21,41,47,48	0
19	CLA	2	2001	51/65	0.66	0.26	-	27,28,29,29	0
21	BCR	1	6023	40/40	0.61	0.40	-	21,28,29,30	0
22	LMU	4	7009	34/35	0.73	0.26	-	22,44,50,50	0
19	CLA	3	3006	25/65	0.75	0.21	-	26,27,28,28	0
19	CLA	3	3014	25/65	0.53	0.52	-	31,31,32,32	0
19	CLA	3	3016	65/65	0.64	0.47	-	23,26,29,31	0
19	CLA	3	3012	25/65	0.57	0.28	-	30,31,31,31	0
19	CLA	2	2003	25/65	0.77	0.38	-	23,24,25,25	0
19	CLA	1	1310	25/65	0.69	0.31	-	27,28,28,28	0
22	LMU	G	7026	35/35	0.75	0.30	-	12,35,46,51	0
19	CLA	3	3008	50/65	0.74	0.35	-	20,26,27,27	0
22	LMU	G	7051	35/35	0.71	0.27	-	20,32,43,44	0
22	LMU	H	7017	35/35	0.74	0.21	-	8,23,39,41	0
22	LMU	H	7011	35/35	0.67	0.27	-	17,32,38,43	0
22	LMU	2	7006	35/35	0.76	0.22	-	22,25,26,27	0
22	LMU	R	7020	35/35	0.77	0.23	-	7,26,40,44	0
22	LMU	4	7019	35/35	0.75	0.22	-	11,25,40,43	0
19	CLA	H	1241	55/65	0.72	0.26	-	23,25,26,26	0
19	CLA	B	1233	51/65	0.66	0.39	-	24,27,27,28	0
22	LMU	N	7049	35/35	0.67	0.29	-	15,28,40,41	0
19	CLA	A	1149	46/65	0.76	0.31	-	22,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
19	CLA	4	4013	25/65	0.83	0.19	-	20,21,21,21	0
22	LMU	B	7040	35/35	0.69	0.22	-	12,26,40,43	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.