



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:26 AM GMT

PDB ID : 3I4M
Title : 8-oxoguanine containing RNA polymerase II elongation complex D
Authors : Damsma, G.E.; Cramer, P.
Deposited on : 2009-07-02
Resolution : 3.70 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

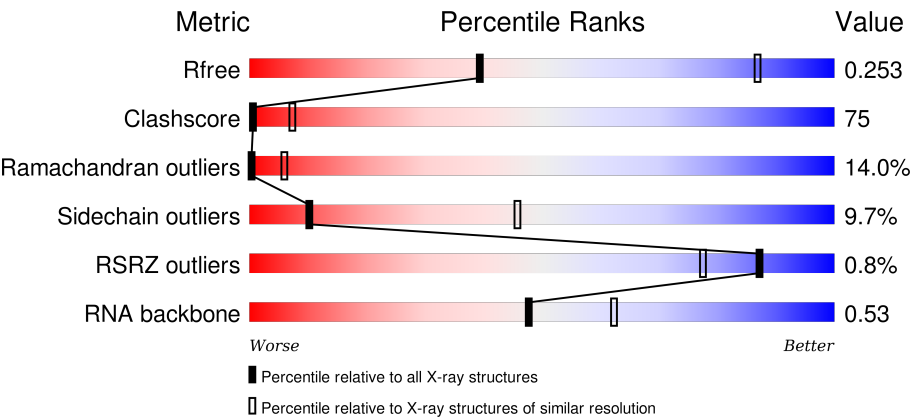
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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	1101 (3.90-3.50)
Clashscore	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (3.90-3.50)
RNA backbone	2183	1067 (4.60-2.80)

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 ≥ 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	1733	<div><div></div><div><div>16%</div><div>53%</div><div>13%</div><div>•</div><div>18%</div></div></div>
2	B	1224	<div><div>%</div><div><div>17%</div><div>58%</div><div>16%</div><div>•</div><div>8%</div></div></div>
3	C	324	<div><div></div><div><div>18%</div><div>50%</div><div>15%</div><div>•</div><div>17%</div></div></div>
4	D	221	<div><div>2%</div><div><div>19%</div><div>51%</div><div>13%</div><div>•</div><div>15%</div></div></div>

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Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	T	26	
14	N	12	
15	P	16	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 32355 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 DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1429	Total	C	N	O	S	0	0	0
			11240	7079	1966	2133	62			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1125	Total	C	N	O	S	0	0	0
			8942	5659	1571	1657	55			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	270	Total	C	N	O	S	0	0	0
			2125	1336	353	422	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	HIS	-	EXPRESSION TAG	UNP P16370
C	-4	HIS	-	EXPRESSION TAG	UNP P16370
C	-3	HIS	-	EXPRESSION TAG	UNP P16370
C	-2	HIS	-	EXPRESSION TAG	UNP P16370
C	-1	HIS	-	EXPRESSION TAG	UNP P16370
C	0	HIS	-	EXPRESSION TAG	UNP P16370

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	187	Total	C	N	O	S	0	0	0
			1504	930	269	301	4			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	88	Total	C	N	O	S	0	0	0
			712	455	120	134	3			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	137	Total	C	N	O	S	0	0	0
			1101	693	185	218	5			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	116	Total	C	N	O	S	0	0	0
			944	581	172	181	10			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	116	Total	C	N	O	S	0	0	0
			929	596	158	173	2			

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	47	Total	C	N	O	S	0	0	0
			370	228	73	65	4			

- Molecule 13 is a DNA chain called DNA (5'-D(*AP*G*CP*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*AP*(8OG)P*GP*CP*CP*(BRU)P*GP*GP*TP*CP*AP*TP*T)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
13	T	21	Total	Br	C	N	O	P	0	0	0
			426	1	203	75	127	20			

- Molecule 14 is a DNA chain called DNA (5'-D(*AP*GP*TP*AP*CP*TP*TP*GP*AP*GP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	11	Total	C	N	O	P	0	0	0
			224	108	42	64	10			

- Molecule 15 is a RNA chain called RNA (5'-R(*UP*GP*CP*AP*UP*C*UP*UP*CP*CP*AP*GP*GP*CP*CP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	P	10	Total	C	N	O	P	0	0	0
			205	93	33	70	9			

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Mg	0	0
			1	1		

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	J	1	Total	Zn	0	0
			1	1		
17	B	1	Total	Zn	0	0
			1	1		
17	I	2	Total	Zn	0	0
			2	2		
17	C	1	Total	Zn	0	0
			1	1		

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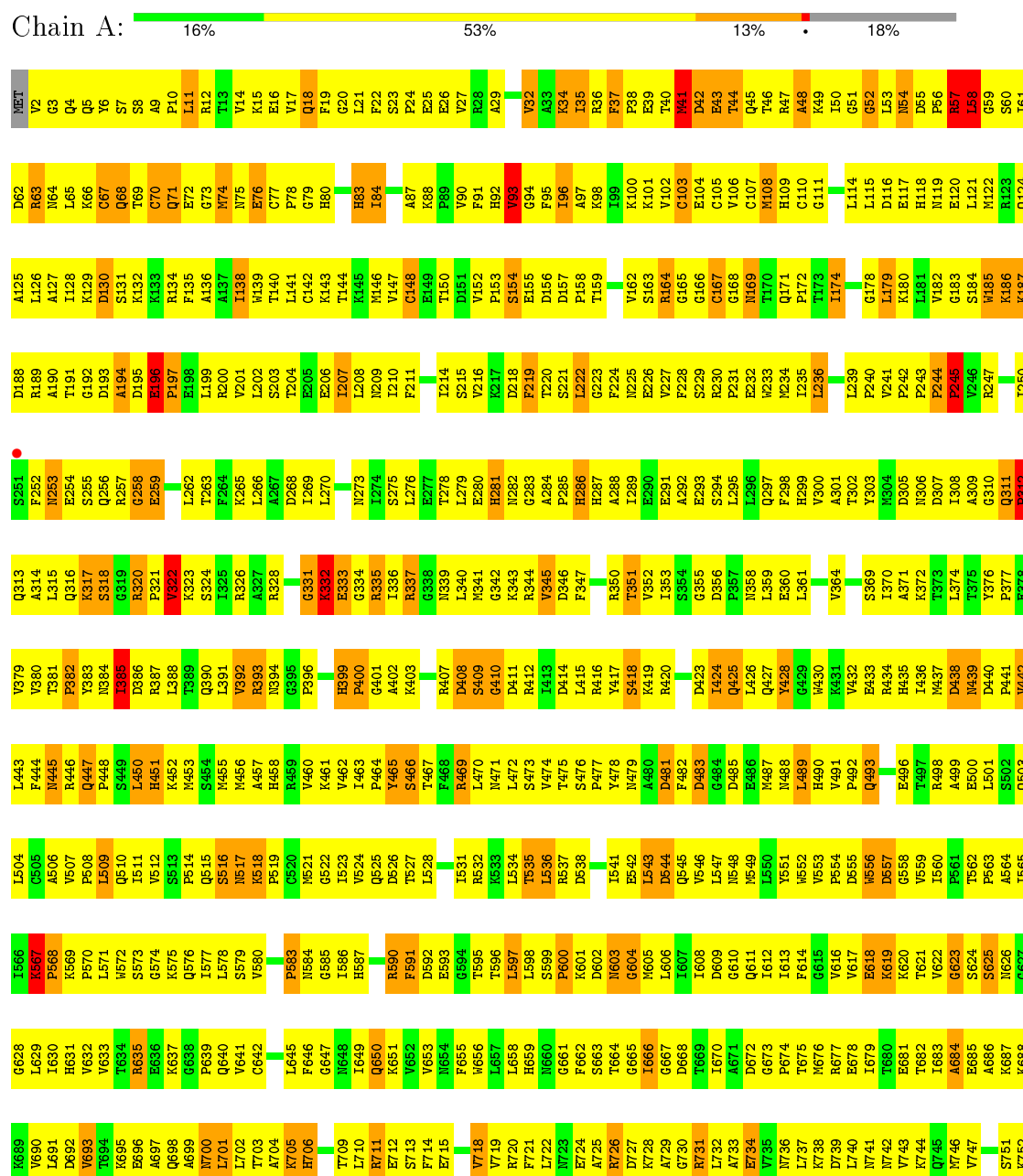
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	2	Total 2	Zn 2	0	0
17	L	1	Total 1	Zn 1	0	0

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.

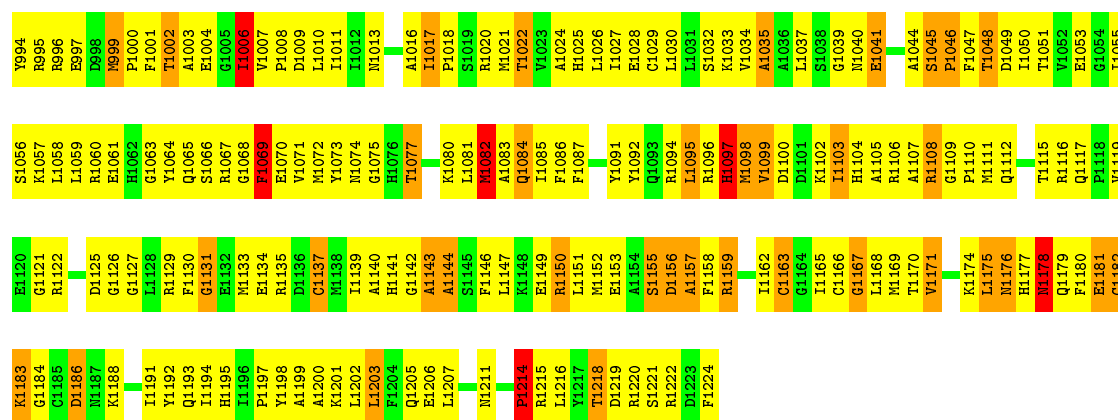
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



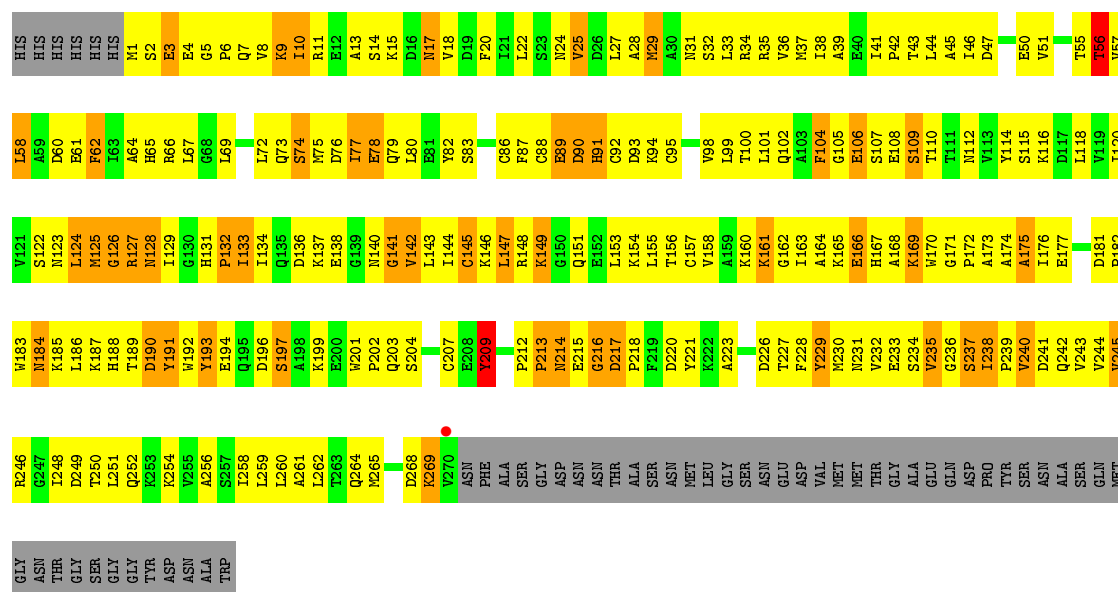
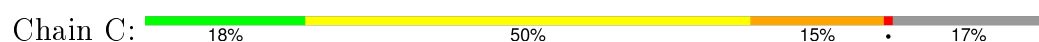
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SER	PRO	PRO	PHE	H1387	I1322	E1256	L1193	Q1130	Q1070	M1009	A944	Q881	M818	S754
SER	SER	SER	ALA	G1388	D1323	E1257	R1194	K1131	S1071	A1010	E945	S882	G820	S755
PRO	PRO	PRO	ALA	F1389	D1257	D1257	L1195	K1132	I1072	Q1011	V946	L883	G819	W756
THR	PRO	PRO	GLY	M1390	P1324	M1259	E1196	L1133	G1073	D1013	F947	D884	R821	W757
SER	THR	THR	GLY	R1391	T1325	M1259	L1197	I1134	E1074	D1012	V948	T885	E822	W758
PRO	SER	PRO	GLY	S1392	R1326	L1260	D1198	I1138	P1075	D1013	D949	L886	I825	W759
SER	THR	SER	ALA	H1393	I1327	K1261	R1199	E1139	A1076	V1015	G950	G887	I826	W760
ASN	PRO	PRO	ASP	Y1394	Y1328	K1262	A1200	E1139	T1077	T1016	E951	G888	D826	W761
THR	PRO	PRO	THR	G1395	Y1329	I1263	A1201	Q1078	Q1078	L1017	A952	S889	A828	W762
SER	THR	THR	GLY	A1396	M1330	E1264	T1141	M1079	F1018	F1017	S893	D890	A828	W763
PRO	PRO	PRO	GLY	L1397	S1331	T1265	T1142	T1080	C1019	C1019	V954	T890	V829	W764
THR	PRO	PRO	ALA	M1398	F1332	T1266	L1143	L1081	T1081	C1020	G954	A891	K830	W765
SER	THR	THR	THR	R1399	I1333	M1267	L1207	ASN	ASN	L1021	P955	E894	T831	W766
PRO	SER	SER	GLY	C1400	D1334	L1268	T1208	THR	THR	L1022	Y958	K895	A832	W767
PRO	PRO	PRO	ILE	S1401	I1335	E1269	M1209	PHE	PHE	L1022	N959	K896	E833	W768
THR	PRO	PRO	THR	F1402	M1270	N1271	G1210	HIS	HIS	R1025	I960	T897	T834	W769
GLY	PRO	PRO	GLY	E1403	Q1211	T1272	V1212	PHE	PHE	L1026	R961	K898	G835	W770
GLN	PRO	PRO	GLY	E1404	V1212	T1273	V1212	ALA	ALA	A1027	R962	V899	X836	W771
ASP	PRO	PRO	GLY	T1405	G1213	L1273	G1213	GLY	GLY	T1028	I963	D900	I837	
GLY	GLY	GLY	GLY	I1408	E1342	G1275	R1215	VAL	VAL	R1029	I964	L901	Q838	W774
GLY	GLY	GLY	GLY	L1409	A1343	V1276	I1216	ALA	ALA	R1030	Q965	L902	R839	W775
THR	THR	THR	VAL	E1410	G1344	E1277	K1217	SER	SER	V1031	N966	N903	R840	W776
PRO	PRO	PRO	THR	E1411	R1345	M1278	Q1218	LVS	LVS	L1032	A967	T904	L841	W777
PRO	PRO	PRO	PRO	A1412	I1279	I1279	T1219	P1456	K1093	Q1033	Q968	D905	V842	W778
GLY	THR	THR	THR	G1413	E1280	E1280	F1220	P1456	V1094	E1034	Q969	E906	K843	W779
GLY	THR	THR	GLY	Y1349	Y1349	M1284	F1221	D1157	T1095	R1036	T970	T907	A844	W780
GLY	THR	THR	GLY	K1350	K1350	M1285	D1222	P1158	S1096	Q1035	F971	L908	L845	W781
ALA	PRO	PRO	GLY	E1351	R1352	M1285	D1222	R1159	G1097	L1037	H972	D909	E846	W782
THR	THR	THR	VAL	V1352	V1352		L1224	S1160	V1098	T1038	N973	P910	D847	W783
SER	SER	SER	SER	F1417	F1353		F1225	V1162	P1099	K1039	D974	S911	I848	W784
SER	SER	SER	SER	L1418	M1354	R1289	F1225	V1162	R1100	Q1040	H975	L912	M849	W785
PRO	PRO	PRO	LEU	D1419	M1354	R1289	V1226	V1163	L1101	A1041		L913	H786	
VAL	PRO	PRO	VAL	D1420	V1355	V1291	I1227	P1164	K1102	F1042		E914	Y852	W787
GLN	THR	THR	ASN	K1421	I1356	P1292	W1228	E1165	E1103	D1043	S979	S915	D853	W788
ASP	SER	SER	ALA	R1422	A1357	S1293	S1229	D1166	I1104	W1044	D980	G916	N854	
ASP	PRO	PRO	ASP	G1423	P1294	E1230	E1230	E1167	L1105	W1045	L981	S917	T855	
LEU	PRO	PRO	LEU	V1424	T1295	T1295	D1231	E1168	N1106	L1046	T982	E918	T856	W790
ASP	THR	THR	ASP	S1425	G1296	G1296	D1232	I1169	V1107	S1047	L983	Y919		
VAL	SER	SER	VAL	E1426	M1364	E1297	D1233	I1170	A1108	N1048	D985		N858	
PRO	PRO	PRO	PRO	N1427	Y1365	V1298	E1234	K1110	K1109	L1049	D985	L923	S859	
THR	THR	THR	THR	V1428	R1366	V1299	K1235	H1173	N1110	E1050	N986	L925	L860	
GLY	PRO	PRO	GLY	H1429	H1367	K1300	L1236	F1174	M1111	A1051	V987	L926	G661	
LEU	PRO	PRO	LEU	L1430	M1368		I1237	S1175	K1112	Q1052		Q926		
MET	PRO	PRO	MET	G1431	A1369		I1238	L1176	T1113	F1053		Y927		
PHE	THR	THR	PHE	Q1432	L1370	E1303	R1239	D1177	P1114	L1054	L993	L928	I864	
SER	SER	SER	SER	M1433	L1371	V1304	R1240	D1178	S1115	R1055	Q994	L929	Q865	
PRO	PRO	PRO	PRO	A1434	V1372	L1306	C1240	E1179	S1116	S1056	N995	D930	F866	
ALA	THR	THR	ALA	P1435	D1373	E1307	R1241	GLU	T1117	V1057	T996	E931	I867	
VAL	THR	THR	VAL	I1436	V1374	T1308	V1242	ALA	V1118	V1058	L997	E932	Y868	
ASP	PRO	PRO	ASP	G1437	M1375	D1309	V1243	GLU	V1119	H1059	L998	Y933	G869	
PRO	PRO	PRO	PRO	T1438	T1376	G1310	R1244	GLN	L1120	P1060	V999	K934	D871	
THR	THR	THR	THR	G1439	T1377	V1311	E1246	SER	E1121	Q1061	L1000	Q935	G872	
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MET	PRO	PRO	MET	M1444	S1383	V1316	GLY	S1189	A1126	L1066	H877	R940	H813	
ALA	PRO	PRO	ALA	I1445	V1384	M1317	THR	P1190	D1127	L1067	I1006	F941	I878	
THR	THR	THR	THR	D1446	T1385	T1318	GLU	W1191	Q1128	A1068	T1007	F942	E879	

- Molecule 2: DNA-directed RNA polymerase II subunit RPB2

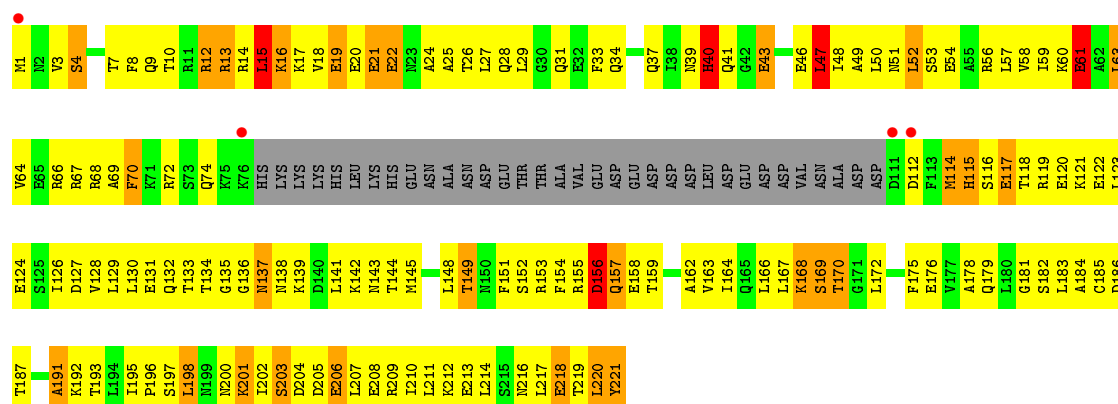
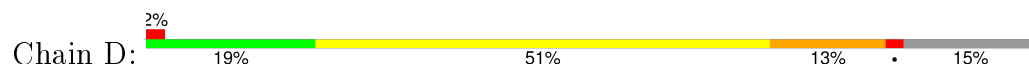




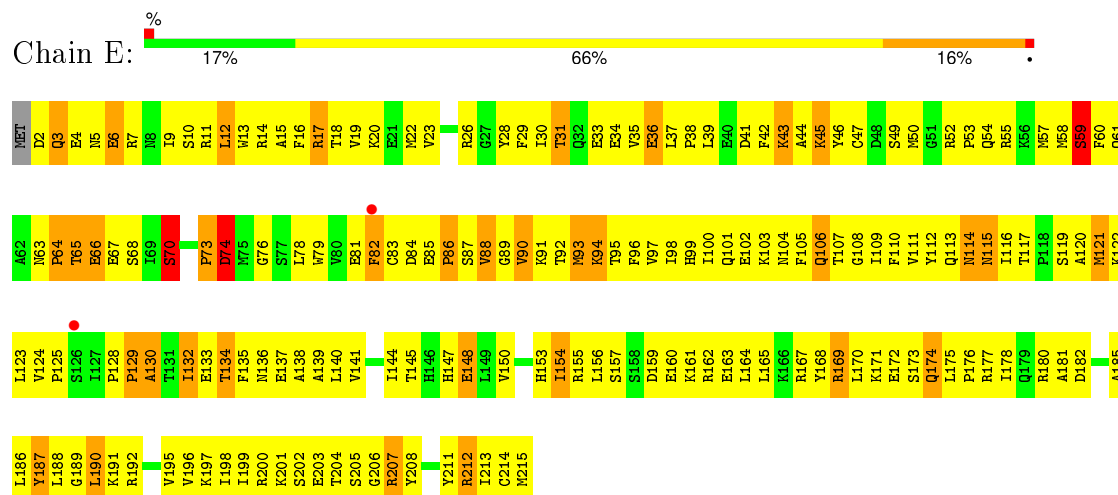
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3



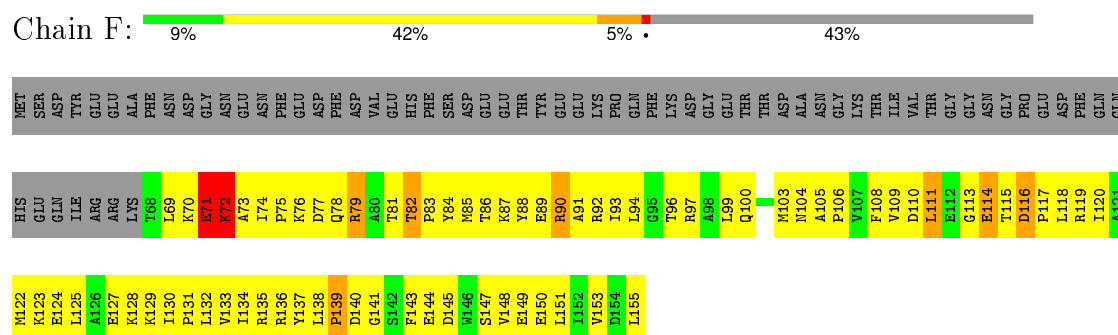
- Molecule 4: DNA-directed RNA polymerase II subunit RPB4



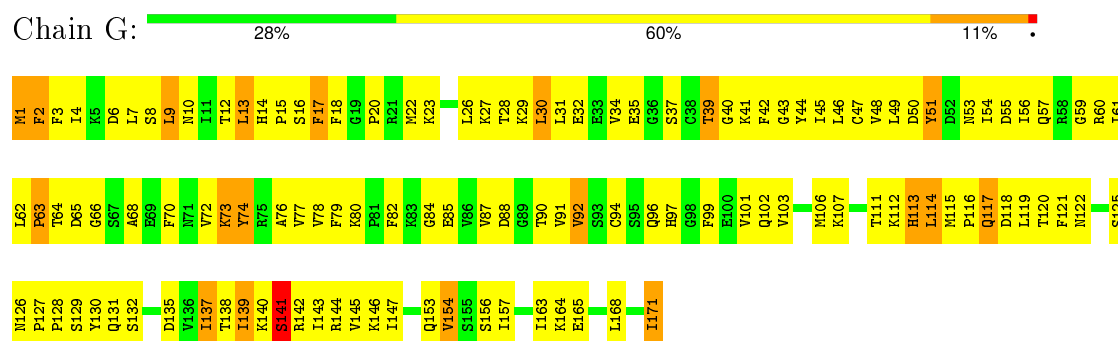
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



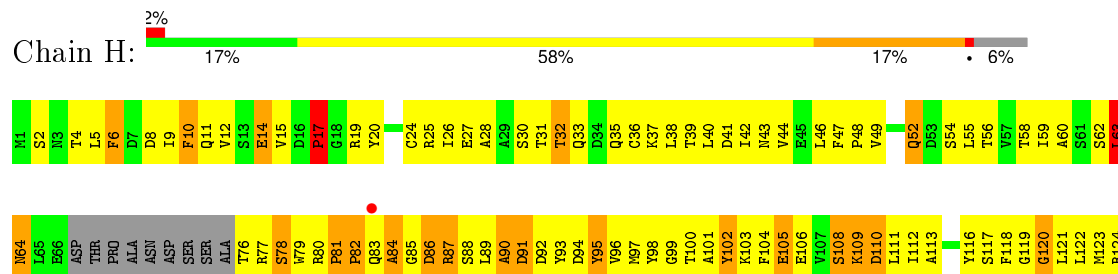
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

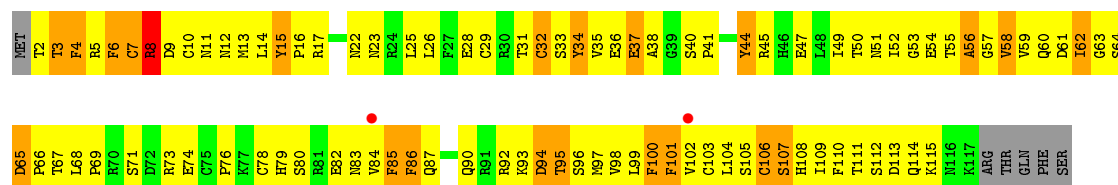
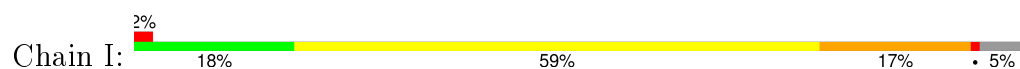


• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

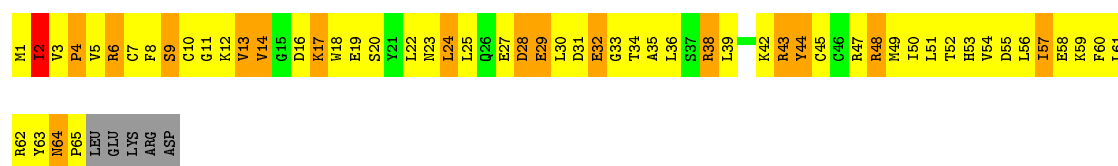
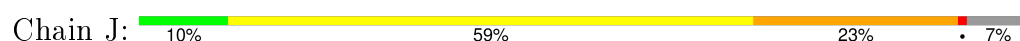




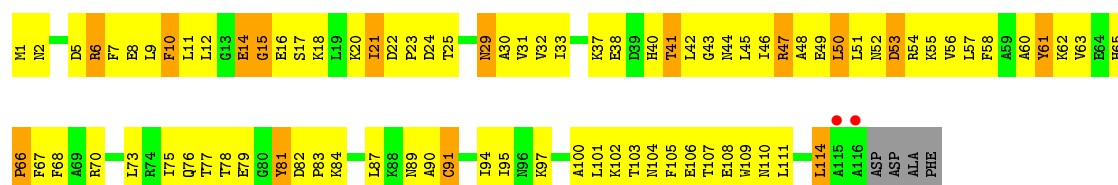
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



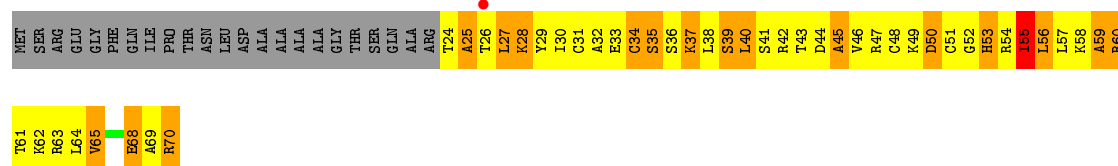
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



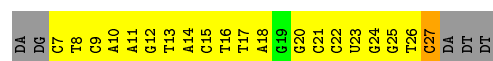
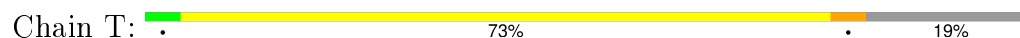
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11



- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



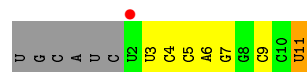
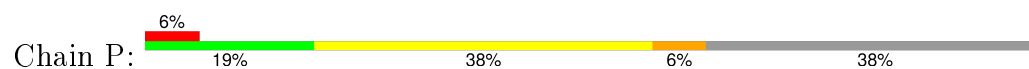
- Molecule 13: DNA (5'-D(*AP*G*CP*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*AP*(8OG)P*GP*CP*CP*(BRU)P*GP*GP*TP*CP*AP*TP*T)-3')



- Molecule 14: DNA (5'-D(*AP*GP*TP*AP*CP*TP*TP*GP*AP*GP*CP*T)-3')



- Molecule 15: RNA (5'-R(*UP*GP*CP*AP*UP*C*UP*UP*CP*CP*AP*GP*GP*CP*CP*U)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	220.65Å 392.00Å 281.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.70 49.00 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-3.70) 100.0 (49.00-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 3.67Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.225 , 0.258 0.227 , 0.253	Depositor DCC
R_{free} test set	2439 reflections (1.92%)	DCC
Wilson B-factor (Å ²)	114.2	Xtriage
Anisotropy	0.492	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 97.9	EDS
Estimated twinning fraction	0.029 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.034 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 129421 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	32355	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: MG, 8OG, ZN, BRU

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	0.44	0/11441	0.74	3/15473 (0.0%)
2	B	0.41	0/9116	0.70	0/12291
3	C	0.42	0/2163	0.69	0/2930
4	D	0.38	0/1516	0.63	0/2031
5	E	0.39	0/1788	0.64	0/2406
6	F	0.52	0/724	0.82	0/977
7	G	0.44	0/1368	0.72	0/1844
8	H	0.37	0/1119	0.68	0/1514
9	I	0.38	0/962	0.66	0/1295
10	J	0.44	0/541	0.74	0/727
11	K	0.46	0/947	0.68	0/1279
12	L	0.39	0/372	0.68	0/495
13	T	0.56	1/426 (0.2%)	0.87	0/650
14	N	0.41	0/251	0.81	0/386
15	P	0.42	0/227	0.80	0/351
All	All	0.43	1/32961 (0.0%)	0.71	3/44649 (0.0%)

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	1
2	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	T	27	DC	C1'-N1	5.98	1.57	1.49

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	567	LYS	C-N-CD	5.82	140.63	128.40
1	A	3	GLY	N-CA-C	-5.75	98.73	113.10
1	A	509	LEU	CA-CB-CG	-5.00	103.79	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1035	TYR	Sidechain
2	B	797	TYR	Sidechain

5.2 Too-close contacts [i](#)

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	11240	0	11311	1819	0
2	B	8942	0	8986	1481	0
3	C	2125	0	2090	340	0
4	D	1504	0	1518	205	0
5	E	1752	0	1776	286	0
6	F	712	0	738	138	0
7	G	1340	0	1357	217	0
8	H	1101	0	1075	206	0
9	I	944	0	901	162	0
10	J	532	0	542	129	0
11	K	929	0	939	135	0
12	L	370	0	394	90	0
13	T	426	0	236	37	0
14	N	224	0	126	11	0
15	P	205	0	109	8	0
16	A	1	0	0	0	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	L	1	0	0	0	0
All	All	32355	0	32098	4821	0

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 75.

All (4821) 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)
2:B:69:LEU:HD13	2:B:429:PHE:CD1	1.39	1.55
2:B:69:LEU:HD13	2:B:429:PHE:CE1	1.66	1.30
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.24	1.17
2:B:806:THR:HG22	2:B:808:ALA:H	1.08	1.16
2:B:340:ALA:HB3	2:B:343:ILE:HG12	1.29	1.15
2:B:69:LEU:CD1	2:B:429:PHE:CD1	2.30	1.14
13:T:16:DT:H2"	13:T:17:DT:H5'	1.29	1.13
2:B:133:LYS:HE3	2:B:135:ARG:HH21	1.13	1.12
1:A:225:ASN:ND2	1:A:228:PHE:H	1.48	1.12
1:A:41:MET:HB2	1:A:49:LYS:HA	1.32	1.12
2:B:639:ILE:HD11	2:B:691:GLU:HG3	1.32	1.11
1:A:825:ILE:HD11	2:B:512:ARG:HB3	1.22	1.11
1:A:567:LYS:HG3	8:H:95:TYR:HA	1.11	1.10
2:B:637:LEU:HD12	2:B:693:ILE:HD12	1.32	1.10
2:B:622:LYS:HE2	9:I:59:VAL:HG22	1.28	1.10
3:C:43:THR:HG22	3:C:44:LEU:H	1.02	1.09
1:A:899:VAL:HB	1:A:929:LEU:HD11	1.14	1.09
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.27	1.09
7:G:138:THR:HG22	7:G:139:ILE:H	1.00	1.07
1:A:53:LEU:HD23	1:A:54:ASN:N	1.70	1.07
6:F:109:VAL:HG11	6:F:123:LYS:HD2	1.30	1.06
3:C:148:ARG:H	3:C:151:GLN:HG3	1.20	1.05
1:A:1244:ARG:HB3	1:A:1245:PRO:HA	1.28	1.05
2:B:506:GLY:HA2	2:B:512:ARG:HH21	1.21	1.05
2:B:244:LEU:HD11	2:B:366:GLN:HE22	1.20	1.05
1:A:666:ILE:H	2:B:1026:LEU:HD13	1.21	1.05
12:L:40:LEU:HD13	12:L:44:ASP:HB3	1.38	1.04
1:A:320:ARG:HB2	1:A:320:ARG:HH11	1.19	1.04
1:A:12:ARG:HB2	2:B:1218:THR:HG22	1.39	1.04
2:B:217:ARG:HE	2:B:405:ARG:HB2	1.20	1.04
8:H:12:VAL:HB	8:H:52:GLN:H	1.21	1.04
5:E:22:MET:HE3	5:E:26:ARG:HH11	1.23	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:81:PRO:HB2	8:H:82:PRO:CD	1.89	1.02
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.40	1.02
2:B:1097:HIS:H	2:B:1098:MET:HE2	1.23	1.02
8:H:64:ASN:HB2	8:H:88:SER:HB2	1.41	1.02
2:B:69:LEU:HB3	2:B:429:PHE:HE1	1.22	1.01
5:E:78:LEU:HA	5:E:107:THR:HB	1.38	1.01
1:A:903:ASN:HD22	1:A:904:THR:N	1.57	1.01
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.41	1.01
5:E:100:ILE:HG23	5:E:105:PHE:HB2	1.41	1.01
1:A:1445:ILE:HD12	1:A:1445:ILE:H	1.26	1.00
1:A:590:ARG:HH11	1:A:590:ARG:HB2	1.24	1.00
3:C:238:ILE:HG23	3:C:242:GLN:HB2	1.43	1.00
12:L:32:ALA:HB2	12:L:55:ILE:HG13	1.44	1.00
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.42	1.00
1:A:535:THR:HG21	1:A:616:VAL:HA	1.44	1.00
1:A:188:ASP:HB3	1:A:191:THR:HB	1.43	0.99
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.43	0.99
3:C:101:LEU:HD13	3:C:118:LEU:HD23	1.41	0.99
1:A:382:PRO:HD3	1:A:428:TYR:HD2	1.27	0.99
2:B:1065:GLN:HE21	2:B:1067:ARG:N	1.60	0.99
9:I:58:VAL:HG13	9:I:62:ILE:HD12	1.44	0.98
2:B:503:GLY:HA3	2:B:507:LYS:HE2	1.45	0.98
5:E:207:ARG:HH11	5:E:207:ARG:HB3	1.28	0.98
6:F:76:LYS:HA	6:F:79:ARG:HD3	1.45	0.98
2:B:69:LEU:CD1	2:B:429:PHE:CE1	2.45	0.98
3:C:148:ARG:N	3:C:151:GLN:HG3	1.78	0.98
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.28	0.97
1:A:567:LYS:HE2	8:H:47:PHE:HB2	1.44	0.97
2:B:810:GLU:HA	2:B:815:ARG:HH22	1.29	0.97
6:F:111:LEU:HD12	6:F:111:LEU:H	1.27	0.97
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.45	0.97
8:H:40:LEU:HD22	8:H:123:MET:HE3	1.46	0.97
1:A:683:ILE:HD13	1:A:801:GLU:HG3	1.46	0.97
2:B:800:GLN:HB3	10:J:52:THR:CG2	1.92	0.96
5:E:124:VAL:HG13	5:E:132:ILE:HG13	1.46	0.96
1:A:1111:MET:HE2	1:A:1331:SER:HA	1.46	0.96
2:B:559:SER:HA	2:B:563:MET:HB3	1.47	0.96
7:G:138:THR:HG22	7:G:139:ILE:N	1.80	0.96
1:A:925:LEU:HD13	1:A:983:ILE:HD12	1.48	0.96
1:A:666:ILE:HD12	1:A:667:GLY:H	1.31	0.95
2:B:800:GLN:HB3	10:J:52:THR:HG21	1.49	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1099:VAL:HG13	2:B:1100:ASP:H	1.32	0.95
1:A:269:ILE:HG12	1:A:299:HIS:HB3	1.48	0.95
5:E:22:MET:CE	5:E:26:ARG:HH11	1.80	0.95
9:I:85:PHE:HD2	9:I:85:PHE:H	1.08	0.95
2:B:515:HIS:HD2	2:B:517:THR:H	1.01	0.95
6:F:73:ALA:HB1	6:F:143:PHE:H	1.31	0.94
8:H:100:THR:HG23	8:H:138:GLU:HA	1.48	0.94
2:B:866:TYR:HB2	2:B:870:ILE:HB	1.49	0.94
5:E:153:HIS:O	5:E:154:ILE:HG13	1.66	0.94
5:E:16:PHE:CZ	5:E:20:LYS:HE2	2.02	0.94
10:J:64:ASN:HB3	10:J:65:PRO:CD	1.97	0.94
1:A:308:ILE:HG22	1:A:309:ALA:H	1.33	0.94
8:H:128:ASN:H	8:H:130:ARG:NH1	1.65	0.94
8:H:12:VAL:HB	8:H:52:GLN:N	1.83	0.94
1:A:754:SER:H	1:A:757:ASN:HD22	1.13	0.94
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.49	0.94
1:A:320:ARG:HB2	1:A:320:ARG:NH1	1.83	0.94
8:H:81:PRO:HB2	8:H:82:PRO:HD3	1.48	0.93
1:A:567:LYS:CG	8:H:95:TYR:HA	1.97	0.93
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.02	0.93
12:L:27:LEU:H	12:L:27:LEU:HD23	1.34	0.93
2:B:1065:GLN:HE21	2:B:1067:ARG:H	0.96	0.93
1:A:541:ILE:HD13	1:A:549:MET:HE1	1.51	0.93
4:D:39:ASN:ND2	4:D:41:GLN:HB2	1.83	0.93
1:A:1144:LYS:HB2	1:A:1268:LEU:O	1.68	0.93
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.51	0.93
11:K:21:ILE:HG23	11:K:33:ILE:HG12	1.51	0.93
1:A:466:SER:HB3	2:B:1103:ILE:HG12	1.52	0.92
7:G:127:PRO:HG2	7:G:138:THR:HG21	1.50	0.92
1:A:901:LEU:H	1:A:926:GLN:NE2	1.67	0.92
1:A:1424:VAL:HG13	1:A:1436:ILE:HD11	1.51	0.92
1:A:720:ARG:O	1:A:724:GLU:HB2	1.70	0.92
8:H:102:TYR:HD2	8:H:102:TYR:H	1.13	0.92
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.48	0.92
2:B:520:GLY:H	2:B:748:ILE:HG22	1.34	0.92
3:C:43:THR:HG22	3:C:44:LEU:N	1.85	0.92
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.34	0.92
8:H:33:GLN:HE21	8:H:35:GLN:HB2	1.31	0.92
7:G:122:ASN:HB2	7:G:131:GLN:HE21	1.34	0.91
2:B:911:ILE:HD11	2:B:941:LEU:HD13	1.52	0.91
2:B:69:LEU:HB3	2:B:429:PHE:CE1	2.05	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:897:TYR:HD2	1:A:936:LEU:HD13	1.34	0.91
1:A:1208:THR:HB	1:A:1211:GLN:HG3	1.52	0.91
1:A:1004:ASN:ND2	5:E:167:ARG:HD2	1.86	0.91
7:G:7:LEU:HB2	7:G:74:TYR:CE2	2.04	0.91
1:A:49:LYS:HZ1	1:A:61:ILE:HG13	1.34	0.91
3:C:203:GLN:HG2	3:C:207:CYS:SG	2.10	0.91
1:A:441:PRO:HG3	1:A:498:ARG:HB2	1.51	0.91
1:A:225:ASN:HD22	1:A:228:PHE:N	1.68	0.91
11:K:12:LEU:H	11:K:12:LEU:HD12	1.33	0.91
1:A:470:LEU:HD13	1:A:487:MET:HE1	1.52	0.90
3:C:258:ILE:HD11	11:K:42:LEU:HD11	1.52	0.90
1:A:335:ARG:HD3	2:B:1202:LEU:HD23	1.54	0.90
2:B:69:LEU:HD22	2:B:429:PHE:CE1	2.07	0.90
1:A:442:VAL:HG12	1:A:490:HIS:O	1.71	0.90
2:B:410:GLY:HA2	2:B:413:LEU:HD12	1.52	0.89
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.54	0.89
2:B:642:ASP:HA	2:B:649:LYS:HA	1.52	0.89
1:A:1409:LEU:HD13	2:B:1207:LEU:HD11	1.54	0.89
11:K:47:ARG:HB3	11:K:47:ARG:HH11	1.34	0.89
2:B:515:HIS:CD2	2:B:517:THR:H	1.90	0.89
4:D:3:VAL:HG21	7:G:10:ASN:HB2	1.52	0.89
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.14	0.89
2:B:384:ARG:HA	2:B:387:LEU:HD22	1.52	0.89
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.55	0.89
1:A:1369:ALA:O	1:A:1372:VAL:HG12	1.72	0.89
5:E:117:THR:HG22	5:E:119:SER:H	1.37	0.89
3:C:77:ILE:H	3:C:129:ILE:HD11	1.36	0.89
3:C:57:VAL:HG11	10:J:60:PHE:HB3	1.53	0.89
1:A:1308:THR:HG23	1:A:1309:ASP:N	1.84	0.89
3:C:43:THR:CG2	3:C:44:LEU:H	1.85	0.88
7:G:138:THR:CG2	7:G:139:ILE:H	1.82	0.88
1:A:18:GLN:HG2	1:A:1418:LEU:HD13	1.55	0.88
1:A:537:ARG:HD2	8:H:20:TYR:HE1	1.37	0.88
1:A:1153:TYR:HB2	1:A:1192:LEU:HD23	1.55	0.88
2:B:193:LYS:NZ	12:L:32:ALA:HB1	1.88	0.88
1:A:1227:ILE:HG22	1:A:1228:TRP:H	1.37	0.88
1:A:335:ARG:HD2	2:B:1206:GLU:OE1	1.73	0.88
1:A:568:PRO:HG2	8:H:46:LEU:HD22	1.55	0.88
1:A:946:VAL:HG13	5:E:201:LYS:HB3	1.55	0.88
5:E:17:ARG:NH1	5:E:17:ARG:HB2	1.88	0.88
2:B:880:THR:HB	2:B:934:LYS:CE	2.04	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1420:ASP:CB	1:A:1422:ARG:HG3	2.02	0.88
5:E:171:LYS:HG2	5:E:174:GLN:OE1	1.74	0.88
1:A:71:GLN:HG3	1:A:72:GLU:HG2	1.56	0.88
4:D:164:ILE:HG23	4:D:168:LYS:HD2	1.56	0.88
1:A:1030:ARG:HG3	1:A:1034:GLU:OE2	1.75	0.88
2:B:539:LEU:H	2:B:539:LEU:HD12	1.38	0.88
2:B:69:LEU:O	2:B:70:ILE:HG13	1.74	0.87
1:A:630:ILE:HD11	1:A:646:PHE:CZ	2.09	0.87
1:A:665:GLY:O	1:A:667:GLY:N	2.06	0.87
5:E:17:ARG:HB2	5:E:17:ARG:HH11	1.37	0.87
2:B:299:GLU:HB3	2:B:571:PRO:HG3	1.57	0.87
1:A:899:VAL:HB	1:A:929:LEU:CD1	2.04	0.87
2:B:1065:GLN:NE2	2:B:1067:ARG:H	1.73	0.87
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.55	0.87
1:A:901:LEU:H	1:A:926:GLN:HE21	1.19	0.87
12:L:61:THR:HG21	12:L:63:ARG:HE	1.38	0.87
3:C:175:ALA:HB2	10:J:10:CYS:HB2	1.57	0.87
1:A:899:VAL:HG13	1:A:908:LEU:HD21	1.55	0.87
12:L:55:ILE:HD13	12:L:55:ILE:H	1.40	0.86
1:A:182:VAL:HG22	1:A:201:VAL:HA	1.55	0.86
2:B:810:GLU:CA	2:B:815:ARG:HH22	1.88	0.86
13:T:15:DC:H2"	13:T:16:DT:H72	1.55	0.86
1:A:1323:ASP:OD1	1:A:1325:THR:HG22	1.74	0.86
1:A:40:THR:HG22	1:A:41:MET:HG3	1.54	0.86
1:A:1242:VAL:HG12	1:A:1243:VAL:H	1.39	0.86
2:B:278:GLN:HG2	2:B:279:ASP:H	1.38	0.86
9:I:82:GLU:HB3	9:I:104:LEU:HD12	1.58	0.86
1:A:567:LYS:HG3	8:H:95:TYR:CA	2.03	0.86
2:B:801:LYS:O	10:J:52:THR:HG23	1.75	0.86
12:L:34:CYS:HB3	12:L:51:CYS:SG	2.15	0.86
5:E:3:GLN:HG3	5:E:5:ASN:H	1.40	0.86
4:D:70:PHE:O	4:D:74:GLN:HG3	1.75	0.85
1:A:616:VAL:HG12	1:A:617:VAL:H	1.42	0.85
6:F:103:MET:CE	7:G:66:GLY:H	1.89	0.85
5:E:85:GLU:HB2	5:E:88:VAL:HG22	1.56	0.85
13:T:15:DC:C2'	13:T:16:DT:H72	2.05	0.85
1:A:34:LYS:HZ1	1:A:57:ARG:NH2	1.74	0.85
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.56	0.85
9:I:65:ASP:HB3	9:I:68:LEU:HD12	1.56	0.85
1:A:298:PHE:HZ	1:A:314:ALA:HB2	1.39	0.85
8:H:100:THR:OG1	8:H:138:GLU:HG3	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:72:LYS:HA	6:F:72:LYS:HE3	1.59	0.85
1:A:738:LYS:HB2	1:A:740:LEU:HG	1.58	0.85
1:A:390:GLN:O	1:A:394:ASN:HB2	1.75	0.85
3:C:244:VAL:O	3:C:248:ILE:HG13	1.75	0.85
1:A:1261:LYS:O	1:A:1264:GLU:HB3	1.76	0.85
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.58	0.85
7:G:45:ILE:HA	7:G:78:VAL:HG12	1.58	0.85
1:A:134:ARG:HG2	1:A:138:ILE:HD11	1.56	0.85
2:B:882:THR:HG22	2:B:884:ARG:HB2	1.56	0.85
11:K:49:GLU:OE2	11:K:97:LYS:HE3	1.76	0.85
5:E:156:LEU:HD12	5:E:195:VAL:HB	1.57	0.84
1:A:913:LEU:HD12	1:A:914:GLU:H	1.40	0.84
2:B:640:VAL:HG22	2:B:651:LEU:HD23	1.57	0.84
1:A:42:ASP:O	1:A:44:THR:N	2.11	0.84
2:B:880:THR:HB	2:B:934:LYS:HD3	1.58	0.84
2:B:289:LEU:HD13	2:B:375:ALA:HB2	1.58	0.84
2:B:1119:VAL:O	2:B:1126:GLY:HA3	1.78	0.84
2:B:69:LEU:HD13	2:B:429:PHE:HD1	1.11	0.84
11:K:65:HIS:CD2	11:K:67:PHE:H	1.96	0.84
2:B:604:ARG:HG3	2:B:611:PRO:HA	1.58	0.84
3:C:147:LEU:HB2	3:C:151:GLN:HB2	1.59	0.84
1:A:49:LYS:HZ1	1:A:61:ILE:N	1.75	0.84
3:C:32:SER:O	3:C:36:VAL:HG23	1.78	0.84
1:A:53:LEU:HD23	1:A:54:ASN:H	1.40	0.84
6:F:73:ALA:CB	6:F:143:PHE:H	1.90	0.84
1:A:414:ASP:OD1	1:A:416:ARG:HG2	1.78	0.84
12:L:55:ILE:O	12:L:56:LEU:HB2	1.77	0.83
1:A:1404:GLU:HB2	1:A:1408:ILE:HD12	1.58	0.83
5:E:19:VAL:O	5:E:23:VAL:HG23	1.77	0.83
2:B:882:THR:CG2	2:B:884:ARG:HB2	2.08	0.83
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.13	0.83
1:A:1420:ASP:HB2	1:A:1422:ARG:HG3	1.59	0.83
2:B:1180:PHE:HB3	2:B:1191:ILE:HD12	1.59	0.83
1:A:981:LEU:HD21	1:A:1039:LYS:HA	1.59	0.83
8:H:64:ASN:HD22	8:H:88:SER:CB	1.90	0.83
3:C:47:ASP:HA	12:L:69:ALA:HB3	1.60	0.83
2:B:652:LYS:O	2:B:689:LEU:HD22	1.78	0.83
2:B:1084:GLN:NE2	2:B:1084:GLN:N	2.26	0.83
8:H:129:TYR:H	8:H:130:ARG:HH11	1.27	0.83
1:A:738:LYS:H	1:A:738:LYS:HD2	1.42	0.83
2:B:526:GLU:HG2	2:B:538:ASN:HD22	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:VAL:O	1:A:57:ARG:HD3	1.78	0.83
1:A:332:LYS:HG3	1:A:333:GLU:OE2	1.77	0.83
2:B:593:PRO:HG2	2:B:617:ARG:CZ	2.09	0.83
2:B:121:ASN:HA	2:B:207:GLY:HA2	1.58	0.83
12:L:32:ALA:CB	12:L:55:ILE:HG13	2.09	0.82
1:A:1189:SER:O	1:A:1241:ARG:HD3	1.79	0.82
2:B:101:MET:HB2	2:B:169:ARG:HH22	1.44	0.82
7:G:1:MET:SD	7:G:2:PHE:N	2.52	0.82
5:E:114:ASN:O	5:E:115:ASN:HB3	1.76	0.82
2:B:309:GLN:OE1	9:I:52:ILE:HD11	1.79	0.82
1:A:1095:THR:HG22	1:A:1100:ARG:HB2	1.61	0.82
2:B:770:GLN:CD	2:B:983:ARG:HA	1.98	0.82
2:B:1084:GLN:HE21	2:B:1084:GLN:H	1.24	0.82
2:B:277:LYS:HG3	2:B:338:GLY:HA2	1.60	0.82
1:A:351:THR:HB	2:B:1103:ILE:CD1	2.09	0.82
1:A:590:ARG:CB	1:A:590:ARG:HH11	1.91	0.82
1:A:709:THR:HG22	1:A:711:ARG:H	1.45	0.82
1:A:196:GLU:HB2	1:A:197:PRO:HD2	1.61	0.82
7:G:62:LEU:HB3	7:G:63:PRO:HD2	1.61	0.82
2:B:815:ARG:HD3	2:B:1041:GLU:OE2	1.79	0.82
1:A:69:THR:O	1:A:71:GLN:N	2.13	0.82
1:A:770:VAL:HA	1:A:822:GLU:OE1	1.79	0.82
2:B:1095:LEU:HD12	2:B:1095:LEU:H	1.45	0.82
2:B:850:LEU:HD12	2:B:851:PHE:N	1.94	0.82
2:B:1099:VAL:HG13	2:B:1100:ASP:N	1.95	0.82
7:G:49:LEU:HD21	7:G:77:VAL:HG23	1.61	0.82
1:A:1244:ARG:HB3	1:A:1245:PRO:CA	2.08	0.82
2:B:515:HIS:HD2	2:B:517:THR:N	1.77	0.82
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.15	0.82
2:B:65:GLU:HG3	2:B:66:ASP:H	1.45	0.82
2:B:1084:GLN:HE21	2:B:1084:GLN:N	1.77	0.82
9:I:26:LEU:HD23	9:I:37:GLU:HA	1.59	0.82
3:C:142:VAL:H	10:J:16:ASP:HB3	1.45	0.82
1:A:855:THR:HG21	1:A:857:ARG:HE	1.44	0.81
1:A:1116:LEU:HB3	1:A:1308:THR:CG2	2.10	0.81
1:A:225:ASN:HD22	1:A:228:PHE:H	0.83	0.81
3:C:133:ILE:HG21	3:C:236:GLY:HA3	1.62	0.81
7:G:87:VAL:HB	7:G:103:VAL:HG11	1.61	0.81
1:A:49:LYS:NZ	1:A:61:ILE:HG13	1.94	0.81
2:B:69:LEU:CB	2:B:429:PHE:HE1	1.93	0.81
1:A:1260:LEU:HD12	1:A:1260:LEU:O	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:LEU:HD22	2:B:429:PHE:CZ	2.16	0.81
1:A:567:LYS:CE	8:H:47:PHE:HB2	2.11	0.81
2:B:622:LYS:CE	9:I:59:VAL:HG22	2.11	0.81
5:E:128:PRO:HA	5:E:129:PRO:O	1.79	0.81
1:A:590:ARG:HB3	1:A:605:MET:H	1.46	0.81
10:J:64:ASN:HB3	10:J:65:PRO:HD2	1.61	0.81
1:A:107:CYS:HA	1:A:171:GLN:OE1	1.79	0.81
1:A:1438:THR:HB	2:B:1144:ALA:HB3	1.63	0.81
2:B:579:ARG:HB2	2:B:586:TRP:NE1	1.95	0.81
7:G:125:SER:OG	7:G:128:PRO:HA	1.80	0.81
2:B:289:LEU:HD13	2:B:375:ALA:CB	2.09	0.81
8:H:93:TYR:HB3	8:H:144:ILE:O	1.80	0.81
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	1.61	0.81
1:A:1002:GLY:HA3	1:A:1007:ILE:HG21	1.60	0.81
2:B:637:LEU:O	2:B:690:VAL:HG13	1.81	0.80
9:I:35:VAL:HG12	9:I:36:GLU:N	1.96	0.80
1:A:180:LYS:HZ2	1:A:294:SER:HB3	1.46	0.80
2:B:1182:CYS:SG	2:B:1182:CYS:O	2.38	0.80
2:B:882:THR:HG21	2:B:935:ARG:HA	1.63	0.80
1:A:321:PRO:O	1:A:322:VAL:HG12	1.81	0.80
2:B:365:THR:OG1	2:B:367:LEU:HG	1.81	0.80
2:B:1002:THR:HG23	2:B:1006:ILE:HG13	1.62	0.80
2:B:1150:ARG:HG3	2:B:1150:ARG:HH11	1.45	0.80
1:A:779:PHE:HE1	1:A:785:PRO:HD3	1.45	0.80
8:H:101:ALA:HB2	8:H:116:TYR:CZ	2.15	0.80
2:B:217:ARG:NE	2:B:405:ARG:HB2	1.97	0.80
6:F:77:ASP:O	6:F:78:GLN:HB2	1.79	0.80
2:B:336:ARG:HE	2:B:348:ARG:HH12	1.25	0.80
1:A:600:PRO:HG2	1:A:601:LYS:H	1.44	0.80
3:C:8:VAL:HG12	3:C:9:LYS:H	1.46	0.80
2:B:957:ASN:HD22	2:B:961:LEU:HB2	1.47	0.80
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.17	0.80
7:G:15:PRO:HA	7:G:18:PHE:CD1	2.17	0.80
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.62	0.80
2:B:1159:ARG:HB3	2:B:1159:ARG:HH11	1.46	0.80
1:A:1444:MET:HE1	6:F:135:ARG:HB2	1.64	0.80
1:A:1130:GLN:HE21	1:A:1134:ILE:HD11	1.47	0.80
5:E:52:ARG:HB3	5:E:53:PRO:HD2	1.64	0.80
1:A:23:SER:HA	1:A:233:TRP:NE1	1.96	0.80
3:C:98:VAL:C	3:C:99:LEU:HD23	2.02	0.80
2:B:422:LYS:O	2:B:426:LYS:HG2	1.80	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:15:DC:H2"	13:T:16:DT:C7	2.12	0.79
4:D:47:LEU:HD13	4:D:48:ILE:H	1.46	0.79
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.64	0.79
12:L:61:THR:HG22	12:L:63:ARG:H	1.47	0.79
1:A:115:LEU:O	1:A:122:MET:HG2	1.83	0.79
2:B:343:ILE:HG23	2:B:347:LYS:HE2	1.62	0.79
6:F:103:MET:HE2	7:G:66:GLY:H	1.47	0.79
10:J:9:SER:HB2	10:J:45:CYS:HB2	1.64	0.79
2:B:824:ILE:HG22	2:B:1087:PHE:CE2	2.18	0.79
1:A:1254:ALA:O	1:A:1255:GLU:HB2	1.81	0.79
1:A:1206:ASP:HB3	1:A:1274:ARG:HH12	1.45	0.79
11:K:53:ASP:HB3	11:K:56:VAL:HG23	1.64	0.79
2:B:133:LYS:HE3	2:B:135:ARG:NH2	1.95	0.79
2:B:46:GLN:HB2	2:B:408:LEU:HD21	1.65	0.79
4:D:8:PHE:CD2	7:G:6:ASP:HB2	2.18	0.79
2:B:995:ARG:HH12	3:C:165:LYS:HG2	1.47	0.79
11:K:6:ARG:O	11:K:9:LEU:HG	1.81	0.79
1:A:21:LEU:HD11	1:A:1414:ALA:HA	1.65	0.79
7:G:7:LEU:HB2	7:G:74:TYR:HE2	1.43	0.79
11:K:12:LEU:N	11:K:12:LEU:HD12	1.97	0.79
2:B:35:SER:HA	2:B:811:TYR:HE2	1.48	0.78
12:L:30:ILE:O	12:L:56:LEU:HA	1.82	0.78
8:H:44:VAL:HG13	8:H:48:PRO:HA	1.63	0.78
3:C:238:ILE:HD11	3:C:246:ARG:HH11	1.47	0.78
3:C:39:ALA:CA	3:C:164:ALA:HB3	2.12	0.78
1:A:148:CYS:O	1:A:168:GLY:HA2	1.82	0.78
3:C:73:GLN:HE21	3:C:74:SER:H	1.29	0.78
7:G:88:ASP:HB3	7:G:144:ARG:HA	1.66	0.78
1:A:92:HIS:HB2	1:A:236:LEU:HD21	1.63	0.78
1:A:982:THR:H	1:A:985:ASP:HB2	1.47	0.78
2:B:880:THR:CB	2:B:934:LYS:HD3	2.12	0.78
1:A:372:LYS:HA	1:A:435:HIS:ND1	1.98	0.78
3:C:235:VAL:HG12	10:J:13:VAL:HG23	1.64	0.78
7:G:128:PRO:O	7:G:138:THR:HG23	1.83	0.78
12:L:28:LYS:HB2	12:L:39:SER:HB2	1.65	0.78
5:E:207:ARG:NH1	5:E:207:ARG:HB3	1.98	0.78
2:B:1162:ILE:HD11	2:B:1194:ILE:HD13	1.64	0.78
8:H:27:GLU:HG2	8:H:39:THR:HA	1.66	0.78
5:E:109:ILE:HG22	5:E:110:PHE:H	1.47	0.78
13:T:13:DT:H2"	13:T:14:DA:OP2	1.83	0.78
2:B:579:ARG:HB2	2:B:586:TRP:HE1	1.46	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ILE:HD11	1:A:270:LEU:HD13	1.65	0.78
10:J:1:MET:N	10:J:57:ILE:H	1.82	0.78
2:B:412:LEU:HB3	2:B:466:TRP:HE1	1.48	0.78
4:D:18:VAL:O	4:D:19:GLU:HB2	1.82	0.78
2:B:613:VAL:HG13	2:B:627:PHE:O	1.84	0.78
2:B:549:THR:HB	2:B:628:THR:OG1	1.84	0.78
1:A:567:LYS:HB3	1:A:568:PRO:HD3	1.65	0.78
8:H:41:ASP:O	8:H:42:ILE:HG13	1.84	0.78
1:A:1004:ASN:HD21	5:E:167:ARG:HD2	1.46	0.78
2:B:294:ASP:O	2:B:296:GLU:N	2.17	0.78
11:K:30:ALA:HB2	11:K:76:GLN:HG3	1.64	0.78
2:B:70:ILE:O	2:B:137:TYR:HB2	1.84	0.78
2:B:880:THR:HB	2:B:934:LYS:CD	2.12	0.78
2:B:882:THR:HG22	2:B:884:ARG:H	1.49	0.78
2:B:244:LEU:HD11	2:B:366:GLN:NE2	1.97	0.78
1:A:320:ARG:CB	1:A:320:ARG:HH11	1.97	0.78
1:A:1100:ARG:NH2	1:A:1351:GLU:HG2	1.99	0.78
8:H:25:ARG:HA	8:H:41:ASP:HA	1.65	0.77
8:H:80:ARG:HH11	11:K:57:LEU:HD21	1.49	0.77
1:A:696:GLU:OE2	1:A:702:LEU:HD21	1.83	0.77
5:E:109:ILE:HG22	5:E:110:PHE:N	1.99	0.77
8:H:128:ASN:H	8:H:130:ARG:HH11	1.30	0.77
4:D:40:HIS:CB	7:G:73:LYS:HZ2	1.97	0.77
2:B:1095:LEU:HD12	2:B:1095:LEU:N	1.99	0.77
2:B:611:PRO:HG2	2:B:685:LEU:HD21	1.67	0.77
1:A:56:PRO:O	1:A:57:ARG:HG3	1.84	0.77
1:A:567:LYS:HD3	1:A:568:PRO:HD3	1.65	0.77
1:A:541:ILE:HD13	1:A:549:MET:CE	2.14	0.77
11:K:55:LYS:HB3	11:K:81:TYR:CD1	2.20	0.77
4:D:139:LYS:HE2	4:D:143:ASN:HD21	1.47	0.77
1:A:629:LEU:O	1:A:633:VAL:HG23	1.83	0.77
1:A:635:ARG:HH11	1:A:635:ARG:HA	1.50	0.77
3:C:46:ILE:HG13	3:C:72:LEU:HD11	1.66	0.77
2:B:277:LYS:O	2:B:278:GLN:HB2	1.83	0.77
3:C:38:ILE:HA	3:C:173:ALA:HB2	1.66	0.77
8:H:130:ARG:N	8:H:130:ARG:HD2	1.98	0.77
9:I:7:CYS:HB3	9:I:14:LEU:HD21	1.66	0.77
1:A:1175:SER:O	1:A:1176:LEU:HB2	1.84	0.77
2:B:723:VAL:HG12	2:B:724:ASP:H	1.49	0.77
1:A:1444:MET:HG3	7:G:60:ARG:HA	1.66	0.77
1:A:1325:THR:O	5:E:148:GLU:HB2	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ALA:C	1:A:286:HIS:H	1.88	0.77
1:A:477:PRO:HG2	1:A:521:MET:HG2	1.67	0.77
1:A:1343:ALA:HB2	5:E:150:VAL:HG22	1.64	0.77
1:A:189:ARG:HA	1:A:195:ASP:HA	1.65	0.77
1:A:49:LYS:NZ	1:A:61:ILE:H	1.82	0.77
11:K:31:VAL:HG12	11:K:32:VAL:H	1.50	0.77
11:K:55:LYS:HB3	11:K:81:TYR:HD1	1.49	0.77
11:K:107:THR:O	11:K:111:LEU:HG	1.85	0.77
1:A:899:VAL:HG22	1:A:1029:ARG:HG2	1.65	0.77
1:A:590:ARG:HH21	1:A:620:LYS:HB3	1.48	0.77
1:A:1115:SER:C	1:A:1308:THR:HG22	2.04	0.77
1:A:11:LEU:HD12	1:A:11:LEU:C	2.05	0.77
15:P:3:U:H2'	15:P:4:C:C6	2.20	0.77
2:B:464:GLY:O	2:B:477:ALA:HA	1.85	0.77
2:B:506:GLY:HA2	2:B:512:ARG:NH2	1.99	0.76
7:G:119:LEU:HD12	7:G:131:GLN:O	1.85	0.76
11:K:31:VAL:HG12	11:K:32:VAL:N	2.00	0.76
2:B:906:SER:O	2:B:941:LEU:HD23	1.83	0.76
1:A:1308:THR:HG23	1:A:1310:GLY:H	1.50	0.76
1:A:1160:SER:HA	1:A:1170:ILE:HD13	1.65	0.76
2:B:800:GLN:HB3	10:J:52:THR:HG22	1.67	0.76
3:C:235:VAL:HG11	10:J:6:ARG:HH21	1.49	0.76
2:B:1069:PHE:HD1	2:B:1069:PHE:H	1.31	0.76
11:K:46:ILE:O	11:K:50:LEU:HB2	1.85	0.76
1:A:343:LYS:NZ	2:B:1151:LEU:HD12	2.00	0.76
2:B:745:PRO:O	2:B:748:ILE:HG12	1.84	0.76
13:T:16:DT:C2'	13:T:17:DT:H5'	2.14	0.76
1:A:12:ARG:HD2	2:B:1218:THR:HB	1.67	0.76
4:D:8:PHE:HD2	7:G:6:ASP:HB2	1.50	0.76
1:A:837:ILE:HA	1:A:840:ARG:HD3	1.67	0.76
2:B:326:ASP:OD2	2:B:328:GLU:HB3	1.85	0.76
1:A:869:GLY:O	5:E:204:THR:HG21	1.86	0.76
2:B:803:LEU:HD12	2:B:1032:SER:HB3	1.67	0.76
1:A:577:ILE:O	1:A:580:VAL:HG23	1.85	0.76
2:B:755:ILE:HG23	2:B:809:MET:HE3	1.65	0.76
2:B:314:LEU:O	2:B:318:VAL:HG23	1.84	0.76
1:A:381:THR:C	1:A:383:TYR:H	1.88	0.76
1:A:754:SER:N	1:A:757:ASN:HD22	1.83	0.76
1:A:115:LEU:HG	1:A:142:CYS:HB3	1.68	0.76
1:A:852:TYR:CD2	1:A:1060:PRO:HB2	2.21	0.76
2:B:821:GLN:HE22	2:B:851:PHE:H	1.33	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:866:PHE:C	1:A:867:ILE:HD12	2.06	0.76
1:A:392:VAL:HG13	1:A:415:LEU:HD11	1.68	0.76
1:A:670:ILE:HG23	1:A:805:LEU:HD21	1.67	0.76
8:H:42:ILE:HG23	8:H:95:TYR:HE1	1.50	0.76
2:B:1224:PHE:CE1	5:E:171:LYS:HG3	2.21	0.76
3:C:92:CYS:SG	3:C:94:LYS:HB2	2.26	0.76
1:A:1101:LEU:HD12	1:A:1101:LEU:O	1.85	0.76
2:B:758:PHE:CE1	2:B:1027:ILE:HG22	2.21	0.75
10:J:57:ILE:HA	10:J:60:PHE:HD2	1.51	0.75
1:A:1315:GLU:C	1:A:1317:MET:H	1.88	0.75
1:A:34:LYS:NZ	1:A:57:ARG:HH21	1.84	0.75
5:E:113:GLN:HA	5:E:137:GLU:HG3	1.68	0.75
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.22	0.75
2:B:834:ASN:HA	2:B:838:SER:O	1.86	0.75
2:B:757:PRO:HG3	2:B:1028:GLU:OE2	1.87	0.75
1:A:504:LEU:HD11	6:F:91:ALA:CB	2.15	0.75
1:A:35:ILE:HG22	1:A:84:ILE:HD12	1.68	0.75
2:B:654:ARG:H	2:B:657:HIS:HD2	1.32	0.75
7:G:1:MET:SD	7:G:79:PHE:HD1	2.09	0.75
1:A:857:ARG:NH1	6:F:139:PRO:HB2	2.00	0.75
2:B:359:GLU:O	2:B:362:PRO:HD3	1.86	0.75
2:B:516:ASN:N	2:B:516:ASN:HD22	1.83	0.75
2:B:777:ALA:HA	2:B:1095:LEU:HA	1.66	0.75
5:E:212:ARG:HH11	5:E:212:ARG:HG3	1.50	0.75
2:B:806:THR:HG22	2:B:808:ALA:N	1.94	0.75
1:A:34:LYS:NZ	1:A:57:ARG:NH2	2.35	0.75
7:G:97:HIS:HA	7:G:112:LYS:HE2	1.68	0.75
4:D:47:LEU:O	4:D:48:ILE:HD13	1.87	0.75
1:A:43:GLU:HB2	1:A:46:THR:HB	1.67	0.75
4:D:40:HIS:HB3	7:G:73:LYS:HZ2	1.52	0.75
1:A:583:PRO:HG2	1:A:586:ILE:HG13	1.69	0.75
2:B:336:ARG:HE	2:B:348:ARG:NH1	1.84	0.75
2:B:97:VAL:HG22	2:B:128:LEU:HG	1.68	0.75
4:D:144:THR:HG21	7:G:46:LEU:HD13	1.69	0.75
2:B:855:PHE:HD1	2:B:856:PHE:N	1.84	0.75
8:H:99:GLY:HA3	8:H:118:PHE:HA	1.69	0.75
3:C:89:GLU:O	3:C:90:ASP:HB3	1.86	0.75
10:J:23:ASN:C	10:J:25:LEU:H	1.90	0.75
13:T:26:DT:H2"	13:T:27:DC:OP2	1.87	0.75
1:A:335:ARG:CD	2:B:1202:LEU:HD23	2.16	0.74
7:G:28:THR:O	7:G:32:GLU:HG3	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:809:THR:H	1:A:812:GLU:HB2	1.52	0.74
5:E:92:THR:O	5:E:95:THR:HB	1.87	0.74
1:A:463:ILE:HB	1:A:464:PRO:HD2	1.70	0.74
1:A:1394:THR:HG21	1:A:1398:MET:SD	2.26	0.74
2:B:69:LEU:CG	2:B:429:PHE:CE1	2.69	0.74
1:A:1255:GLU:OE1	1:A:1258:HIS:HB2	1.88	0.74
3:C:36:VAL:HG21	3:C:251:LEU:HB2	1.68	0.74
3:C:242:GLN:HA	3:C:245:VAL:HG23	1.68	0.74
5:E:23:VAL:HG13	5:E:78:LEU:HD13	1.70	0.74
10:J:44:TYR:HD2	10:J:44:TYR:H	1.31	0.74
2:B:850:LEU:HD12	2:B:851:PHE:H	1.52	0.74
2:B:957:ASN:O	2:B:959:ASP:N	2.20	0.74
1:A:298:PHE:CZ	1:A:314:ALA:HB2	2.22	0.74
1:A:940:ARG:HH11	1:A:940:ARG:HG2	1.51	0.74
11:K:7:PHE:HB2	11:K:11:LEU:HD23	1.69	0.74
3:C:93:ASP:OD1	3:C:122:SER:HB2	1.88	0.74
1:A:1280:GLU:O	1:A:1309:ASP:HB3	1.88	0.74
1:A:22:PHE:HB2	2:B:1211:ASN:OD1	1.88	0.74
1:A:132:LYS:HE2	1:A:1411:GLU:OE1	1.87	0.74
12:L:28:LYS:HD2	12:L:39:SER:OG	1.87	0.74
2:B:378:LEU:O	2:B:382:ILE:HG13	1.87	0.74
2:B:1180:PHE:HB3	2:B:1191:ILE:CD1	2.17	0.74
15:P:3:U:H2'	15:P:4:C:H6	1.53	0.74
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.23	0.74
1:A:1006:ILE:HD11	5:E:163:GLU:HG3	1.70	0.73
1:A:464:PRO:HG2	1:A:465:TYR:HD1	1.52	0.73
2:B:526:GLU:HG2	2:B:538:ASN:ND2	2.03	0.73
1:A:483:ASP:OD2	15:P:11:U:H5''	1.88	0.73
1:A:105:CYS:O	1:A:114:LEU:HG	1.88	0.73
1:A:7:SER:CB	2:B:1175:LEU:HD22	2.17	0.73
5:E:180:ARG:HH21	5:E:192:ARG:HB2	1.52	0.73
1:A:889:SER:HB3	1:A:1297:GLU:HG3	1.70	0.73
1:A:825:ILE:HD11	2:B:512:ARG:CB	2.13	0.73
2:B:1006:ILE:HG22	10:J:45:CYS:HB3	1.69	0.73
1:A:1391:ARG:C	1:A:1391:ARG:HD2	2.08	0.73
1:A:239:LEU:HD12	1:A:240:PRO:HD2	1.70	0.73
11:K:61:TYR:C	11:K:61:TYR:CD2	2.61	0.73
3:C:50:GLU:HG2	12:L:64:LEU:HD22	1.71	0.73
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.69	0.73
3:C:128:ASN:O	3:C:129:ILE:HG13	1.88	0.73
8:H:109:LYS:HD2	8:H:111:LEU:HD11	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:60:ARG:HH21	12:L:65:VAL:HG21	1.52	0.73
1:A:450:LEU:HD13	1:A:1074:GLU:HG2	1.69	0.73
1:A:288:ALA:HA	1:A:291:GLU:OE2	1.87	0.73
1:A:351:THR:HB	2:B:1103:ILE:HD12	1.69	0.73
1:A:591:PHE:HA	1:A:595:THR:HG21	1.70	0.73
3:C:112:ASN:HB3	3:C:114:TYR:CE1	2.24	0.73
1:A:14:VAL:N	1:A:1432:GLN:HE22	1.85	0.73
1:A:1219:THR:HG21	1:A:1271:ILE:HD11	1.71	0.73
9:I:111:THR:HG22	9:I:112:SER:H	1.54	0.73
1:A:49:LYS:HZ1	1:A:61:ILE:H	1.32	0.73
6:F:79:ARG:NH2	6:F:150:GLU:OE1	2.22	0.73
1:A:10:PRO:HB3	4:D:3:VAL:HA	1.71	0.73
3:C:22:LEU:HD13	3:C:230:MET:CE	2.19	0.73
8:H:100:THR:HG22	8:H:101:ALA:N	2.03	0.72
1:A:506:ALA:HB1	1:A:508:PRO:HD2	1.71	0.72
1:A:438:ASP:OD2	1:A:461:LYS:HD2	1.89	0.72
1:A:464:PRO:HG2	1:A:465:TYR:CD1	2.23	0.72
1:A:682:THR:CG2	1:A:728:LYS:HE3	2.19	0.72
2:B:708:GLU:HG3	2:B:709:ASP:H	1.53	0.72
1:A:34:LYS:HB3	1:A:36:ARG:HH21	1.52	0.72
2:B:1097:HIS:N	2:B:1098:MET:HE2	2.02	0.72
1:A:896:ARG:NH2	1:A:1030:ARG:HE	1.86	0.72
1:A:1116:LEU:N	1:A:1308:THR:HG22	2.03	0.72
11:K:65:HIS:HD2	11:K:67:PHE:H	1.36	0.72
2:B:193:LYS:HZ1	12:L:32:ALA:HB1	1.54	0.72
1:A:535:THR:HG23	1:A:575:LYS:HG2	1.71	0.72
10:J:1:MET:N	10:J:56:LEU:N	2.36	0.72
2:B:364:ILE:O	2:B:365:THR:HB	1.89	0.72
1:A:335:ARG:HE	1:A:335:ARG:HA	1.54	0.72
1:A:511:ILE:HA	1:A:521:MET:HE3	1.69	0.72
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.29	0.72
1:A:534:LEU:O	1:A:574:GLY:HA3	1.90	0.72
1:A:1420:ASP:O	1:A:1421:CYS:HB2	1.88	0.72
1:A:802:ASN:ND2	2:B:728:ARG:HB2	2.04	0.72
5:E:190:LEU:HD12	5:E:214:CYS:HB2	1.72	0.72
1:A:50:ILE:O	1:A:52:GLY:N	2.23	0.72
5:E:61:GLN:HG3	5:E:78:LEU:O	1.89	0.72
1:A:1101:LEU:HD11	1:A:1105:LEU:HD11	1.72	0.72
8:H:129:TYR:H	8:H:130:ARG:NH1	1.87	0.72
1:A:967:ALA:HA	1:A:1044:TRP:CZ3	2.24	0.72
4:D:119:ARG:HD3	4:D:221:TYR:CD2	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:23:VAL:O	5:E:28:TYR:HB2	1.89	0.72
1:A:399:HIS:CB	1:A:400:PRO:HD3	2.20	0.72
1:A:1193:LEU:HB2	1:A:1260:LEU:HD11	1.71	0.72
2:B:1150:ARG:CG	2:B:1150:ARG:HH11	2.03	0.72
1:A:382:PRO:HB3	1:A:428:TYR:HE2	1.53	0.72
6:F:79:ARG:HG3	6:F:144:GLU:HG2	1.72	0.72
4:D:24:ALA:C	4:D:26:THR:H	1.92	0.72
1:A:557:ASP:OD2	1:A:559:VAL:HB	1.88	0.72
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.54	0.72
3:C:44:LEU:HB2	3:C:77:ILE:HD11	1.71	0.72
1:A:470:LEU:HD23	1:A:470:LEU:H	1.51	0.72
1:A:1152:ILE:HD11	9:I:44:TYR:CD2	2.25	0.72
2:B:810:GLU:HA	2:B:815:ARG:NH2	2.02	0.72
12:L:30:ILE:O	12:L:56:LEU:HD23	1.90	0.72
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.72	0.72
2:B:906:SER:HA	2:B:946:ASN:HB2	1.70	0.72
2:B:547:VAL:HG12	2:B:612:GLU:OE2	1.89	0.71
4:D:119:ARG:HG2	4:D:120:GLU:N	2.04	0.71
1:A:763:ALA:O	1:A:803:SER:HB3	1.90	0.71
3:C:236:GLY:O	3:C:238:ILE:N	2.23	0.71
6:F:99:LEU:O	6:F:103:MET:HG2	1.90	0.71
9:I:105:SER:O	9:I:106:CYS:HB3	1.89	0.71
5:E:195:VAL:HG12	5:E:196:VAL:H	1.54	0.71
2:B:1106:ARG:NH1	2:B:1110:PRO:HG2	2.05	0.71
1:A:722:LEU:H	1:A:722:LEU:HD12	1.53	0.71
3:C:22:LEU:HD13	3:C:230:MET:HE3	1.73	0.71
3:C:75:MET:HB3	3:C:128:ASN:HB3	1.72	0.71
1:A:903:ASN:HD22	1:A:904:THR:H	1.39	0.71
1:A:356:ASP:HB2	1:A:469:ARG:NH1	2.05	0.71
13:T:9:DC:H2"	13:T:10:DA:C8	2.25	0.71
9:I:74:GLU:HA	9:I:80:SER:O	1.90	0.71
2:B:862:GLN:HG2	2:B:963:PHE:HD1	1.56	0.71
8:H:64:ASN:OD1	8:H:90:ALA:N	2.20	0.71
1:A:1436:ILE:HD13	2:B:1139:ILE:HG23	1.73	0.71
1:A:1116:LEU:HD13	1:A:1329:THR:HB	1.73	0.71
12:L:61:THR:HG21	12:L:63:ARG:NE	2.05	0.71
2:B:582:VAL:HB	2:B:587:HIS:HD2	1.54	0.71
1:A:32:VAL:HG23	1:A:57:ARG:HB2	1.71	0.71
8:H:101:ALA:HB2	8:H:116:TYR:CE2	2.24	0.71
8:H:89:LEU:HB3	8:H:91:ASP:OD1	1.90	0.71
1:A:567:LYS:HD2	8:H:95:TYR:CD2	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:147:LEU:HB2	3:C:151:GLN:CB	2.21	0.71
9:I:76:PRO:HD2	9:I:108:HIS:HD2	1.54	0.71
5:E:44:ALA:O	5:E:45:LYS:HB2	1.90	0.71
2:B:60:GLN:O	2:B:63:ILE:HG22	1.90	0.71
2:B:412:LEU:HB3	2:B:466:TRP:NE1	2.06	0.71
6:F:79:ARG:HB2	6:F:79:ARG:HH11	1.55	0.71
1:A:868:TYR:OH	1:A:1366:ARG:HD3	1.89	0.71
2:B:126:SER:OG	2:B:172:ILE:HD11	1.91	0.71
1:A:853:ASP:O	1:A:854:ASN:HB2	1.89	0.71
9:I:71:SER:OG	9:I:83:ASN:HB2	1.90	0.71
1:A:524:VAL:HG12	1:A:525:GLN:N	2.04	0.71
1:A:816:HIS:CD2	2:B:764:SER:HB2	2.26	0.71
5:E:63:ASN:HB3	5:E:64:PRO:HD2	1.73	0.71
9:I:58:VAL:HG13	9:I:62:ILE:CD1	2.20	0.71
1:A:1032:LEU:O	1:A:1036:ARG:HD3	1.91	0.71
1:A:96:ILE:CG2	1:A:97:ALA:N	2.53	0.71
1:A:184:SER:HB3	1:A:199:LEU:HD23	1.73	0.71
1:A:225:ASN:ND2	1:A:228:PHE:N	2.31	0.71
8:H:95:TYR:CE2	8:H:97:MET:HG3	2.26	0.71
6:F:109:VAL:HG12	6:F:110:ASP:N	2.06	0.71
12:L:61:THR:CG2	12:L:63:ARG:HE	2.03	0.71
1:A:963:ILE:HD11	1:A:1048:ASN:CB	2.21	0.71
1:A:438:ASP:O	1:A:439:ASN:HB2	1.90	0.71
1:A:356:ASP:HB2	1:A:469:ARG:HH12	1.56	0.71
14:N:3:DT:H1'	14:N:4:DA:C8	2.25	0.71
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.71	0.71
1:A:34:LYS:HZ1	1:A:57:ARG:HH21	1.34	0.71
3:C:73:GLN:NE2	3:C:74:SER:H	1.87	0.71
2:B:713:ALA:HB1	2:B:714:GLU:OE1	1.91	0.71
2:B:583:ASN:ND2	2:B:628:THR:HG22	2.05	0.70
7:G:23:LYS:HG3	7:G:56:ILE:HD11	1.73	0.70
1:A:960:ILE:O	1:A:963:ILE:HG22	1.91	0.70
1:A:722:LEU:HD23	1:A:799:PHE:CD1	2.26	0.70
1:A:1006:ILE:CD1	5:E:163:GLU:HG3	2.21	0.70
1:A:1107:VAL:HG12	1:A:1107:VAL:O	1.91	0.70
1:A:117:GLU:H	1:A:117:GLU:CD	1.93	0.70
2:B:291:ILE:HD13	2:B:300:HIS:NE2	2.05	0.70
1:A:41:MET:HB2	1:A:49:LYS:CA	2.17	0.70
1:A:616:VAL:HG12	1:A:617:VAL:N	2.05	0.70
2:B:977:GLY:HA3	2:B:1099:VAL:HB	1.73	0.70
8:H:64:ASN:HD22	8:H:88:SER:HB2	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:903:ASN:ND2	1:A:904:THR:N	2.37	0.70
1:A:381:THR:O	1:A:383:TYR:N	2.24	0.70
4:D:9:GLN:NE2	4:D:31:GLN:HE21	1.89	0.70
2:B:294:ASP:C	2:B:296:GLU:H	1.95	0.70
9:I:13:MET:CE	9:I:14:LEU:H	2.04	0.70
1:A:515:GLN:HA	1:A:1367:HIS:HE2	1.57	0.70
1:A:49:LYS:HZ1	1:A:61:ILE:CG1	2.04	0.70
1:A:567:LYS:CB	1:A:568:PRO:HD3	2.21	0.70
1:A:535:THR:CG2	1:A:616:VAL:HA	2.20	0.70
1:A:144:THR:O	1:A:146:MET:HG3	1.90	0.70
1:A:1027:ALA:O	1:A:1031:VAL:HG23	1.91	0.70
11:K:63:VAL:O	11:K:63:VAL:HG23	1.92	0.70
1:A:466:SER:HB2	2:B:1099:VAL:CG2	2.21	0.70
4:D:119:ARG:HD3	4:D:221:TYR:CE2	2.26	0.70
1:A:834:THR:HG21	1:A:1077:THR:HG23	1.72	0.70
2:B:613:VAL:HG22	2:B:628:THR:HA	1.73	0.70
5:E:22:MET:HE3	5:E:26:ARG:NH1	2.04	0.70
8:H:129:TYR:N	8:H:130:ARG:HH11	1.89	0.70
1:A:896:ARG:NH2	1:A:1030:ARG:HH21	1.89	0.70
6:F:132:LEU:HD21	7:G:61:ILE:HD11	1.72	0.70
2:B:112:LEU:HD12	2:B:113:TYR:H	1.57	0.70
2:B:603:LEU:HD13	2:B:608:ASP:HB3	1.74	0.70
1:A:37:PHE:HD1	1:A:37:PHE:N	1.89	0.70
12:L:38:LEU:O	12:L:39:SER:HB3	1.92	0.70
1:A:382:PRO:HD3	1:A:428:TYR:CD2	2.19	0.70
9:I:85:PHE:HD2	9:I:85:PHE:N	1.87	0.70
9:I:35:VAL:HG12	9:I:36:GLU:H	1.56	0.70
1:A:885:THR:O	1:A:885:THR:HG22	1.91	0.70
2:B:229:ALA:HB1	2:B:231:PRO:HD2	1.72	0.70
10:J:24:LEU:HD12	10:J:39:LEU:HD11	1.73	0.70
2:B:69:LEU:CD2	2:B:429:PHE:CE1	2.74	0.70
2:B:244:LEU:HD21	2:B:366:GLN:HE21	1.56	0.70
9:I:111:THR:HG22	9:I:112:SER:N	2.06	0.70
1:A:332:LYS:H	1:A:337:ARG:CB	2.05	0.70
1:A:1057:VAL:HG12	1:A:1058:VAL:N	2.06	0.70
1:A:1066:VAL:O	1:A:1070:GLN:HG3	1.91	0.70
3:C:5:GLY:O	3:C:7:GLN:HG3	1.92	0.70
3:C:107:SER:O	3:C:109:SER:N	2.23	0.70
2:B:918:ILE:HD12	2:B:935:ARG:CZ	2.22	0.70
3:C:73:GLN:HE21	3:C:75:MET:N	1.89	0.70
1:A:1420:ASP:HB3	1:A:1422:ARG:HG3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.74	0.70
1:A:1036:ARG:HH11	1:A:1036:ARG:HG2	1.56	0.70
1:A:774:ARG:NH1	1:A:797:LYS:HG3	2.07	0.70
1:A:230:ARG:H	1:A:233:TRP:HE3	1.38	0.70
1:A:1149:ALA:HB2	9:I:47:GLU:HA	1.74	0.70
1:A:252:PHE:O	1:A:256:GLN:HB2	1.92	0.70
8:H:118:PHE:O	8:H:120:GLY:N	2.25	0.70
7:G:122:ASN:ND2	7:G:125:SER:HB3	2.07	0.70
8:H:125:LEU:HG	8:H:126:GLU:H	1.55	0.70
3:C:259:LEU:HD21	11:K:91:CYS:HB3	1.73	0.70
1:A:596:THR:C	1:A:598:LEU:H	1.95	0.69
2:B:172:ILE:HD13	2:B:178:ASN:HD22	1.56	0.69
1:A:317:LYS:O	1:A:318:SER:HB3	1.92	0.69
1:A:35:ILE:O	1:A:35:ILE:HG22	1.92	0.69
12:L:53:HIS:HB3	12:L:55:ILE:CD1	2.22	0.69
1:A:567:LYS:HB2	8:H:96:VAL:H	1.56	0.69
6:F:147:SER:OG	6:F:150:GLU:HG3	1.91	0.69
5:E:153:HIS:HB3	5:E:196:VAL:CG1	2.22	0.69
1:A:332:LYS:H	1:A:337:ARG:HB2	1.57	0.69
1:A:1116:LEU:HB3	1:A:1308:THR:HG21	1.73	0.69
2:B:1095:LEU:CD1	2:B:1095:LEU:H	2.03	0.69
1:A:885:THR:O	1:A:940:ARG:HD2	1.91	0.69
1:A:96:ILE:HG22	1:A:97:ALA:H	1.57	0.69
2:B:637:LEU:HD21	2:B:742:GLU:OE2	1.92	0.69
1:A:12:ARG:HB2	2:B:1218:THR:CG2	2.20	0.69
2:B:405:ARG:NE	2:B:632:ARG:HG2	2.07	0.69
5:E:117:THR:HG22	5:E:119:SER:N	2.07	0.69
2:B:1007:VAL:CG2	2:B:1008:PRO:HD2	2.22	0.69
1:A:883:LEU:HD11	1:A:1017:LEU:HD11	1.75	0.69
8:H:38:LEU:HD12	8:H:124:ARG:O	1.92	0.69
8:H:15:VAL:HG13	8:H:26:ILE:HG12	1.72	0.69
8:H:104:PHE:CZ	8:H:136:LYS:HA	2.27	0.69
1:A:202:LEU:HA	1:A:206:GLU:OE1	1.92	0.69
2:B:189:LEU:HD13	2:B:196:PRO:HA	1.74	0.69
2:B:1215:ARG:O	2:B:1216:LEU:HD23	1.91	0.69
8:H:106:GLU:HG2	8:H:112:ILE:HG12	1.71	0.69
2:B:654:ARG:H	2:B:657:HIS:CD2	2.10	0.69
2:B:746:SER:HB2	2:B:1046:PRO:HG2	1.74	0.69
1:A:1081:LEU:HD11	1:A:1097:GLY:HA3	1.73	0.69
1:A:829:VAL:C	1:A:831:THR:H	1.93	0.69
2:B:175:ARG:HH11	2:B:175:ARG:HG2	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:173:SER:O	5:E:175:LEU:N	2.24	0.69
1:A:1164:PRO:HG2	1:A:1165:GLU:H	1.55	0.69
2:B:911:ILE:HD11	2:B:941:LEU:CD1	2.23	0.69
2:B:999:MET:HB3	2:B:1007:VAL:HG21	1.73	0.69
4:D:155:ARG:HD3	4:D:221:TYR:CZ	2.27	0.69
12:L:53:HIS:O	12:L:55:ILE:HD13	1.91	0.69
1:A:913:LEU:CD1	1:A:914:GLU:H	2.06	0.69
1:A:49:LYS:NZ	1:A:61:ILE:N	2.41	0.69
1:A:608:ILE:HB	1:A:613:ILE:HD11	1.73	0.69
12:L:26:THR:HG23	12:L:62:LYS:NZ	2.07	0.69
7:G:30:LEU:HD13	7:G:72:VAL:HG11	1.73	0.69
2:B:497:ARG:HH22	2:B:775:LYS:CE	2.04	0.69
3:C:212:PRO:HB3	3:C:213:PRO:HD2	1.74	0.69
10:J:48:ARG:HE	10:J:49:MET:HE2	1.57	0.69
2:B:430:ARG:O	2:B:434:ARG:HD2	1.93	0.69
1:A:567:LYS:CG	1:A:568:PRO:HD3	2.22	0.69
7:G:127:PRO:HG3	7:G:139:ILE:CD1	2.23	0.69
7:G:139:ILE:HG22	7:G:140:LYS:HD3	1.75	0.69
1:A:852:TYR:CD1	6:F:136:ARG:HB3	2.28	0.69
3:C:137:LYS:HB2	3:C:138:GLU:OE1	1.92	0.69
2:B:1000:PRO:O	2:B:1007:VAL:HG23	1.92	0.69
2:B:213:ILE:HD11	2:B:497:ARG:HB3	1.74	0.69
2:B:1142:GLY:HA3	6:F:88:TYR:HE2	1.58	0.69
1:A:552:TRP:HE3	1:A:651:LYS:HB3	1.57	0.69
6:F:106:PRO:HG2	7:G:18:PHE:O	1.93	0.68
1:A:870:GLU:O	5:E:205:SER:HB3	1.93	0.68
1:A:709:THR:HB	1:A:712:GLU:H	1.58	0.68
6:F:75:PRO:HG2	6:F:77:ASP:O	1.93	0.68
3:C:235:VAL:HG11	10:J:6:ARG:NH2	2.07	0.68
1:A:630:ILE:HD11	1:A:646:PHE:HZ	1.55	0.68
4:D:134:THR:HG22	4:D:136:GLY:H	1.58	0.68
2:B:1159:ARG:HB3	2:B:1159:ARG:NH1	2.08	0.68
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.75	0.68
1:A:90:VAL:HG13	1:A:297:GLN:CD	2.13	0.68
3:C:100:THR:HG22	3:C:101:LEU:H	1.57	0.68
2:B:273:LEU:HD12	2:B:276:ILE:HD12	1.75	0.68
2:B:751:VAL:HG13	2:B:812:LEU:HD22	1.75	0.68
2:B:100:PRO:HA	2:B:125:SER:O	1.93	0.68
1:A:504:LEU:HD11	6:F:91:ALA:HB1	1.75	0.68
2:B:879:ARG:NH1	2:B:883:LEU:HD22	2.07	0.68
2:B:955:THR:CG2	2:B:956:THR:N	2.56	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:THR:HG23	1:A:476:SER:N	2.08	0.68
3:C:184:ASN:ND2	3:C:187:LYS:HA	2.08	0.68
2:B:273:LEU:CB	2:B:276:ILE:HD12	2.21	0.68
2:B:364:ILE:HG12	2:B:585:VAL:HG13	1.76	0.68
1:A:866:PHE:HE1	5:E:211:TYR:H	1.41	0.68
1:A:382:PRO:HB3	1:A:428:TYR:CE2	2.27	0.68
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.58	0.68
2:B:852:ARG:HH22	12:L:70:ARG:C	1.97	0.68
14:N:2:DG:H4'	14:N:3:DT:OP1	1.94	0.68
4:D:170:THR:C	4:D:172:LEU:H	1.97	0.68
2:B:863:GLU:OE2	2:B:873:THR:HA	1.94	0.68
8:H:84:ALA:HB2	8:H:87:ARG:HD2	1.75	0.68
1:A:2:VAL:HG11	2:B:1157:ALA:HB1	1.74	0.68
1:A:883:LEU:HD23	1:A:1021:LEU:HD13	1.76	0.68
2:B:497:ARG:HH22	2:B:775:LYS:HE2	1.58	0.68
2:B:638:PHE:HA	2:B:690:VAL:HG22	1.74	0.68
5:E:111:VAL:HG12	5:E:137:GLU:HG2	1.76	0.68
1:A:857:ARG:HD3	1:A:861:GLY:O	1.94	0.68
2:B:423:LYS:HA	2:B:426:LYS:HE2	1.76	0.68
3:C:66:ARG:NH2	10:J:3:VAL:O	2.25	0.68
6:F:109:VAL:HG11	6:F:123:LYS:CD	2.15	0.68
1:A:427:GLN:HB2	1:A:430:TRP:CD1	2.28	0.68
1:A:852:TYR:CE2	1:A:1060:PRO:HB2	2.27	0.68
11:K:87:LEU:O	11:K:91:CYS:HB2	1.94	0.68
1:A:658:LEU:HD23	1:A:659:HIS:CE1	2.29	0.68
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	1.76	0.68
1:A:285:PRO:HG2	1:A:288:ALA:HB3	1.75	0.68
1:A:1339:LEU:HD13	5:E:147:HIS:CD2	2.29	0.68
2:B:520:GLY:N	2:B:748:ILE:HG22	2.09	0.68
1:A:528:LEU:O	1:A:531:ILE:HG22	1.93	0.68
8:H:111:LEU:HA	8:H:127:GLY:O	1.93	0.68
2:B:167:ILE:HD12	2:B:167:ILE:N	2.09	0.68
2:B:60:GLN:NE2	2:B:95:ILE:HG22	2.08	0.68
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.76	0.68
1:A:11:LEU:HD12	1:A:11:LEU:O	1.94	0.68
2:B:582:VAL:HA	2:B:626:ILE:HB	1.74	0.68
7:G:102:GLN:HG3	7:G:106:MET:O	1.94	0.68
3:C:80:LEU:HD11	3:C:95:CYS:C	2.14	0.67
1:A:1308:THR:HG21	1:A:1310:GLY:O	1.94	0.67
1:A:910:PRO:HB3	1:A:916:GLY:HA3	1.75	0.67
2:B:519:TRP:HE1	2:B:635:ARG:NH2	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ILE:HG23	1:A:84:ILE:O	1.93	0.67
1:A:825:ILE:CG2	1:A:826:ASP:N	2.58	0.67
3:C:146:LYS:HB2	10:J:61:LEU:HD11	1.77	0.67
12:L:40:LEU:HD22	12:L:44:ASP:CG	2.15	0.67
1:A:903:ASN:HD22	1:A:903:ASN:C	1.97	0.67
1:A:1262:LYS:C	1:A:1264:GLU:H	1.97	0.67
1:A:1127:ASP:CG	1:A:1130:GLN:HB2	2.15	0.67
1:A:981:LEU:CD2	1:A:1039:LYS:HA	2.23	0.67
2:B:855:PHE:HD1	2:B:855:PHE:C	1.97	0.67
1:A:402:ALA:CB	1:A:434:ARG:HA	2.25	0.67
1:A:447:GLN:NE2	13:T:20:DG:H4'	2.09	0.67
3:C:193:TYR:HD2	3:C:197:SER:HB3	1.60	0.67
8:H:89:LEU:C	8:H:91:ASP:H	1.98	0.67
3:C:123:ASN:HD21	3:C:125:MET:HA	1.60	0.67
1:A:353:ILE:HD13	1:A:487:MET:HE2	1.75	0.67
1:A:216:VAL:O	1:A:219:PHE:HB2	1.94	0.67
2:B:408:LEU:HD22	2:B:545:ILE:HD12	1.77	0.67
8:H:4:THR:HG22	8:H:5:LEU:H	1.59	0.67
3:C:77:ILE:N	3:C:129:ILE:HD11	2.08	0.67
5:E:195:VAL:HG12	5:E:196:VAL:N	2.09	0.67
1:A:1224:LEU:HD11	1:A:1240:CYS:HB2	1.75	0.67
2:B:1181:GLU:O	2:B:1182:CYS:HB3	1.93	0.67
3:C:99:LEU:HD22	3:C:120:ILE:HG12	1.75	0.67
3:C:77:ILE:HG22	3:C:78:GLU:N	2.09	0.67
7:G:96:GLN:O	7:G:112:LYS:HD3	1.94	0.67
5:E:15:ALA:O	5:E:19:VAL:HG23	1.94	0.67
2:B:98:THR:O	2:B:126:SER:HB2	1.95	0.67
4:D:69:ALA:HA	4:D:72:ARG:HD2	1.77	0.67
2:B:168:GLY:HA2	2:B:454:THR:OG1	1.94	0.67
2:B:810:GLU:CB	2:B:815:ARG:HH22	2.06	0.67
2:B:193:LYS:HZ2	12:L:32:ALA:HB1	1.57	0.67
3:C:238:ILE:CG2	3:C:242:GLN:HB2	2.20	0.67
2:B:288:ALA:HA	2:B:331:LEU:HD12	1.74	0.67
5:E:154:ILE:H	5:E:196:VAL:HG13	1.58	0.67
1:A:446:ARG:HB2	1:A:487:MET:SD	2.33	0.67
4:D:39:ASN:HD22	4:D:41:GLN:HB2	1.60	0.67
2:B:999:MET:HA	2:B:999:MET:HE2	1.77	0.67
9:I:17:ARG:HG3	9:I:28:GLU:OE1	1.95	0.67
2:B:25:ILE:HG23	2:B:658:ILE:HD11	1.76	0.67
8:H:55:LEU:HB3	8:H:144:ILE:HG23	1.76	0.67
2:B:515:HIS:H	2:B:518:HIS:CD2	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:36:LEU:HB2	10:J:47:ARG:HH12	1.60	0.67
2:B:999:MET:HA	2:B:999:MET:CE	2.25	0.67
1:A:416:ARG:NH1	1:A:417:TYR:HE2	1.93	0.67
2:B:596:LEU:O	2:B:600:LEU:HG	1.94	0.67
2:B:133:LYS:CE	2:B:135:ARG:HH21	2.01	0.67
1:A:37:PHE:N	1:A:37:PHE:CD1	2.60	0.67
3:C:56:THR:HG21	3:C:145:CYS:SG	2.34	0.67
1:A:606:LEU:HG	1:A:613:ILE:HB	1.76	0.67
2:B:744:HIS:HD2	2:B:746:SER:OG	1.78	0.67
2:B:1084:GLN:HG2	3:C:201:TRP:HZ2	1.59	0.67
2:B:546:SER:OG	2:B:631:GLY:N	2.27	0.67
2:B:383:ASN:C	2:B:387:LEU:HD13	2.15	0.67
1:A:1264:GLU:HG3	1:A:1265:ASN:N	2.10	0.67
7:G:48:VAL:HA	7:G:76:ALA:HB2	1.75	0.67
1:A:855:THR:HG21	1:A:857:ARG:NE	2.08	0.67
1:A:552:TRP:CE3	1:A:651:LYS:HB3	2.29	0.67
2:B:616:ILE:HD12	2:B:616:ILE:N	2.10	0.67
2:B:29:ASP:CG	2:B:658:ILE:HD13	2.14	0.67
5:E:157:SER:OG	5:E:160:GLU:HG3	1.95	0.67
1:A:1227:ILE:HG22	1:A:1228:TRP:N	2.07	0.67
3:C:35:ARG:NH1	11:K:41:THR:OG1	2.27	0.67
1:A:802:ASN:HD21	2:B:729:ILE:H	1.41	0.67
1:A:1148:ILE:HD11	1:A:1198:ASP:HA	1.76	0.67
2:B:1201:LYS:HE2	2:B:1205:GLN:OE1	1.94	0.67
2:B:822:ASN:HD21	10:J:52:THR:HG21	1.60	0.66
9:I:73:ARG:HH12	9:I:112:SER:HB3	1.60	0.66
1:A:1151:GLU:OE2	9:I:45:ARG:HD2	1.96	0.66
4:D:8:PHE:CZ	4:D:37:GLN:HB2	2.30	0.66
11:K:45:LEU:HG	11:K:94:ILE:HD13	1.77	0.66
11:K:67:PHE:C	11:K:68:PHE:HD2	1.98	0.66
8:H:15:VAL:HA	8:H:26:ILE:HG23	1.76	0.66
1:A:1313:LEU:HD23	1:A:1338:VAL:HG21	1.75	0.66
1:A:451:HIS:O	2:B:1137:CYS:SG	2.52	0.66
3:C:3:GLU:HG3	11:K:104:ASN:OD1	1.95	0.66
3:C:238:ILE:CD1	3:C:246:ARG:HH11	2.08	0.66
5:E:124:VAL:CG1	5:E:132:ILE:HG13	2.23	0.66
2:B:593:PRO:HA	2:B:596:LEU:HB3	1.76	0.66
4:D:208:GLU:HG3	4:D:212:LYS:HE3	1.77	0.66
2:B:1080:LYS:HD2	3:C:188:HIS:HB2	1.77	0.66
1:A:929:LEU:HD23	1:A:983:ILE:CG2	2.26	0.66
6:F:136:ARG:O	6:F:143:PHE:HB2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.60	0.66
2:B:755:ILE:HG23	2:B:809:MET:CE	2.26	0.66
1:A:524:VAL:HG12	1:A:525:GLN:H	1.59	0.66
3:C:73:GLN:HE21	3:C:75:MET:H	1.43	0.66
2:B:273:LEU:O	2:B:276:ILE:HB	1.95	0.66
8:H:102:TYR:N	8:H:102:TYR:HD2	1.91	0.66
1:A:1191:TRP:HB3	1:A:1260:LEU:HD23	1.77	0.66
4:D:40:HIS:HB2	7:G:73:LYS:CE	2.26	0.66
1:A:345:VAL:HG21	2:B:1150:ARG:HH22	1.61	0.66
3:C:36:VAL:HG21	3:C:251:LEU:HD13	1.77	0.66
4:D:53:SER:HB3	4:D:152:SER:HB2	1.78	0.66
1:A:698:GLN:HA	9:I:97:MET:O	1.96	0.66
1:A:833:GLU:HG2	1:A:1102:LYS:HD2	1.76	0.66
2:B:527:THR:OG1	2:B:528:PRO:HD2	1.95	0.66
1:A:1291:VAL:HG13	1:A:1292:PRO:HD2	1.77	0.66
1:A:1057:VAL:HG12	1:A:1058:VAL:H	1.61	0.66
2:B:230:ALA:N	2:B:231:PRO:HD2	2.11	0.66
2:B:511:PRO:O	2:B:513:GLN:N	2.28	0.66
8:H:100:THR:HG23	8:H:138:GLU:CA	2.22	0.66
3:C:115:SER:O	3:C:118:LEU:HG	1.96	0.66
2:B:859:TYR:CZ	2:B:941:LEU:HD12	2.29	0.66
1:A:1124:HIS:HB2	1:A:1130:GLN:HG2	1.78	0.66
10:J:24:LEU:HA	10:J:28:ASP:HB2	1.77	0.66
1:A:116:ASP:OD2	1:A:164:ARG:HD2	1.95	0.66
2:B:487:THR:HG22	2:B:488:TYR:N	2.10	0.66
10:J:1:MET:H1	10:J:57:ILE:H	1.40	0.66
5:E:23:VAL:HG13	5:E:78:LEU:CD1	2.25	0.66
1:A:903:ASN:ND2	1:A:905:ASP:H	1.93	0.66
6:F:76:LYS:HA	6:F:79:ARG:CD	2.25	0.66
1:A:456:MET:HE2	1:A:507:VAL:HA	1.76	0.66
1:A:106:VAL:HG12	1:A:107:CYS:H	1.58	0.66
9:I:13:MET:HE2	9:I:14:LEU:H	1.59	0.66
2:B:102:VAL:HB	2:B:110:HIS:HB3	1.76	0.66
2:B:583:ASN:HD21	2:B:628:THR:CG2	2.08	0.66
2:B:1072:MET:CE	2:B:1085:ILE:HB	2.25	0.66
2:B:276:ILE:HA	2:B:337:ARG:O	1.95	0.66
1:A:14:VAL:H	1:A:1432:GLN:NE2	1.92	0.66
1:A:567:LYS:CD	1:A:568:PRO:HD3	2.25	0.66
1:A:899:VAL:CG1	1:A:908:LEU:HD21	2.25	0.66
2:B:827:ILE:O	2:B:828:ALA:HB2	1.95	0.66
3:C:181:ASP:CG	3:C:186:LEU:HD13	2.15	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:144:ILE:HG13	5:E:145:THR:N	2.10	0.66
1:A:596:THR:O	1:A:598:LEU:N	2.28	0.66
1:A:265:LYS:HD3	1:A:302:THR:HG23	1.76	0.66
2:B:860:MET:HG3	2:B:965:LYS:HG2	1.78	0.66
2:B:996:ARG:NH1	3:C:38:ILE:HG23	2.11	0.66
3:C:166:GLU:HG3	11:K:10:PHE:HZ	1.60	0.66
2:B:648:HIS:CG	2:B:649:LYS:H	2.13	0.66
1:A:372:LYS:HA	1:A:435:HIS:HD1	1.57	0.66
7:G:49:LEU:HG	7:G:76:ALA:HA	1.78	0.66
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.78	0.66
1:A:79:GLY:HA3	1:A:243:PRO:CG	2.26	0.66
13:T:21:DC:H2''	13:T:22:DC:H5'	1.76	0.66
1:A:979:SER:OG	1:A:980:ASP:N	2.28	0.66
2:B:853:SER:O	2:B:854:LEU:HD23	1.96	0.66
1:A:1312:ASN:O	1:A:1316:VAL:HG23	1.95	0.66
2:B:613:VAL:HG13	2:B:628:THR:HA	1.78	0.66
1:A:41:MET:CB	1:A:49:LYS:HA	2.18	0.66
3:C:238:ILE:HG22	3:C:243:VAL:HG23	1.77	0.66
6:F:111:LEU:H	6:F:111:LEU:CD1	2.07	0.66
10:J:48:ARG:HD2	10:J:49:MET:N	2.10	0.66
2:B:1202:LEU:O	2:B:1206:GLU:HG3	1.96	0.66
1:A:442:VAL:O	1:A:457:ALA:HA	1.96	0.66
2:B:1108:ARG:HG2	2:B:1109:GLY:N	2.11	0.66
2:B:975:GLN:O	2:B:990:ILE:HD12	1.95	0.66
4:D:148:LEU:O	4:D:152:SER:HB3	1.95	0.66
1:A:129:LYS:O	1:A:130:ASP:HB2	1.95	0.66
8:H:135:LEU:HD22	8:H:137:GLN:HE21	1.61	0.66
2:B:220:GLY:O	2:B:222:ILE:HG13	1.96	0.66
3:C:239:PRO:HB2	3:C:241:ASP:OD1	1.96	0.65
10:J:9:SER:CB	10:J:45:CYS:HB2	2.25	0.65
9:I:31:THR:O	9:I:32:CYS:HB3	1.96	0.65
1:A:96:ILE:HG22	1:A:97:ALA:N	2.11	0.65
2:B:345:LYS:O	2:B:348:ARG:HG2	1.96	0.65
1:A:38:PRO:HA	1:A:270:LEU:HD23	1.76	0.65
1:A:57:ARG:HH11	1:A:57:ARG:HG2	1.60	0.65
3:C:83:SER:HA	3:C:95:CYS:HB2	1.78	0.65
2:B:515:HIS:CD2	2:B:516:ASN:N	2.64	0.65
1:A:310:GLY:O	1:A:312:PRO:HD2	1.95	0.65
1:A:547:LEU:HD22	11:K:58:PHE:CE1	2.32	0.65
11:K:7:PHE:C	11:K:9:LEU:H	2.00	0.65
1:A:1438:THR:HB	2:B:1144:ALA:CB	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1198:ASP:HB3	1:A:1201:ALA:HB3	1.77	0.65
4:D:130:LEU:O	4:D:132:GLN:N	2.28	0.65
3:C:161:LYS:HG3	3:C:162:GLY:N	2.12	0.65
5:E:96:PHE:O	5:E:99:HIS:HB3	1.96	0.65
2:B:314:LEU:O	2:B:317:CYS:HB3	1.97	0.65
1:A:1237:ILE:HG22	1:A:1238:ILE:N	2.11	0.65
11:K:50:LEU:HD11	11:K:75:ILE:HD13	1.77	0.65
1:A:1028:THR:O	1:A:1032:LEU:HD12	1.96	0.65
1:A:7:SER:HB3	2:B:1175:LEU:HD22	1.78	0.65
2:B:464:GLY:C	2:B:465:ASN:HD22	1.99	0.65
3:C:18:VAL:HG23	3:C:240:VAL:CG1	2.26	0.65
1:A:253:ASN:HD22	1:A:256:GLN:NE2	1.94	0.65
2:B:605:ARG:NH1	2:B:639:ILE:HG21	2.10	0.65
2:B:282:ILE:HD11	2:B:317:CYS:SG	2.36	0.65
1:A:1225:PHE:CZ	1:A:1227:ILE:HD11	2.32	0.65
1:A:836:TYR:CD2	1:A:840:ARG:HD2	2.31	0.65
2:B:102:VAL:O	2:B:102:VAL:HG12	1.96	0.65
1:A:55:ASP:C	1:A:57:ARG:H	2.00	0.65
12:L:55:ILE:HG12	12:L:56:LEU:N	2.11	0.65
5:E:28:TYR:C	5:E:65:THR:HG22	2.17	0.65
2:B:978:ASP:OD2	2:B:1098:MET:HG2	1.96	0.65
1:A:1447:GLU:OE2	7:G:23:LYS:HB2	1.97	0.65
7:G:1:MET:HG2	7:G:85:GLU:OE2	1.96	0.65
11:K:53:ASP:HB3	11:K:56:VAL:CG2	2.27	0.65
1:A:1392:SER:O	1:A:1394:THR:N	2.29	0.65
2:B:773:MET:SD	2:B:987:LYS:HG2	2.37	0.65
2:B:806:THR:HG23	2:B:1046:PRO:HD3	1.78	0.65
2:B:955:THR:HG22	2:B:956:THR:O	1.96	0.65
8:H:64:ASN:CB	8:H:88:SER:HB2	2.21	0.65
1:A:858:ASN:HD22	1:A:858:ASN:C	1.98	0.65
1:A:7:SER:HB2	2:B:1175:LEU:HD22	1.77	0.65
5:E:198:ILE:HD12	5:E:198:ILE:H	1.60	0.65
1:A:276:LEU:HD13	1:A:293:GLU:HA	1.79	0.65
8:H:40:LEU:HD13	8:H:123:MET:HB2	1.77	0.65
1:A:466:SER:HB2	2:B:1099:VAL:HG21	1.79	0.65
5:E:124:VAL:N	5:E:125:PRO:HD2	2.12	0.65
1:A:630:ILE:HG23	1:A:631:HIS:N	2.11	0.65
1:A:848:ILE:HA	1:A:857:ARG:O	1.95	0.65
9:I:8:ARG:HG3	9:I:34:TYR:CE1	2.32	0.65
2:B:508:LEU:O	2:B:509:ALA:HB2	1.97	0.65
5:E:7:ARG:HD2	5:E:7:ARG:C	2.17	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:ILE:HG22	1:A:565:ILE:O	1.97	0.65
11:K:18:LYS:NZ	11:K:38:GLU:HG2	2.11	0.65
2:B:589:VAL:HG12	2:B:590:HIS:N	2.12	0.65
1:A:739:ASP:OD2	8:H:19:ARG:HD2	1.97	0.65
11:K:12:LEU:HD23	11:K:16:GLU:O	1.96	0.65
2:B:843:GLN:N	2:B:994:TYR:O	2.19	0.65
1:A:855:THR:CG2	1:A:857:ARG:HE	2.10	0.65
9:I:7:CYS:N	9:I:14:LEU:HD21	2.12	0.65
2:B:1162:ILE:HD11	2:B:1194:ILE:CD1	2.26	0.65
13:T:7:DC:H2"	13:T:8:DT:C5	2.32	0.65
1:A:91:PHE:HB3	1:A:96:ILE:HD12	1.79	0.65
8:H:135:LEU:HD22	8:H:137:GLN:NE2	2.12	0.65
5:E:197:LYS:HG2	5:E:199:ILE:HG13	1.78	0.65
1:A:785:PRO:HG2	1:A:786:HIS:CD2	2.32	0.65
1:A:35:ILE:HB	1:A:83:HIS:O	1.97	0.65
1:A:898:ARG:HD2	1:A:899:VAL:N	2.12	0.65
7:G:13:LEU:HD23	7:G:14:HIS:H	1.60	0.65
2:B:165:VAL:HG11	2:B:448:ILE:CD1	2.27	0.65
2:B:449:ASN:O	2:B:451:LYS:N	2.30	0.65
1:A:767:GLN:HB2	1:A:799:PHE:HD1	1.60	0.65
4:D:123:LEU:O	4:D:127:ASP:HB2	1.97	0.65
2:B:38:PHE:HD1	2:B:811:TYR:CD2	2.15	0.65
1:A:567:LYS:HZ3	8:H:95:TYR:CB	2.09	0.65
6:F:70:LYS:O	6:F:72:LYS:HD2	1.96	0.65
1:A:1208:THR:HB	1:A:1211:GLN:CG	2.26	0.65
3:C:167:HIS:ND1	3:C:169:LYS:HG2	2.11	0.65
5:E:198:ILE:HD12	5:E:198:ILE:N	2.12	0.65
2:B:867:GLY:C	2:B:869:SER:H	1.99	0.65
1:A:954:TRP:HB3	1:A:955:PRO:HD2	1.78	0.65
2:B:26:THR:HA	2:B:708:GLU:OE1	1.96	0.64
1:A:35:ILE:CG2	1:A:84:ILE:HD12	2.27	0.64
8:H:100:THR:HG22	8:H:101:ALA:H	1.60	0.64
5:E:111:VAL:CG1	5:E:137:GLU:HG2	2.27	0.64
7:G:59:GLY:HA3	7:G:70:PHE:CD2	2.31	0.64
11:K:21:ILE:CG2	11:K:33:ILE:HG12	2.26	0.64
5:E:202:SER:OG	5:E:204:THR:HG22	1.97	0.64
1:A:962:ARG:HA	1:A:965:GLN:HB2	1.77	0.64
2:B:100:PRO:HD2	2:B:180:TYR:CE1	2.32	0.64
2:B:766:ARG:HG3	2:B:1022:THR:HG23	1.78	0.64
1:A:565:ILE:O	1:A:570:PRO:HA	1.97	0.64
3:C:261:ALA:O	3:C:265:MET:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LYS:CB	1:A:36:ARG:HH21	2.10	0.64
11:K:102:LYS:O	11:K:106:GLU:HG3	1.97	0.64
1:A:381:THR:HG23	1:A:382:PRO:HD2	1.78	0.64
1:A:469:ARG:HB3	1:A:469:ARG:HH11	1.60	0.64
1:A:967:ALA:HA	1:A:1044:TRP:HZ3	1.62	0.64
1:A:172:PRO:HD3	1:A:185:TRP:NE1	2.12	0.64
1:A:828:ALA:HB2	2:B:530:GLY:HA2	1.79	0.64
2:B:1099:VAL:CG1	2:B:1100:ASP:H	2.08	0.64
6:F:79:ARG:HG3	6:F:144:GLU:CG	2.27	0.64
1:A:1341:ILE:HG23	1:A:1342:GLU:N	2.11	0.64
1:A:474:VAL:HG22	1:A:474:VAL:O	1.96	0.64
8:H:44:VAL:HG12	8:H:44:VAL:O	1.96	0.64
3:C:56:THR:HG22	3:C:57:VAL:H	1.61	0.64
12:L:28:LYS:CB	12:L:39:SER:HB2	2.27	0.64
2:B:870:ILE:HG22	2:B:917:PRO:HG2	1.78	0.64
11:K:68:PHE:HB3	11:K:70:ARG:NH1	2.12	0.64
2:B:597:MET:HA	2:B:597:MET:CE	2.27	0.64
4:D:22:GLU:H	4:D:22:GLU:CD	2.01	0.64
2:B:90:ILE:HD12	2:B:432:MET:SD	2.38	0.64
1:A:1242:VAL:HG12	1:A:1243:VAL:N	2.12	0.64
1:A:590:ARG:HB3	1:A:605:MET:N	2.12	0.64
11:K:50:LEU:HD11	11:K:75:ILE:CD1	2.28	0.64
1:A:106:VAL:HG12	1:A:107:CYS:N	2.13	0.64
1:A:1438:THR:HG23	6:F:92:ARG:HB2	1.79	0.64
1:A:809:THR:HG23	1:A:812:GLU:OE1	1.97	0.64
1:A:315:LEU:HD13	2:B:471:LYS:HB3	1.78	0.64
1:A:172:PRO:HB3	1:A:185:TRP:CD2	2.33	0.64
1:A:370:ILE:HG12	2:B:1105:ALA:HB2	1.79	0.64
2:B:865:LYS:HG3	2:B:961:LEU:HD21	1.77	0.64
2:B:243:ALA:CB	2:B:251:ILE:HG12	2.28	0.64
2:B:1002:THR:HG21	2:B:1006:ILE:HD12	1.80	0.64
1:A:506:ALA:HB3	1:A:509:LEU:HD12	1.79	0.64
2:B:1186:ASP:O	4:D:17:LYS:HE2	1.97	0.64
2:B:51:PHE:O	2:B:54:PHE:HB3	1.97	0.64
2:B:604:ARG:C	2:B:606:LYS:H	1.98	0.64
2:B:918:ILE:CG2	2:B:919:SER:N	2.61	0.64
2:B:288:ALA:HA	2:B:331:LEU:CD1	2.27	0.64
7:G:13:LEU:HD21	7:G:17:PHE:CD1	2.33	0.64
2:B:642:ASP:CA	2:B:649:LYS:HG3	2.28	0.64
1:A:675:THR:OG1	1:A:736:ASN:ND2	2.29	0.64
2:B:863:GLU:O	2:B:961:LEU:HD22	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:91:ASP:O	8:H:93:TYR:N	2.25	0.64
2:B:502:ILE:HD12	2:B:502:ILE:H	1.62	0.64
5:E:54:GLN:O	5:E:57:MET:HB3	1.97	0.64
2:B:891:ASP:C	2:B:893:LEU:H	2.00	0.64
2:B:123:THR:OG1	2:B:458:LYS:HE2	1.98	0.64
2:B:1174:LYS:O	2:B:1176:ASN:N	2.31	0.64
1:A:185:TRP:H	1:A:185:TRP:HE3	1.46	0.64
1:A:637:LYS:HB3	1:A:641:VAL:HG21	1.79	0.64
9:I:2:THR:HG22	9:I:3:THR:N	2.13	0.64
1:A:135:PHE:CD1	1:A:222:LEU:HD22	2.33	0.64
2:B:25:ILE:HD11	2:B:653:VAL:C	2.18	0.64
2:B:822:ASN:ND2	10:J:52:THR:HG21	2.13	0.64
1:A:39:GLU:OE1	1:A:50:ILE:HD12	1.98	0.64
1:A:900:ASP:HA	1:A:926:GLN:NE2	2.12	0.64
1:A:666:ILE:HD12	1:A:667:GLY:N	2.08	0.64
1:A:666:ILE:N	2:B:1026:LEU:HD13	2.03	0.64
2:B:515:HIS:CD2	2:B:516:ASN:H	2.16	0.64
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.78	0.64
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.33	0.64
2:B:1110:PRO:HG3	2:B:1125:ASP:HB3	1.78	0.64
2:B:1159:ARG:HE	2:B:1193:GLN:HE21	1.44	0.64
2:B:855:PHE:CD1	2:B:855:PHE:C	2.69	0.64
1:A:90:VAL:HG13	1:A:297:GLN:OE1	1.97	0.64
11:K:82:ASP:OD1	11:K:84:LYS:HG3	1.98	0.64
2:B:135:ARG:HB2	2:B:137:TYR:CE1	2.33	0.64
2:B:387:LEU:O	2:B:392:ARG:HB2	1.98	0.64
1:A:547:LEU:HD22	11:K:58:PHE:CD1	2.32	0.64
2:B:953:LEU:HD23	2:B:965:LYS:O	1.98	0.64
1:A:1130:GLN:O	1:A:1134:ILE:HG13	1.97	0.64
4:D:60:LYS:CE	4:D:126:ILE:HD11	2.28	0.64
3:C:8:VAL:O	3:C:9:LYS:HD2	1.98	0.64
2:B:791:THR:HA	2:B:858:SER:HB2	1.79	0.64
2:B:758:PHE:CZ	2:B:1044:ALA:HA	2.33	0.63
1:A:1191:TRP:HA	1:A:1191:TRP:CE3	2.32	0.63
2:B:899:ILE:CD1	2:B:911:ILE:HA	2.28	0.63
2:B:847:ASP:C	2:B:849:GLY:H	2.00	0.63
11:K:47:ARG:HH11	11:K:47:ARG:CB	2.09	0.63
1:A:963:ILE:HD11	1:A:1048:ASN:HB2	1.78	0.63
4:D:9:GLN:HE21	4:D:31:GLN:NE2	1.95	0.63
2:B:1034:VAL:HG12	2:B:1035:ALA:N	2.14	0.63
12:L:32:ALA:HB3	12:L:33:GLU:OE2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:139:ASN:O	8:H:140:ALA:HB2	1.97	0.63
3:C:242:GLN:HA	3:C:245:VAL:CG2	2.28	0.63
2:B:1002:THR:CG2	2:B:1006:ILE:HG13	2.27	0.63
1:A:1308:THR:HG23	1:A:1309:ASP:H	1.62	0.63
4:D:9:GLN:HE21	4:D:31:GLN:HE21	1.43	0.63
4:D:56:ARG:NH2	4:D:155:ARG:HA	2.12	0.63
1:A:515:GLN:HA	1:A:1367:HIS:NE2	2.13	0.63
1:A:1364:ASN:HD22	1:A:1365:TYR:N	1.97	0.63
8:H:142:LEU:C	8:H:143:LEU:HD12	2.18	0.63
3:C:148:ARG:H	3:C:151:GLN:CG	2.06	0.63
1:A:1187:GLN:HG3	1:A:1188:GLN:HG3	1.79	0.63
1:A:1142:THR:HA	1:A:1273:LEU:HD13	1.78	0.63
10:J:14:VAL:HG12	10:J:14:VAL:O	1.96	0.63
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.80	0.63
2:B:1096:ARG:O	2:B:1097:HIS:HB2	1.98	0.63
5:E:165:LEU:HD23	5:E:165:LEU:N	2.13	0.63
5:E:204:THR:HG23	5:E:205:SER:N	2.13	0.63
4:D:139:LYS:HE2	4:D:143:ASN:ND2	2.13	0.63
2:B:637:LEU:C	2:B:690:VAL:HG13	2.19	0.63
2:B:343:ILE:HG23	2:B:347:LYS:CE	2.28	0.63
2:B:114:PRO:HG2	2:B:115:GLN:H	1.63	0.63
2:B:217:ARG:C	2:B:217:ARG:HD2	2.19	0.63
2:B:1096:ARG:O	2:B:1097:HIS:CB	2.47	0.63
1:A:1100:ARG:HH22	1:A:1111:MET:CE	2.11	0.63
1:A:93:VAL:HG21	1:A:301:ALA:O	1.99	0.63
2:B:99:LYS:HA	2:B:178:ASN:HD21	1.63	0.63
4:D:60:LYS:HE3	4:D:126:ILE:HD11	1.79	0.63
12:L:26:THR:HG23	12:L:62:LYS:HZ3	1.64	0.63
1:A:55:ASP:CG	1:A:55:ASP:O	2.36	0.63
1:A:901:LEU:N	1:A:926:GLN:HE21	1.95	0.63
5:E:117:THR:HB	5:E:120:ALA:CB	2.29	0.63
5:E:180:ARG:NH2	5:E:192:ARG:HD2	2.14	0.63
1:A:1364:ASN:C	1:A:1364:ASN:HD22	1.98	0.63
5:E:116:ILE:HG22	5:E:117:THR:N	2.12	0.63
7:G:34:VAL:CG1	7:G:45:ILE:HG21	2.28	0.63
1:A:535:THR:HG22	1:A:575:LYS:HE2	1.81	0.63
2:B:244:LEU:HD21	2:B:366:GLN:NE2	2.14	0.63
2:B:363:HIS:O	2:B:364:ILE:HB	1.98	0.63
1:A:877:HIS:ND1	1:A:1056:SER:HA	2.14	0.63
5:E:204:THR:HG23	5:E:205:SER:H	1.64	0.63
2:B:686:ASN:C	2:B:688:GLY:H	2.02	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:276:ILE:HD13	2:B:280:ILE:HD11	1.80	0.63
2:B:383:ASN:O	2:B:387:LEU:HD13	1.98	0.63
5:E:159:ASP:HA	5:E:162:ARG:NH2	2.13	0.63
5:E:167:ARG:O	5:E:168:TYR:HD2	1.82	0.63
1:A:332:LYS:C	1:A:334:GLY:H	2.02	0.63
7:G:27:LYS:O	7:G:31:LEU:HG	1.98	0.63
5:E:198:ILE:HD11	5:E:212:ARG:HB2	1.81	0.63
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.79	0.63
3:C:13:ALA:O	11:K:114:LEU:HD13	1.99	0.63
2:B:857:ARG:HD2	2:B:945:GLU:OE1	1.97	0.63
2:B:90:ILE:HG23	2:B:133:LYS:O	1.99	0.62
1:A:41:MET:SD	1:A:42:ASP:N	2.71	0.62
8:H:144:ILE:HG22	8:H:145:ARG:N	2.14	0.62
2:B:357:GLN:O	2:B:366:GLN:HA	1.98	0.62
1:A:1094:VAL:HG12	1:A:1113:THR:HG21	1.80	0.62
8:H:36:CYS:HA	8:H:126:GLU:O	1.98	0.62
1:A:343:LYS:HE2	2:B:1156:ASP:HB2	1.81	0.62
1:A:278:THR:HG23	1:A:282:ASN:HD22	1.63	0.62
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.33	0.62
6:F:118:LEU:O	6:F:122:MET:HG3	1.99	0.62
3:C:209:TYR:H	3:C:209:TYR:HD1	1.47	0.62
2:B:578:THR:H	2:B:589:VAL:CG1	2.12	0.62
3:C:238:ILE:HD13	3:C:246:ARG:HD2	1.80	0.62
2:B:596:LEU:HD11	2:B:600:LEU:HD11	1.81	0.62
7:G:142:ARG:HB3	7:G:171:ILE:HD11	1.80	0.62
2:B:351:TYR:O	2:B:355:ILE:HG13	2.00	0.62
5:E:93:MET:HE1	5:E:123:LEU:HB2	1.81	0.62
1:A:266:LEU:HD21	1:A:303:TYR:CE1	2.35	0.62
1:A:1436:ILE:O	1:A:1437:GLY:C	2.37	0.62
1:A:847:ASP:O	1:A:858:ASN:HA	2.00	0.62
5:E:168:TYR:HB3	5:E:170:LEU:HG	1.81	0.62
8:H:105:GLU:O	8:H:112:ILE:HG23	1.99	0.62
1:A:645:LEU:O	1:A:649:ILE:HG13	2.00	0.62
2:B:797:TYR:HE1	2:B:971:THR:HG23	1.64	0.62
2:B:1072:MET:HE3	2:B:1085:ILE:HB	1.81	0.62
9:I:86:PHE:CE1	9:I:100:PHE:HB2	2.34	0.62
3:C:31:ASN:O	3:C:35:ARG:HG3	2.00	0.62
1:A:335:ARG:O	1:A:339:ASN:HB2	1.97	0.62
2:B:862:GLN:HG2	2:B:963:PHE:CD1	2.34	0.62
1:A:79:GLY:HA3	1:A:243:PRO:HG3	1.80	0.62
2:B:614:SER:HB3	2:B:694:ASP:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:LEU:CB	2:B:429:PHE:CE1	2.74	0.62
12:L:55:ILE:O	12:L:56:LEU:CB	2.48	0.62
5:E:145:THR:HG21	5:E:187:TYR:CE2	2.34	0.62
1:A:427:GLN:HG3	1:A:430:TRP:CZ2	2.33	0.62
8:H:32:THR:HG22	8:H:33:GLN:H	1.65	0.62
2:B:449:ASN:O	2:B:450:ALA:C	2.38	0.62
8:H:4:THR:HG22	8:H:5:LEU:N	2.15	0.62
3:C:65:HIS:CE1	3:C:69:LEU:HD11	2.35	0.62
1:A:475:THR:CG2	1:A:476:SER:N	2.62	0.62
1:A:472:LEU:O	1:A:475:THR:HB	1.99	0.62
2:B:232:SER:O	2:B:261:ARG:HD3	1.99	0.62
1:A:466:SER:O	2:B:1103:ILE:HD11	1.98	0.62
8:H:30:SER:HB2	8:H:36:CYS:HB3	1.81	0.62
1:A:646:PHE:O	1:A:650:GLN:HB2	1.99	0.62
2:B:284:ILE:HD13	2:B:333:PHE:CD2	2.35	0.62
7:G:23:LYS:HG3	7:G:56:ILE:CD1	2.30	0.62
2:B:871:THR:O	2:B:917:PRO:HG3	1.98	0.62
1:A:1424:VAL:HG11	2:B:1139:ILE:HD13	1.79	0.62
1:A:1152:ILE:HD11	9:I:44:TYR:HD2	1.64	0.62
2:B:898:LEU:HD13	2:B:952:VAL:HG11	1.80	0.62
9:I:80:SER:OG	9:I:105:SER:HB2	2.00	0.62
2:B:510:LYS:CB	2:B:511:PRO:HD3	2.30	0.62
2:B:105:SER:O	2:B:106:ASP:HB2	1.99	0.62
2:B:221:ASN:N	2:B:241:ARG:O	2.31	0.62
2:B:768:THR:O	2:B:771:SER:HB2	1.99	0.62
1:A:247:ARG:NH1	1:A:263:THR:HG23	2.15	0.62
7:G:145:VAL:HG12	7:G:146:LYS:N	2.15	0.62
1:A:399:HIS:HB3	1:A:400:PRO:CD	2.25	0.62
1:A:1161:THR:HG22	1:A:1163:ILE:N	2.11	0.62
2:B:1177:HIS:C	2:B:1178:ASN:HD22	2.03	0.62
1:A:1109:LYS:O	1:A:1110:ASN:HB3	2.00	0.62
2:B:196:PRO:HG2	2:B:197:PHE:H	1.65	0.62
2:B:916:THR:HB	2:B:935:ARG:CG	2.30	0.62
1:A:899:VAL:CG2	1:A:1029:ARG:HG2	2.29	0.62
2:B:258:LEU:HG	2:B:258:LEU:O	2.00	0.62
2:B:282:ILE:HD12	2:B:382:ILE:HD13	1.82	0.62
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.35	0.62
6:F:72:LYS:CA	6:F:72:LYS:HE3	2.30	0.62
11:K:21:ILE:HG22	11:K:31:VAL:CG1	2.29	0.62
2:B:99:LYS:HB3	2:B:100:PRO:HD2	1.81	0.62
1:A:110:CYS:HB3	1:A:167:CYS:SG	2.40	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1118:VAL:HG12	1:A:1327:ILE:HG13	1.81	0.62
2:B:549:THR:HG22	2:B:550:ASP:H	1.64	0.62
2:B:801:LYS:O	10:J:52:THR:CG2	2.47	0.62
8:H:40:LEU:HG	8:H:41:ASP:O	1.98	0.62
8:H:82:PRO:HG3	11:K:54:ARG:HH11	1.65	0.62
7:G:18:PHE:HA	7:G:22:MET:CE	2.30	0.62
1:A:188:ASP:CB	1:A:191:THR:HB	2.25	0.62
1:A:1345:ARG:NH1	5:E:200:ARG:HH22	1.98	0.62
1:A:1329:THR:CG2	1:A:1335:ILE:HG13	2.30	0.62
2:B:128:LEU:HB2	2:B:167:ILE:O	2.00	0.62
9:I:78:CYS:O	9:I:80:SER:N	2.32	0.62
1:A:1371:LEU:O	1:A:1375:MET:HG3	2.00	0.62
2:B:351:TYR:CZ	2:B:355:ILE:HD11	2.35	0.61
12:L:55:ILE:HG12	12:L:56:LEU:H	1.65	0.61
5:E:89:GLY:HA2	5:E:117:THR:OG1	1.99	0.61
1:A:847:ASP:HB3	1:A:1424:VAL:HG23	1.81	0.61
2:B:903:VAL:HG12	2:B:904:ARG:N	2.15	0.61
11:K:41:THR:HG22	11:K:42:LEU:N	2.14	0.61
5:E:83:CYS:C	5:E:85:GLU:H	2.04	0.61
2:B:593:PRO:HG2	2:B:617:ARG:NH1	2.15	0.61
11:K:61:TYR:HD2	11:K:61:TYR:C	2.02	0.61
8:H:4:THR:HA	8:H:60:ALA:HB2	1.80	0.61
11:K:60:ALA:O	11:K:73:LEU:HD12	1.99	0.61
2:B:807:ARG:HG2	2:B:1045:SER:OG	1.99	0.61
1:A:929:LEU:HD23	1:A:983:ILE:HG23	1.82	0.61
2:B:243:ALA:HA	2:B:250:PHE:O	2.00	0.61
5:E:100:ILE:CG2	5:E:105:PHE:HB2	2.25	0.61
1:A:1100:ARG:HH21	1:A:1351:GLU:CG	2.12	0.61
11:K:7:PHE:O	11:K:9:LEU:N	2.33	0.61
9:I:6:PHE:HB3	9:I:12:ASN:O	2.00	0.61
1:A:523:ILE:HG23	1:A:527:THR:HB	1.82	0.61
6:F:86:THR:OG1	6:F:89:GLU:HG3	2.00	0.61
2:B:286:PHE:HA	2:B:289:LEU:HD12	1.83	0.61
2:B:378:LEU:HD12	2:B:378:LEU:O	2.00	0.61
9:I:53:GLY:HA2	9:I:56:ALA:HB2	1.82	0.61
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.83	0.61
4:D:40:HIS:CB	7:G:73:LYS:NZ	2.63	0.61
11:K:12:LEU:H	11:K:12:LEU:CD1	2.10	0.61
1:A:1276:VAL:HG12	1:A:1277:GLU:H	1.65	0.61
1:A:1018:PHE:O	1:A:1021:LEU:HB3	2.01	0.61
1:A:986:ILE:HD12	1:A:1032:LEU:HD11	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:14:GLU:HG2	8:H:15:VAL:N	2.13	0.61
1:A:1315:GLU:O	1:A:1317:MET:N	2.33	0.61
2:B:510:LYS:HG3	2:B:511:PRO:HD3	1.81	0.61
2:B:393:LYS:HA	2:B:393:LYS:HE3	1.81	0.61
13:T:15:DC:H2"	13:T:16:DT:OP2	2.01	0.61
5:E:103:LYS:HB3	5:E:105:PHE:CE2	2.35	0.61
2:B:273:LEU:HB2	2:B:276:ILE:CD1	2.24	0.61
1:A:1155:ASP:OD2	1:A:1161:THR:HA	2.01	0.61
4:D:63:LEU:HD13	4:D:133:THR:OG1	2.00	0.61
4:D:144:THR:O	4:D:148:LEU:HB2	2.00	0.61
1:A:233:TRP:C	1:A:235:ILE:H	2.03	0.61
11:K:1:MET:HG3	11:K:2:ASN:N	2.15	0.61
2:B:56:ASP:HB2	2:B:57:TYR:HD1	1.65	0.61
2:B:190:TYR:CE2	10:J:62:ARG:HB3	2.34	0.61
1:A:830:LYS:HE2	1:A:1081:LEU:HB2	1.82	0.61
5:E:129:PRO:O	5:E:130:ALA:C	2.39	0.61
9:I:69:PRO:HG2	9:I:85:PHE:CD2	2.36	0.61
10:J:64:ASN:HD22	10:J:65:PRO:HD3	1.64	0.61
1:A:115:LEU:O	1:A:122:MET:HE2	2.00	0.61
11:K:44:ASN:N	11:K:61:TYR:CE1	2.68	0.61
2:B:497:ARG:NH2	2:B:775:LYS:HE2	2.14	0.61
2:B:737:THR:CG2	9:I:66:PRO:HA	2.31	0.61
1:A:1199:ARG:NH2	1:A:1234:GLU:HA	2.16	0.61
1:A:849:MET:HE1	1:A:1061:GLY:HA2	1.82	0.61
2:B:651:LEU:C	2:B:653:VAL:H	2.03	0.61
1:A:18:GLN:NE2	1:A:228:PHE:HE1	1.99	0.61
1:A:901:LEU:N	1:A:926:GLN:NE2	2.44	0.61
7:G:112:LYS:O	7:G:115:MET:HG2	2.00	0.61
2:B:559:SER:CA	2:B:563:MET:HB3	2.26	0.61
11:K:7:PHE:HA	11:K:10:PHE:CE2	2.35	0.61
1:A:1035:TYR:HD1	1:A:1037:LEU:HD23	1.64	0.61
1:A:196:GLU:CB	1:A:197:PRO:HD2	2.29	0.61
1:A:98:LYS:HE2	1:A:224:PHE:CZ	2.35	0.61
2:B:1201:LYS:HE2	2:B:1205:GLN:NE2	2.15	0.61
2:B:1080:LYS:HB2	3:C:188:HIS:HB3	1.80	0.61
1:A:1450:LEU:HG	1:A:1450:LEU:O	2.01	0.61
1:A:1214:GLU:HA	1:A:1214:GLU:OE1	2.01	0.61
1:A:225:ASN:ND2	1:A:227:VAL:H	1.99	0.61
1:A:43:GLU:HG3	1:A:48:ALA:HB3	1.82	0.61
3:C:66:ARG:HH21	10:J:5:VAL:H	1.49	0.61
2:B:1065:GLN:HB3	2:B:1069:PHE:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1154:TYR:HD1	1:A:1191:TRP:CZ3	2.19	0.61
2:B:944:THR:HG21	2:B:1122:ARG:NH2	2.14	0.61
2:B:261:ARG:HH11	2:B:262:GLU:H	1.48	0.61
2:B:259:TYR:HB2	2:B:268:THR:HG23	1.83	0.61
1:A:590:ARG:NH1	1:A:590:ARG:HB2	2.08	0.61
2:B:999:MET:HB3	2:B:1007:VAL:CG2	2.30	0.61
2:B:573:GLN:O	2:B:575:PRO:HD3	2.00	0.61
1:A:1039:LYS:HE3	1:A:1043:ASP:OD2	2.01	0.61
1:A:1149:ALA:CB	9:I:47:GLU:HA	2.31	0.61
6:F:94:LEU:HD21	6:F:122:MET:HA	1.81	0.61
2:B:776:GLN:OE1	15:P:9:C:H4'	2.01	0.61
1:A:152:VAL:CG1	1:A:153:PRO:HD2	2.31	0.61
3:C:177:GLU:HG3	3:C:231:ASN:HB3	1.83	0.61
1:A:882:SER:H	1:A:1025:ARG:NH2	1.98	0.61
1:A:382:PRO:CD	1:A:428:TYR:HD2	2.09	0.61
1:A:403:LYS:O	1:A:415:LEU:HB2	2.00	0.61
4:D:56:ARG:HB2	4:D:148:LEU:HD22	1.82	0.61
2:B:352:ALA:HA	2:B:355:ILE:HD12	1.83	0.61
1:A:573:SER:O	1:A:576:GLN:HB3	2.01	0.61
1:A:665:GLY:O	1:A:666:ILE:HD12	2.00	0.61
1:A:741:ASN:ND2	1:A:744:LYS:H	1.99	0.61
4:D:53:SER:H	4:D:148:LEU:CD2	2.13	0.61
6:F:130:ILE:O	6:F:148:VAL:HG21	2.01	0.61
1:A:74:MET:CE	1:A:74:MET:H	2.13	0.60
3:C:66:ARG:NH1	10:J:2:ILE:HG21	2.16	0.60
7:G:17:PHE:N	7:G:17:PHE:CD2	2.68	0.60
8:H:26:ILE:HG22	8:H:27:GLU:H	1.66	0.60
1:A:695:LYS:HG2	1:A:698:GLN:OE1	2.01	0.60
10:J:12:LYS:O	10:J:14:VAL:HG23	2.00	0.60
2:B:680:THR:OG1	2:B:681:TRP:N	2.33	0.60
2:B:653:VAL:HA	2:B:657:HIS:CD2	2.35	0.60
8:H:40:LEU:HD22	8:H:123:MET:CE	2.27	0.60
2:B:1072:MET:HG3	2:B:1085:ILE:HD13	1.81	0.60
2:B:236:HIS:CE1	2:B:389:ALA:HA	2.35	0.60
8:H:32:THR:HG22	8:H:33:GLN:N	2.16	0.60
1:A:1427:ASN:H	1:A:1427:ASN:HD22	1.50	0.60
4:D:119:ARG:HG2	4:D:120:GLU:H	1.64	0.60
1:A:20:GLY:O	1:A:21:LEU:HD23	2.01	0.60
2:B:582:VAL:HB	2:B:587:HIS:CD2	2.35	0.60
2:B:1201:LYS:HE2	2:B:1205:GLN:CD	2.21	0.60
1:A:930:ASP:O	1:A:934:LYS:HG2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:327:ARG:O	2:B:331:LEU:HD13	2.02	0.60
7:G:56:ILE:O	7:G:57:GLN:HB2	2.01	0.60
5:E:154:ILE:O	5:E:196:VAL:HA	2.01	0.60
1:A:1173:HIS:CD2	1:A:1227:ILE:HG23	2.36	0.60
2:B:900:ALA:HB3	12:L:61:THR:OG1	2.02	0.60
9:I:35:VAL:CG1	9:I:36:GLU:N	2.65	0.60
1:A:679:ILE:HG12	1:A:732:LEU:HD12	1.83	0.60
5:E:182:ASP:HB3	5:E:185:ALA:HB2	1.83	0.60
1:A:154:SER:HB3	1:A:162:VAL:HG23	1.82	0.60
6:F:125:LEU:HG	6:F:125:LEU:O	2.01	0.60
8:H:91:ASP:C	8:H:93:TYR:H	2.03	0.60
2:B:277:LYS:CG	2:B:338:GLY:HA2	2.31	0.60
1:A:857:ARG:NH2	6:F:139:PRO:HG3	2.16	0.60
3:C:98:VAL:O	3:C:99:LEU:HD23	2.00	0.60
1:A:512:VAL:HA	1:A:519:PRO:HA	1.83	0.60
2:B:579:ARG:CB	2:B:586:TRP:HE1	2.13	0.60
2:B:20:ASP:C	2:B:22:SER:H	2.04	0.60
2:B:611:PRO:CG	2:B:685:LEU:HD11	2.31	0.60
8:H:24:CYS:HB2	8:H:44:VAL:HG21	1.83	0.60
2:B:314:LEU:HD21	2:B:386:LEU:HD11	1.83	0.60
7:G:14:HIS:ND1	7:G:15:PRO:HD2	2.17	0.60
5:E:46:TYR:O	5:E:54:GLN:HG2	2.02	0.60
8:H:30:SER:CB	8:H:36:CYS:HB3	2.31	0.60
1:A:544:ASP:CG	1:A:545:GLN:H	2.05	0.60
9:I:14:LEU:HA	9:I:28:GLU:O	2.01	0.60
1:A:1313:LEU:O	1:A:1315:GLU:N	2.34	0.60
5:E:4:GLU:C	5:E:6:GLU:N	2.55	0.60
2:B:446:LEU:O	2:B:447:ALA:HB3	2.02	0.60
2:B:639:ILE:HD11	2:B:691:GLU:CG	2.22	0.60
3:C:101:LEU:CD1	3:C:118:LEU:HD23	2.26	0.60
1:A:666:ILE:HD11	2:B:1067:ARG:O	2.00	0.60
5:E:46:TYR:CD2	5:E:58:MET:HG2	2.36	0.60
2:B:941:LEU:HD21	2:B:946:ASN:HA	1.82	0.60
1:A:343:LYS:HZ2	2:B:1151:LEU:HD12	1.65	0.60
1:A:832:ALA:HA	13:T:18:DA:N7	2.15	0.60
1:A:722:LEU:N	1:A:722:LEU:HD12	2.16	0.60
1:A:746:MET:CE	2:B:1018:PRO:HG2	2.32	0.60
1:A:731:ARG:O	1:A:734:GLU:HB3	2.00	0.60
12:L:68:GLU:N	12:L:68:GLU:OE1	2.31	0.60
1:A:18:GLN:NE2	1:A:228:PHE:CE1	2.70	0.60
12:L:44:ASP:O	12:L:45:ALA:HB3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:361:LEU:HD21	2:B:377:PHE:CD2	2.36	0.60
1:A:1453:TYR:O	1:A:1454:MET:HB3	2.01	0.60
3:C:173:ALA:O	3:C:174:ALA:HB3	2.01	0.60
7:G:1:MET:SD	7:G:79:PHE:CD1	2.93	0.60
2:B:723:VAL:HG12	2:B:724:ASP:N	2.14	0.60
1:A:1319:VAL:O	1:A:1322:ILE:HG12	2.02	0.60
1:A:186:LYS:O	1:A:194:ALA:HB1	2.02	0.60
8:H:40:LEU:CD1	8:H:123:MET:HB2	2.32	0.60
5:E:55:ARG:C	5:E:57:MET:H	2.02	0.60
10:J:7:CYS:HA	10:J:49:MET:HE3	1.84	0.60
1:A:1152:ILE:HG23	1:A:1193:LEU:HD13	1.84	0.60
1:A:441:PRO:CG	1:A:498:ARG:HB2	2.30	0.60
1:A:91:PHE:HB3	1:A:96:ILE:CD1	2.31	0.60
2:B:616:ILE:HD13	2:B:625:LYS:HB2	1.83	0.60
1:A:154:SER:HB3	1:A:162:VAL:CG2	2.31	0.60
1:A:150:THR:HG23	1:A:165:GLY:O	2.01	0.60
1:A:369:SER:CB	11:K:2:ASN:HD21	2.15	0.60
4:D:195:ILE:HG22	4:D:198:LEU:HG	1.83	0.60
1:A:420:ARG:HG2	1:A:423:ASP:HB3	1.84	0.60
2:B:654:ARG:N	2:B:657:HIS:HD2	1.98	0.60
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.37	0.60
1:A:339:ASN:O	1:A:343:LYS:HG2	2.01	0.60
9:I:2:THR:HG22	9:I:3:THR:H	1.66	0.60
2:B:135:ARG:HB2	2:B:137:TYR:HE1	1.67	0.60
11:K:21:ILE:HG22	11:K:31:VAL:HG11	1.84	0.60
2:B:642:ASP:N	2:B:649:LYS:HG3	2.16	0.60
1:A:946:VAL:HG22	5:E:201:LYS:HD2	1.82	0.60
2:B:127:GLY:C	2:B:128:LEU:HD12	2.22	0.60
11:K:18:LYS:HZ2	11:K:38:GLU:HG2	1.66	0.60
3:C:261:ALA:HA	3:C:264:GLN:OE1	2.02	0.60
1:A:172:PRO:HG3	1:A:185:TRP:CZ2	2.37	0.60
1:A:784:LEU:HB3	1:A:785:PRO:HD2	1.84	0.59
5:E:136:ASN:O	5:E:140:LEU:HG	2.01	0.59
5:E:79:TRP:HE1	5:E:81:GLU:HB2	1.67	0.59
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	1.84	0.59
4:D:56:ARG:HA	4:D:148:LEU:HD13	1.83	0.59
1:A:1315:GLU:C	1:A:1317:MET:N	2.55	0.59
3:C:3:GLU:CB	11:K:104:ASN:HD21	2.15	0.59
7:G:132:SER:HB3	7:G:135:ASP:HB2	1.83	0.59
2:B:758:PHE:CE2	2:B:1044:ALA:HA	2.37	0.59
2:B:35:SER:O	2:B:39:ARG:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:604:ARG:C	2:B:606:LYS:N	2.55	0.59
1:A:1187:GLN:O	1:A:1244:ARG:HG3	2.02	0.59
1:A:1193:LEU:HD12	1:A:1194:ARG:N	2.17	0.59
4:D:63:LEU:HD12	4:D:129:LEU:HG	1.84	0.59
2:B:510:LYS:CG	2:B:511:PRO:HD3	2.31	0.59
2:B:944:THR:HG21	2:B:1122:ARG:CZ	2.32	0.59
4:D:50:LEU:HD11	7:G:4:ILE:HD11	1.83	0.59
2:B:1047:PHE:O	2:B:1048:THR:HG23	2.01	0.59
1:A:1157:ASP:C	1:A:1159:ARG:H	2.05	0.59
1:A:56:PRO:O	1:A:57:ARG:CG	2.49	0.59
12:L:34:CYS:SG	12:L:34:CYS:O	2.60	0.59
1:A:567:LYS:HZ3	8:H:95:TYR:HB2	1.67	0.59
8:H:42:ILE:O	8:H:44:VAL:HG23	2.02	0.59
6:F:103:MET:O	6:F:104:ASN:HB2	2.02	0.59
5:E:153:HIS:C	5:E:154:ILE:HG13	2.22	0.59
2:B:65:GLU:HG3	2:B:66:ASP:OD1	2.03	0.59
3:C:18:VAL:HG23	3:C:240:VAL:HG12	1.82	0.59
2:B:67:SER:HB2	2:B:92:PHE:HD1	1.67	0.59
2:B:842:ASN:HD22	2:B:845:SER:CB	2.15	0.59
1:A:49:LYS:HE2	1:A:61:ILE:HD12	1.84	0.59
7:G:143:ILE:HG22	7:G:144:ARG:N	2.17	0.59
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.85	0.59
1:A:829:VAL:C	1:A:831:THR:N	2.56	0.59
1:A:1277:GLU:O	1:A:1279:ILE:N	2.34	0.59
1:A:986:ILE:HG22	1:A:987:VAL:N	2.16	0.59
4:D:134:THR:HG22	4:D:135:GLY:N	2.16	0.59
1:A:115:LEU:CG	1:A:142:CYS:HB3	2.32	0.59
1:A:115:LEU:CD1	1:A:142:CYS:HB3	2.32	0.59
1:A:697:ALA:HB2	1:A:702:LEU:HD12	1.84	0.59
5:E:190:LEU:HD13	5:E:191:LYS:H	1.68	0.59
4:D:207:LEU:HA	4:D:210:ILE:HD12	1.85	0.59
2:B:992:ILE:CD1	11:K:66:PRO:HB2	2.32	0.59
4:D:114:MET:CE	4:D:114:MET:HA	2.32	0.59
1:A:564:ALA:O	8:H:97:MET:HA	2.02	0.59
2:B:798:TYR:HD2	2:B:798:TYR:N	2.01	0.59
7:G:13:LEU:CD2	7:G:17:PHE:HB2	2.32	0.59
1:A:590:ARG:CG	1:A:590:ARG:HH11	2.15	0.59
1:A:337:ARG:HD3	1:A:839:ARG:NH2	2.18	0.59
11:K:7:PHE:HB2	11:K:11:LEU:CD2	2.31	0.59
1:A:1121:GLU:HG2	1:A:1122:PRO:HD2	1.84	0.59
1:A:511:ILE:HA	1:A:521:MET:CE	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:47:LEU:HD11	7:G:3:PHE:CD2	2.38	0.59
1:A:756:ILE:O	1:A:759:ALA:HB3	2.01	0.59
2:B:31:TRP:HA	2:B:31:TRP:CE3	2.37	0.59
2:B:652:LYS:HD3	2:B:688:GLY:O	2.01	0.59
1:A:537:ARG:HD2	8:H:20:TYR:CE1	2.28	0.59
3:C:147:LEU:N	3:C:147:LEU:HD23	2.17	0.59
1:A:666:ILE:CD1	1:A:667:GLY:H	2.10	0.59
1:A:845:LEU:O	1:A:846:GLU:C	2.41	0.59
2:B:830:TYR:HE2	2:B:1000:PRO:HD3	1.66	0.59
11:K:11:LEU:N	11:K:11:LEU:HD22	2.17	0.59
1:A:456:MET:CE	1:A:507:VAL:HG13	2.32	0.59
7:G:30:LEU:HD13	7:G:72:VAL:CG1	2.32	0.59
2:B:992:ILE:HD11	11:K:66:PRO:HB2	1.84	0.59
1:A:409:SER:O	1:A:411:ASP:N	2.36	0.59
1:A:785:PRO:HG2	1:A:786:HIS:HD2	1.68	0.59
2:B:235:SER:C	2:B:236:HIS:HD2	2.06	0.59
2:B:331:LEU:CD2	2:B:353:LYS:HG2	2.33	0.59
8:H:128:ASN:N	8:H:130:ARG:NH1	2.45	0.59
12:L:27:LEU:N	12:L:27:LEU:HD23	2.13	0.59
2:B:891:ASP:O	2:B:893:LEU:N	2.35	0.59
1:A:1030:ARG:HG3	1:A:1034:GLU:CD	2.23	0.59
4:D:3:VAL:HG12	4:D:4:SER:N	2.17	0.59
2:B:172:ILE:HD13	2:B:178:ASN:ND2	2.18	0.59
1:A:853:ASP:OD1	1:A:855:THR:HB	2.03	0.59
2:B:483:LEU:HD11	2:B:491:THR:CG2	2.32	0.59
1:A:69:THR:C	1:A:71:GLN:N	2.55	0.59
1:A:898:ARG:HD3	1:A:933:TYR:CD1	2.37	0.59
12:L:49:LYS:O	12:L:50:ASP:HB2	2.03	0.59
2:B:333:PHE:CE1	2:B:337:ARG:NH2	2.70	0.59
2:B:516:ASN:ND2	2:B:516:ASN:N	2.49	0.59
6:F:82:THR:CG2	6:F:84:TYR:H	2.16	0.59
2:B:123:THR:O	2:B:125:SER:N	2.35	0.59
1:A:700:ASN:ND2	9:I:115:LYS:HD2	2.17	0.59
1:A:523:ILE:HB	1:A:622:VAL:CG2	2.33	0.59
9:I:64:SER:O	9:I:66:PRO:HD3	2.01	0.59
2:B:498:THR:O	2:B:536:VAL:HA	2.03	0.59
1:A:323:LYS:H	1:A:323:LYS:HD2	1.68	0.59
2:B:557:PHE:HZ	2:B:603:LEU:HD21	1.67	0.59
1:A:475:THR:CG2	1:A:476:SER:H	2.15	0.59
3:C:124:LEU:HD21	3:C:129:ILE:O	2.03	0.59
2:B:563:MET:CE	2:B:580:VAL:HB	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1130:GLN:HG3	1:A:1134:ILE:HD11	1.84	0.59
1:A:401:GLY:C	1:A:435:HIS:HD2	2.05	0.59
6:F:138:LEU:HB3	6:F:139:PRO:HD2	1.84	0.59
10:J:35:ALA:O	10:J:38:ARG:HB3	2.02	0.59
2:B:732:SER:HB2	2:B:734:HIS:CE1	2.38	0.59
2:B:956:THR:HG22	2:B:957:ASN:H	1.68	0.59
1:A:528:LEU:O	1:A:528:LEU:HD12	2.02	0.59
1:A:567:LYS:HD2	8:H:95:TYR:CG	2.38	0.59
8:H:95:TYR:O	8:H:143:LEU:HA	2.03	0.59
2:B:308:TRP:HA	2:B:311:LEU:HD12	1.84	0.59
1:A:867:ILE:HG22	1:A:872:GLY:H	1.66	0.59
1:A:353:ILE:HG21	1:A:487:MET:HE3	1.84	0.59
3:C:112:ASN:CB	3:C:114:TYR:HE1	2.15	0.59
4:D:40:HIS:HB3	7:G:6:ASP:HB3	1.85	0.59
2:B:180:TYR:HD1	2:B:180:TYR:H	1.51	0.59
1:A:731:ARG:HG3	1:A:755:PHE:CE1	2.38	0.59
5:E:182:ASP:O	5:E:185:ALA:HB3	2.03	0.59
2:B:1215:ARG:CZ	4:D:15:LEU:HD21	2.33	0.59
9:I:95:THR:HG22	9:I:96:SER:O	2.03	0.59
1:A:208:LEU:HD23	1:A:208:LEU:C	2.24	0.59
1:A:471:ASN:OD1	1:A:472:LEU:N	2.36	0.58
8:H:64:ASN:ND2	8:H:88:SER:HB2	2.18	0.58
1:A:1445:ILE:HD12	7:G:59:GLY:O	2.03	0.58
2:B:864:LYS:HB2	2:B:872:GLU:HG3	1.85	0.58
8:H:110:ASP:HB2	8:H:128:ASN:ND2	2.17	0.58
1:A:340:LEU:HD21	2:B:1199:ALA:HB3	1.85	0.58
2:B:553:PRO:O	2:B:557:PHE:HB2	2.03	0.58
2:B:797:TYR:HB3	2:B:798:TYR:CD2	2.39	0.58
3:C:82:TYR:CE1	3:C:161:LYS:HG2	2.37	0.58
3:C:232:VAL:HG21	3:C:244:VAL:HG22	1.84	0.58
2:B:1006:ILE:HG23	10:J:43:ARG:HG3	1.85	0.58
1:A:1173:HIS:ND1	1:A:1173:HIS:O	2.36	0.58
1:A:1224:LEU:HG	1:A:1226:VAL:HG23	1.85	0.58
4:D:59:ILE:O	4:D:63:LEU:HB2	2.03	0.58
1:A:164:ARG:HG3	1:A:165:GLY:H	1.68	0.58
5:E:67:GLU:O	5:E:70:SER:HB2	2.03	0.58
2:B:25:ILE:HD11	2:B:653:VAL:O	2.03	0.58
2:B:827:ILE:O	2:B:1085:ILE:HG23	2.03	0.58
2:B:274:PRO:CG	2:B:359:GLU:HB3	2.32	0.58
1:A:590:ARG:O	1:A:591:PHE:HB2	2.03	0.58
5:E:85:GLU:O	5:E:88:VAL:HG23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:SER:HA	1:A:233:TRP:CD1	2.38	0.58
7:G:106:MET:HG2	7:G:107:LYS:N	2.18	0.58
4:D:127:ASP:OD2	4:D:142:LYS:HE3	2.02	0.58
1:A:523:ILE:HB	1:A:622:VAL:HG22	1.85	0.58
2:B:164:LYS:HD3	2:B:164:LYS:N	2.18	0.58
2:B:20:ASP:O	2:B:22:SER:N	2.35	0.58
1:A:525:GLN:OE1	2:B:836:GLU:HG2	2.02	0.58
7:G:91:VAL:HG23	7:G:141:SER:O	2.03	0.58
2:B:357:GLN:HG2	2:B:366:GLN:O	2.04	0.58
5:E:22:MET:HG3	5:E:187:TYR:CD1	2.38	0.58
2:B:515:HIS:H	2:B:518:HIS:HD2	1.49	0.58
1:A:709:THR:HG22	1:A:710:LEU:N	2.18	0.58
8:H:5:LEU:O	8:H:133:ASN:HB3	2.03	0.58
2:B:1169:MET:HE3	2:B:1201:LYS:HG2	1.84	0.58
2:B:56:ASP:HB2	2:B:57:TYR:CD1	2.38	0.58
4:D:116:SER:O	4:D:118:THR:HG23	2.03	0.58
1:A:901:LEU:HG	1:A:926:GLN:HE21	1.67	0.58
1:A:901:LEU:HD11	1:A:983:ILE:HD13	1.85	0.58
6:F:117:PRO:C	6:F:119:ARG:H	2.06	0.58
1:A:1101:LEU:C	1:A:1101:LEU:HD12	2.23	0.58
1:A:295:LEU:O	1:A:298:PHE:HB3	2.03	0.58
1:A:853:ASP:OD1	1:A:855:THR:N	2.33	0.58
1:A:164:ARG:HG3	1:A:165:GLY:N	2.18	0.58
2:B:603:LEU:HB3	2:B:609:ILE:HD11	1.86	0.58
2:B:811:TYR:N	2:B:811:TYR:CD1	2.71	0.58
2:B:916:THR:HB	2:B:935:ARG:HG3	1.86	0.58
12:L:30:ILE:C	12:L:56:LEU:HD23	2.24	0.58
7:G:140:LYS:O	7:G:141:SER:C	2.42	0.58
9:I:50:THR:HB	9:I:92:ARG:NH1	2.18	0.58
1:A:1036:ARG:HG2	1:A:1036:ARG:NH1	2.19	0.58
2:B:1163:CYS:HB2	2:B:1182:CYS:SG	2.43	0.58
1:A:278:THR:HG23	1:A:282:ASN:ND2	2.19	0.58
2:B:615:MET:HA	2:B:625:LYS:O	2.04	0.58
2:B:1115:THR:HG22	2:B:1117:GLN:HG3	1.85	0.58
4:D:49:ALA:HB1	4:D:178:ALA:HB2	1.86	0.58
1:A:814:PHE:CE1	2:B:519:TRP:HA	2.38	0.58
2:B:798:TYR:CD2	2:B:798:TYR:N	2.72	0.58
2:B:326:ASP:C	2:B:328:GLU:H	2.06	0.58
1:A:427:GLN:HB2	1:A:430:TRP:CG	2.39	0.58
5:E:98:ILE:HG22	5:E:102:GLU:HG3	1.86	0.58
1:A:456:MET:HE1	1:A:507:VAL:HG13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:774:ARG:O	1:A:775:ILE:C	2.41	0.58
1:A:583:PRO:O	1:A:610:GLY:HA3	2.03	0.58
10:J:39:LEU:N	10:J:39:LEU:HD12	2.18	0.58
2:B:641:GLU:HB2	2:B:643:ASP:OD2	2.03	0.58
1:A:998:LEU:HD12	1:A:998:LEU:H	1.69	0.58
2:B:918:ILE:HG22	2:B:919:SER:N	2.19	0.58
7:G:88:ASP:CB	7:G:144:ARG:HA	2.33	0.58
5:E:99:HIS:CE1	5:E:103:LYS:HG3	2.39	0.58
2:B:274:PRO:HG2	2:B:359:GLU:HB3	1.85	0.58
1:A:860:LEU:HD11	1:A:1393:ASN:ND2	2.18	0.58
1:A:860:LEU:O	2:B:1224:PHE:HE2	1.86	0.58
1:A:1143:LEU:HD23	1:A:1267:MET:HB3	1.85	0.58
1:A:2:VAL:HG11	2:B:1157:ALA:CB	2.33	0.58
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.69	0.58
2:B:1177:HIS:CB	2:B:1179:GLN:HE21	2.17	0.58
1:A:984:LYS:O	1:A:988:LEU:HB2	2.04	0.58
2:B:345:LYS:C	2:B:348:ARG:HG2	2.24	0.58
1:A:568:PRO:CG	8:H:46:LEU:HD22	2.29	0.58
2:B:1006:ILE:HD13	10:J:44:TYR:CE2	2.39	0.58
1:A:17:VAL:HB	1:A:1419:ASP:HB3	1.84	0.58
1:A:180:LYS:NZ	1:A:294:SER:HB3	2.16	0.58
1:A:317:LYS:HA	2:B:471:LYS:HE2	1.86	0.58
2:B:708:GLU:O	2:B:710:LEU:N	2.36	0.58
2:B:918:ILE:HD12	2:B:935:ARG:NH1	2.19	0.58
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.86	0.58
2:B:899:ILE:CG2	2:B:949:VAL:HG21	2.34	0.58
2:B:95:ILE:HB	2:B:130:VAL:HG22	1.85	0.58
7:G:85:GLU:HB3	7:G:147:ILE:HD12	1.86	0.58
2:B:770:GLN:OE1	2:B:983:ARG:HA	2.04	0.58
1:A:7:SER:C	1:A:9:ALA:H	2.07	0.58
13:T:7:DC:H2"	13:T:8:DT:C7	2.34	0.58
2:B:479:VAL:HG12	2:B:480:SER:H	1.69	0.58
1:A:947:PHE:CE2	1:A:954:TRP:CE2	2.92	0.58
1:A:825:ILE:CD1	2:B:512:ARG:HB3	2.15	0.57
3:C:189:THR:HG22	3:C:190:ASP:N	2.19	0.57
9:I:51:ASN:O	9:I:54:GLU:HG3	2.03	0.57
1:A:381:THR:C	1:A:383:TYR:N	2.56	0.57
1:A:265:LYS:O	1:A:269:ILE:HG13	2.04	0.57
1:A:302:THR:HA	1:A:305:ASP:O	2.04	0.57
1:A:353:ILE:HG21	1:A:487:MET:HG3	1.84	0.57
3:C:112:ASN:CB	3:C:114:TYR:CE1	2.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:44:TYR:N	10:J:44:TYR:CD2	2.69	0.57
3:C:34:ARG:O	3:C:38:ILE:HG13	2.04	0.57
2:B:1181:GLU:H	2:B:1188:LYS:HG3	1.69	0.57
2:B:615:MET:O	2:B:697:GLU:HG3	2.04	0.57
6:F:85:MET:HB3	6:F:155:LEU:HD11	1.86	0.57
2:B:216:GLU:OE1	2:B:537:LYS:HE3	2.04	0.57
4:D:25:ALA:C	4:D:27:LEU:H	2.08	0.57
1:A:62:ASP:O	1:A:63:ARG:C	2.42	0.57
2:B:953:LEU:HB3	12:L:57:LEU:HD23	1.86	0.57
1:A:1035:TYR:O	1:A:1036:ARG:C	2.41	0.57
1:A:147:VAL:HG13	1:A:168:GLY:O	2.04	0.57
1:A:434:ARG:HH11	1:A:434:ARG:HG2	1.69	0.57
3:C:66:ARG:NH1	10:J:2:ILE:CG2	2.67	0.57
1:A:1427:ASN:O	1:A:1430:LEU:N	2.37	0.57
3:C:167:HIS:CD2	12:L:70:ARG:HB3	2.39	0.57
1:A:1053:PHE:O	1:A:1056:SER:N	2.37	0.57
1:A:469:ARG:HB3	1:A:469:ARG:NH1	2.19	0.57
2:B:1165:ILE:CD1	4:D:17:LYS:HD3	2.34	0.57
1:A:523:ILE:CG2	1:A:527:THR:HB	2.34	0.57
6:F:85:MET:HB3	6:F:155:LEU:CD1	2.34	0.57
2:B:39:ARG:HG2	2:B:39:ARG:HH11	1.69	0.57
1:A:826:ASP:HB2	1:A:830:LYS:HD3	1.86	0.57
3:C:100:THR:HG22	3:C:101:LEU:N	2.19	0.57
9:I:76:PRO:HD2	9:I:108:HIS:CD2	2.36	0.57
1:A:897:TYR:CD2	1:A:936:LEU:HD13	2.27	0.57
11:K:49:GLU:HG3	11:K:94:ILE:HG12	1.87	0.57
2:B:1178:ASN:O	2:B:1179:GLN:C	2.43	0.57
2:B:487:THR:CG2	2:B:488:TYR:N	2.66	0.57
1:A:864:ILE:HG21	1:A:1374:VAL:HG22	1.85	0.57
3:C:24:ASN:O	3:C:25:VAL:HG13	2.04	0.57
2:B:640:VAL:CG2	2:B:651:LEU:HD23	2.32	0.57
2:B:640:VAL:HG13	2:B:650:GLU:C	2.24	0.57
1:A:41:MET:O	1:A:42:ASP:O	2.23	0.57
1:A:67:CYS:C	1:A:68:GLN:HG3	2.23	0.57
7:G:91:VAL:HB	7:G:139:ILE:O	2.05	0.57
5:E:106:GLN:HA	5:E:130:ALA:CB	2.35	0.57
1:A:618:GLU:O	1:A:620:LYS:N	2.38	0.57
6:F:74:ILE:HD12	6:F:144:GLU:HG3	1.85	0.57
1:A:1100:ARG:O	1:A:1103:GLU:HB3	2.04	0.57
1:A:896:ARG:HH21	1:A:1030:ARG:NE	2.01	0.57
2:B:642:ASP:HB3	2:B:649:LYS:HG3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1017:LEU:HD23	5:E:204:THR:O	2.05	0.57
1:A:775:ILE:HD12	1:A:818:MET:SD	2.44	0.57
1:A:709:THR:HG21	9:I:93:LYS:O	2.04	0.57
1:A:701:LEU:O	1:A:702:LEU:HG	2.03	0.57
10:J:23:ASN:C	10:J:25:LEU:N	2.58	0.57
1:A:1142:THR:HB	1:A:1271:ILE:O	2.04	0.57
2:B:1167:GLY:HA3	2:B:1216:LEU:H	1.68	0.57
1:A:804:TYR:HE1	2:B:1021:MET:HE3	1.69	0.57
2:B:351:TYR:CE1	2:B:355:ILE:HD11	2.40	0.57
2:B:265:SER:O	2:B:267:ARG:N	2.37	0.57
1:A:1445:ILE:HD12	1:A:1445:ILE:N	2.09	0.57
5:E:10:SER:O	5:E:13:TRP:HB3	2.04	0.57
5:E:85:GLU:C	5:E:87:SER:H	2.08	0.57
2:B:204:ILE:C	2:B:205:ILE:HD12	2.24	0.57
4:D:60:LYS:HZ3	4:D:115:HIS:CE1	2.22	0.57
1:A:189:ARG:O	1:A:190:ALA:HB3	2.05	0.57
5:E:178:ILE:HB	5:E:212:ARG:HD2	1.86	0.57
3:C:18:VAL:HG12	3:C:20:PHE:HD2	1.70	0.57
6:F:132:LEU:CD2	7:G:61:ILE:HD11	2.34	0.57
2:B:1121:GLY:HA2	13:T:22:DC:OP2	2.05	0.57
7:G:44:TYR:HE1	7:G:157:ILE:H	1.52	0.57
2:B:603:LEU:CD1	2:B:608:ASP:HB3	2.34	0.57
2:B:794:ASN:C	2:B:795:ILE:HD12	2.24	0.57
7:G:146:LYS:HB2	7:G:168:LEU:HD11	1.84	0.57
1:A:590:ARG:HG2	1:A:591:PHE:N	2.19	0.57
3:C:164:ALA:HA	3:C:167:HIS:O	2.04	0.57
4:D:31:GLN:O	4:D:34:GLN:HG3	2.03	0.57
7:G:51:TYR:O	7:G:54:ILE:HG13	2.04	0.57
1:A:1322:ILE:O	1:A:1324:PRO:HD3	2.05	0.57
13:T:25:DG:H2''	13:T:26:DT:H5'	1.86	0.57
2:B:950:ASP:O	2:B:951:GLN:HB3	2.04	0.57
3:C:82:TYR:CD1	3:C:161:LYS:HG2	2.40	0.57
10:J:1:MET:H1	10:J:56:LEU:HB2	1.69	0.57
6:F:109:VAL:HG12	6:F:110:ASP:H	1.67	0.57
1:A:470:LEU:CD1	1:A:487:MET:HE1	2.31	0.57
1:A:873:MET:C	1:A:1058:VAL:HG23	2.24	0.57
1:A:356:ASP:OD2	11:K:65:HIS:HE1	1.87	0.57
1:A:416:ARG:HG3	1:A:417:TYR:CE2	2.39	0.57
1:A:11:LEU:HB2	2:B:1193:GLN:O	2.04	0.57
8:H:26:ILE:HD13	8:H:49:VAL:HG11	1.87	0.57
13:T:24:DG:H2'	13:T:25:DG:C8	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:130:LEU:C	4:D:132:GLN:H	2.08	0.57
8:H:11:GLN:O	8:H:28:ALA:HB1	2.05	0.57
1:A:898:ARG:HD2	1:A:899:VAL:H	1.68	0.57
7:G:115:MET:HB2	7:G:116:PRO:HD2	1.86	0.57
1:A:1453:TYR:CE2	6:F:129:LYS:HA	2.39	0.57
7:G:18:PHE:HA	7:G:22:MET:HE3	1.86	0.57
9:I:58:VAL:HG12	9:I:58:VAL:O	2.03	0.57
1:A:860:LEU:HD11	1:A:1393:ASN:HD22	1.69	0.57
4:D:159:THR:O	4:D:163:VAL:HG23	2.05	0.57
2:B:558:LEU:HD21	2:B:600:LEU:HD11	1.87	0.57
2:B:653:VAL:CG2	2:B:689:LEU:HB3	2.33	0.57
2:B:186:GLU:CG	10:J:62:ARG:HH22	2.18	0.57
7:G:127:PRO:HG3	7:G:139:ILE:HG13	1.86	0.57
7:G:15:PRO:HA	7:G:18:PHE:CE1	2.39	0.57
2:B:864:LYS:HG3	2:B:872:GLU:OE1	2.04	0.57
1:A:331:GLY:O	1:A:332:LYS:HB3	2.05	0.57
1:A:336:ILE:HD13	1:A:340:LEU:HD12	1.86	0.57
2:B:648:HIS:CG	2:B:649:LYS:N	2.71	0.57
3:C:36:VAL:HG21	3:C:251:LEU:CD1	2.35	0.57
1:A:236:LEU:HD23	1:A:236:LEU:N	2.20	0.57
1:A:682:THR:HG23	1:A:728:LYS:HE3	1.85	0.57
1:A:1106:ASN:O	1:A:1107:VAL:HB	2.04	0.57
3:C:214:ASN:HB3	3:C:217:ASP:OD2	2.04	0.57
6:F:87:LYS:HA	6:F:155:LEU:HD22	1.87	0.57
4:D:214:LEU:C	4:D:216:ASN:H	2.09	0.57
1:A:567:LYS:NZ	8:H:47:PHE:HB2	2.20	0.56
3:C:132:PRO:O	3:C:134:ILE:HG13	2.05	0.56
1:A:768:GLN:CG	1:A:816:HIS:HA	2.17	0.56
5:E:22:MET:HE3	5:E:26:ARG:HD2	1.86	0.56
5:E:59:SER:HB3	5:E:81:GLU:HA	1.85	0.56
2:B:165:VAL:HG12	2:B:166:PHE:N	2.20	0.56
2:B:126:SER:CB	2:B:172:ILE:HD11	2.34	0.56
6:F:75:PRO:O	6:F:77:ASP:O	2.23	0.56
5:E:180:ARG:HH21	5:E:192:ARG:HD2	1.70	0.56
3:C:229:TYR:CD1	3:C:229:TYR:N	2.72	0.56
2:B:1116:ARG:HG3	2:B:1198:TYR:CE2	2.40	0.56
2:B:1130:PHE:CE1	2:B:1134:GLU:HB3	2.40	0.56
1:A:1293:SER:OG	1:A:1295:THR:HG23	2.05	0.56
1:A:542:GLU:O	1:A:546:VAL:HG23	2.05	0.56
1:A:1161:THR:C	1:A:1163:ILE:H	2.07	0.56
2:B:750:GLY:O	2:B:751:VAL:C	2.42	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:CYS:HB2	1:A:169:ASN:ND2	2.20	0.56
9:I:4:PHE:CE1	9:I:6:PHE:HE2	2.23	0.56
3:C:212:PRO:CB	3:C:213:PRO:HD2	2.35	0.56
2:B:604:ARG:NH2	2:B:613:VAL:O	2.35	0.56
1:A:798:GLY:HA2	1:A:815:PHE:HD1	1.69	0.56
2:B:343:ILE:HD12	2:B:347:LYS:NZ	2.21	0.56
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.86	0.56
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.36	0.56
8:H:118:PHE:C	8:H:120:GLY:H	2.07	0.56
3:C:61:GLU:HA	3:C:64:ALA:HB3	1.86	0.56
7:G:127:PRO:HG3	7:G:139:ILE:HD11	1.85	0.56
5:E:156:LEU:HD12	5:E:195:VAL:CB	2.31	0.56
8:H:127:GLY:O	8:H:128:ASN:HB2	2.05	0.56
10:J:36:LEU:HD12	10:J:47:ARG:NH1	2.20	0.56
1:A:1226:VAL:HG22	1:A:1240:CYS:HB3	1.87	0.56
7:G:34:VAL:HG12	7:G:45:ILE:HG21	1.85	0.56
4:D:3:VAL:CG2	7:G:10:ASN:HB2	2.32	0.56
2:B:299:GLU:CB	2:B:571:PRO:HG3	2.32	0.56
12:L:60:ARG:NH2	12:L:65:VAL:HG21	2.20	0.56
5:E:9:ILE:HD11	5:E:53:PRO:HD3	1.88	0.56
1:A:388:LEU:O	1:A:392:VAL:HG23	2.05	0.56
1:A:881:GLN:NE2	1:A:958:VAL:O	2.39	0.56
1:A:134:ARG:HG2	1:A:138:ILE:CD1	2.31	0.56
7:G:35:GLU:HG2	7:G:48:VAL:HG23	1.88	0.56
2:B:1017:ILE:CB	2:B:1018:PRO:HD3	2.33	0.56
1:A:584:ASN:C	1:A:586:ILE:H	2.07	0.56
2:B:465:ASN:HB3	2:B:475:SER:OG	2.05	0.56
1:A:503:GLN:HE21	6:F:90:ARG:HH21	1.54	0.56
9:I:71:SER:HG	9:I:101:PHE:HD2	1.53	0.56
9:I:106:CYS:O	9:I:107:SER:HB2	2.05	0.56
13:T:21:DC:H2''	13:T:22:DC:C5'	2.35	0.56
1:A:639:PRO:HG2	1:A:640:GLN:N	2.20	0.56
2:B:839:MET:HG3	2:B:1010:LEU:HD11	1.87	0.56
2:B:997:GLU:H	2:B:997:GLU:CD	2.06	0.56
1:A:794:PRO:HG2	1:A:795:GLU:OE2	2.06	0.56
1:A:865:GLN:HE21	1:A:1370:LEU:HA	1.71	0.56
1:A:35:ILE:HA	1:A:52:GLY:O	2.06	0.56
1:A:69:THR:C	1:A:71:GLN:H	2.07	0.56
2:B:879:ARG:O	2:B:934:LYS:HE2	2.05	0.56
2:B:957:ASN:O	2:B:957:ASN:CG	2.42	0.56
5:E:17:ARG:CB	5:E:17:ARG:HH11	2.14	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:PRO:CG	1:A:521:MET:HG2	2.35	0.56
1:A:711:ARG:O	1:A:714:PHE:HB3	2.05	0.56
4:D:155:ARG:HD3	4:D:221:TYR:CE1	2.40	0.56
1:A:503:GLN:HE21	6:F:90:ARG:NH2	2.04	0.56
9:I:101:PHE:N	9:I:101:PHE:CD1	2.73	0.56
1:A:140:THR:HA	1:A:143:LYS:HE2	1.87	0.56
1:A:108:MET:N	1:A:108:MET:SD	2.78	0.56
3:C:243:VAL:HG12	3:C:243:VAL:O	2.05	0.56
1:A:1313:LEU:HD11	1:A:1317:MET:HE2	1.87	0.56
2:B:616:ILE:HG12	2:B:697:GLU:HA	1.85	0.56
2:B:603:LEU:HB3	2:B:609:ILE:CD1	2.35	0.56
8:H:99:GLY:HA3	8:H:117:SER:O	2.06	0.56
3:C:89:GLU:O	3:C:90:ASP:CB	2.54	0.56
2:B:235:SER:HB3	2:B:258:LEU:HG	1.88	0.56
3:C:169:LYS:HE3	3:C:170:TRP:CH2	2.40	0.56
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.86	0.56
1:A:1050:GLU:O	1:A:1053:PHE:HB3	2.05	0.56
7:G:29:LYS:HD2	7:G:32:GLU:OE1	2.06	0.56
1:A:1322:ILE:O	1:A:1322:ILE:HG13	2.06	0.56
2:B:792:MET:HA	2:B:856:PHE:O	2.05	0.56
10:J:34:THR:O	10:J:35:ALA:C	2.44	0.56
4:D:217:LEU:O	4:D:219:THR:N	2.39	0.56
1:A:64:ASN:H	1:A:74:MET:CE	2.19	0.56
9:I:50:THR:CG2	9:I:52:ILE:HG12	2.35	0.56
3:C:39:ALA:HA	3:C:164:ALA:CB	2.31	0.56
3:C:2:SER:O	3:C:3:GLU:HB2	2.05	0.56
1:A:821:ARG:HB2	1:A:821:ARG:NH1	2.20	0.56
2:B:613:VAL:HG13	2:B:627:PHE:C	2.26	0.56
1:A:57:ARG:O	1:A:58:LEU:O	2.23	0.56
8:H:84:ALA:O	8:H:89:LEU:HD21	2.06	0.56
8:H:98:TYR:HE1	8:H:139:ASN:HA	1.69	0.56
2:B:785:TYR:CE1	2:B:795:ILE:HG12	2.41	0.56
3:C:242:GLN:C	3:C:244:VAL:H	2.07	0.56
1:A:1029:ARG:HG3	1:A:1029:ARG:HH11	1.71	0.56
3:C:138:GLU:OE1	3:C:138:GLU:N	2.39	0.56
1:A:332:LYS:HG3	1:A:333:GLU:CD	2.26	0.56
1:A:93:VAL:CG2	1:A:301:ALA:HA	2.34	0.56
1:A:715:GLU:OE1	1:A:774:ARG:HD3	2.05	0.56
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.06	0.56
2:B:824:ILE:HG22	2:B:1087:PHE:HE2	1.71	0.56
1:A:1356:ILE:HD12	1:A:1368:MET:SD	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1141:THR:HA	1:A:1205:LYS:HZ3	1.71	0.56
2:B:707:PRO:HA	2:B:741:CYS:SG	2.46	0.56
5:E:117:THR:HB	5:E:120:ALA:HB2	1.86	0.56
1:A:269:ILE:CG1	1:A:299:HIS:HB3	2.31	0.56
1:A:1220:PHE:O	1:A:1221:LYS:HB2	2.06	0.56
6:F:86:THR:HG23	6:F:89:GLU:OE1	2.05	0.56
2:B:973:ILE:CG2	2:B:974:PRO:HD2	2.36	0.56
2:B:562:GLY:HA3	2:B:590:HIS:ND1	2.21	0.56
10:J:1:MET:H1	10:J:56:LEU:N	2.02	0.56
1:A:899:VAL:HG13	1:A:908:LEU:CD2	2.32	0.56
1:A:1437:GLY:O	1:A:1439:GLY:N	2.39	0.56
1:A:340:LEU:CD2	2:B:1199:ALA:HB3	2.36	0.56
2:B:834:ASN:CA	2:B:838:SER:O	2.54	0.56
11:K:68:PHE:HB3	11:K:70:ARG:HH11	1.70	0.56
3:C:18:VAL:O	3:C:18:VAL:HG12	2.05	0.56
10:J:24:LEU:O	10:J:30:LEU:HB2	2.06	0.56
2:B:1169:MET:HE1	2:B:1201:LYS:HA	1.88	0.56
1:A:172:PRO:HB3	1:A:185:TRP:CE3	2.41	0.56
1:A:1289:ARG:HD2	1:A:1303:GLU:OE2	2.06	0.56
1:A:125:ALA:C	1:A:127:ALA:H	2.08	0.56
2:B:1147:LEU:HD23	2:B:1147:LEU:C	2.26	0.56
1:A:61:ILE:HG22	1:A:62:ASP:N	2.21	0.55
1:A:567:LYS:HB3	1:A:568:PRO:CD	2.36	0.55
8:H:100:THR:CG2	8:H:101:ALA:N	2.70	0.55
3:C:58:LEU:N	3:C:58:LEU:HD22	2.21	0.55
3:C:77:ILE:HG23	3:C:161:LYS:NZ	2.21	0.55
1:A:919:ILE:HG21	1:A:983:ILE:HD11	1.88	0.55
5:E:128:PRO:HA	5:E:129:PRO:C	2.25	0.55
5:E:136:ASN:OD1	5:E:137:GLU:N	2.38	0.55
5:E:114:ASN:O	5:E:115:ASN:CB	2.47	0.55
2:B:467:GLY:O	2:B:469:GLN:N	2.39	0.55
2:B:402:GLY:HA2	2:B:695:ALA:HB3	1.87	0.55
2:B:662:MET:HA	2:B:665:GLU:HB2	1.88	0.55
8:H:129:TYR:HA	8:H:131:ASN:ND2	2.21	0.55
12:L:27:LEU:HB3	12:L:37:LYS:HB3	1.88	0.55
2:B:1109:GLY:O	2:B:1111:MET:HG2	2.06	0.55
11:K:65:HIS:CD2	11:K:67:PHE:HB2	2.41	0.55
1:A:818:MET:HG2	2:B:514:LEU:HG	1.87	0.55
1:A:1317:MET:O	1:A:1322:ILE:HD11	2.06	0.55
2:B:855:PHE:CD1	2:B:856:PHE:N	2.73	0.55
11:K:44:ASN:N	11:K:61:TYR:HE1	2.03	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:104:PHE:CE2	8:H:136:LYS:HG2	2.41	0.55
1:A:150:THR:O	1:A:150:THR:HG22	2.05	0.55
1:A:849:MET:HB2	1:A:1062:GLU:O	2.05	0.55
4:D:137:ASN:N	4:D:137:ASN:HD22	2.03	0.55
1:A:903:ASN:ND2	1:A:903:ASN:C	2.58	0.55
10:J:64:ASN:CB	10:J:65:PRO:CD	2.80	0.55
5:E:173:SER:C	5:E:175:LEU:H	2.09	0.55
1:A:913:LEU:HD12	1:A:914:GLU:N	2.18	0.55
7:G:51:TYR:C	7:G:51:TYR:CD2	2.80	0.55
1:A:107:CYS:SG	1:A:148:CYS:HB2	2.47	0.55
2:B:344:LYS:O	2:B:345:LYS:C	2.44	0.55
1:A:915:SER:O	1:A:919:ILE:HG13	2.07	0.55
9:I:50:THR:HB	9:I:92:ARG:HH12	1.71	0.55
5:E:154:ILE:HG22	5:E:155:ARG:O	2.05	0.55
8:H:108:SER:O	8:H:110:ASP:N	2.39	0.55
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	2.06	0.55
1:A:1262:LYS:C	1:A:1264:GLU:N	2.59	0.55
4:D:53:SER:HA	4:D:56:ARG:HB3	1.88	0.55
5:E:4:GLU:C	5:E:6:GLU:H	2.08	0.55
2:B:594:ALA:HB2	9:I:61:ASP:OD1	2.06	0.55
3:C:176:ILE:HG22	3:C:177:GLU:N	2.22	0.55
3:C:252:GLN:HG3	11:K:95:ILE:HG23	1.87	0.55
5:E:109:ILE:CG2	5:E:110:PHE:H	2.16	0.55
1:A:886:ILE:HG23	1:A:887:GLY:N	2.21	0.55
4:D:40:HIS:HD2	7:G:73:LYS:CG	2.19	0.55
9:I:34:TYR:CD2	9:I:35:VAL:N	2.75	0.55
1:A:21:LEU:HD12	1:A:229:SER:HB2	1.89	0.55
1:A:639:PRO:HG2	1:A:640:GLN:H	1.72	0.55
1:A:104:GLU:HG3	1:A:174:ILE:HD12	1.88	0.55
2:B:549:THR:HG22	2:B:550:ASP:N	2.22	0.55
1:A:35:ILE:HG13	1:A:241:VAL:HG21	1.88	0.55
10:J:6:ARG:HB3	10:J:11:GLY:O	2.07	0.55
2:B:244:LEU:HD12	2:B:250:PHE:H	1.71	0.55
2:B:243:ALA:HB2	2:B:251:ILE:HG12	1.89	0.55
2:B:284:ILE:HG23	2:B:324:ILE:HD13	1.89	0.55
9:I:73:ARG:HH12	9:I:112:SER:CB	2.19	0.55
9:I:52:ILE:HG13	9:I:52:ILE:O	2.05	0.55
5:E:55:ARG:C	5:E:57:MET:N	2.60	0.55
3:C:196:ASP:HB3	3:C:199:LYS:HB2	1.87	0.55
1:A:535:THR:HG21	1:A:616:VAL:CA	2.28	0.55
5:E:133:GLU:HG2	5:E:135:PHE:HE1	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:99:LEU:O	9:I:111:THR:HG23	2.07	0.55
1:A:1423:GLY:HA3	1:A:1426:GLU:HG2	1.88	0.55
4:D:40:HIS:HB2	7:G:73:LYS:HD3	1.88	0.55
1:A:1373:ASP:O	1:A:1377:THR:HG23	2.07	0.55
1:A:1284:MET:HA	1:A:1306:LEU:HD23	1.89	0.55
1:A:1342:GLU:CD	5:E:198:ILE:HG21	2.26	0.55
3:C:6:PRO:HB2	11:K:101:LEU:HD12	1.89	0.55
5:E:38:PRO:HG2	5:E:41:ASP:HB2	1.87	0.55
1:A:935:GLN:HE22	1:A:938:LYS:HD2	1.71	0.55
2:B:579:ARG:HD2	2:B:586:TRP:CZ2	2.42	0.55
6:F:116:ASP:O	6:F:120:ILE:HG13	2.06	0.55
5:E:206:GLY:O	5:E:207:ARG:HG2	2.07	0.55
5:E:90:VAL:CA	5:E:120:ALA:HB2	2.37	0.55
5:E:153:HIS:HB3	5:E:196:VAL:HG11	1.87	0.55
4:D:163:VAL:O	4:D:166:LEU:HB3	2.06	0.55
5:E:52:ARG:HB3	5:E:53:PRO:CD	2.35	0.55
2:B:526:GLU:OE1	2:B:752:ALA:HB3	2.07	0.55
1:A:224:PHE:CD2	1:A:231:PRO:HG3	2.42	0.55
1:A:98:LYS:O	1:A:102:VAL:HG23	2.06	0.55
2:B:1115:THR:O	2:B:1116:ARG:HB2	2.06	0.55
8:H:10:PHE:N	8:H:10:PHE:CD1	2.75	0.55
2:B:69:LEU:CD1	2:B:429:PHE:HD1	1.89	0.55
2:B:873:THR:O	2:B:914:LYS:HA	2.07	0.55
1:A:929:LEU:HD13	1:A:929:LEU:O	2.06	0.55
6:F:99:LEU:O	6:F:103:MET:CG	2.55	0.55
4:D:8:PHE:CE1	4:D:37:GLN:HB2	2.41	0.55
1:A:1341:ILE:HG23	1:A:1342:GLU:H	1.70	0.55
5:E:177:ARG:C	5:E:212:ARG:HD3	2.27	0.55
8:H:5:LEU:O	8:H:6:PHE:HB2	2.06	0.55
1:A:849:MET:CE	1:A:1061:GLY:HA2	2.35	0.55
2:B:842:ASN:HD22	2:B:845:SER:HB3	1.71	0.55
1:A:1318:THR:HB	5:E:141:VAL:HG11	1.87	0.55
2:B:708:GLU:HG3	2:B:709:ASP:N	2.22	0.55
2:B:278:GLN:CG	2:B:279:ASP:H	2.13	0.55
1:A:590:ARG:CD	1:A:604:GLY:HA2	2.37	0.55
7:G:7:LEU:O	7:G:73:LYS:HE2	2.07	0.55
2:B:620:ARG:NH1	9:I:68:LEU:HD21	2.23	0.55
1:A:154:SER:C	1:A:156:ASP:H	2.10	0.55
1:A:1141:THR:OG1	1:A:1205:LYS:HD3	2.07	0.55
2:B:696:GLU:O	2:B:699:GLU:HB2	2.07	0.55
2:B:613:VAL:CG2	2:B:628:THR:HA	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:807:ARG:HB3	2:B:807:ARG:NH1	2.22	0.54
1:A:55:ASP:C	1:A:57:ARG:N	2.58	0.54
2:B:390:LEU:O	2:B:392:ARG:N	2.40	0.54
7:G:22:MET:O	7:G:23:LYS:C	2.46	0.54
1:A:1330:ASN:O	1:A:1332:PHE:N	2.40	0.54
11:K:31:VAL:CG1	11:K:32:VAL:H	2.18	0.54
1:A:1152:ILE:HG22	1:A:1192:LEU:O	2.06	0.54
2:B:893:LEU:HD22	2:B:897:GLY:C	2.27	0.54
1:A:134:ARG:O	1:A:138:ILE:HG13	2.07	0.54
9:I:35:VAL:CG1	9:I:36:GLU:H	2.18	0.54
1:A:1074:GLU:HB3	1:A:1075:PRO:CD	2.36	0.54
4:D:14:ARG:O	4:D:16:LYS:HG2	2.07	0.54
1:A:41:MET:CB	1:A:50:ILE:H	2.19	0.54
9:I:55:THR:HG21	9:I:109:ILE:HD13	1.88	0.54
5:E:124:VAL:N	5:E:125:PRO:CD	2.70	0.54
5:E:39:LEU:O	5:E:42:PHE:HB3	2.07	0.54
2:B:847:ASP:C	2:B:849:GLY:N	2.59	0.54
1:A:1308:THR:CG2	1:A:1309:ASP:N	2.57	0.54
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.41	0.54
1:A:1081:LEU:HD12	1:A:1098:VAL:HG23	1.89	0.54
9:I:59:VAL:HG12	9:I:60:GLN:H	1.72	0.54
3:C:148:ARG:HG2	3:C:149:LYS:N	2.23	0.54
1:A:658:LEU:HD23	1:A:659:HIS:HE1	1.69	0.54
2:B:205:ILE:N	2:B:205:ILE:HD12	2.23	0.54
1:A:1001:ARG:O	1:A:1002:GLY:O	2.25	0.54
1:A:9:ALA:HB3	2:B:1193:GLN:HB2	1.88	0.54
5:E:185:ALA:O	5:E:190:LEU:HB2	2.08	0.54
4:D:203:SER:OG	4:D:206:GLU:HB2	2.08	0.54
2:B:305:VAL:HG12	2:B:305:VAL:O	2.07	0.54
2:B:936:ASP:OD1	2:B:937:ALA:N	2.40	0.54
7:G:96:GLN:HA	7:G:121:PHE:CZ	2.41	0.54
2:B:360:PHE:O	2:B:361:LEU:C	2.46	0.54
1:A:427:GLN:HB2	1:A:430:TRP:CE2	2.42	0.54
1:A:427:GLN:HG3	1:A:430:TRP:CE2	2.42	0.54
5:E:89:GLY:C	5:E:91:LYS:H	2.10	0.54
1:A:1161:THR:C	1:A:1163:ILE:N	2.61	0.54
1:A:1114:PRO:O	1:A:1115:SER:O	2.24	0.54
1:A:967:ALA:CA	1:A:1044:TRP:HZ3	2.21	0.54
1:A:746:MET:HE3	2:B:1018:PRO:HG2	1.90	0.54
3:C:7:GLN:HG2	11:K:104:ASN:ND2	2.23	0.54
2:B:68:THR:HG23	2:B:91:SER:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:707:PRO:HG2	2:B:708:GLU:H	1.72	0.54
12:L:55:ILE:CG1	12:L:56:LEU:H	2.21	0.54
10:J:60:PHE:O	10:J:63:TYR:HD1	1.90	0.54
1:A:1223:ASP:HA	1:A:1243:VAL:HG11	1.88	0.54
5:E:153:HIS:O	5:E:154:ILE:CG1	2.48	0.54
1:A:1019:CYS:O	1:A:1022:LEU:HB3	2.07	0.54
2:B:455:SER:O	2:B:456:GLY:C	2.46	0.54
9:I:12:ASN:OD1	9:I:31:THR:HG21	2.08	0.54
9:I:7:CYS:HB3	9:I:14:LEU:CD2	2.38	0.54
1:A:728:LYS:CA	1:A:731:ARG:HH21	2.20	0.54
1:A:316:GLN:O	1:A:317:LYS:C	2.45	0.54
1:A:185:TRP:CZ3	1:A:200:ARG:HB3	2.43	0.54
8:H:76:THR:O	8:H:77:ARG:HB2	2.08	0.54
1:A:254:GLU:HB2	2:B:935:ARG:NH2	2.23	0.54
3:C:91:HIS:ND1	3:C:158:VAL:HG11	2.22	0.54
3:C:184:ASN:HD21	3:C:187:LYS:HA	1.72	0.54
8:H:62:SER:OG	8:H:63:LEU:N	2.41	0.54
1:A:688:LYS:HA	1:A:691:LEU:HB3	1.88	0.54
5:E:93:MET:O	5:E:95:THR:N	2.41	0.54
7:G:34:VAL:HG11	7:G:74:TYR:HE1	1.72	0.54
1:A:343:LYS:HZ3	2:B:1151:LEU:HD12	1.69	0.54
1:A:831:THR:HG23	1:A:832:ALA:N	2.23	0.54
5:E:85:GLU:HB2	5:E:88:VAL:CG2	2.35	0.54
4:D:170:THR:C	4:D:172:LEU:N	2.61	0.54
2:B:68:THR:HG22	2:B:69:LEU:H	1.71	0.54
1:A:602:ASP:HB3	1:A:616:VAL:HG23	1.88	0.54
1:A:578:LEU:HD23	1:A:612:ILE:CD1	2.38	0.54
8:H:19:ARG:O	8:H:20:TYR:HD2	1.91	0.54
1:A:898:ARG:HA	1:A:933:TYR:CD1	2.42	0.54
1:A:852:TYR:CD2	1:A:1060:PRO:CB	2.89	0.54
1:A:1254:ALA:O	1:A:1255:GLU:CB	2.54	0.54
2:B:170:LEU:HD12	2:B:170:LEU:C	2.27	0.54
4:D:66:ARG:HD2	4:D:133:THR:HB	1.90	0.54
1:A:111:GLY:O	1:A:214:ILE:HA	2.07	0.54
9:I:4:PHE:HD1	9:I:4:PHE:C	2.11	0.54
8:H:38:LEU:HD12	8:H:39:THR:H	1.73	0.54
2:B:616:ILE:CG2	2:B:700:SER:OG	2.56	0.54
3:C:177:GLU:CG	3:C:231:ASN:HB3	2.37	0.54
4:D:207:LEU:HD23	4:D:207:LEU:C	2.28	0.54
2:B:711:GLU:HB2	2:B:712:PRO:CD	2.38	0.54
2:B:658:ILE:HG22	2:B:662:MET:HE2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:802:PRO:HG2	2:B:805:THR:HG22	1.89	0.54
1:A:1418:LEU:HB3	2:B:1222:ARG:NH1	2.23	0.54
8:H:145:ARG:O	8:H:146:ARG:HB2	2.08	0.54
2:B:63:ILE:HA	2:B:421:PHE:CE2	2.43	0.54
1:A:105:CYS:SG	1:A:139:TRP:HA	2.48	0.54
3:C:14:SER:HA	11:K:114:LEU:HD22	1.89	0.54
1:A:152:VAL:HG12	1:A:153:PRO:HD2	1.90	0.54
1:A:193:ASP:O	1:A:194:ALA:HB3	2.08	0.54
2:B:38:PHE:CD1	2:B:811:TYR:CD2	2.96	0.54
8:H:81:PRO:CB	8:H:82:PRO:CD	2.74	0.54
2:B:326:ASP:O	2:B:328:GLU:N	2.41	0.54
1:A:590:ARG:HH21	1:A:620:LYS:CB	2.19	0.54
1:A:407:ARG:HG2	1:A:430:TRP:CH2	2.42	0.54
1:A:1156:PRO:HA	1:A:1190:PRO:CB	2.38	0.54
1:A:738:LYS:H	1:A:738:LYS:CD	2.15	0.54
1:A:874:ASP:N	1:A:1058:VAL:HG23	2.23	0.54
1:A:968:GLN:HE22	1:A:1035:TYR:HB2	1.72	0.54
1:A:729:ALA:HA	1:A:732:LEU:HD12	1.88	0.54
2:B:230:ALA:N	2:B:231:PRO:CD	2.70	0.54
3:C:213:PRO:O	3:C:214:ASN:CB	2.55	0.54
1:A:556:TRP:CE3	1:A:558:GLY:HA2	2.42	0.54
2:B:850:LEU:CD2	2:B:1009:ASP:HB3	2.38	0.54
1:A:18:GLN:HG2	1:A:1418:LEU:CD1	2.34	0.54
1:A:1446:ASP:O	1:A:1447:GLU:C	2.45	0.54
5:E:13:TRP:CZ3	5:E:39:LEU:HB2	2.43	0.54
11:K:31:VAL:CG1	11:K:32:VAL:N	2.69	0.54
1:A:1063:MET:CG	1:A:1436:ILE:HG23	2.38	0.54
1:A:1153:TYR:CD2	1:A:1163:ILE:HD11	2.43	0.54
3:C:34:ARG:HA	3:C:37:MET:HE2	1.89	0.54
2:B:60:GLN:NE2	2:B:94:LYS:HA	2.23	0.54
2:B:95:ILE:CG1	2:B:130:VAL:HG22	2.38	0.54
10:J:27:GLU:O	10:J:29:GLU:HG3	2.07	0.54
2:B:124:TYR:HH	2:B:179:CYS:HG	1.55	0.54
1:A:974:ASP:OD2	1:A:976:THR:OG1	2.26	0.54
1:A:551:TYR:CZ	11:K:62:LYS:HE2	2.43	0.54
1:A:1386:ARG:HB2	1:A:1403:GLU:OE1	2.08	0.54
1:A:567:LYS:CB	1:A:568:PRO:CD	2.86	0.53
3:C:102:GLN:HG2	3:C:154:LYS:HG2	1.90	0.53
6:F:119:ARG:HH11	6:F:119:ARG:HG3	1.72	0.53
2:B:1098:MET:H	2:B:1098:MET:HE3	1.73	0.53
1:A:269:ILE:HD13	1:A:300:VAL:HG22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:LEU:HD12	1:A:328:ARG:NH2	2.23	0.53
11:K:23:PRO:HA	11:K:31:VAL:HG13	1.90	0.53
1:A:884:ASP:O	1:A:886:ILE:N	2.41	0.53
3:C:165:LYS:O	11:K:6:ARG:NH1	2.39	0.53
1:A:444:PHE:HB3	1:A:458:HIS:HD2	1.73	0.53
2:B:97:VAL:CG2	2:B:128:LEU:HG	2.38	0.53
7:G:51:TYR:HD2	7:G:51:TYR:C	2.12	0.53
2:B:1171:VAL:HA	2:B:1182:CYS:HB2	1.90	0.53
1:A:583:PRO:HG2	1:A:586:ILE:CG1	2.38	0.53
4:D:24:ALA:C	4:D:26:THR:N	2.60	0.53
13:T:22:DC:H2'	13:T:23:BRU:H6	1.90	0.53
1:A:64:ASN:O	1:A:65:LEU:C	2.46	0.53
8:H:42:ILE:HG12	8:H:97:MET:HE1	1.90	0.53
3:C:235:VAL:HG12	10:J:13:VAL:CG2	2.37	0.53
7:G:99:PHE:HZ	7:G:163:ILE:HD13	1.73	0.53
10:J:7:CYS:SG	10:J:49:MET:HE3	2.48	0.53
4:D:40:HIS:CD2	7:G:73:LYS:HZ3	2.26	0.53
11:K:7:PHE:C	11:K:9:LEU:N	2.62	0.53
1:A:1120:LEU:HD22	1:A:1124:HIS:O	2.09	0.53
1:A:396:PRO:HB3	1:A:403:LYS:HA	1.90	0.53
4:D:126:ILE:HD13	4:D:145:MET:HE2	1.91	0.53
4:D:139:LYS:HG3	4:D:143:ASN:ND2	2.23	0.53
2:B:57:TYR:CD1	2:B:57:TYR:N	2.76	0.53
1:A:1230:GLU:C	1:A:1232:ASN:H	2.11	0.53
1:A:371:ALA:HB2	1:A:462:VAL:HG13	1.90	0.53
2:B:685:LEU:HG	2:B:686:ASN:N	2.24	0.53
1:A:825:ILE:HG22	1:A:826:ASP:N	2.22	0.53
3:C:74:SER:OG	3:C:237:SER:HB2	2.07	0.53
5:E:121:MET:O	5:E:124:VAL:HG23	2.09	0.53
1:A:1103:GLU:O	1:A:1108:ALA:HB2	2.08	0.53
2:B:563:MET:HE3	2:B:580:VAL:HB	1.91	0.53
2:B:899:ILE:HG23	2:B:903:VAL:HG21	1.89	0.53
1:A:384:ASN:OD1	1:A:388:LEU:HD12	2.07	0.53
1:A:233:TRP:C	1:A:235:ILE:N	2.61	0.53
2:B:1073:TYR:CE2	2:B:1080:LYS:HG2	2.43	0.53
2:B:39:ARG:HH21	2:B:665:GLU:CD	2.11	0.53
2:B:880:THR:HB	2:B:934:LYS:HE2	1.88	0.53
1:A:525:GLN:O	1:A:528:LEU:N	2.42	0.53
3:C:245:VAL:O	3:C:249:ASP:N	2.40	0.53
2:B:377:PHE:O	2:B:380:TYR:N	2.42	0.53
8:H:64:ASN:ND2	8:H:88:SER:C	2.61	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:PHE:HA	1:A:595:THR:CG2	2.37	0.53
1:A:353:ILE:CD1	1:A:487:MET:HE2	2.36	0.53
1:A:340:LEU:HD21	2:B:1200:ALA:N	2.23	0.53
2:B:900:ALA:CB	12:L:61:THR:OG1	2.56	0.53
1:A:1008:GLN:O	1:A:1011:GLN:HB3	2.09	0.53
2:B:1106:ARG:HH12	2:B:1110:PRO:HG2	1.72	0.53
1:A:463:ILE:HD11	1:A:469:ARG:HG3	1.89	0.53
4:D:52:LEU:O	4:D:54:GLU:N	2.39	0.53
4:D:60:LYS:O	4:D:64:VAL:HG23	2.08	0.53
2:B:465:ASN:N	2:B:465:ASN:ND2	2.55	0.53
3:C:193:TYR:HD1	3:C:193:TYR:O	1.91	0.53
2:B:616:ILE:HG23	2:B:700:SER:OG	2.08	0.53
2:B:753:ALA:HA	2:B:756:ILE:CD1	2.39	0.53
2:B:659:ALA:HA	2:B:662:MET:HE2	1.91	0.53
2:B:637:LEU:CD1	2:B:693:ILE:HD12	2.22	0.53
1:A:70:CYS:O	1:A:72:GLU:HG2	2.08	0.53
2:B:284:ILE:HG23	2:B:324:ILE:CD1	2.38	0.53
2:B:899:ILE:O	2:B:952:VAL:HG21	2.09	0.53
1:A:913:LEU:HG	1:A:914:GLU:N	2.23	0.53
1:A:92:HIS:O	1:A:94:GLY:N	2.42	0.53
2:B:469:GLN:CG	2:B:470:LYS:H	2.22	0.53
1:A:676:MET:O	1:A:679:ILE:HB	2.08	0.53
5:E:178:ILE:HG13	5:E:182:ASP:OD2	2.08	0.53
2:B:984:HIS:NE2	2:B:1025:HIS:HA	2.23	0.53
12:L:24:THR:O	12:L:25:ALA:HB3	2.08	0.53
1:A:1397:LEU:O	1:A:1400:CYS:HB3	2.09	0.53
2:B:802:PRO:HG2	2:B:805:THR:CG2	2.39	0.53
2:B:955:THR:HG23	2:B:956:THR:H	1.74	0.53
8:H:89:LEU:C	8:H:91:ASP:N	2.62	0.53
1:A:687:LYS:O	1:A:690:VAL:HB	2.08	0.53
1:A:311:GLN:O	1:A:312:PRO:C	2.46	0.53
1:A:896:ARG:NH2	1:A:1030:ARG:NH2	2.56	0.53
1:A:473:SER:HG	1:A:646:PHE:HD2	1.56	0.53
1:A:182:VAL:CG2	1:A:201:VAL:HA	2.32	0.53
1:A:963:ILE:HD11	1:A:1048:ASN:HB3	1.89	0.53
1:A:997:LEU:HD13	1:A:1018:PHE:CE2	2.43	0.53
2:B:1178:ASN:O	2:B:1180:PHE:CD1	2.61	0.53
1:A:613:ILE:O	1:A:614:PHE:HB3	2.08	0.53
1:A:682:THR:HG22	1:A:728:LYS:HE3	1.91	0.53
5:E:212:ARG:HH11	5:E:212:ARG:CG	2.20	0.53
3:C:209:TYR:N	3:C:209:TYR:CD1	2.76	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1058:LEU:N	2:B:1058:LEU:HD23	2.23	0.53
1:A:1187:GLN:HA	1:A:1244:ARG:HD2	1.91	0.53
5:E:110:PHE:HE2	5:E:112:TYR:HB3	1.72	0.53
2:B:265:SER:O	2:B:266:ALA:C	2.47	0.53
7:G:13:LEU:HD22	7:G:17:PHE:HB2	1.90	0.53
1:A:1163:ILE:HG22	1:A:1165:GLU:HG2	1.91	0.53
9:I:44:TYR:CD1	9:I:45:ARG:N	2.77	0.53
1:A:740:LEU:HD12	1:A:741:ASN:N	2.24	0.53
4:D:126:ILE:HD13	4:D:145:MET:CE	2.39	0.53
4:D:66:ARG:HG3	7:G:51:TYR:CD1	2.43	0.53
1:A:178:GLY:C	1:A:179:LEU:HD23	2.28	0.53
1:A:940:ARG:NH1	1:A:940:ARG:HG2	2.20	0.53
2:B:222:ILE:O	2:B:240:ILE:HA	2.08	0.53
1:A:947:PHE:CD1	1:A:947:PHE:N	2.76	0.53
1:A:408:ASP:O	1:A:410:GLY:N	2.42	0.53
10:J:31:ASP:O	10:J:32:GLU:C	2.47	0.53
1:A:798:GLY:HA2	1:A:815:PHE:CD1	2.44	0.53
2:B:506:GLY:CA	2:B:512:ARG:HH21	2.07	0.53
5:E:112:TYR:CZ	5:E:136:ASN:HB2	2.44	0.53
2:B:309:GLN:CD	9:I:52:ILE:HD11	2.29	0.53
1:A:343:LYS:HD3	2:B:1155:SER:OG	2.09	0.53
2:B:896:ASP:OD2	12:L:58:LYS:HE3	2.09	0.53
1:A:1015:VAL:CG1	1:A:1019:CYS:SG	2.96	0.53
4:D:51:ASN:O	4:D:52:LEU:O	2.27	0.53
2:B:294:ASP:HB2	9:I:12:ASN:HA	1.91	0.53
4:D:137:ASN:ND2	4:D:137:ASN:H	2.06	0.53
1:A:704:ALA:O	1:A:705:LYS:C	2.46	0.53
2:B:745:PRO:C	2:B:747:MET:H	2.13	0.53
2:B:882:THR:HG21	2:B:934:LYS:O	2.09	0.53
10:J:16:ASP:OD1	10:J:17:LYS:HD2	2.09	0.53
3:C:181:ASP:OD2	3:C:184:ASN:HA	2.08	0.53
5:E:22:MET:O	5:E:26:ARG:HB2	2.09	0.53
2:B:273:LEU:HD12	2:B:276:ILE:CD1	2.37	0.53
1:A:1446:ASP:HB2	6:F:133:VAL:CG2	2.38	0.53
7:G:17:PHE:HD2	7:G:17:PHE:N	2.07	0.53
1:A:1100:ARG:O	1:A:1104:ILE:HG13	2.08	0.53
1:A:858:ASN:ND2	1:A:858:ASN:C	2.62	0.53
3:C:174:ALA:O	3:C:175:ALA:HB2	2.08	0.53
5:E:14:ARG:HA	5:E:17:ARG:HG2	1.91	0.53
5:E:9:ILE:CD1	5:E:53:PRO:HD3	2.38	0.53
2:B:63:ILE:HD12	2:B:421:PHE:CE2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:PHE:CG	1:A:231:PRO:HG3	2.43	0.53
1:A:278:THR:CG2	1:A:282:ASN:HD22	2.21	0.53
1:A:675:THR:O	1:A:679:ILE:HG13	2.09	0.53
1:A:734:GLU:C	1:A:736:ASN:H	2.10	0.53
1:A:135:PHE:HD1	1:A:222:LEU:HD22	1.74	0.53
6:F:85:MET:O	6:F:155:LEU:HD21	2.08	0.53
4:D:50:LEU:HD11	7:G:4:ILE:CD1	2.38	0.53
4:D:7:THR:HB	7:G:42:PHE:CZ	2.43	0.53
2:B:215:GLN:HA	2:B:215:GLN:NE2	2.24	0.53
2:B:62:ILE:HG23	2:B:418:LYS:HG3	1.91	0.53
2:B:133:LYS:HG3	2:B:135:ARG:HE	1.73	0.53
2:B:589:VAL:HG12	2:B:590:HIS:H	1.73	0.53
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.90	0.53
2:B:879:ARG:CZ	2:B:883:LEU:HD22	2.38	0.53
2:B:955:THR:OG1	12:L:55:ILE:HA	2.09	0.53
8:H:100:THR:CG2	8:H:101:ALA:H	2.22	0.53
3:C:123:ASN:CG	3:C:125:MET:H	2.11	0.53
3:C:148:ARG:HG2	3:C:149:LYS:H	1.74	0.53
5:E:86:PRO:HA	5:E:113:GLN:HB2	1.90	0.53
5:E:63:ASN:HB3	5:E:64:PRO:CD	2.38	0.53
2:B:272:THR:O	2:B:273:LEU:HD23	2.09	0.53
1:A:598:LEU:O	1:A:599:SER:C	2.47	0.53
1:A:1351:GLU:O	1:A:1355:VAL:HG23	2.09	0.53
1:A:308:ILE:HG22	1:A:309:ALA:N	2.12	0.53
1:A:1276:VAL:HG12	1:A:1277:GLU:N	2.23	0.53
1:A:401:GLY:C	1:A:435:HIS:CD2	2.82	0.53
4:D:60:LYS:NZ	4:D:115:HIS:CE1	2.76	0.53
2:B:1159:ARG:HD2	2:B:1159:ARG:C	2.29	0.53
1:A:1206:ASP:HB3	1:A:1274:ARG:NH1	2.19	0.53
1:A:1272:THR:C	1:A:1273:LEU:HD12	2.30	0.53
8:H:135:LEU:HD13	8:H:137:GLN:HE21	1.73	0.53
2:B:221:ASN:OD1	2:B:242:SER:HA	2.09	0.53
1:A:75:ASN:O	1:A:76:GLU:CB	2.56	0.53
2:B:605:ARG:CZ	2:B:639:ILE:HD13	2.38	0.52
2:B:687:GLU:HB3	2:B:689:LEU:HG	1.90	0.52
8:H:80:ARG:NH1	11:K:57:LEU:HD21	2.20	0.52
2:B:1065:GLN:NE2	2:B:1066:SER:N	2.57	0.52
2:B:1085:ILE:HD12	2:B:1085:ILE:N	2.23	0.52
2:B:318:VAL:C	2:B:320:ASP:N	2.62	0.52
5:E:94:LYS:HG3	5:E:98:ILE:CD1	2.39	0.52
1:A:867:ILE:HG13	1:A:1000:LEU:HD21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:64:VAL:C	4:D:66:ARG:N	2.62	0.52
1:A:107:CYS:N	1:A:114:LEU:HD21	2.24	0.52
1:A:168:GLY:O	1:A:169:ASN:C	2.46	0.52
3:C:22:LEU:HD13	3:C:230:MET:HE1	1.90	0.52
3:C:69:LEU:N	3:C:69:LEU:HD12	2.24	0.52
7:G:112:LYS:HA	7:G:115:MET:CE	2.40	0.52
2:B:273:LEU:CD1	2:B:276:ILE:HD12	2.39	0.52
2:B:313:MET:CE	2:B:390:LEU:HD21	2.39	0.52
5:E:162:ARG:HB3	5:E:162:ARG:CZ	2.39	0.52
2:B:859:TYR:HD1	2:B:859:TYR:H	1.57	0.52
1:A:23:SER:HB3	1:A:233:TRP:CZ2	2.45	0.52
1:A:21:LEU:HG	1:A:1413:GLY:O	2.09	0.52
14:N:3:DT:OP2	14:N:3:DT:H3'	2.09	0.52
1:A:523:ILE:HD12	1:A:622:VAL:HG21	1.91	0.52
2:B:192:LEU:O	2:B:193:LYS:HB2	2.09	0.52
2:B:955:THR:HG23	2:B:956:THR:N	2.24	0.52
1:A:825:ILE:HG22	1:A:826:ASP:H	1.73	0.52
3:C:189:THR:HG22	3:C:190:ASP:H	1.73	0.52
1:A:322:VAL:O	1:A:322:VAL:CG1	2.58	0.52
1:A:618:GLU:OE2	1:A:620:LYS:HB2	2.09	0.52
1:A:334:GLY:O	1:A:335:ARG:C	2.48	0.52
9:I:7:CYS:SG	9:I:8:ARG:O	2.67	0.52
2:B:460:ALA:HB1	2:B:466:TRP:CZ3	2.44	0.52
2:B:1167:GLY:O	2:B:1215:ARG:HA	2.10	0.52
1:A:954:TRP:CZ3	5:E:203:GLU:HB2	2.43	0.52
2:B:597:MET:HE2	2:B:597:MET:HA	1.90	0.52
1:A:452:LYS:HG3	2:B:1140:ALA:HB1	1.90	0.52
1:A:677:ARG:HD2	1:A:678:GLU:N	2.25	0.52
2:B:542:MET:HG2	2:B:747:MET:HB3	1.91	0.52
2:B:613:VAL:CG1	2:B:628:THR:HA	2.39	0.52
2:B:805:THR:HB	2:B:809:MET:SD	2.49	0.52
2:B:956:THR:HG22	2:B:960:GLY:HA2	1.91	0.52
12:L:33:GLU:C	12:L:35:SER:H	2.13	0.52
5:E:134:THR:C	5:E:135:PHE:HD1	2.13	0.52
2:B:260:GLY:O	2:B:267:ARG:NH1	2.43	0.52
2:B:368:GLU:O	2:B:370:PHE:N	2.38	0.52
2:B:952:VAL:HG12	2:B:953:LEU:N	2.24	0.52
1:A:884:ASP:HB3	1:A:896:ARG:HH12	1.74	0.52
7:G:34:VAL:HG11	7:G:74:TYR:CE1	2.45	0.52
1:A:507:VAL:N	1:A:508:PRO:CD	2.72	0.52
4:D:34:GLN:O	4:D:47:LEU:HD23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:90:ARG:HH11	6:F:90:ARG:HB2	1.73	0.52
1:A:1394:THR:CG2	1:A:1398:MET:SD	2.97	0.52
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	1.90	0.52
2:B:175:ARG:NH1	2:B:175:ARG:HG2	2.23	0.52
2:B:1053:GLU:HB3	2:B:1057:LYS:HE3	1.90	0.52
2:B:1030:LEU:HD11	2:B:1059:LEU:HD22	1.92	0.52
2:B:376:PHE:O	2:B:586:TRP:HZ3	1.93	0.52
2:B:745:PRO:O	2:B:747:MET:N	2.43	0.52
1:A:63:ARG:HG3	1:A:63:ARG:O	2.09	0.52
1:A:64:ASN:H	1:A:74:MET:HE1	1.74	0.52
1:A:575:LYS:HB3	1:A:612:ILE:HG21	1.92	0.52
3:C:132:PRO:O	3:C:133:ILE:C	2.47	0.52
5:E:22:MET:HE1	5:E:26:ARG:HH11	1.71	0.52
8:H:64:ASN:OD1	8:H:90:ALA:CB	2.58	0.52
5:E:91:LYS:C	5:E:93:MET:H	2.11	0.52
1:A:1063:MET:HG3	1:A:1436:ILE:HG23	1.92	0.52
2:B:648:HIS:CD2	2:B:649:LYS:H	2.28	0.52
1:A:913:LEU:CG	1:A:914:GLU:N	2.72	0.52
4:D:179:GLN:O	4:D:183:LEU:HB2	2.10	0.52
1:A:853:ASP:OD1	1:A:855:THR:CB	2.58	0.52
1:A:219:PHE:CE2	1:A:231:PRO:HD2	2.45	0.52
1:A:179:LEU:O	1:A:180:LYS:HG3	2.09	0.52
1:A:1313:LEU:C	1:A:1315:GLU:H	2.13	0.52
5:E:178:ILE:HG23	5:E:178:ILE:O	2.08	0.52
8:H:135:LEU:HD13	8:H:137:GLN:NE2	2.24	0.52
2:B:485:ARG:CZ	2:B:782:LEU:HD11	2.40	0.52
1:A:555:ASP:O	1:A:556:TRP:O	2.27	0.52
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.92	0.52
2:B:755:ILE:HG22	2:B:755:ILE:O	2.09	0.52
3:C:154:LYS:O	3:C:155:LEU:HD23	2.10	0.52
1:A:919:ILE:HG21	1:A:983:ILE:CD1	2.39	0.52
6:F:103:MET:HE3	7:G:66:GLY:H	1.74	0.52
9:I:85:PHE:N	9:I:85:PHE:CD2	2.57	0.52
1:A:1225:PHE:HZ	1:A:1227:ILE:HD11	1.73	0.52
1:A:333:GLU:N	1:A:333:GLU:OE2	2.43	0.52
4:D:159:THR:O	4:D:162:ALA:HB3	2.09	0.52
9:I:82:GLU:O	9:I:104:LEU:HG	2.09	0.52
2:B:1150:ARG:NH1	2:B:1150:ARG:HB3	2.25	0.52
2:B:724:ASP:HB3	2:B:727:LYS:HG3	1.91	0.52
9:I:95:THR:HG22	9:I:96:SER:N	2.25	0.52
1:A:1299:VAL:HG12	1:A:1300:LYS:N	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:808:LEU:HD23	1:A:813:PHE:HA	1.90	0.52
2:B:120:ARG:HE	2:B:955:THR:HG21	1.73	0.52
1:A:567:LYS:HG3	8:H:94:ASP:O	2.10	0.52
1:A:919:ILE:HG23	1:A:925:LEU:HD12	1.91	0.52
5:E:65:THR:O	5:E:68:SER:N	2.42	0.52
6:F:71:GLU:O	6:F:72:LYS:C	2.48	0.52
3:C:136:ASP:CB	3:C:141:GLY:H	2.23	0.52
1:A:1224:LEU:HD12	1:A:1225:PHE:N	2.25	0.52
2:B:1106:ARG:HD3	2:B:1127:GLY:CA	2.40	0.52
1:A:1438:THR:O	1:A:1438:THR:HG22	2.10	0.52
8:H:15:VAL:HG21	8:H:49:VAL:HG12	1.91	0.52
14:N:6:DT:H2"	14:N:7:DT:OP2	2.10	0.52
13:T:11:DA:H2"	13:T:12:DG:C8	2.45	0.52
1:A:606:LEU:HG	1:A:613:ILE:HD12	1.90	0.52
1:A:1316:VAL:HG12	1:A:1316:VAL:O	2.10	0.52
3:C:123:ASN:ND2	3:C:125:MET:HA	2.25	0.52
2:B:309:GLN:O	2:B:310:MET:C	2.47	0.52
1:A:1434:ALA:O	1:A:1436:ILE:N	2.42	0.52
1:A:1263:ILE:O	1:A:1263:ILE:HG22	2.09	0.52
12:L:29:TYR:HA	12:L:57:LEU:O	2.10	0.52
2:B:995:ARG:NH1	3:C:165:LYS:HA	2.25	0.52
9:I:82:GLU:HB3	9:I:104:LEU:CD1	2.37	0.52
5:E:85:GLU:O	5:E:87:SER:N	2.43	0.52
1:A:298:PHE:O	1:A:301:ALA:HB3	2.10	0.52
2:B:496:ARG:HD2	2:B:751:VAL:CG2	2.40	0.52
2:B:203:PHE:HB3	2:B:205:ILE:CD1	2.39	0.52
7:G:1:MET:HE1	7:G:80:LYS:O	2.09	0.52
1:A:244:PRO:HB2	1:A:245:PRO:HD3	1.92	0.52
1:A:157:ASP:C	1:A:159:THR:H	2.13	0.52
2:B:31:TRP:CZ3	2:B:34:ILE:HD12	2.45	0.52
1:A:41:MET:HE1	1:A:42:ASP:HB2	1.90	0.52
3:C:66:ARG:NH2	10:J:5:VAL:HG23	2.24	0.52
3:C:73:GLN:HG3	3:C:74:SER:N	2.25	0.52
5:E:124:VAL:H	5:E:125:PRO:HD2	1.74	0.52
6:F:70:LYS:C	6:F:72:LYS:H	2.13	0.52
3:C:136:ASP:HB2	3:C:141:GLY:H	1.74	0.52
10:J:48:ARG:C	10:J:48:ARG:HD2	2.30	0.52
1:A:1423:GLY:CA	1:A:1426:GLU:HG2	2.39	0.52
1:A:1389:PHE:CD1	1:A:1390:ASN:N	2.78	0.52
1:A:1038:THR:HG23	1:A:1041:ALA:HB2	1.92	0.52
6:F:140:ASP:OD1	6:F:141:GLY:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1001:ARG:HH11	1:A:1001:ARG:HG2	1.73	0.52
14:N:5:DC:H2"	14:N:6:DT:O5'	2.10	0.52
3:C:11:ARG:NH2	3:C:229:TYR:HD2	2.08	0.52
2:B:616:ILE:CG1	2:B:697:GLU:HA	2.40	0.52
1:A:369:SER:HB3	11:K:2:ASN:HD21	1.75	0.52
9:I:40:SER:OG	9:I:41:PRO:HD2	2.10	0.52
1:A:61:ILE:HG22	1:A:62:ASP:H	1.74	0.52
8:H:80:ARG:NH1	11:K:57:LEU:HD11	2.25	0.52
7:G:125:SER:C	7:G:126:ASN:HD22	2.13	0.52
8:H:63:LEU:HD13	8:H:64:ASN:H	1.74	0.52
1:A:593:GLU:C	1:A:595:THR:H	2.14	0.52
1:A:942:PHE:HZ	5:E:207:ARG:CG	2.23	0.52
1:A:1100:ARG:HH22	1:A:1111:MET:HE1	1.74	0.52
10:J:8:PHE:H	10:J:49:MET:CE	2.23	0.52
1:A:1121:GLU:HB3	1:A:1124:HIS:NE2	2.24	0.52
2:B:990:ILE:HG22	2:B:991:GLY:N	2.25	0.52
1:A:865:GLN:NE2	1:A:1370:LEU:HA	2.24	0.52
1:A:1402:PHE:O	1:A:1403:GLU:HB2	2.09	0.52
10:J:53:HIS:CD2	10:J:54:VAL:N	2.78	0.52
2:B:68:THR:HG22	2:B:69:LEU:N	2.25	0.51
3:C:242:GLN:C	3:C:244:VAL:N	2.63	0.51
5:E:65:THR:O	5:E:66:GLU:C	2.48	0.51
2:B:331:LEU:HD23	2:B:353:LYS:HG2	1.91	0.51
9:I:58:VAL:CG1	9:I:62:ILE:HD12	2.29	0.51
1:A:445:ASN:CB	1:A:455:MET:HG2	2.29	0.51
2:B:1039:GLY:HA2	10:J:51:LEU:HD21	1.92	0.51
2:B:60:GLN:HE22	2:B:94:LYS:HA	1.75	0.51
1:A:700:ASN:HB2	9:I:98:VAL:HG21	1.92	0.51
1:A:698:GLN:O	9:I:98:VAL:HG13	2.10	0.51
1:A:947:PHE:N	1:A:947:PHE:HD1	2.08	0.51
4:D:206:GLU:O	4:D:210:ILE:HG13	2.11	0.51
1:A:481:ASP:CG	1:A:485:ASP:OD2	2.49	0.51
2:B:638:PHE:HB3	2:B:651:LEU:HD22	1.90	0.51
1:A:40:THR:HB	1:A:41:MET:CE	2.40	0.51
2:B:120:ARG:NH1	12:L:54:ARG:HH11	2.08	0.51
3:C:77:ILE:O	3:C:79:GLN:N	2.43	0.51
3:C:204:SER:H	3:C:207:CYS:HG	1.56	0.51
2:B:1102:LYS:O	2:B:1103:ILE:C	2.48	0.51
8:H:110:ASP:HB2	8:H:128:ASN:HD22	1.76	0.51
2:B:1002:THR:HG21	2:B:1006:ILE:CD1	2.40	0.51
2:B:952:VAL:HG13	2:B:966:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:31:ASN:OD1	3:C:34:ARG:HD3	2.10	0.51
1:A:343:LYS:HZ2	2:B:1151:LEU:CD1	2.23	0.51
1:A:630:ILE:CG2	1:A:631:HIS:N	2.72	0.51
1:A:722:LEU:CD1	1:A:722:LEU:H	2.22	0.51
1:A:767:GLN:HA	1:A:799:PHE:HA	1.92	0.51
4:D:56:ARG:HD3	4:D:149:THR:HA	1.92	0.51
9:I:4:PHE:CD1	9:I:4:PHE:C	2.82	0.51
8:H:14:GLU:O	8:H:26:ILE:HG23	2.10	0.51
11:K:109:TRP:C	11:K:111:LEU:H	2.13	0.51
4:D:118:THR:OG1	4:D:121:LYS:HB2	2.10	0.51
1:A:743:VAL:O	1:A:747:VAL:HG23	2.10	0.51
2:B:298:LEU:N	2:B:298:LEU:HD22	2.26	0.51
2:B:120:ARG:NH1	12:L:54:ARG:NH1	2.58	0.51
1:A:1098:VAL:HB	1:A:1099:PRO:CD	2.40	0.51
2:B:244:LEU:O	2:B:249:ARG:HG2	2.10	0.51
6:F:103:MET:CE	7:G:66:GLY:N	2.68	0.51
1:A:544:ASP:CG	1:A:545:GLN:N	2.62	0.51
10:J:36:LEU:HB2	10:J:47:ARG:NH1	2.24	0.51
9:I:82:GLU:HB3	9:I:104:LEU:HB2	1.91	0.51
1:A:1017:LEU:O	1:A:1017:LEU:HD12	2.10	0.51
2:B:100:PRO:HD2	2:B:180:TYR:HE1	1.72	0.51
4:D:63:LEU:HD23	7:G:47:CYS:SG	2.50	0.51
11:K:78:THR:O	11:K:81:TYR:HB3	2.10	0.51
10:J:27:GLU:O	10:J:29:GLU:N	2.43	0.51
1:A:450:LEU:HB2	1:A:838:GLN:HE21	1.74	0.51
3:C:3:GLU:HG3	11:K:104:ASN:CG	2.31	0.51
2:B:508:LEU:O	2:B:509:ALA:CB	2.57	0.51
2:B:942:ARG:O	2:B:943:SER:C	2.48	0.51
1:A:817:ALA:O	1:A:820:GLY:N	2.43	0.51
2:B:562:GLY:O	2:B:590:HIS:ND1	2.43	0.51
2:B:746:SER:CB	2:B:1046:PRO:HG2	2.39	0.51
1:A:567:LYS:CG	1:A:568:PRO:CD	2.87	0.51
3:C:124:LEU:O	3:C:126:GLY:N	2.44	0.51
1:A:306:ASN:ND2	1:A:322:VAL:HG12	2.26	0.51
1:A:466:SER:HB2	2:B:1099:VAL:HG22	1.91	0.51
9:I:62:ILE:HD13	9:I:102:VAL:HG11	1.93	0.51
1:A:896:ARG:HH21	1:A:1030:ARG:HE	1.53	0.51
3:C:31:ASN:ND2	3:C:35:ARG:HD2	2.26	0.51
1:A:343:LYS:NZ	2:B:1151:LEU:CD1	2.70	0.51
5:E:5:ASN:O	5:E:9:ILE:HG13	2.10	0.51
1:A:877:HIS:CD2	1:A:877:HIS:N	2.78	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:ILE:HB	1:A:464:PRO:CD	2.40	0.51
4:D:145:MET:O	4:D:149:THR:HB	2.11	0.51
13:T:12:DG:H2"	13:T:13:DT:O5'	2.09	0.51
1:A:284:ALA:O	1:A:286:HIS:N	2.41	0.51
1:A:1167:GLU:HA	1:A:1170:ILE:HD12	1.92	0.51
1:A:1102:LYS:O	1:A:1106:ASN:ND2	2.43	0.51
1:A:74:MET:HE2	1:A:74:MET:H	1.75	0.51
2:B:884:ARG:O	2:B:936:ASP:HB2	2.10	0.51
1:A:562:THR:HG21	8:H:98:TYR:CD2	2.46	0.51
3:C:82:TYR:CZ	3:C:161:LYS:HG2	2.45	0.51
10:J:1:MET:H1	10:J:57:ILE:N	2.05	0.51
1:A:901:LEU:HD13	1:A:919:ILE:CG2	2.41	0.51
7:G:119:LEU:HA	7:G:131:GLN:O	2.09	0.51
1:A:591:PHE:HA	1:A:595:THR:CB	2.41	0.51
5:E:117:THR:HG22	5:E:120:ALA:H	1.74	0.51
2:B:866:TYR:O	2:B:868:MET:N	2.41	0.51
1:A:543:LEU:O	1:A:546:VAL:N	2.44	0.51
2:B:899:ILE:HG21	2:B:949:VAL:HG21	1.92	0.51
1:A:1120:LEU:H	1:A:1120:LEU:HD12	1.75	0.51
1:A:477:PRO:HG2	1:A:521:MET:CG	2.40	0.51
1:A:767:GLN:NE2	1:A:797:LYS:O	2.42	0.51
9:I:6:PHE:HA	9:I:14:LEU:HG	1.93	0.51
13:T:8:DT:H2"	13:T:9:DC:OP2	2.10	0.51
1:A:284:ALA:HB1	1:A:289:ILE:HD11	1.91	0.51
1:A:725:ALA:HA	1:A:728:LYS:HE2	1.93	0.51
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.41	0.51
1:A:1102:LYS:HG2	1:A:1106:ASN:HD21	1.75	0.51
2:B:737:THR:HG21	9:I:66:PRO:HA	1.91	0.51
2:B:730:ARG:NH2	2:B:1047:PHE:HB3	2.26	0.51
1:A:104:GLU:CG	1:A:174:ILE:HD12	2.41	0.51
8:H:10:PHE:O	8:H:54:SER:HA	2.09	0.51
2:B:781:PHE:O	2:B:782:LEU:HG	2.10	0.51
2:B:1044:ALA:O	2:B:1045:SER:O	2.29	0.51
2:B:186:GLU:HG3	10:J:62:ARG:NH2	2.26	0.51
2:B:882:THR:HG22	2:B:884:ARG:CB	2.35	0.51
1:A:830:LYS:HG3	1:A:1098:VAL:HG11	1.91	0.51
2:B:797:TYR:HB3	2:B:798:TYR:HD2	1.76	0.51
2:B:391:ASP:HB2	9:I:92:ARG:HG3	1.91	0.51
1:A:1446:ASP:HB2	6:F:133:VAL:HG21	1.91	0.51
1:A:598:LEU:O	1:A:598:LEU:HD23	2.11	0.51
3:C:168:ALA:O	3:C:171:GLY:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ARG:O	1:A:231:PRO:C	2.49	0.51
10:J:23:ASN:O	10:J:25:LEU:N	2.43	0.51
1:A:765:VAL:HG23	1:A:802:ASN:O	2.11	0.51
2:B:582:VAL:HG22	2:B:626:ILE:HG21	1.92	0.51
2:B:510:LYS:HB2	2:B:511:PRO:HD3	1.92	0.51
1:A:556:TRP:CZ3	1:A:558:GLY:HA2	2.45	0.51
2:B:69:LEU:CD1	2:B:429:PHE:HE1	2.19	0.51
1:A:535:THR:CG2	1:A:575:LYS:HE2	2.39	0.51
1:A:574:GLY:O	1:A:575:LYS:C	2.49	0.51
2:B:798:TYR:CE1	10:J:4:PRO:HA	2.46	0.51
1:A:898:ARG:O	1:A:1029:ARG:NH1	2.44	0.51
2:B:515:HIS:O	2:B:518:HIS:HB2	2.11	0.51
1:A:843:LYS:HD3	1:A:846:GLU:OE2	2.11	0.51
1:A:498:ARG:HG3	1:A:499:ALA:N	2.26	0.51
1:A:1345:ARG:NH1	1:A:1373:ASP:OD1	2.44	0.51
1:A:387:ARG:O	1:A:390:GLN:HB3	2.10	0.51
1:A:1001:ARG:HH11	1:A:1001:ARG:CG	2.24	0.51
9:I:6:PHE:N	9:I:6:PHE:CD2	2.75	0.51
1:A:432:VAL:O	1:A:433:GLU:C	2.47	0.51
1:A:637:LYS:HB3	1:A:641:VAL:HG11	1.93	0.51
9:I:61:ASP:C	9:I:63:GLY:H	2.13	0.51
6:F:93:ILE:HD13	6:F:148:VAL:HG12	1.93	0.51
4:D:137:ASN:N	4:D:137:ASN:ND2	2.58	0.51
1:A:76:GLU:O	1:A:78:PRO:HD3	2.11	0.51
1:A:524:VAL:CG1	1:A:525:GLN:N	2.73	0.51
8:H:101:ALA:HB2	8:H:116:TYR:CE1	2.46	0.51
9:I:50:THR:HG22	9:I:51:ASN:N	2.26	0.51
7:G:55:ASP:OD1	7:G:57:GLN:HG3	2.10	0.51
1:A:427:GLN:HB2	1:A:430:TRP:CD2	2.46	0.51
9:I:69:PRO:HB2	9:I:85:PHE:CE2	2.46	0.51
5:E:153:HIS:HB3	5:E:196:VAL:HG13	1.93	0.51
12:L:36:SER:O	12:L:37:LYS:C	2.48	0.51
1:A:1425:SER:HA	1:A:1428:VAL:CG2	2.40	0.51
4:D:8:PHE:CD2	7:G:6:ASP:O	2.64	0.51
1:A:832:ALA:HA	13:T:18:DA:C8	2.45	0.51
3:C:51:VAL:HB	12:L:65:VAL:HG23	1.93	0.51
1:A:1048:ASN:O	1:A:1052:GLN:HB2	2.11	0.51
3:C:36:VAL:CG2	3:C:251:LEU:HD13	2.41	0.51
1:A:284:ALA:C	1:A:286:HIS:N	2.59	0.51
10:J:25:LEU:O	10:J:29:GLU:HA	2.10	0.51
9:I:74:GLU:O	9:I:74:GLU:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:857:ARG:HH21	2:B:942:ARG:NH2	2.09	0.51
2:B:842:ASN:O	2:B:846:ILE:HG13	2.11	0.51
1:A:677:ARG:HD2	1:A:677:ARG:C	2.31	0.51
2:B:601:ARG:HH11	2:B:605:ARG:NH2	2.08	0.51
1:A:42:ASP:OD1	1:A:47:ARG:HA	2.10	0.51
2:B:114:PRO:O	2:B:116:GLU:N	2.44	0.51
2:B:797:TYR:C	2:B:798:TYR:HD2	2.15	0.51
1:A:900:ASP:HA	1:A:926:GLN:HE22	1.75	0.51
7:G:112:LYS:HA	7:G:115:MET:HE3	1.93	0.51
6:F:114:GLU:HA	6:F:114:GLU:OE2	2.11	0.51
2:B:521:LEU:HD22	2:B:633:VAL:CG1	2.27	0.51
5:E:98:ILE:HA	5:E:101:GLN:HB3	1.93	0.51
5:E:124:VAL:HA	5:E:132:ILE:CD1	2.40	0.51
1:A:1151:GLU:HG2	9:I:45:ARG:HB2	1.93	0.51
1:A:391:LEU:HD22	1:A:401:GLY:O	2.10	0.51
1:A:1015:VAL:O	1:A:1017:LEU:N	2.44	0.51
2:B:95:ILE:CB	2:B:130:VAL:HG22	2.40	0.51
7:G:48:VAL:HA	7:G:76:ALA:CB	2.40	0.51
5:E:181:ALA:O	5:E:182:ASP:C	2.49	0.51
1:A:130:ASP:O	1:A:132:LYS:N	2.44	0.51
2:B:912:ILE:O	2:B:938:SER:HA	2.10	0.51
2:B:1166:CYS:O	2:B:1168:LEU:N	2.33	0.51
2:B:190:TYR:HD2	10:J:62:ARG:O	1.92	0.51
2:B:969:ARG:HG2	2:B:970:THR:N	2.25	0.51
2:B:276:ILE:O	2:B:278:GLN:N	2.37	0.51
1:A:1445:ILE:HD13	7:G:70:PHE:CZ	2.46	0.51
5:E:16:PHE:HE2	5:E:37:LEU:HD23	1.76	0.51
1:A:1388:GLY:O	1:A:1391:ARG:HG3	2.11	0.51
2:B:95:ILE:HG13	2:B:129:PHE:O	2.11	0.51
2:B:293:PRO:O	2:B:297:ILE:HG13	2.11	0.51
13:T:11:DA:H2"	13:T:12:DG:H8	1.76	0.51
1:A:1272:THR:HG22	1:A:1273:LEU:N	2.26	0.51
1:A:172:PRO:HD3	1:A:185:TRP:CE2	2.45	0.51
2:B:992:ILE:HG12	2:B:993:THR:N	2.26	0.51
1:A:19:PHE:O	1:A:1416:ALA:HA	2.11	0.51
2:B:606:LYS:HD3	2:B:608:ASP:HB2	1.93	0.50
2:B:685:LEU:HD12	2:B:685:LEU:C	2.31	0.50
1:A:531:ILE:HD11	1:A:578:LEU:HD21	1.93	0.50
7:G:127:PRO:HG3	7:G:139:ILE:CG1	2.40	0.50
7:G:143:ILE:CG2	7:G:144:ARG:N	2.74	0.50
12:L:38:LEU:O	12:L:39:SER:CB	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:116:ILE:CG2	5:E:117:THR:N	2.74	0.50
2:B:891:ASP:C	2:B:893:LEU:N	2.64	0.50
1:A:896:ARG:HH22	1:A:1030:ARG:HH21	1.57	0.50
3:C:168:ALA:O	3:C:170:TRP:N	2.44	0.50
2:B:1182:CYS:O	2:B:1183:LYS:O	2.29	0.50
2:B:1158:PHE:CG	2:B:1159:ARG:N	2.79	0.50
2:B:229:ALA:CB	2:B:231:PRO:HD2	2.39	0.50
7:G:142:ARG:CB	7:G:171:ILE:HD11	2.41	0.50
12:L:68:GLU:CD	12:L:68:GLU:H	2.15	0.50
1:A:787:PHE:CE1	1:A:796:SER:HA	2.46	0.50
7:G:39:THR:O	7:G:43:GLY:HA2	2.11	0.50
1:A:37:PHE:CD2	1:A:50:ILE:HG21	2.46	0.50
2:B:189:LEU:O	2:B:192:LEU:N	2.45	0.50
8:H:84:ALA:HA	8:H:87:ARG:HG3	1.92	0.50
2:B:619:ILE:O	2:B:622:LYS:N	2.44	0.50
2:B:785:TYR:HD2	2:B:785:TYR:N	2.09	0.50
3:C:248:ILE:HD13	11:K:102:LYS:HA	1.94	0.50
1:A:1187:GLN:CD	1:A:1188:GLN:HE21	2.15	0.50
2:B:258:LEU:O	2:B:258:LEU:CG	2.59	0.50
2:B:307:ASP:O	2:B:309:GLN:N	2.44	0.50
2:B:644:GLU:OE2	2:B:646:LEU:HB2	2.11	0.50
2:B:778:MET:HE2	2:B:1094:ARG:HG2	1.93	0.50
2:B:464:GLY:C	2:B:465:ASN:ND2	2.63	0.50
2:B:469:GLN:HG3	2:B:470:LYS:H	1.74	0.50
2:B:1115:THR:HG22	2:B:1117:GLN:CG	2.41	0.50
2:B:542:MET:SD	2:B:747:MET:HE2	2.52	0.50
2:B:811:TYR:H	2:B:811:TYR:HD1	1.58	0.50
2:B:877:PRO:C	2:B:878:GLN:HG3	2.31	0.50
7:G:88:ASP:HB3	7:G:144:ARG:CA	2.40	0.50
2:B:864:LYS:O	2:B:871:THR:HG23	2.11	0.50
1:A:1191:TRP:CB	1:A:1260:LEU:HD23	2.40	0.50
3:C:8:VAL:HG12	3:C:9:LYS:N	2.22	0.50
1:A:699:ALA:HB3	1:A:701:LEU:HG	1.92	0.50
1:A:286:HIS:C	1:A:288:ALA:H	2.15	0.50
1:A:125:ALA:O	1:A:127:ALA:N	2.45	0.50
2:B:654:ARG:O	2:B:656:GLY:N	2.45	0.50
1:A:58:LEU:HA	1:A:80:HIS:HB2	1.93	0.50
8:H:44:VAL:CG1	8:H:48:PRO:HA	2.38	0.50
2:B:969:ARG:HD3	3:C:61:GLU:OE2	2.11	0.50
10:J:16:ASP:O	10:J:18:TRP:N	2.45	0.50
9:I:111:THR:HG22	9:I:113:ASP:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:ARG:CG	1:A:590:ARG:NH1	2.74	0.50
7:G:45:ILE:HD13	7:G:78:VAL:CG1	2.41	0.50
2:B:847:ASP:O	2:B:849:GLY:N	2.44	0.50
3:C:169:LYS:HE3	3:C:170:TRP:CZ2	2.47	0.50
1:A:506:ALA:CB	1:A:508:PRO:HD2	2.39	0.50
2:B:593:PRO:O	2:B:596:LEU:N	2.44	0.50
2:B:983:ARG:HD2	2:B:1091:TYR:HB3	1.92	0.50
4:D:54:GLU:O	4:D:58:VAL:HG23	2.11	0.50
1:A:282:ASN:O	1:A:284:ALA:N	2.44	0.50
2:B:706:GLN:NE2	2:B:730:ARG:HH11	2.09	0.50
4:D:14:ARG:O	4:D:16:LYS:N	2.42	0.50
1:A:25:GLU:OE1	1:A:25:GLU:N	2.20	0.50
1:A:40:THR:HB	1:A:41:MET:HE2	1.93	0.50
2:B:785:TYR:CD2	2:B:785:TYR:N	2.80	0.50
3:C:88:CYS:SG	3:C:91:HIS:C	2.90	0.50
5:E:186:LEU:O	5:E:189:GLY:N	2.41	0.50
2:B:278:GLN:HG2	2:B:279:ASP:N	2.18	0.50
2:B:331:LEU:HD12	2:B:331:LEU:N	2.26	0.50
2:B:860:MET:CG	2:B:965:LYS:HG2	2.41	0.50
3:C:174:ALA:O	10:J:10:CYS:O	2.29	0.50
11:K:7:PHE:O	11:K:11:LEU:HD23	2.11	0.50
1:A:345:VAL:HG21	2:B:1150:ARG:NH2	2.24	0.50
1:A:461:LYS:O	1:A:463:ILE:HG23	2.12	0.50
1:A:1396:ALA:HA	1:A:1399:ARG:NH2	2.27	0.50
1:A:767:GLN:OE1	1:A:799:PHE:HB2	2.12	0.50
9:I:33:SER:O	9:I:35:VAL:HG23	2.11	0.50
1:A:402:ALA:HB2	1:A:434:ARG:HA	1.94	0.50
2:B:54:PHE:O	2:B:58:THR:HB	2.11	0.50
2:B:57:TYR:N	2:B:57:TYR:HD1	2.10	0.50
2:B:660:LYS:HB3	2:B:679:TYR:CE2	2.46	0.50
2:B:1050:ILE:N	2:B:1050:ILE:HD12	2.26	0.50
1:A:909:ASP:O	1:A:911:SER:N	2.42	0.50
2:B:68:THR:CG2	2:B:91:SER:HB3	2.41	0.50
2:B:914:LYS:HD3	2:B:937:ALA:O	2.11	0.50
3:C:146:LYS:C	3:C:147:LEU:HD23	2.32	0.50
10:J:5:VAL:HG12	10:J:6:ARG:CG	2.29	0.50
1:A:1453:TYR:O	1:A:1454:MET:CB	2.59	0.50
5:E:42:PHE:HZ	5:E:58:MET:HE1	1.77	0.50
1:A:1138:ILE:C	1:A:1275:GLY:HA2	2.32	0.50
4:D:59:ILE:HG21	4:D:145:MET:SD	2.52	0.50
1:A:699:ALA:O	1:A:700:ASN:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ALA:CB	1:A:276:LEU:HD23	2.42	0.50
1:A:418:SER:C	1:A:420:ARG:H	2.14	0.50
1:A:125:ALA:HA	1:A:128:ILE:HG13	1.93	0.50
2:B:34:ILE:HG12	2:B:542:MET:HE1	1.94	0.50
2:B:637:LEU:HD22	2:B:741:CYS:O	2.12	0.50
2:B:800:GLN:CB	10:J:52:THR:HG22	2.39	0.50
2:B:193:LYS:HD3	2:B:787:VAL:HG11	1.93	0.50
1:A:575:LYS:HB3	1:A:612:ILE:CG2	2.42	0.50
3:C:101:LEU:O	3:C:102:GLN:HG3	2.11	0.50
3:C:82:TYR:O	3:C:83:SER:C	2.49	0.50
1:A:929:LEU:HD23	1:A:983:ILE:HG21	1.94	0.50
2:B:1069:PHE:HA	2:B:1085:ILE:O	2.11	0.50
2:B:313:MET:O	2:B:316:PRO:HD2	2.11	0.50
1:A:1218:GLN:O	1:A:1221:LYS:HE3	2.12	0.50
1:A:1259:MET:C	1:A:1261:LYS:H	2.15	0.50
1:A:441:PRO:HD2	1:A:498:ARG:CZ	2.41	0.50
3:C:166:GLU:O	3:C:167:HIS:HB2	2.12	0.50
2:B:170:LEU:O	2:B:172:ILE:HG13	2.11	0.50
8:H:26:ILE:O	8:H:27:GLU:HG3	2.12	0.50
14:N:4:DA:H2"	14:N:5:DC:C5	2.46	0.50
1:A:728:LYS:HB3	1:A:731:ARG:HH21	1.77	0.50
1:A:1443:VAL:CG1	6:F:132:LEU:HD13	2.42	0.50
1:A:523:ILE:CD1	1:A:649:ILE:HG21	2.41	0.50
2:B:839:MET:HG3	2:B:1010:LEU:CD1	2.41	0.50
1:A:244:PRO:HG2	1:A:245:PRO:HD3	1.94	0.50
7:G:153:GLN:O	7:G:154:VAL:C	2.50	0.50
3:C:268:ASP:O	3:C:269:LYS:HB2	2.11	0.50
4:D:153:ARG:NH2	4:D:184:ALA:HA	2.27	0.50
2:B:547:VAL:N	2:B:612:GLU:OE2	2.38	0.50
2:B:744:HIS:CG	2:B:745:PRO:HD2	2.47	0.50
2:B:810:GLU:CA	2:B:815:ARG:NH2	2.66	0.50
1:A:65:LEU:O	1:A:66:LYS:C	2.49	0.50
8:H:101:ALA:HA	8:H:116:TYR:HA	1.94	0.50
8:H:89:LEU:O	8:H:91:ASP:N	2.45	0.50
3:C:249:ASP:O	3:C:250:THR:C	2.48	0.50
2:B:390:LEU:O	2:B:392:ARG:HG3	2.12	0.50
5:E:121:MET:C	5:E:123:LEU:H	2.15	0.50
1:A:265:LYS:HG2	1:A:303:TYR:HA	1.94	0.50
1:A:262:LEU:HD22	1:A:303:TYR:HE1	1.77	0.50
6:F:70:LYS:O	6:F:72:LYS:NZ	2.42	0.50
3:C:112:ASN:HB2	3:C:114:TYR:HE1	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:826:ALA:HB2	2:B:1008:PRO:HB3	1.92	0.50
4:D:3:VAL:HG12	4:D:4:SER:H	1.77	0.50
1:A:741:ASN:HD22	1:A:744:LYS:HB2	1.75	0.50
1:A:960:ILE:HA	1:A:963:ILE:HG22	1.91	0.50
1:A:219:PHE:CD2	1:A:231:PRO:HD2	2.47	0.50
1:A:1141:THR:CG2	1:A:1205:LYS:HD3	2.42	0.50
2:B:785:TYR:CD1	2:B:795:ILE:HG12	2.47	0.50
2:B:244:LEU:HB2	2:B:249:ARG:HA	1.93	0.50
12:L:61:THR:HG22	12:L:63:ARG:N	2.24	0.50
1:A:870:GLU:HB2	5:E:204:THR:HG21	1.94	0.50
2:B:1178:ASN:N	2:B:1178:ASN:ND2	2.59	0.50
2:B:558:LEU:O	2:B:560:GLU:N	2.30	0.50
4:D:155:ARG:HG3	4:D:155:ARG:HH11	1.77	0.50
9:I:5:ARG:HG3	9:I:14:LEU:HD12	1.92	0.50
5:E:197:LYS:HE2	5:E:199:ILE:HD11	1.94	0.50
1:A:548:ASN:HA	11:K:60:ALA:HB1	1.92	0.50
2:B:731:VAL:HG12	2:B:732:SER:N	2.27	0.50
4:D:153:ARG:HB3	4:D:154:PHE:CD1	2.46	0.50
4:D:153:ARG:HB3	4:D:154:PHE:CE1	2.47	0.50
1:A:491:VAL:HG12	1:A:492:PRO:O	2.12	0.50
4:D:57:LEU:O	4:D:61:GLU:HB2	2.11	0.50
1:A:347:PHE:CE2	1:A:493:GLN:OE1	2.65	0.50
1:A:220:THR:O	1:A:221:SER:C	2.50	0.50
1:A:786:HIS:NE2	2:B:742:GLU:OE1	2.45	0.49
2:B:863:GLU:OE1	2:B:962:LYS:HB2	2.11	0.49
3:C:105:GLY:HA3	3:C:149:LYS:O	2.12	0.49
3:C:76:ASP:OD2	3:C:127:ARG:HB2	2.11	0.49
2:B:243:ALA:HB1	2:B:251:ILE:HG12	1.92	0.49
1:A:1111:MET:HB2	1:A:1113:THR:O	2.12	0.49
3:C:114:TYR:HB2	3:C:116:LYS:HG2	1.94	0.49
4:D:40:HIS:HB2	7:G:73:LYS:NZ	2.27	0.49
1:A:1114:PRO:HB2	1:A:1311:VAL:HG23	1.93	0.49
4:D:47:LEU:CD1	4:D:48:ILE:H	2.20	0.49
4:D:138:ASN:HD21	7:G:35:GLU:HB3	1.76	0.49
1:A:1341:ILE:O	1:A:1344:GLY:N	2.45	0.49
10:J:27:GLU:C	10:J:29:GLU:H	2.15	0.49
1:A:95:PHE:O	1:A:96:ILE:C	2.51	0.49
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.93	0.49
1:A:1402:PHE:CD1	1:A:1403:GLU:HG3	2.47	0.49
2:B:298:LEU:N	2:B:298:LEU:CD2	2.75	0.49
2:B:49:ASP:HA	2:B:52:ASN:HD22	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:821:GLN:HE22	2:B:851:PHE:N	2.06	0.49
2:B:118:ARG:HH22	2:B:194:GLU:CD	2.16	0.49
3:C:236:GLY:O	3:C:237:SER:C	2.51	0.49
2:B:405:ARG:CZ	2:B:632:ARG:HG2	2.41	0.49
5:E:26:ARG:HA	5:E:188:LEU:HD23	1.93	0.49
9:I:73:ARG:NH1	9:I:112:SER:HB3	2.27	0.49
2:B:455:SER:O	2:B:458:LYS:N	2.44	0.49
9:I:28:GLU:HG3	9:I:29:CYS:N	2.27	0.49
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.94	0.49
1:A:452:LYS:HG3	2:B:1140:ALA:CB	2.42	0.49
2:B:49:ASP:HA	2:B:52:ASN:ND2	2.27	0.49
2:B:609:ILE:O	2:B:609:ILE:HG13	2.12	0.49
2:B:654:ARG:O	2:B:657:HIS:N	2.45	0.49
2:B:958:GLN:C	2:B:960:GLY:H	2.15	0.49
8:H:84:ALA:CB	8:H:87:ARG:HD2	2.42	0.49
8:H:82:PRO:HG3	11:K:54:ARG:NH1	2.26	0.49
3:C:124:LEU:C	3:C:126:GLY:H	2.14	0.49
7:G:138:THR:HG22	7:G:139:ILE:HG13	1.95	0.49
2:B:235:SER:C	2:B:236:HIS:CD2	2.86	0.49
1:A:866:PHE:O	1:A:867:ILE:HD12	2.10	0.49
5:E:161:LYS:HG3	5:E:195:VAL:HG21	1.94	0.49
1:A:543:LEU:O	1:A:544:ASP:C	2.50	0.49
1:A:741:ASN:ND2	1:A:744:LYS:N	2.60	0.49
1:A:345:VAL:HG23	1:A:346:ASP:O	2.13	0.49
1:A:889:SER:HA	1:A:1297:GLU:N	2.27	0.49
1:A:1273:LEU:N	1:A:1273:LEU:HD12	2.27	0.49
2:B:291:ILE:HG22	2:B:291:ILE:O	2.11	0.49
2:B:1215:ARG:C	2:B:1216:LEU:HD23	2.31	0.49
1:A:402:ALA:HB1	1:A:433:GLU:O	2.12	0.49
1:A:1291:VAL:HG13	1:A:1292:PRO:CD	2.40	0.49
2:B:661:LEU:C	2:B:663:ALA:N	2.66	0.49
2:B:579:ARG:N	2:B:589:VAL:HG13	2.27	0.49
2:B:542:MET:HB3	2:B:636:PRO:CD	2.42	0.49
3:C:124:LEU:O	3:C:127:ARG:HG2	2.12	0.49
8:H:62:SER:OG	8:H:63:LEU:HD12	2.13	0.49
1:A:884:ASP:C	1:A:886:ILE:H	2.16	0.49
1:A:334:GLY:O	1:A:336:ILE:N	2.46	0.49
1:A:836:TYR:HB2	13:T:18:DA:H5'	1.93	0.49
2:B:1156:ASP:OD2	2:B:1199:ALA:HB2	2.12	0.49
1:A:655:PHE:O	1:A:658:LEU:HB3	2.12	0.49
1:A:1120:LEU:O	1:A:1323:ASP:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:ILE:HD11	1:A:646:PHE:HE1	1.76	0.49
1:A:741:ASN:HD22	1:A:744:LYS:CB	2.26	0.49
2:B:205:ILE:O	2:B:207:GLY:N	2.44	0.49
2:B:65:GLU:HG3	2:B:66:ASP:N	2.19	0.49
1:A:1313:LEU:HD11	1:A:1317:MET:CE	2.43	0.49
5:E:190:LEU:CD1	5:E:214:CYS:HB2	2.42	0.49
2:B:102:VAL:N	2:B:110:HIS:O	2.45	0.49
1:A:761:MET:HA	1:A:804:TYR:HB2	1.94	0.49
9:I:10:CYS:SG	9:I:10:CYS:O	2.70	0.49
8:H:144:ILE:HG22	8:H:145:ARG:H	1.77	0.49
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.52	0.49
2:B:1084:GLN:NE2	2:B:1084:GLN:H	1.91	0.49
5:E:61:GLN:NE2	5:E:105:PHE:CZ	2.79	0.49
1:A:416:ARG:NH1	1:A:417:TYR:CE2	2.76	0.49
1:A:11:LEU:CD1	1:A:11:LEU:C	2.75	0.49
1:A:608:ILE:C	1:A:610:GLY:N	2.66	0.49
1:A:731:ARG:HA	1:A:734:GLU:HB3	1.95	0.49
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.95	0.49
2:B:102:VAL:CG2	2:B:112:LEU:HB2	2.43	0.49
2:B:240:ILE:CG2	2:B:254:LEU:HB3	2.42	0.49
9:I:61:ASP:O	9:I:63:GLY:N	2.45	0.49
1:A:795:GLU:CD	1:A:795:GLU:H	2.15	0.49
2:B:485:ARG:NH1	2:B:782:LEU:HD11	2.28	0.49
1:A:492:PRO:HB3	1:A:501:LEU:CD1	2.42	0.49
5:E:31:THR:HG23	5:E:34:GLU:HB2	1.94	0.49
1:A:344:ARG:HA	2:B:1129:ARG:HA	1.94	0.49
2:B:281:PRO:O	2:B:283:VAL:N	2.46	0.49
2:B:372:SER:O	2:B:376:PHE:HB2	2.13	0.49
2:B:37:PHE:CE1	2:B:41:LYS:HG3	2.47	0.49
2:B:343:ILE:HG23	2:B:347:LYS:CD	2.42	0.49
2:B:348:ARG:HG3	2:B:349:ILE:N	2.28	0.49
2:B:244:LEU:HD13	2:B:247:GLY:O	2.13	0.49
5:E:109:ILE:CG2	5:E:110:PHE:N	2.69	0.49
2:B:1096:ARG:O	2:B:1097:HIS:CG	2.66	0.49
1:A:681:GLU:C	1:A:683:ILE:N	2.65	0.49
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.92	0.49
1:A:1054:LEU:O	1:A:1057:VAL:HG23	2.12	0.49
1:A:412:ARG:HH22	2:B:1108:ARG:NH2	2.10	0.49
1:A:189:ARG:O	1:A:190:ALA:CB	2.61	0.49
2:B:614:SER:HB3	2:B:694:ASP:CB	2.42	0.49
9:I:61:ASP:O	9:I:64:SER:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:5:C:O2'	15:P:6:A:H5'	2.12	0.49
1:A:780:VAL:O	1:A:780:VAL:HG12	2.12	0.49
1:A:270:LEU:O	1:A:273:ASN:HB3	2.13	0.49
2:B:531:GLN:HG3	2:B:532:ALA:H	1.77	0.49
5:E:89:GLY:CA	5:E:117:THR:OG1	2.60	0.49
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.94	0.49
11:K:45:LEU:HG	11:K:94:ILE:CD1	2.41	0.49
1:A:412:ARG:NH2	2:B:1108:ARG:NH2	2.60	0.49
2:B:558:LEU:C	2:B:560:GLU:H	2.12	0.49
2:B:203:PHE:HB3	2:B:205:ILE:HD11	1.94	0.49
2:B:210:LYS:HG3	2:B:461:LEU:O	2.12	0.49
7:G:1:MET:HE1	7:G:3:PHE:HE1	1.77	0.49
1:A:23:SER:O	1:A:24:PRO:C	2.49	0.49
13:T:7:DC:H2"	13:T:8:DT:H71	1.94	0.49
1:A:1148:ILE:HG12	1:A:1198:ASP:HB2	1.95	0.49
4:D:204:ASP:O	4:D:208:GLU:HB2	2.12	0.49
1:A:208:LEU:HD23	1:A:209:ASN:N	2.28	0.49
1:A:639:PRO:CG	1:A:640:GLN:N	2.76	0.49
2:B:1221:SER:HB3	4:D:12:ARG:HE	1.77	0.49
2:B:579:ARG:HH11	2:B:579:ARG:HG2	1.77	0.49
2:B:22:SER:HA	2:B:654:ARG:CB	2.43	0.49
1:A:49:LYS:HD2	1:A:55:ASP:HB3	1.94	0.49
2:B:882:THR:HG22	2:B:884:ARG:N	2.23	0.49
12:L:53:HIS:HB3	12:L:55:ILE:HD12	1.92	0.49
8:H:143:LEU:N	8:H:143:LEU:HD12	2.27	0.49
2:B:1072:MET:HE3	2:B:1085:ILE:CB	2.42	0.49
5:E:100:ILE:O	5:E:100:ILE:HG22	2.13	0.49
1:A:381:THR:CG2	1:A:382:PRO:HD2	2.42	0.49
5:E:156:LEU:HA	5:E:160:GLU:OE1	2.13	0.49
1:A:1125:ALA:C	1:A:1127:ASP:H	2.14	0.49
2:B:95:ILE:HG13	2:B:130:VAL:HG22	1.95	0.49
4:D:52:LEU:O	4:D:53:SER:OG	2.28	0.49
7:G:50:ASP:OD1	7:G:50:ASP:O	2.30	0.49
1:A:6:TYR:CD1	1:A:7:SER:N	2.81	0.49
1:A:730:GLY:O	1:A:731:ARG:C	2.50	0.49
2:B:529:GLU:OE1	2:B:769:TYR:HE1	1.96	0.49
10:J:14:VAL:CG1	10:J:50:ILE:HD11	2.42	0.49
1:A:374:LEU:O	1:A:436:ILE:HG12	2.13	0.49
7:G:117:GLN:OE1	7:G:117:GLN:N	2.46	0.49
2:B:601:ARG:NH1	2:B:605:ARG:NH2	2.61	0.49
2:B:115:GLN:HG2	2:B:193:LYS:CB	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:190:TYR:CD2	10:J:62:ARG:HB3	2.48	0.49
2:B:880:THR:O	2:B:880:THR:HG22	2.13	0.49
3:C:101:LEU:C	3:C:102:GLN:HG3	2.33	0.49
3:C:124:LEU:C	3:C:126:GLY:N	2.66	0.49
6:F:120:ILE:O	6:F:124:GLU:HG3	2.13	0.49
2:B:259:TYR:HD1	2:B:259:TYR:H	1.61	0.49
8:H:102:TYR:N	8:H:102:TYR:CD2	2.63	0.49
1:A:1053:PHE:O	1:A:1055:ARG:N	2.46	0.49
2:B:592:ASN:HD21	2:B:595:ARG:NH1	2.11	0.49
1:A:774:ARG:CZ	1:A:797:LYS:HG3	2.42	0.49
6:F:138:LEU:CB	6:F:139:PRO:HD2	2.43	0.49
1:A:670:ILE:HA	1:A:805:LEU:HD22	1.94	0.49
9:I:25:LEU:HB3	9:I:38:ALA:HB2	1.93	0.49
1:A:528:LEU:HA	1:A:531:ILE:HG22	1.94	0.49
1:A:535:THR:HG22	1:A:536:LEU:N	2.28	0.49
3:C:83:SER:HA	3:C:95:CYS:CB	2.43	0.49
7:G:138:THR:CG2	7:G:139:ILE:N	2.53	0.49
2:B:276:ILE:HG22	2:B:278:GLN:O	2.13	0.49
2:B:361:LEU:N	2:B:362:PRO:CD	2.75	0.49
9:I:111:THR:CG2	9:I:112:SER:H	2.25	0.49
5:E:161:LYS:HD2	5:E:195:VAL:HG23	1.95	0.49
5:E:11:ARG:C	5:E:13:TRP:N	2.66	0.49
7:G:37:SER:OG	7:G:45:ILE:HG13	2.12	0.49
3:C:38:ILE:HA	3:C:173:ALA:CB	2.40	0.49
13:T:18:DA:H8	13:T:18:DA:O5'	1.95	0.49
1:A:1348:LEU:HG	1:A:1372:VAL:HG23	1.95	0.49
1:A:391:LEU:O	1:A:394:ASN:HB3	2.13	0.49
2:B:792:MET:O	2:B:793:ALA:HB2	2.13	0.49
6:F:85:MET:C	6:F:155:LEU:HD11	2.32	0.49
1:A:55:ASP:N	1:A:56:PRO:HD3	2.28	0.48
2:B:956:THR:CG2	2:B:960:GLY:HA2	2.43	0.48
2:B:865:LYS:HE3	2:B:961:LEU:HD21	1.94	0.48
3:C:76:ASP:OD2	3:C:128:ASN:N	2.46	0.48
2:B:1097:HIS:H	2:B:1098:MET:CE	2.09	0.48
1:A:605:MET:HG2	1:A:621:THR:CG2	2.43	0.48
10:J:9:SER:OG	10:J:48:ARG:NH2	2.46	0.48
1:A:1197:LEU:O	1:A:1236:LEU:HD12	2.12	0.48
1:A:1237:ILE:CG2	1:A:1238:ILE:N	2.75	0.48
1:A:1211:GLN:O	1:A:1212:VAL:C	2.52	0.48
1:A:1120:LEU:N	1:A:1120:LEU:HD12	2.27	0.48
1:A:1134:ILE:O	1:A:1138:ILE:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:TYR:CZ	1:A:1064:VAL:HG11	2.48	0.48
1:A:1389:PHE:CG	1:A:1390:ASN:N	2.80	0.48
7:G:1:MET:HA	7:G:1:MET:HE2	1.94	0.48
2:B:46:GLN:HG3	2:B:47:GLN:H	1.78	0.48
1:A:728:LYS:HG3	1:A:729:ALA:N	2.28	0.48
1:A:1074:GLU:C	1:A:1076:ALA:H	2.16	0.48
1:A:1450:LEU:HD11	6:F:108:PHE:CZ	2.48	0.48
6:F:130:ILE:O	6:F:148:VAL:CG2	2.61	0.48
7:G:44:TYR:OH	7:G:156:SER:HA	2.12	0.48
4:D:7:THR:HB	7:G:42:PHE:CE2	2.48	0.48
2:B:295:GLY:N	2:B:298:LEU:HD23	2.28	0.48
2:B:225:VAL:HA	2:B:237:VAL:O	2.13	0.48
11:K:48:ALA:O	11:K:51:LEU:N	2.45	0.48
2:B:44:VAL:O	2:B:45:SER:C	2.51	0.48
2:B:802:PRO:HA	2:B:822:ASN:OD1	2.13	0.48
2:B:343:ILE:CG2	2:B:347:LYS:HG3	2.43	0.48
2:B:873:THR:CG2	2:B:874:PHE:N	2.76	0.48
2:B:120:ARG:NE	2:B:955:THR:HG21	2.28	0.48
1:A:560:ILE:HG13	8:H:79:TRP:H	1.78	0.48
8:H:91:ASP:C	8:H:93:TYR:N	2.66	0.48
3:C:238:ILE:HG22	3:C:243:VAL:CG2	2.40	0.48
2:B:1082:MET:HA	3:C:189:THR:HA	1.95	0.48
2:B:326:ASP:C	2:B:328:GLU:N	2.66	0.48
6:F:71:GLU:N	6:F:71:GLU:OE1	2.46	0.48
1:A:543:LEU:O	1:A:545:GLN:N	2.46	0.48
2:B:1007:VAL:HG22	2:B:1008:PRO:CD	2.43	0.48
2:B:751:VAL:O	2:B:752:ALA:C	2.52	0.48
2:B:451:LYS:O	2:B:455:SER:OG	2.30	0.48
4:D:53:SER:H	4:D:148:LEU:HD22	1.78	0.48
1:A:114:LEU:N	1:A:114:LEU:HD23	2.28	0.48
2:B:1077:THR:HG22	11:K:44:ASN:ND2	2.28	0.48
2:B:1215:ARG:NH1	4:D:15:LEU:HD21	2.28	0.48
1:A:187:LYS:O	1:A:194:ALA:HB3	2.13	0.48
4:D:214:LEU:C	4:D:216:ASN:N	2.64	0.48
5:E:33:GLU:OE1	5:E:33:GLU:N	2.41	0.48
8:H:58:THR:C	8:H:59:ILE:HG13	2.34	0.48
2:B:34:ILE:O	2:B:37:PHE:HB3	2.14	0.48
1:A:55:ASP:OD2	1:A:55:ASP:O	2.31	0.48
1:A:57:ARG:O	1:A:68:GLN:HG2	2.13	0.48
2:B:798:TYR:HD1	10:J:4:PRO:HB3	1.78	0.48
9:I:90:GLN:HE21	9:I:92:ARG:HB2	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:VAL:HG21	1:A:430:TRP:HB2	1.94	0.48
5:E:173:SER:OG	5:E:174:GLN:N	2.46	0.48
1:A:1191:TRP:HA	1:A:1191:TRP:HE3	1.76	0.48
2:B:890:TYR:CE2	2:B:910:VAL:HG21	2.49	0.48
5:E:168:TYR:CB	5:E:170:LEU:HG	2.42	0.48
1:A:384:ASN:O	1:A:385:ILE:C	2.52	0.48
1:A:1271:ILE:HG22	1:A:1271:ILE:O	2.13	0.48
4:D:22:GLU:N	4:D:22:GLU:CD	2.65	0.48
1:A:556:TRP:C	1:A:558:GLY:H	2.15	0.48
2:B:1055:ILE:O	2:B:1058:LEU:N	2.46	0.48
1:A:247:ARG:HH11	1:A:263:THR:HG23	1.77	0.48
8:H:84:ALA:HA	8:H:87:ARG:CG	2.43	0.48
1:A:1187:GLN:HA	1:A:1244:ARG:CD	2.44	0.48
1:A:1105:LEU:HD22	1:A:1384:VAL:HG21	1.96	0.48
1:A:310:GLY:C	1:A:312:PRO:HD2	2.34	0.48
10:J:7:CYS:CA	10:J:49:MET:HE3	2.42	0.48
3:C:168:ALA:O	3:C:169:LYS:C	2.50	0.48
1:A:1115:SER:O	1:A:1311:VAL:HG22	2.13	0.48
13:T:10:DA:H2"	13:T:11:DA:C8	2.47	0.48
1:A:679:ILE:HG12	1:A:732:LEU:CD1	2.43	0.48
1:A:730:GLY:O	1:A:732:LEU:N	2.46	0.48
11:K:63:VAL:O	11:K:63:VAL:CG2	2.61	0.48
3:C:260:LEU:O	3:C:264:GLN:HG3	2.13	0.48
1:A:639:PRO:CG	1:A:640:GLN:H	2.26	0.48
1:A:121:LEU:O	1:A:124:GLN:HB2	2.14	0.48
2:B:909:ASP:N	2:B:909:ASP:OD1	2.47	0.48
1:A:41:MET:N	1:A:41:MET:HE3	2.28	0.48
8:H:43:ASN:OD1	8:H:46:LEU:N	2.45	0.48
2:B:797:TYR:O	10:J:1:MET:HG2	2.12	0.48
3:C:79:GLN:HG3	3:C:127:ARG:HD2	1.94	0.48
10:J:1:MET:H1	10:J:56:LEU:CA	2.27	0.48
10:J:2:ILE:HG12	10:J:57:ILE:HD12	1.95	0.48
1:A:666:ILE:CD1	1:A:667:GLY:N	2.75	0.48
1:A:266:LEU:HD21	1:A:303:TYR:CZ	2.48	0.48
1:A:843:LYS:HZ3	2:B:1135:ARG:HH12	1.61	0.48
2:B:50:SER:OG	2:B:411:PRO:HD3	2.13	0.48
1:A:358:ASN:ND2	2:B:833:TYR:OH	2.46	0.48
2:B:1177:HIS:HB2	2:B:1179:GLN:HE21	1.77	0.48
1:A:710:LEU:HD12	1:A:710:LEU:N	2.28	0.48
10:J:24:LEU:CD1	10:J:38:ARG:HG2	2.44	0.48
1:A:88:LYS:HD2	1:A:293:GLU:OE2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1030:LEU:CD1	2:B:1059:LEU:HD22	2.44	0.48
1:A:244:PRO:CB	1:A:245:PRO:HD3	2.43	0.48
1:A:481:ASP:N	1:A:481:ASP:OD2	2.45	0.48
2:B:319:GLU:HA	2:B:322:PHE:HB2	1.96	0.48
2:B:653:VAL:O	2:B:654:ARG:HD3	2.14	0.48
2:B:39:ARG:NH2	2:B:665:GLU:HG2	2.27	0.48
1:A:785:PRO:O	2:B:702:LEU:HD12	2.14	0.48
7:G:144:ARG:HG2	7:G:168:LEU:HD23	1.96	0.48
2:B:1072:MET:CG	2:B:1085:ILE:HD13	2.43	0.48
1:A:427:GLN:O	1:A:428:TYR:C	2.51	0.48
2:B:864:LYS:HD2	2:B:872:GLU:OE2	2.14	0.48
10:J:36:LEU:HD11	10:J:51:LEU:HB2	1.95	0.48
1:A:1329:THR:HG23	1:A:1335:ILE:HG13	1.95	0.48
1:A:444:PHE:HB3	1:A:458:HIS:CD2	2.48	0.48
1:A:1057:VAL:CG1	1:A:1058:VAL:N	2.76	0.48
2:B:450:ALA:O	2:B:451:LYS:C	2.51	0.48
4:D:134:THR:CG2	4:D:135:GLY:N	2.75	0.48
14:N:4:DA:H2"	14:N:5:DC:C6	2.48	0.48
1:A:79:GLY:CA	1:A:243:PRO:HG3	2.44	0.48
2:B:731:VAL:HG12	2:B:732:SER:H	1.79	0.48
2:B:1166:CYS:O	2:B:1166:CYS:SG	2.71	0.48
1:A:587:HIS:CE1	1:A:609:ASP:H	2.31	0.48
2:B:35:SER:HA	2:B:811:TYR:CE2	2.38	0.48
2:B:687:GLU:CB	2:B:689:LEU:HG	2.43	0.48
2:B:707:PRO:O	2:B:708:GLU:O	2.32	0.48
8:H:139:ASN:O	8:H:140:ALA:CB	2.61	0.48
1:A:567:LYS:HZ1	8:H:47:PHE:HB2	1.78	0.48
3:C:62:PHE:HD2	3:C:62:PHE:C	2.17	0.48
12:L:43:THR:C	12:L:45:ALA:H	2.16	0.48
11:K:42:LEU:HD21	11:K:46:ILE:HD12	1.94	0.48
12:L:61:THR:CG2	12:L:63:ARG:HB2	2.44	0.48
1:A:993:LEU:HD23	1:A:1022:LEU:HD11	1.94	0.48
1:A:356:ASP:OD1	1:A:358:ASN:N	2.35	0.48
2:B:595:ARG:HH11	2:B:595:ARG:HG3	1.78	0.48
1:A:586:ILE:HD11	1:A:633:VAL:HA	1.95	0.48
5:E:198:ILE:H	5:E:198:ILE:CD1	2.27	0.48
1:A:29:ALA:HB1	2:B:1184:GLY:CA	2.43	0.48
2:B:705:MET:N	2:B:710:LEU:HD12	2.28	0.48
1:A:40:THR:CG2	1:A:41:MET:HE2	2.44	0.48
3:C:88:CYS:O	3:C:90:ASP:N	2.47	0.48
2:B:373:ARG:HG2	2:B:566:LEU:HD23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:SER:CB	2:B:1103:ILE:HG12	2.35	0.48
9:I:102:VAL:HA	9:I:108:HIS:O	2.14	0.48
2:B:502:ILE:HD12	2:B:502:ILE:N	2.26	0.48
1:A:866:PHE:N	5:E:208:TYR:OH	2.43	0.48
1:A:334:GLY:C	1:A:336:ILE:N	2.64	0.48
5:E:4:GLU:OE1	5:E:4:GLU:HA	2.14	0.48
2:B:597:MET:O	2:B:599:THR:N	2.46	0.48
1:A:1067:LEU:O	1:A:1068:ALA:C	2.51	0.48
2:B:345:LYS:O	2:B:346:GLU:C	2.51	0.48
3:C:66:ARG:HH21	10:J:5:VAL:HG23	1.77	0.48
2:B:262:GLU:HA	2:B:267:ARG:NH2	2.29	0.48
5:E:90:VAL:O	5:E:90:VAL:HG22	2.14	0.48
1:A:859:SER:HB2	1:A:1422:ARG:HB2	1.96	0.48
1:A:1224:LEU:HD12	1:A:1241:ARG:O	2.13	0.48
2:B:895:ASP:C	2:B:897:GLY:H	2.16	0.48
1:A:1123:GLY:O	1:A:1125:ALA:N	2.47	0.48
1:A:1130:GLN:HE21	1:A:1134:ILE:CD1	2.21	0.48
2:B:123:THR:CB	2:B:458:LYS:HE2	2.44	0.48
4:D:47:LEU:HD13	4:D:48:ILE:N	2.22	0.48
2:B:1016:ALA:HA	2:B:1020:ARG:NH1	2.29	0.48
3:C:6:PRO:CB	11:K:101:LEU:HD12	2.44	0.48
1:A:787:PHE:CZ	1:A:796:SER:HA	2.49	0.48
1:A:865:GLN:NE2	1:A:1370:LEU:HD13	2.29	0.48
1:A:514:PRO:C	1:A:516:SER:H	2.16	0.48
3:C:15:LYS:HG2	3:C:15:LYS:O	2.14	0.48
4:D:151:PHE:HZ	7:G:90:THR:HG1	1.60	0.48
2:B:745:PRO:C	2:B:747:MET:N	2.67	0.48
2:B:542:MET:HG2	2:B:747:MET:HE3	1.95	0.48
2:B:358:LYS:HA	2:B:366:GLN:HB3	1.96	0.48
2:B:1084:GLN:OE1	3:C:189:THR:CG2	2.61	0.48
1:A:341:MET:CE	2:B:1135:ARG:NH1	2.77	0.48
1:A:1161:THR:HG22	1:A:1163:ILE:HG13	1.95	0.48
1:A:1193:LEU:HD12	1:A:1193:LEU:C	2.34	0.48
2:B:899:ILE:HD11	2:B:910:VAL:O	2.14	0.48
1:A:441:PRO:HD2	1:A:498:ARG:NH2	2.29	0.48
2:B:1156:ASP:O	2:B:1157:ALA:O	2.32	0.48
1:A:1376:THR:O	1:A:1377:THR:C	2.52	0.48
4:D:164:ILE:CG2	4:D:168:LYS:HD2	2.38	0.48
2:B:539:LEU:H	2:B:539:LEU:CD1	2.17	0.48
1:A:509:LEU:C	1:A:511:ILE:H	2.17	0.48
1:A:509:LEU:O	1:A:511:ILE:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1163:CYS:SG	2:B:1165:ILE:HB	2.54	0.48
2:B:430:ARG:O	2:B:434:ARG:CD	2.62	0.48
1:A:1290:LYS:O	1:A:1291:VAL:HG23	2.14	0.48
1:A:150:THR:OG1	1:A:166:GLY:HA2	2.13	0.48
1:A:1450:LEU:HD13	6:F:131:PRO:HG3	1.95	0.48
1:A:1230:GLU:C	1:A:1232:ASN:N	2.67	0.48
1:A:668:ASP:CG	1:A:742:ASN:HD22	2.18	0.48
2:B:578:THR:C	2:B:589:VAL:HG13	2.34	0.47
2:B:603:LEU:HD12	2:B:609:ILE:HG12	1.96	0.47
2:B:519:TRP:NE1	2:B:635:ARG:NH2	2.61	0.47
2:B:708:GLU:CG	2:B:709:ASP:H	2.19	0.47
2:B:345:LYS:O	2:B:347:LYS:N	2.47	0.47
3:C:91:HIS:C	3:C:91:HIS:CD2	2.86	0.47
7:G:115:MET:SD	7:G:119:LEU:HD23	2.53	0.47
2:B:405:ARG:HA	2:B:631:GLY:O	2.14	0.47
1:A:549:MET:HE2	1:A:656:TRP:HD1	1.78	0.47
1:A:1424:VAL:HG13	1:A:1436:ILE:CD1	2.35	0.47
1:A:341:MET:HE1	2:B:1135:ARG:NH1	2.29	0.47
1:A:1422:ARG:HH12	2:B:1224:PHE:HD2	1.62	0.47
11:K:46:ILE:O	11:K:46:ILE:HG22	2.14	0.47
1:A:331:GLY:O	1:A:332:LYS:O	2.31	0.47
1:A:392:VAL:HG21	1:A:426:LEU:HD11	1.96	0.47
2:B:976:ILE:O	2:B:990:ILE:HB	2.13	0.47
1:A:107:CYS:HB2	1:A:171:GLN:NE2	2.29	0.47
3:C:8:VAL:HG21	11:K:105:PHE:HA	1.96	0.47
4:D:198:LEU:HA	4:D:201:LYS:HD2	1.95	0.47
2:B:174:LEU:HD22	2:B:202:TYR:CE1	2.49	0.47
4:D:10:THR:O	4:D:10:THR:HG23	2.13	0.47
2:B:613:VAL:HG13	2:B:628:THR:CA	2.43	0.47
2:B:186:GLU:HG3	10:J:62:ARG:NH1	2.29	0.47
10:J:16:ASP:CG	10:J:17:LYS:HD2	2.34	0.47
12:L:43:THR:O	12:L:43:THR:HG22	2.13	0.47
2:B:324:ILE:HD11	2:B:329:THR:O	2.14	0.47
1:A:592:ASP:N	1:A:595:THR:OG1	2.46	0.47
1:A:596:THR:C	1:A:598:LEU:N	2.62	0.47
2:B:642:ASP:CB	2:B:649:LYS:HG3	2.43	0.47
1:A:1038:THR:HG23	1:A:1041:ALA:CB	2.44	0.47
2:B:128:LEU:N	2:B:128:LEU:HD12	2.29	0.47
7:G:62:LEU:CB	7:G:63:PRO:HD2	2.33	0.47
1:A:1313:LEU:CD1	1:A:1327:ILE:HD13	2.44	0.47
1:A:1198:ASP:HB3	1:A:1201:ALA:CB	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1058:LEU:O	2:B:1061:GLU:HB2	2.14	0.47
2:B:52:ASN:O	2:B:55:VAL:N	2.44	0.47
5:E:33:GLU:O	5:E:36:GLU:N	2.47	0.47
2:B:605:ARG:HB3	2:B:688:GLY:CA	2.45	0.47
1:A:44:THR:O	1:A:45:GLN:HB2	2.15	0.47
1:A:600:PRO:CG	1:A:601:LYS:H	2.20	0.47
3:C:76:ASP:O	3:C:78:GLU:N	2.44	0.47
7:G:96:GLN:HA	7:G:121:PHE:CE2	2.49	0.47
2:B:1033:LYS:NZ	2:B:1068:GLY:O	2.47	0.47
1:A:322:VAL:O	1:A:322:VAL:HG13	2.13	0.47
2:B:306:ASN:C	2:B:308:TRP:H	2.17	0.47
5:E:117:THR:CG2	5:E:119:SER:HB2	2.43	0.47
8:H:36:CYS:HB2	8:H:130:ARG:HH22	1.79	0.47
8:H:130:ARG:N	8:H:130:ARG:CD	2.73	0.47
5:E:173:SER:C	5:E:175:LEU:N	2.67	0.47
7:G:8:SER:O	7:G:9:LEU:HB2	2.14	0.47
1:A:1054:LEU:HD13	6:F:84:TYR:OH	2.13	0.47
1:A:853:ASP:C	1:A:853:ASP:OD1	2.52	0.47
2:B:762:ASN:HD21	2:B:1024:ALA:HB3	1.79	0.47
2:B:1167:GLY:HA3	2:B:1215:ARG:HB3	1.95	0.47
1:A:90:VAL:CG1	1:A:297:GLN:HA	2.43	0.47
2:B:239:GLU:HA	2:B:254:LEU:O	2.14	0.47
1:A:185:TRP:CE3	1:A:185:TRP:N	2.82	0.47
1:A:1199:ARG:HH21	1:A:1234:GLU:HA	1.78	0.47
1:A:1159:ARG:HD3	1:A:1174:PHE:CZ	2.49	0.47
1:A:518:LYS:HE2	1:A:624:SER:O	2.14	0.47
2:B:39:ARG:HG2	2:B:39:ARG:NH1	2.29	0.47
2:B:635:ARG:HB2	2:B:636:PRO:HD2	1.96	0.47
6:F:109:VAL:CG1	6:F:110:ASP:N	2.76	0.47
3:C:183:TRP:O	3:C:184:ASN:HB3	2.14	0.47
3:C:190:ASP:O	3:C:191:TYR:C	2.52	0.47
5:E:157:SER:C	5:E:159:ASP:N	2.67	0.47
2:B:911:ILE:O	2:B:911:ILE:HG22	2.14	0.47
1:A:1430:LEU:HB3	1:A:1432:GLN:HG3	1.95	0.47
1:A:506:ALA:O	1:A:509:LEU:HB2	2.14	0.47
1:A:958:VAL:CG2	1:A:1053:PHE:HA	2.44	0.47
4:D:47:LEU:HD11	7:G:3:PHE:HD2	1.78	0.47
1:A:725:ALA:O	1:A:728:LYS:HG2	2.14	0.47
10:J:27:GLU:C	10:J:29:GLU:N	2.67	0.47
2:B:766:ARG:HG3	2:B:1022:THR:CG2	2.41	0.47
1:A:1273:LEU:CD1	1:A:1273:LEU:N	2.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:GLN:HE22	13:T:20:DG:H4'	1.79	0.47
4:D:68:ARG:O	4:D:72:ARG:HG3	2.14	0.47
1:A:645:LEU:HG	1:A:649:ILE:HD11	1.95	0.47
5:E:138:ALA:HA	5:E:141:VAL:HG23	1.96	0.47
9:I:25:LEU:CB	9:I:38:ALA:HB2	2.45	0.47
3:C:86:CYS:SG	3:C:87:PHE:N	2.87	0.47
1:A:628:GLY:O	1:A:632:VAL:HG23	2.14	0.47
2:B:1081:LEU:O	2:B:1083:ALA:N	2.48	0.47
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.97	0.47
2:B:604:ARG:O	2:B:606:LYS:N	2.47	0.47
2:B:686:ASN:C	2:B:688:GLY:N	2.68	0.47
7:G:139:ILE:HG22	7:G:140:LYS:N	2.29	0.47
1:A:1243:VAL:HG22	1:A:1244:ARG:H	1.80	0.47
1:A:1243:VAL:HG22	1:A:1244:ARG:N	2.28	0.47
2:B:261:ARG:NH1	2:B:262:GLU:H	2.13	0.47
2:B:288:ALA:N	2:B:330:ALA:HB1	2.29	0.47
2:B:370:PHE:HD2	2:B:373:ARG:HD2	1.79	0.47
9:I:111:THR:CG2	9:I:112:SER:N	2.76	0.47
6:F:135:ARG:HG2	6:F:137:TYR:CE1	2.48	0.47
1:A:381:THR:HG22	1:A:383:TYR:CD2	2.49	0.47
5:E:90:VAL:HB	5:E:120:ALA:HB2	1.96	0.47
1:A:1332:PHE:N	1:A:1332:PHE:CD2	2.83	0.47
2:B:412:LEU:HD13	2:B:479:VAL:HG11	1.96	0.47
1:A:728:LYS:O	1:A:732:LEU:HG	2.14	0.47
1:A:1443:VAL:HG11	6:F:132:LEU:HD13	1.96	0.47
2:B:867:GLY:C	2:B:869:SER:N	2.67	0.47
5:E:30:ILE:HG23	5:E:34:GLU:OE1	2.15	0.47
1:A:777:PHE:C	1:A:779:PHE:H	2.17	0.47
1:A:399:HIS:CB	1:A:400:PRO:CD	2.84	0.47
1:A:605:MET:HG2	1:A:621:THR:HG23	1.97	0.47
1:A:852:TYR:HD2	1:A:1060:PRO:CB	2.27	0.47
5:E:164:LEU:C	5:E:165:LEU:HD23	2.34	0.47
5:E:45:LYS:HB3	5:E:46:TYR:CD1	2.49	0.47
4:D:40:HIS:HB2	7:G:73:LYS:CD	2.44	0.47
1:A:1129:GLU:O	1:A:1130:GLN:C	2.51	0.47
1:A:230:ARG:HG3	1:A:233:TRP:CZ3	2.49	0.47
8:H:26:ILE:HG22	8:H:27:GLU:N	2.28	0.47
1:A:280:GLU:C	1:A:282:ASN:H	2.16	0.47
2:B:1104:HIS:CG	2:B:1122:ARG:HB2	2.50	0.47
5:E:73:PRO:HB2	5:E:74:ASP:OD1	2.15	0.47
2:B:557:PHE:CZ	2:B:603:LEU:HD21	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:336:ARG:NE	2:B:348:ARG:HH12	2.03	0.47
2:B:955:THR:HG22	2:B:956:THR:N	2.30	0.47
2:B:114:PRO:O	2:B:115:GLN:C	2.53	0.47
1:A:822:GLU:O	1:A:825:ILE:HG22	2.15	0.47
1:A:572:TRP:HA	1:A:576:GLN:OE1	2.14	0.47
2:B:618:ASP:O	2:B:622:LYS:N	2.47	0.47
5:E:78:LEU:HD23	5:E:79:TRP:N	2.29	0.47
1:A:1448:GLU:O	1:A:1449:SER:C	2.51	0.47
2:B:515:HIS:CD2	2:B:517:THR:HG23	2.49	0.47
2:B:898:LEU:HD13	2:B:952:VAL:CG1	2.44	0.47
1:A:1378:GLN:OE1	1:A:1378:GLN:HA	2.15	0.47
2:B:539:LEU:N	2:B:539:LEU:HD12	2.17	0.47
1:A:134:ARG:C	1:A:136:ALA:N	2.68	0.47
1:A:1389:PHE:O	1:A:1391:ARG:N	2.44	0.47
1:A:1037:LEU:HD13	1:A:1041:ALA:CB	2.43	0.47
2:B:496:ARG:HD2	2:B:751:VAL:HG23	1.97	0.47
2:B:591:ARG:O	2:B:593:PRO:HD3	2.15	0.47
1:A:233:TRP:O	1:A:235:ILE:N	2.47	0.47
1:A:890:ASP:OD2	1:A:1296:GLY:HA2	2.14	0.47
2:B:54:PHE:HE1	2:B:414:ALA:HA	1.79	0.47
8:H:11:GLN:O	8:H:28:ALA:CB	2.63	0.47
4:D:12:ARG:HG3	4:D:14:ARG:NH2	2.30	0.47
2:B:1053:GLU:O	2:B:1057:LYS:HG3	2.15	0.47
4:D:157:GLN:O	4:D:158:GLU:C	2.53	0.47
1:A:38:PRO:HG2	1:A:39:GLU:N	2.30	0.47
8:H:84:ALA:C	8:H:86:ASP:N	2.68	0.47
3:C:238:ILE:CD1	3:C:246:ARG:HD2	2.44	0.47
1:A:933:TYR:O	1:A:937:VAL:HG23	2.15	0.47
1:A:1063:MET:SD	1:A:1436:ILE:HG12	2.55	0.47
1:A:1209:MET:SD	1:A:1236:LEU:HB3	2.55	0.47
1:A:1399:ARG:HB3	1:A:1408:ILE:CD1	2.44	0.47
1:A:1399:ARG:HB3	1:A:1408:ILE:HD13	1.97	0.47
2:B:203:PHE:N	2:B:203:PHE:CD1	2.83	0.47
2:B:130:VAL:HG23	2:B:167:ILE:HD13	1.95	0.47
9:I:14:LEU:HD22	9:I:28:GLU:O	2.15	0.47
1:A:7:SER:O	1:A:9:ALA:N	2.48	0.47
1:A:635:ARG:HA	1:A:635:ARG:NH1	2.24	0.47
1:A:755:PHE:O	1:A:758:ILE:HG13	2.15	0.47
3:C:107:SER:C	3:C:109:SER:N	2.65	0.47
5:E:138:ALA:HA	5:E:141:VAL:CG2	2.45	0.47
1:A:1362:TYR:CD1	1:A:1363:VAL:N	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:ILE:HD11	1:A:578:LEU:CD2	2.44	0.47
3:C:105:GLY:HA3	3:C:148:ARG:O	2.15	0.47
3:C:62:PHE:CD2	3:C:62:PHE:C	2.88	0.47
2:B:318:VAL:C	2:B:320:ASP:H	2.18	0.47
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.97	0.47
1:A:829:VAL:O	1:A:831:THR:N	2.48	0.47
1:A:1366:ARG:HG2	1:A:1366:ARG:HH11	1.79	0.47
6:F:82:THR:HG23	6:F:84:TYR:H	1.79	0.47
1:A:1035:TYR:CD1	1:A:1037:LEU:HD23	2.47	0.47
2:B:294:ASP:C	2:B:296:GLU:N	2.62	0.47
1:A:9:ALA:CB	2:B:1193:GLN:HB2	2.44	0.47
9:I:101:PHE:N	9:I:101:PHE:HD1	2.13	0.47
1:A:783:THR:HB	1:A:787:PHE:CD1	2.50	0.47
1:A:352:VAL:O	1:A:467:THR:HG22	2.15	0.47
1:A:489:LEU:HD12	1:A:489:LEU:C	2.35	0.47
2:B:540:SER:HB3	2:B:747:MET:O	2.15	0.47
2:B:705:MET:H	2:B:710:LEU:CD1	2.27	0.47
10:J:56:LEU:O	10:J:59:LYS:N	2.48	0.47
1:A:929:LEU:CD1	1:A:929:LEU:O	2.63	0.47
1:A:191:THR:HG22	1:A:192:GLY:N	2.30	0.47
5:E:108:GLY:HA3	5:E:132:ILE:HG22	1.96	0.47
8:H:113:ALA:HB1	8:H:125:LEU:O	2.14	0.47
3:C:258:ILE:O	3:C:262:LEU:HG	2.14	0.47
11:K:89:ASN:C	11:K:91:CYS:N	2.68	0.47
1:A:1345:ARG:HD2	1:A:1373:ASP:OD1	2.14	0.47
5:E:47:CYS:HA	5:E:52:ARG:O	2.15	0.47
3:C:29:MET:HA	11:K:45:LEU:HD13	1.96	0.47
5:E:169:ARG:HB3	6:F:140:ASP:OD2	2.14	0.47
1:A:146:MET:HB3	1:A:171:GLN:O	2.15	0.47
8:H:103:LYS:HG2	8:H:104:PHE:N	2.29	0.47
1:A:162:VAL:HG12	1:A:163:SER:N	2.29	0.47
1:A:953:ASN:C	1:A:954:TRP:CD1	2.89	0.47
2:B:973:ILE:HG23	2:B:974:PRO:HD2	1.96	0.47
1:A:108:MET:HB3	1:A:210:ILE:CD1	2.45	0.47
9:I:16:PRO:HB2	9:I:25:LEU:HD11	1.97	0.47
2:B:810:GLU:CB	2:B:815:ARG:NH2	2.77	0.46
2:B:185:THR:O	2:B:186:GLU:C	2.53	0.46
12:L:55:ILE:H	12:L:55:ILE:CD1	2.19	0.46
8:H:82:PRO:HG2	8:H:83:GLN:N	2.30	0.46
3:C:104:PHE:HB3	3:C:106:GLU:OE1	2.14	0.46
3:C:125:MET:HG3	3:C:127:ARG:NH2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:563:MET:HE1	2:B:580:VAL:HB	1.97	0.46
1:A:1236:LEU:C	1:A:1237:ILE:HG13	2.36	0.46
1:A:1259:MET:O	1:A:1263:ILE:HD12	2.14	0.46
1:A:1030:ARG:O	1:A:1034:GLU:HB2	2.15	0.46
1:A:896:ARG:HD3	1:A:897:TYR:HE1	1.79	0.46
1:A:1140:HIS:HA	1:A:1275:GLY:HA3	1.97	0.46
12:L:60:ARG:HG2	12:L:61:THR:H	1.80	0.46
11:K:65:HIS:HD2	11:K:67:PHE:N	2.07	0.46
1:A:606:LEU:CG	1:A:613:ILE:HD12	2.44	0.46
11:K:110:ASN:O	11:K:111:LEU:HD23	2.15	0.46
2:B:453:ILE:O	2:B:454:THR:C	2.53	0.46
5:E:4:GLU:HB3	5:E:7:ARG:HE	1.80	0.46
6:F:89:GLU:HB3	6:F:134:ILE:CD1	2.45	0.46
2:B:1055:ILE:O	2:B:1057:LYS:N	2.48	0.46
1:A:342:GLY:HA3	2:B:1131:GLY:HA2	1.97	0.46
4:D:29:LEU:HD22	7:G:82:PHE:CE2	2.50	0.46
2:B:611:PRO:O	2:B:692:TYR:HB2	2.16	0.46
1:A:84:ILE:CG2	1:A:84:ILE:O	2.63	0.46
3:C:115:SER:HB3	3:C:142:VAL:HB	1.96	0.46
7:G:88:ASP:HA	7:G:144:ARG:HA	1.97	0.46
2:B:1065:GLN:NE2	2:B:1067:ARG:N	2.43	0.46
2:B:1068:GLY:O	2:B:1069:PHE:O	2.33	0.46
2:B:235:SER:HB2	2:B:267:ARG:HH12	1.80	0.46
2:B:311:LEU:O	2:B:312:GLU:C	2.53	0.46
9:I:100:PHE:CD1	9:I:100:PHE:N	2.83	0.46
2:B:309:GLN:HG3	9:I:52:ILE:CD1	2.44	0.46
1:A:1451:VAL:C	1:A:1453:TYR:H	2.17	0.46
7:G:13:LEU:HD21	7:G:17:PHE:HB2	1.97	0.46
2:B:871:THR:HG22	2:B:872:GLU:O	2.15	0.46
1:A:1143:LEU:O	1:A:1146:VAL:HG23	2.15	0.46
1:A:1265:ASN:C	1:A:1267:MET:N	2.68	0.46
1:A:1011:GLN:NE2	1:A:1015:VAL:HG21	2.31	0.46
1:A:993:LEU:CD2	1:A:1022:LEU:HD11	2.45	0.46
1:A:695:LYS:HA	1:A:698:GLN:HB2	1.97	0.46
5:E:178:ILE:HG22	5:E:213:ILE:O	2.15	0.46
2:B:483:LEU:CD1	2:B:491:THR:HG23	2.45	0.46
2:B:53:GLN:HG2	2:B:547:VAL:CG2	2.46	0.46
2:B:547:VAL:HG13	2:B:548:GLY:N	2.30	0.46
2:B:806:THR:HB	2:B:809:MET:HG3	1.98	0.46
2:B:934:LYS:HG2	2:B:934:LYS:O	2.14	0.46
1:A:575:LYS:HD2	8:H:120:GLY:HA2	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1445:ILE:HD11	7:G:68:ALA:HB1	1.96	0.46
1:A:332:LYS:C	1:A:334:GLY:N	2.69	0.46
2:B:1125:ASP:OD1	2:B:1125:ASP:O	2.34	0.46
1:A:1040:GLN:O	1:A:1041:ALA:C	2.54	0.46
2:B:126:SER:HB3	2:B:172:ILE:HD11	1.98	0.46
2:B:458:LYS:O	2:B:459:TYR:C	2.53	0.46
4:D:46:GLU:HG2	4:D:47:LEU:N	2.31	0.46
1:A:1441:PHE:CE1	6:F:92:ARG:HG2	2.50	0.46
1:A:289:ILE:O	1:A:292:ALA:N	2.32	0.46
1:A:670:ILE:HG22	1:A:676:MET:HE2	1.98	0.46
11:K:77:THR:HG21	11:K:83:PRO:HA	1.97	0.46
2:B:498:THR:N	2:B:537:LYS:O	2.49	0.46
1:A:623:GLY:C	1:A:625:SER:H	2.17	0.46
2:B:397:ASP:OD1	2:B:399:ASP:N	2.38	0.46
3:C:228:PHE:N	3:C:228:PHE:CD1	2.83	0.46
2:B:1060:ARG:HA	2:B:1060:ARG:HD2	1.68	0.46
1:A:40:THR:C	1:A:41:MET:HG3	2.34	0.46
2:B:1065:GLN:HB2	3:C:201:TRP:CZ3	2.50	0.46
2:B:261:ARG:O	2:B:263:GLY:N	2.48	0.46
2:B:287:ARG:HH11	2:B:324:ILE:HG22	1.81	0.46
1:A:1152:ILE:HD11	9:I:44:TYR:CE2	2.50	0.46
2:B:1001:PHE:CE2	3:C:34:ARG:CZ	2.99	0.46
4:D:4:SER:O	7:G:9:LEU:HD13	2.15	0.46
1:A:874:ASP:CA	1:A:1058:VAL:HG23	2.46	0.46
6:F:82:THR:HG22	6:F:84:TYR:H	1.80	0.46
4:D:119:ARG:HD3	4:D:221:TYR:HE2	1.80	0.46
1:A:144:THR:O	1:A:146:MET:CE	2.63	0.46
1:A:889:SER:CB	1:A:1297:GLU:HG3	2.44	0.46
2:B:581:PHE:O	2:B:626:ILE:HB	2.16	0.46
2:B:509:ALA:O	2:B:510:LYS:C	2.54	0.46
1:A:949:ASP:OD2	1:A:951:GLU:HB2	2.15	0.46
2:B:435:THR:CG2	2:B:437:GLU:HB2	2.45	0.46
6:F:117:PRO:C	6:F:119:ARG:N	2.69	0.46
5:E:29:PHE:N	5:E:65:THR:HG22	2.31	0.46
2:B:307:ASP:C	2:B:309:GLN:N	2.69	0.46
2:B:326:ASP:CG	2:B:328:GLU:HB3	2.36	0.46
7:G:18:PHE:HZ	7:G:68:ALA:HB2	1.80	0.46
1:A:427:GLN:HB2	1:A:430:TRP:NE1	2.31	0.46
6:F:111:LEU:N	6:F:111:LEU:HD12	2.10	0.46
4:D:8:PHE:HZ	4:D:37:GLN:HB2	1.79	0.46
1:A:857:ARG:CZ	6:F:139:PRO:CB	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:608:ILE:CB	1:A:613:ILE:HD11	2.42	0.46
1:A:1284:MET:O	1:A:1285:MET:HG2	2.15	0.46
1:A:1341:ILE:CG2	1:A:1342:GLU:N	2.76	0.46
1:A:802:ASN:HD21	2:B:728:ARG:HB2	1.76	0.46
1:A:203:SER:O	1:A:206:GLU:HB3	2.16	0.46
1:A:369:SER:HB2	11:K:2:ASN:HD21	1.81	0.46
9:I:61:ASP:C	9:I:63:GLY:N	2.68	0.46
1:A:159:THR:O	1:A:159:THR:HG22	2.16	0.46
9:I:25:LEU:CG	9:I:38:ALA:HB2	2.46	0.46
1:A:226:GLU:HG2	1:A:226:GLU:O	2.14	0.46
1:A:83:HIS:CD2	1:A:83:HIS:C	2.89	0.46
3:C:82:TYR:CG	3:C:161:LYS:HG2	2.51	0.46
7:G:145:VAL:HG12	7:G:146:LYS:H	1.80	0.46
6:F:114:GLU:OE2	6:F:119:ARG:HG2	2.15	0.46
5:E:145:THR:HG21	5:E:187:TYR:CD2	2.50	0.46
7:G:59:GLY:CA	7:G:70:PHE:CD2	2.97	0.46
9:I:62:ILE:HG12	9:I:62:ILE:O	2.15	0.46
5:E:17:ARG:HG3	5:E:18:THR:N	2.31	0.46
1:A:870:GLU:O	1:A:871:ASP:HB3	2.15	0.46
2:B:205:ILE:N	2:B:205:ILE:CD1	2.79	0.46
1:A:218:ASP:O	1:A:219:PHE:C	2.54	0.46
1:A:280:GLU:C	1:A:282:ASN:N	2.69	0.46
2:B:529:GLU:OE2	2:B:769:TYR:CE1	2.68	0.46
2:B:762:ASN:OD1	2:B:1022:THR:HA	2.14	0.46
10:J:14:VAL:CG1	10:J:14:VAL:O	2.63	0.46
3:C:13:ALA:O	11:K:114:LEU:HD22	2.14	0.46
1:A:642:CYS:O	1:A:645:LEU:HB3	2.16	0.46
2:B:753:ALA:O	2:B:756:ILE:HG13	2.15	0.46
9:I:25:LEU:HG	9:I:38:ALA:HB2	1.97	0.46
1:A:751:SER:O	1:A:752:LYS:HG2	2.15	0.46
1:A:393:ARG:CB	1:A:393:ARG:HH11	2.27	0.46
3:C:58:LEU:N	3:C:58:LEU:CD2	2.79	0.46
2:B:827:ILE:HD12	2:B:1086:PHE:CD2	2.51	0.46
5:E:186:LEU:O	5:E:187:TYR:C	2.53	0.46
1:A:1444:MET:HG3	7:G:59:GLY:O	2.16	0.46
1:A:852:TYR:CE1	6:F:136:ARG:HG2	2.51	0.46
5:E:35:VAL:C	5:E:37:LEU:H	2.19	0.46
1:A:720:ARG:HB3	1:A:720:ARG:CZ	2.46	0.46
2:B:860:MET:HG2	2:B:861:ASP:H	1.80	0.46
2:B:895:ASP:C	2:B:897:GLY:N	2.69	0.46
2:B:844:SER:O	2:B:847:ASP:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1140:HIS:HB2	1:A:1276:VAL:O	2.16	0.46
1:A:372:LYS:HA	1:A:435:HIS:CE1	2.50	0.46
1:A:1438:THR:O	6:F:92:ARG:NH1	2.49	0.46
3:C:99:LEU:HD23	3:C:99:LEU:N	2.30	0.46
1:A:1340:GLY:O	1:A:1342:GLU:N	2.48	0.46
11:K:61:TYR:HD2	11:K:61:TYR:O	1.98	0.46
1:A:184:SER:HB3	1:A:199:LEU:CD2	2.44	0.46
1:A:79:GLY:H	2:B:1205:GLN:HE22	1.64	0.46
2:B:641:GLU:C	2:B:643:ASP:H	2.18	0.46
1:A:1067:LEU:HD13	1:A:1067:LEU:C	2.36	0.46
1:A:516:SER:O	1:A:518:LYS:HB3	2.16	0.46
1:A:672:ASP:OD2	1:A:674:PRO:HG2	2.16	0.46
1:A:826:ASP:C	1:A:828:ALA:N	2.68	0.46
2:B:292:ILE:HG23	2:B:326:ASP:HA	1.98	0.46
2:B:333:PHE:O	2:B:333:PHE:CD2	2.69	0.46
9:I:55:THR:O	9:I:55:THR:HG22	2.16	0.46
10:J:64:ASN:ND2	10:J:65:PRO:HD3	2.31	0.46
1:A:1258:HIS:HB3	1:A:1259:MET:CE	2.46	0.46
2:B:890:TYR:O	2:B:893:LEU:HB2	2.16	0.46
1:A:897:TYR:CD1	1:A:897:TYR:N	2.83	0.46
1:A:932:GLU:O	1:A:936:LEU:HG	2.16	0.46
3:C:35:ARG:HH11	11:K:41:THR:CA	2.29	0.46
11:K:89:ASN:O	11:K:91:CYS:N	2.49	0.46
2:B:834:ASN:O	2:B:838:SER:O	2.32	0.46
1:A:1345:ARG:NH1	5:E:200:ARG:NH2	2.64	0.46
1:A:875:ALA:HA	1:A:878:ILE:CD1	2.45	0.46
2:B:100:PRO:HD3	2:B:172:ILE:HD13	1.98	0.46
4:D:155:ARG:CZ	4:D:155:ARG:HB2	2.45	0.46
2:B:240:ILE:HG23	2:B:240:ILE:O	2.15	0.46
4:D:29:LEU:HD22	7:G:82:PHE:CD2	2.51	0.46
3:C:226:ASP:O	3:C:227:THR:HB	2.16	0.46
1:A:718:VAL:O	1:A:721:PHE:HB2	2.16	0.46
4:D:185:CYS:HB2	4:D:211:LEU:HD21	1.96	0.46
5:E:82:PHE:CD1	5:E:82:PHE:N	2.83	0.46
2:B:579:ARG:HA	2:B:589:VAL:HG22	1.98	0.46
2:B:552:MET:N	2:B:553:PRO:HD2	2.30	0.46
2:B:654:ARG:C	2:B:656:GLY:N	2.68	0.46
8:H:25:ARG:HB2	8:H:41:ASP:OD1	2.15	0.46
3:C:245:VAL:HA	3:C:248:ILE:HD12	1.98	0.46
6:F:116:ASP:C	6:F:116:ASP:OD1	2.54	0.46
12:L:39:SER:O	12:L:40:LEU:HG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:22:MET:CE	5:E:26:ARG:HD2	2.46	0.46
1:A:407:ARG:HA	1:A:430:TRP:CD2	2.51	0.46
1:A:896:ARG:HH21	1:A:1030:ARG:CZ	2.29	0.46
2:B:1106:ARG:HD3	2:B:1127:GLY:N	2.31	0.46
3:C:10:ILE:HG13	11:K:108:GLU:HB3	1.98	0.46
2:B:1020:ARG:HG3	2:B:1020:ARG:HH11	1.80	0.46
2:B:291:ILE:HD13	2:B:300:HIS:CD2	2.51	0.46
11:K:82:ASP:OD1	11:K:84:LYS:N	2.46	0.46
6:F:148:VAL:HA	6:F:151:LEU:HD12	1.96	0.46
1:A:377:PRO:HG3	1:A:493:GLN:HG3	1.98	0.46
2:B:334:ILE:C	2:B:336:ARG:H	2.20	0.46
1:A:1418:LEU:HB3	2:B:1222:ARG:HH11	1.79	0.46
12:L:30:ILE:HG22	12:L:31:CYS:N	2.31	0.46
1:A:616:VAL:CG1	1:A:617:VAL:H	2.19	0.46
3:C:46:ILE:HD12	3:C:67:LEU:O	2.16	0.46
7:G:127:PRO:HG2	7:G:138:THR:CG2	2.34	0.46
2:B:1065:GLN:HG3	2:B:1067:ARG:H	1.80	0.46
1:A:1111:MET:CE	1:A:1331:SER:HA	2.31	0.46
5:E:195:VAL:CG1	5:E:196:VAL:N	2.78	0.46
8:H:37:LYS:HD2	8:H:126:GLU:OE1	2.16	0.46
1:A:1261:LYS:HE3	9:I:44:TYR:CE2	2.51	0.46
5:E:167:ARG:HD3	5:E:167:ARG:HA	1.66	0.46
7:G:34:VAL:HG13	7:G:45:ILE:HG21	1.98	0.46
1:A:1372:VAL:O	1:A:1376:THR:HG23	2.16	0.46
1:A:1018:PHE:O	1:A:1021:LEU:N	2.49	0.46
11:K:68:PHE:N	11:K:68:PHE:CD2	2.84	0.46
2:B:591:ARG:O	2:B:592:ASN:C	2.55	0.46
4:D:119:ARG:HD3	4:D:221:TYR:HD2	1.76	0.46
7:G:51:TYR:HD2	7:G:51:TYR:O	1.98	0.46
8:H:15:VAL:HG22	8:H:26:ILE:CG2	2.45	0.46
1:A:1118:VAL:O	1:A:1305:VAL:HG13	2.16	0.46
5:E:190:LEU:HD12	5:E:214:CYS:CB	2.45	0.46
2:B:1221:SER:HB3	4:D:12:ARG:NE	2.30	0.46
1:A:1402:PHE:CG	1:A:1402:PHE:O	2.67	0.46
2:B:756:ILE:O	2:B:759:PRO:HD3	2.16	0.46
2:B:1081:LEU:C	2:B:1083:ALA:N	2.69	0.46
1:A:619:LYS:O	1:A:623:GLY:HA3	2.16	0.46
3:C:215:GLU:O	3:C:216:GLY:C	2.54	0.46
2:B:25:ILE:HG23	2:B:658:ILE:CD1	2.43	0.45
2:B:601:ARG:NH1	2:B:605:ARG:HH22	2.14	0.45
2:B:601:ARG:O	2:B:605:ARG:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:693:ILE:HD13	2:B:701:ILE:HD13	1.97	0.45
1:A:42:ASP:C	1:A:44:THR:N	2.69	0.45
12:L:34:CYS:O	12:L:35:SER:C	2.52	0.45
1:A:560:ILE:CG1	8:H:79:TRP:H	2.29	0.45
2:B:235:SER:OG	2:B:236:HIS:CD2	2.69	0.45
2:B:286:PHE:HE1	2:B:382:ILE:HD12	1.81	0.45
6:F:103:MET:CE	7:G:65:ASP:HB2	2.45	0.45
7:G:13:LEU:HD23	7:G:14:HIS:N	2.27	0.45
1:A:590:ARG:HD3	1:A:592:ASP:OD2	2.16	0.45
5:E:164:LEU:HD11	5:E:211:TYR:CE1	2.51	0.45
1:A:1239:ARG:HB3	1:A:1239:ARG:NH1	2.30	0.45
3:C:35:ARG:NH1	11:K:41:THR:CA	2.79	0.45
1:A:1427:ASN:ND2	1:A:1427:ASN:H	2.14	0.45
2:B:1007:VAL:HG23	2:B:1008:PRO:HD2	1.97	0.45
2:B:128:LEU:O	2:B:167:ILE:HD12	2.16	0.45
2:B:459:TYR:CD2	2:B:459:TYR:C	2.88	0.45
4:D:51:ASN:O	4:D:52:LEU:C	2.54	0.45
6:F:77:ASP:O	6:F:78:GLN:CB	2.55	0.45
2:B:479:VAL:HG12	2:B:480:SER:N	2.31	0.45
1:A:699:ALA:O	1:A:700:ASN:CB	2.64	0.45
1:A:584:ASN:C	1:A:586:ILE:N	2.69	0.45
1:A:503:GLN:NE2	6:F:90:ARG:HH21	2.12	0.45
8:H:4:THR:HG22	8:H:6:PHE:H	1.81	0.45
2:B:680:THR:HG23	2:B:683:SER:H	1.81	0.45
11:K:100:ALA:O	11:K:103:THR:HB	2.17	0.45
1:A:944:ARG:NE	1:A:1298:TYR:HE1	2.14	0.45
2:B:656:GLY:O	2:B:657:HIS:C	2.53	0.45
8:H:93:TYR:CD1	8:H:143:LEU:HD23	2.51	0.45
3:C:133:ILE:HG13	3:C:237:SER:H	1.80	0.45
10:J:56:LEU:O	10:J:57:ILE:C	2.55	0.45
1:A:1262:LYS:O	1:A:1264:GLU:N	2.49	0.45
1:A:896:ARG:HH21	1:A:1030:ARG:NH2	2.14	0.45
1:A:1051:ALA:O	1:A:1055:ARG:HG3	2.16	0.45
7:G:50:ASP:O	7:G:51:TYR:C	2.53	0.45
2:B:1181:GLU:HG2	2:B:1188:LYS:HD2	1.98	0.45
11:K:107:THR:HG22	11:K:108:GLU:N	2.30	0.45
11:K:110:ASN:C	11:K:111:LEU:HD23	2.36	0.45
1:A:728:LYS:HA	1:A:731:ARG:HH21	1.80	0.45
1:A:239:LEU:HA	1:A:240:PRO:HD2	1.81	0.45
2:B:102:VAL:HG23	2:B:110:HIS:O	2.16	0.45
1:A:150:THR:O	1:A:163:SER:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:LYS:HG3	1:A:276:LEU:HD21	1.98	0.45
1:A:1110:ASN:CG	1:A:1110:ASN:O	2.55	0.45
2:B:59:LEU:HD12	2:B:417:PHE:CD2	2.51	0.45
1:A:54:ASN:HA	1:A:247:ARG:HH22	1.82	0.45
2:B:882:THR:C	2:B:884:ARG:H	2.20	0.45
3:C:56:THR:CG2	3:C:58:LEU:HD23	2.46	0.45
1:A:684:ALA:O	1:A:687:LYS:HB2	2.16	0.45
1:A:1332:PHE:H	1:A:1332:PHE:HD2	1.61	0.45
2:B:1039:GLY:HA2	10:J:51:LEU:CD2	2.47	0.45
1:A:332:LYS:H	1:A:337:ARG:HB3	1.81	0.45
2:B:834:ASN:ND2	2:B:1013:ASN:HA	2.31	0.45
1:A:509:LEU:C	1:A:511:ILE:N	2.70	0.45
2:B:570:VAL:HB	2:B:573:GLN:HB3	1.99	0.45
2:B:128:LEU:HD11	2:B:170:LEU:HB3	1.98	0.45
7:G:1:MET:CE	7:G:80:LYS:O	2.64	0.45
1:A:7:SER:C	1:A:9:ALA:N	2.70	0.45
2:B:469:GLN:O	2:B:470:LYS:HB2	2.16	0.45
1:A:524:VAL:CG1	1:A:525:GLN:H	2.28	0.45
3:C:91:HIS:HA	3:C:95:CYS:SG	2.56	0.45
2:B:324:ILE:HG23	2:B:325:GLN:N	2.30	0.45
5:E:11:ARG:O	5:E:13:TRP:N	2.49	0.45
1:A:1166:ASP:OD2	1:A:1239:ARG:NE	2.40	0.45
1:A:1191:TRP:HD1	1:A:1256:GLU:HB3	1.80	0.45
11:K:40:HIS:O	11:K:41:THR:C	2.55	0.45
9:I:82:GLU:C	9:I:104:LEU:HG	2.37	0.45
5:E:50:MET:HB3	5:E:52:ARG:NH1	2.32	0.45
1:A:964:ILE:O	1:A:967:ALA:N	2.48	0.45
2:B:558:LEU:C	2:B:560:GLU:N	2.70	0.45
13:T:10:DA:H2"	13:T:11:DA:OP2	2.16	0.45
4:D:208:GLU:O	4:D:212:LYS:HG3	2.16	0.45
2:B:487:THR:H	2:B:490:SER:HB3	1.79	0.45
1:A:821:ARG:HH11	1:A:821:ARG:HB2	1.81	0.45
2:B:782:LEU:HB3	2:B:784:ASN:OD1	2.16	0.45
1:A:1402:PHE:O	1:A:1403:GLU:CB	2.64	0.45
4:D:191:ALA:O	4:D:193:THR:N	2.49	0.45
2:B:1149:GLU:HA	2:B:1153:GLU:OE1	2.16	0.45
9:I:15:TYR:CD1	9:I:15:TYR:N	2.83	0.45
2:B:880:THR:HB	2:B:934:LYS:HE3	1.95	0.45
1:A:600:PRO:C	1:A:602:ASP:H	2.20	0.45
7:G:94:CYS:HA	7:G:99:PHE:HA	1.98	0.45
6:F:116:ASP:OD1	6:F:119:ARG:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:383:ASN:ND2	2:B:387:LEU:HD11	2.32	0.45
2:B:503:GLY:HA3	2:B:507:LYS:CE	2.32	0.45
2:B:502:ILE:HG22	2:B:507:LYS:CG	2.47	0.45
1:A:1100:ARG:NH2	1:A:1351:GLU:CG	2.72	0.45
1:A:896:ARG:NH2	1:A:1030:ARG:NE	2.55	0.45
1:A:996:ASN:HB3	1:A:1050:GLU:OE2	2.17	0.45
2:B:180:TYR:N	2:B:180:TYR:CD1	2.78	0.45
1:A:1313:LEU:CD2	1:A:1338:VAL:HG21	2.43	0.45
2:B:529:GLU:CD	2:B:769:TYR:HE1	2.18	0.45
2:B:766:ARG:NH1	2:B:766:ARG:HG2	2.30	0.45
2:B:498:THR:HG22	2:B:498:THR:O	2.15	0.45
2:B:131:ASP:HA	2:B:164:LYS:N	2.32	0.45
1:A:108:MET:SD	1:A:210:ILE:HD13	2.56	0.45
15:P:6:A:H2'	15:P:7:G:C8	2.51	0.45
15:P:6:A:H2'	15:P:7:G:H8	1.82	0.45
8:H:58:THR:HG22	8:H:59:ILE:N	2.31	0.45
1:A:424:ILE:C	1:A:425:GLN:OE1	2.55	0.45
1:A:1012:ARG:O	1:A:1013:ASP:C	2.54	0.45
1:A:663:SER:OG	1:A:664:THR:N	2.48	0.45
1:A:1131:ALA:O	1:A:1132:LYS:C	2.54	0.45
2:B:20:ASP:C	2:B:22:SER:N	2.70	0.45
1:A:254:GLU:O	1:A:255:SER:OG	2.32	0.45
2:B:186:GLU:HG3	10:J:62:ARG:HH22	1.80	0.45
1:A:531:ILE:HG23	1:A:532:ARG:N	2.32	0.45
3:C:77:ILE:C	3:C:79:GLN:H	2.20	0.45
5:E:22:MET:CE	5:E:26:ARG:NH1	2.64	0.45
2:B:361:LEU:O	2:B:363:HIS:O	2.35	0.45
9:I:50:THR:HG22	9:I:52:ILE:H	1.81	0.45
9:I:90:GLN:NE2	9:I:92:ARG:HD2	2.31	0.45
1:A:867:ILE:CG2	1:A:872:GLY:H	2.30	0.45
1:A:877:HIS:C	1:A:878:ILE:HG13	2.37	0.45
2:B:975:GLN:HG2	2:B:976:ILE:H	1.82	0.45
1:A:767:GLN:HE22	1:A:797:LYS:C	2.20	0.45
4:D:136:GLY:C	4:D:138:ASN:H	2.20	0.45
1:A:1441:PHE:HE1	6:F:92:ARG:HG2	1.81	0.45
2:B:408:LEU:HA	2:B:408:LEU:HD12	1.74	0.45
1:A:982:THR:C	1:A:984:LYS:N	2.66	0.45
1:A:1176:LEU:O	1:A:1176:LEU:HD23	2.17	0.45
7:G:92:VAL:CG2	7:G:102:GLN:HB2	2.46	0.45
1:A:402:ALA:HB1	1:A:434:ARG:HA	1.96	0.45
6:F:93:ILE:CD1	6:F:148:VAL:HG12	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:210:ILE:H	4:D:210:ILE:HG13	1.42	0.45
3:C:6:PRO:HB3	3:C:25:VAL:HG12	1.98	0.45
2:B:38:PHE:HD1	2:B:811:TYR:HD2	1.60	0.45
2:B:806:THR:HG21	2:B:808:ALA:HB3	1.99	0.45
2:B:806:THR:HG22	2:B:807:ARG:N	2.32	0.45
3:C:64:ALA:HA	3:C:67:LEU:HD12	1.97	0.45
7:G:111:THR:O	7:G:112:LYS:C	2.55	0.45
6:F:116:ASP:OD1	6:F:119:ARG:N	2.50	0.45
2:B:290:GLY:HA2	2:B:327:ARG:HD2	1.98	0.45
5:E:45:LYS:HD3	5:E:46:TYR:HE1	1.81	0.45
2:B:876:LYS:HD2	2:B:893:LEU:O	2.17	0.45
4:D:8:PHE:HD2	7:G:6:ASP:O	1.99	0.45
1:A:1427:ASN:O	1:A:1431:GLY:N	2.47	0.45
1:A:1140:HIS:N	1:A:1275:GLY:HA3	2.32	0.45
7:G:27:LYS:HG2	7:G:54:ILE:HD12	1.98	0.45
9:I:34:TYR:C	9:I:34:TYR:CD2	2.89	0.45
1:A:11:LEU:HD22	2:B:1195:HIS:CD2	2.52	0.45
1:A:7:SER:O	4:D:1:MET:HG3	2.17	0.45
1:A:700:ASN:HD22	9:I:115:LYS:HD2	1.81	0.45
1:A:418:SER:O	1:A:420:ARG:N	2.45	0.45
2:B:1081:LEU:O	2:B:1083:ALA:O	2.34	0.45
2:B:199:MET:N	2:B:199:MET:SD	2.88	0.45
1:A:786:HIS:CE1	2:B:705:MET:SD	3.10	0.45
2:B:638:PHE:HB2	2:B:741:CYS:HB3	1.99	0.45
2:B:541:LEU:HB2	2:B:747:MET:HE3	1.99	0.45
2:B:785:TYR:HE2	10:J:60:PHE:CE1	2.35	0.45
3:C:241:ASP:O	3:C:245:VAL:HG22	2.16	0.45
5:E:78:LEU:HD23	5:E:78:LEU:C	2.37	0.45
1:A:350:ARG:O	1:A:351:THR:HG22	2.17	0.45
1:A:1444:MET:HG3	7:G:60:ARG:CA	2.41	0.45
1:A:1436:ILE:O	1:A:1439:GLY:N	2.39	0.45
1:A:1194:ARG:HG3	1:A:1237:ILE:CG2	2.46	0.45
2:B:906:SER:O	2:B:907:GLY:O	2.33	0.45
12:L:60:ARG:HG2	12:L:61:THR:N	2.32	0.45
6:F:82:THR:HA	6:F:83:PRO:HD3	1.71	0.45
1:A:345:VAL:CG2	2:B:1150:ARG:HH22	2.29	0.45
1:A:794:PRO:C	1:A:796:SER:H	2.20	0.45
1:A:1350:LYS:O	1:A:1354:ASN:ND2	2.50	0.45
2:B:29:ASP:HB3	2:B:658:ILE:CD1	2.46	0.45
2:B:547:VAL:HG13	2:B:548:GLY:H	1.82	0.45
1:A:41:MET:HB2	1:A:50:ILE:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:98:TYR:CE1	8:H:139:ASN:HA	2.51	0.45
1:A:665:GLY:C	1:A:666:ILE:HD12	2.37	0.45
2:B:383:ASN:O	2:B:385:LEU:N	2.49	0.45
7:G:14:HIS:ND1	7:G:15:PRO:CD	2.80	0.45
3:C:33:LEU:O	3:C:34:ARG:C	2.54	0.45
11:K:10:PHE:CD2	11:K:10:PHE:N	2.84	0.45
1:A:134:ARG:C	1:A:136:ALA:H	2.20	0.45
11:K:49:GLU:HA	11:K:52:ASN:ND2	2.31	0.45
2:B:100:PRO:CG	2:B:180:TYR:HE1	2.30	0.45
7:G:27:LYS:HD3	7:G:51:TYR:CE2	2.52	0.45
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	1.97	0.45
2:B:529:GLU:CD	2:B:769:TYR:CE1	2.91	0.45
5:E:180:ARG:HB2	5:E:215:MET:OXT	2.16	0.45
1:A:369:SER:HB2	11:K:2:ASN:OD1	2.17	0.45
1:A:323:LYS:HD2	1:A:323:LYS:N	2.30	0.45
5:E:74:ASP:N	5:E:74:ASP:OD1	2.49	0.45
3:C:80:LEU:O	3:C:80:LEU:HG	2.16	0.45
12:L:44:ASP:O	12:L:45:ALA:CB	2.65	0.45
1:A:306:ASN:HB2	1:A:324:SER:HB3	1.98	0.45
2:B:266:ALA:C	2:B:268:THR:H	2.20	0.45
2:B:274:PRO:C	2:B:276:ILE:H	2.20	0.45
2:B:304:ASP:OD1	2:B:306:ASN:N	2.51	0.45
1:A:1437:GLY:C	1:A:1439:GLY:H	2.21	0.45
1:A:1161:THR:OG1	1:A:1239:ARG:NH2	2.50	0.45
2:B:826:ALA:O	2:B:1011:ILE:HA	2.17	0.45
2:B:570:VAL:HA	2:B:571:PRO:HD2	1.85	0.45
9:I:68:LEU:HB3	9:I:84:VAL:HG23	1.99	0.45
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.47	0.45
2:B:593:PRO:CA	2:B:596:LEU:HB3	2.46	0.45
1:A:21:LEU:CD1	1:A:229:SER:HB2	2.47	0.45
13:T:12:DG:N2	14:N:6:DT:C2	2.85	0.45
1:A:608:ILE:HD12	1:A:613:ILE:CD1	2.47	0.45
1:A:1175:SER:O	1:A:1176:LEU:CB	2.59	0.45
1:A:1167:GLU:O	1:A:1170:ILE:HG13	2.17	0.45
1:A:675:THR:O	1:A:675:THR:HG22	2.17	0.45
13:T:25:DG:H2''	13:T:26:DT:C5'	2.47	0.45
12:L:26:THR:HG23	12:L:62:LYS:HZ1	1.82	0.45
1:A:647:GLY:O	1:A:651:LYS:HG3	2.17	0.45
2:B:1034:VAL:O	2:B:1037:LEU:N	2.36	0.45
1:A:645:LEU:CG	1:A:649:ILE:HD11	2.47	0.45
2:B:641:GLU:HB2	2:B:643:ASP:CG	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:39:THR:HG22	7:G:40:GLY:H	1.82	0.45
1:A:29:ALA:HB1	2:B:1184:GLY:HA3	1.98	0.45
4:D:124:GLU:O	4:D:128:VAL:HG23	2.17	0.45
1:A:41:MET:CE	1:A:42:ASP:HB2	2.47	0.44
1:A:567:LYS:CB	8:H:96:VAL:H	2.26	0.44
3:C:239:PRO:O	3:C:241:ASP:N	2.50	0.44
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.47	0.44
12:L:40:LEU:HB3	12:L:41:SER:H	1.56	0.44
5:E:84:ASP:O	5:E:86:PRO:HD3	2.17	0.44
1:A:1447:GLU:O	1:A:1448:GLU:C	2.56	0.44
5:E:92:THR:HG22	5:E:92:THR:O	2.17	0.44
5:E:11:ARG:C	5:E:13:TRP:H	2.20	0.44
8:H:128:ASN:O	8:H:128:ASN:OD1	2.35	0.44
3:C:114:TYR:OH	10:J:19:GLU:OE1	2.34	0.44
1:A:1151:GLU:HG2	9:I:45:ARG:CB	2.47	0.44
2:B:789:MET:HE2	2:B:953:LEU:HD21	1.98	0.44
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.99	0.44
1:A:871:ASP:O	1:A:873:MET:N	2.50	0.44
2:B:451:LYS:O	2:B:452:THR:C	2.55	0.44
1:A:608:ILE:C	1:A:610:GLY:H	2.19	0.44
1:A:288:ALA:HA	1:A:291:GLU:CD	2.37	0.44
1:A:1341:ILE:CG2	1:A:1342:GLU:H	2.29	0.44
4:D:185:CYS:CB	4:D:211:LEU:HD21	2.47	0.44
3:C:220:ASP:OD1	3:C:223:ALA:N	2.50	0.44
2:B:814:PHE:C	2:B:816:GLU:N	2.68	0.44
1:A:661:GLY:O	1:A:662:PHE:HB2	2.16	0.44
1:A:364:VAL:O	1:A:364:VAL:HG13	2.17	0.44
2:B:693:ILE:HD11	2:B:740:HIS:CD2	2.52	0.44
2:B:701:ILE:HB	2:B:739:THR:OG1	2.17	0.44
2:B:335:GLY:HA3	2:B:348:ARG:HB2	1.99	0.44
10:J:2:ILE:HG23	10:J:3:VAL:O	2.18	0.44
6:F:97:ARG:HG3	6:F:124:GLU:OE1	2.17	0.44
2:B:318:VAL:O	2:B:320:ASP:N	2.50	0.44
1:A:618:GLU:O	1:A:621:THR:N	2.44	0.44
6:F:69:LEU:C	6:F:71:GLU:H	2.21	0.44
5:E:13:TRP:CH2	5:E:39:LEU:HB2	2.52	0.44
3:C:173:ALA:O	3:C:174:ALA:CB	2.65	0.44
2:B:980:PHE:HE1	2:B:990:ILE:HD11	1.82	0.44
1:A:1383:SER:O	1:A:1388:GLY:HA3	2.17	0.44
1:A:968:GLN:O	1:A:970:THR:N	2.51	0.44
1:A:722:LEU:HB3	1:A:799:PHE:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:853:ASP:OD1	1:A:855:THR:HG22	2.17	0.44
9:I:33:SER:O	9:I:34:TYR:C	2.55	0.44
11:K:29:ASN:O	11:K:76:GLN:HG3	2.16	0.44
2:B:1201:LYS:HE2	2:B:1205:GLN:HE22	1.80	0.44
1:A:186:LYS:O	1:A:187:LYS:HB3	2.16	0.44
3:C:6:PRO:HB3	3:C:25:VAL:CG1	2.47	0.44
2:B:986:GLN:OE1	2:B:986:GLN:HA	2.18	0.44
1:A:47:ARG:O	1:A:48:ALA:HB2	2.17	0.44
12:L:47:ARG:HG2	12:L:54:ARG:HG2	1.99	0.44
1:A:770:VAL:O	1:A:771:GLU:HB2	2.16	0.44
7:G:138:THR:O	7:G:139:ILE:C	2.56	0.44
7:G:163:ILE:HA	7:G:168:LEU:HD13	2.00	0.44
1:A:666:ILE:HD11	2:B:1086:PHE:HE1	1.83	0.44
2:B:827:ILE:O	2:B:828:ALA:CB	2.61	0.44
3:C:181:ASP:OD2	3:C:185:LYS:N	2.50	0.44
5:E:26:ARG:HG2	5:E:28:TYR:HE1	1.82	0.44
1:A:683:ILE:O	1:A:686:ALA:N	2.44	0.44
2:B:516:ASN:C	2:B:518:HIS:H	2.20	0.44
11:K:21:ILE:HG22	11:K:31:VAL:HG12	1.98	0.44
1:A:858:ASN:ND2	1:A:860:LEU:H	2.15	0.44
1:A:1220:PHE:O	1:A:1221:LYS:CB	2.65	0.44
3:C:258:ILE:N	3:C:258:ILE:HD12	2.32	0.44
1:A:1409:LEU:O	1:A:1412:ALA:HB3	2.17	0.44
1:A:1404:GLU:HB2	1:A:1408:ILE:CD1	2.40	0.44
2:B:172:ILE:HG22	2:B:173:MET:O	2.17	0.44
14:N:5:DC:H2'	14:N:6:DT:H72	1.98	0.44
1:A:700:ASN:HB2	9:I:98:VAL:CG2	2.48	0.44
5:E:212:ARG:NH1	5:E:212:ARG:CG	2.78	0.44
4:D:22:GLU:OE1	4:D:22:GLU:N	2.38	0.44
6:F:85:MET:CB	6:F:155:LEU:HD11	2.46	0.44
1:A:16:GLU:CD	2:B:1220:ARG:HA	2.37	0.44
3:C:143:LEU:HD21	3:C:146:LYS:HE3	1.99	0.44
12:L:40:LEU:CD1	12:L:44:ASP:HB3	2.28	0.44
2:B:312:GLU:O	2:B:315:LYS:HB2	2.17	0.44
1:A:843:LYS:HA	1:A:843:LYS:HD3	1.82	0.44
2:B:953:LEU:HB3	12:L:57:LEU:CD2	2.47	0.44
2:B:1001:PHE:CD2	3:C:34:ARG:NH2	2.85	0.44
4:D:167:LEU:O	4:D:169:SER:N	2.50	0.44
5:E:49:SER:C	5:E:50:MET:HE2	2.38	0.44
7:G:63:PRO:HG2	7:G:64:THR:H	1.82	0.44
1:A:119:ASN:O	1:A:122:MET:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:TYR:CE1	4:D:1:MET:HG3	2.52	0.44
1:A:1392:SER:C	1:A:1394:THR:H	2.21	0.44
1:A:315:LEU:HD13	2:B:471:LYS:O	2.18	0.44
1:A:116:ASP:C	1:A:118:HIS:N	2.68	0.44
1:A:1159:ARG:HD3	1:A:1174:PHE:HZ	1.81	0.44
4:D:176:GLU:C	4:D:178:ALA:N	2.71	0.44
1:A:75:ASN:O	1:A:76:GLU:HB2	2.18	0.44
2:B:425:THR:O	2:B:428:ILE:HD12	2.17	0.44
9:I:22:ASN:O	9:I:23:ASN:HB2	2.15	0.44
1:A:879:GLU:OE2	1:A:959:ASN:ND2	2.48	0.44
1:A:34:LYS:N	1:A:34:LYS:HD3	2.33	0.44
3:C:77:ILE:HG23	3:C:161:LYS:HZ2	1.81	0.44
3:C:83:SER:OG	3:C:160:LYS:HD3	2.18	0.44
7:G:91:VAL:HA	7:G:101:VAL:HA	2.00	0.44
2:B:827:ILE:HD12	2:B:1086:PHE:HD2	1.83	0.44
9:I:100:PHE:N	9:I:100:PHE:HD1	2.15	0.44
2:B:401:PHE:HB2	2:B:517:THR:OG1	2.17	0.44
5:E:55:ARG:O	5:E:57:MET:N	2.51	0.44
2:B:1200:ALA:HA	2:B:1203:LEU:HB3	1.99	0.44
1:A:1120:LEU:CD1	1:A:1120:LEU:H	2.29	0.44
1:A:1125:ALA:C	1:A:1127:ASP:N	2.70	0.44
1:A:134:ARG:CG	1:A:138:ILE:HD11	2.37	0.44
1:A:914:GLU:C	1:A:916:GLY:H	2.21	0.44
2:B:1107:ALA:O	2:B:1108:ARG:O	2.36	0.44
7:G:26:LEU:HA	7:G:26:LEU:HD23	1.85	0.44
1:A:106:VAL:HG21	1:A:214:ILE:HD13	2.00	0.44
1:A:280:GLU:O	1:A:282:ASN:N	2.50	0.44
1:A:734:GLU:C	1:A:736:ASN:N	2.70	0.44
1:A:130:ASP:C	1:A:132:LYS:H	2.21	0.44
9:I:83:ASN:OD1	9:I:103:CYS:HA	2.17	0.44
1:A:1107:VAL:CG1	1:A:1107:VAL:O	2.63	0.44
2:B:615:MET:CE	2:B:615:MET:O	2.66	0.44
2:B:784:ASN:O	2:B:788:ARG:HG3	2.17	0.44
8:H:77:ARG:O	8:H:78:SER:O	2.34	0.44
7:G:41:LYS:HD3	7:G:42:PHE:CE1	2.52	0.44
7:G:39:THR:HB	7:G:42:PHE:H	1.83	0.44
3:C:268:ASP:O	3:C:269:LYS:CB	2.65	0.44
2:B:426:LYS:O	2:B:429:PHE:HB2	2.18	0.44
1:A:472:LEU:HD11	2:B:835:GLN:NE2	2.33	0.44
2:B:797:TYR:CE1	2:B:971:THR:HG23	2.48	0.44
2:B:797:TYR:HE2	3:C:62:PHE:HA	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:798:TYR:HE1	10:J:4:PRO:HA	1.83	0.44
3:C:181:ASP:OD2	3:C:186:LEU:HD13	2.18	0.44
12:L:40:LEU:HD11	12:L:49:LYS:NZ	2.32	0.44
2:B:304:ASP:OD1	2:B:306:ASN:HB2	2.17	0.44
2:B:516:ASN:C	2:B:518:HIS:N	2.71	0.44
5:E:159:ASP:HA	5:E:162:ARG:HH22	1.80	0.44
1:A:1217:LYS:O	1:A:1221:LYS:N	2.50	0.44
5:E:83:CYS:C	5:E:85:GLU:N	2.70	0.44
5:E:202:SER:C	5:E:204:THR:H	2.19	0.44
2:B:129:PHE:CE2	2:B:166:PHE:HD1	2.36	0.44
4:D:115:HIS:CD2	4:D:115:HIS:H	2.36	0.44
1:A:500:GLU:OE1	2:B:1143:ALA:C	2.56	0.44
1:A:7:SER:OG	2:B:1193:GLN:NE2	2.51	0.44
1:A:608:ILE:CG1	1:A:613:ILE:HD11	2.47	0.44
1:A:811:GLN:O	1:A:812:GLU:C	2.55	0.44
10:J:24:LEU:HD12	10:J:39:LEU:CD1	2.44	0.44
10:J:20:SER:O	10:J:24:LEU:HG	2.18	0.44
10:J:24:LEU:CD1	10:J:39:LEU:HD11	2.45	0.44
2:B:1142:GLY:HA3	6:F:88:TYR:CE2	2.46	0.44
2:B:522:VAL:HG12	2:B:523:CYS:N	2.33	0.44
2:B:53:GLN:HG2	2:B:547:VAL:HG23	2.00	0.44
2:B:650:GLU:HG3	2:B:651:LEU:N	2.32	0.44
2:B:541:LEU:HB2	2:B:747:MET:CE	2.48	0.44
1:A:49:LYS:HZ2	1:A:60:SER:HA	1.82	0.44
8:H:82:PRO:HG2	8:H:83:GLN:H	1.82	0.44
3:C:72:LEU:O	3:C:237:SER:HB3	2.17	0.44
5:E:137:GLU:C	5:E:139:ALA:H	2.21	0.44
2:B:276:ILE:O	2:B:276:ILE:HG22	2.18	0.44
8:H:64:ASN:ND2	8:H:88:SER:O	2.50	0.44
1:A:1100:ARG:HH12	1:A:1111:MET:CE	2.30	0.44
2:B:871:THR:HG22	2:B:872:GLU:N	2.32	0.44
2:B:903:VAL:CG1	2:B:904:ARG:N	2.79	0.44
4:D:40:HIS:HD2	7:G:73:LYS:HG3	1.81	0.44
1:A:1329:THR:HG22	1:A:1335:ILE:HG13	2.00	0.44
4:D:56:ARG:HH21	4:D:155:ARG:HA	1.79	0.44
1:A:857:ARG:CZ	6:F:139:PRO:HB2	2.47	0.44
2:B:791:THR:O	2:B:792:MET:CB	2.66	0.44
3:C:22:LEU:HD23	3:C:22:LEU:C	2.38	0.44
2:B:1167:GLY:CA	2:B:1216:LEU:H	2.30	0.44
7:G:92:VAL:HG21	7:G:102:GLN:HB2	1.99	0.44
1:A:447:GLN:H	1:A:447:GLN:HG3	1.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:GLY:HA3	1:A:243:PRO:HG2	1.96	0.44
2:B:1080:LYS:HD2	3:C:188:HIS:CB	2.46	0.44
4:D:130:LEU:C	4:D:132:GLN:N	2.71	0.44
2:B:825:VAL:HG21	2:B:1092:TYR:CE1	2.53	0.44
1:A:108:MET:CE	1:A:210:ILE:HD13	2.48	0.44
1:A:1141:THR:CB	1:A:1205:LYS:HZ3	2.31	0.44
1:A:492:PRO:HB3	1:A:501:LEU:HD11	1.99	0.44
1:A:693:VAL:HG21	1:A:721:PHE:HE1	1.83	0.44
1:A:1381:LEU:HA	1:A:1381:LEU:HD23	1.71	0.44
2:B:758:PHE:HB3	2:B:761:HIS:HD2	1.82	0.44
1:A:532:ARG:HG2	1:A:532:ARG:NH1	2.33	0.44
1:A:1244:ARG:CB	1:A:1245:PRO:CA	2.89	0.44
9:I:86:PHE:HE1	9:I:100:PHE:HB2	1.80	0.44
9:I:76:PRO:HG2	9:I:110:PHE:HB3	1.99	0.44
5:E:93:MET:C	5:E:95:THR:N	2.71	0.44
1:A:446:ARG:HB3	1:A:478:TYR:HB3	1.99	0.44
1:A:1220:PHE:CD1	1:A:1224:LEU:HD23	2.53	0.44
1:A:1208:THR:HG22	1:A:1210:GLY:N	2.32	0.44
4:D:166:LEU:HG	4:D:167:LEU:HD23	2.00	0.44
2:B:620:ARG:HD2	9:I:68:LEU:HD11	1.99	0.44
1:A:910:PRO:HB3	1:A:917:SER:N	2.33	0.44
1:A:982:THR:HB	1:A:985:ASP:H	1.83	0.44
1:A:203:SER:OG	1:A:206:GLU:HB2	2.18	0.44
6:F:94:LEU:CD2	6:F:122:MET:HA	2.46	0.44
2:B:846:ILE:HG23	2:B:974:PRO:HG2	2.00	0.44
2:B:132:VAL:H	2:B:164:LYS:N	2.16	0.44
1:A:1293:SER:O	1:A:1294:PRO:C	2.54	0.44
1:A:258:GLY:O	1:A:259:GLU:O	2.36	0.44
2:B:40:GLU:OE1	2:B:682:SER:HB2	2.17	0.44
2:B:346:GLU:HG2	2:B:347:LYS:N	2.32	0.44
2:B:188:ASP:O	2:B:192:LEU:HD12	2.18	0.44
8:H:40:LEU:CD2	8:H:123:MET:HE3	2.31	0.44
3:C:88:CYS:SG	3:C:91:HIS:CA	3.06	0.44
2:B:1064:TYR:O	2:B:1065:GLN:C	2.56	0.44
1:A:320:ARG:HG2	1:A:322:VAL:H	1.83	0.44
5:E:108:GLY:O	5:E:132:ILE:HG22	2.18	0.44
5:E:90:VAL:HA	5:E:93:MET:HB2	1.99	0.44
5:E:42:PHE:O	5:E:43:LYS:C	2.56	0.44
1:A:1265:ASN:O	1:A:1267:MET:N	2.51	0.44
1:A:496:GLU:O	1:A:499:ALA:HB3	2.18	0.44
1:A:332:LYS:HG3	1:A:333:GLU:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:410:GLY:O	2:B:411:PRO:C	2.56	0.44
1:A:994:GLN:HG2	1:A:1022:LEU:HD23	2.00	0.44
2:B:210:LYS:HE2	2:B:461:LEU:O	2.17	0.44
4:D:64:VAL:C	4:D:66:ARG:H	2.21	0.44
2:B:766:ARG:HH21	2:B:1020:ARG:HG2	1.83	0.44
2:B:616:ILE:CD1	2:B:625:LYS:HB2	2.48	0.44
1:A:71:GLN:CG	1:A:72:GLU:N	2.80	0.43
1:A:262:LEU:CD2	1:A:303:TYR:CE1	3.01	0.43
1:A:543:LEU:CD1	1:A:547:LEU:HG	2.48	0.43
1:A:15:LYS:O	1:A:1420:ASP:O	2.35	0.43
1:A:1377:THR:OG1	1:A:1378:GLN:N	2.51	0.43
3:C:20:PHE:CE1	3:C:230:MET:HB2	2.52	0.43
2:B:224:GLN:HA	2:B:396:ASP:OD2	2.18	0.43
2:B:257:LYS:N	2:B:270:LYS:O	2.51	0.43
2:B:562:GLY:HA3	2:B:590:HIS:CE1	2.53	0.43
1:A:784:LEU:HD11	1:A:815:PHE:CE2	2.53	0.43
1:A:71:GLN:HG3	1:A:72:GLU:N	2.32	0.43
2:B:865:LYS:CG	2:B:961:LEU:HD21	2.46	0.43
8:H:56:THR:HB	8:H:145:ARG:HG2	2.00	0.43
7:G:112:LYS:HE3	7:G:113:HIS:CE1	2.53	0.43
2:B:258:LEU:O	2:B:259:TYR:O	2.36	0.43
2:B:1098:MET:O	2:B:1099:VAL:C	2.55	0.43
1:A:595:THR:C	1:A:596:THR:HG23	2.38	0.43
8:H:129:TYR:C	8:H:130:ARG:HD2	2.38	0.43
1:A:1194:ARG:HG3	1:A:1237:ILE:HG23	2.00	0.43
2:B:1202:LEU:C	2:B:1206:GLU:HG3	2.37	0.43
1:A:658:LEU:HD12	2:B:830:TYR:CD1	2.53	0.43
2:B:570:VAL:CG2	2:B:573:GLN:HB3	2.48	0.43
1:A:384:ASN:HB3	1:A:387:ARG:HH21	1.82	0.43
1:A:883:LEU:CD2	1:A:1021:LEU:HB2	2.48	0.43
5:E:204:THR:CG2	5:E:205:SER:N	2.79	0.43
2:B:205:ILE:HG12	2:B:461:LEU:HB3	2.00	0.43
2:B:615:MET:HE2	2:B:697:GLU:CD	2.38	0.43
1:A:276:LEU:HD11	1:A:293:GLU:HB2	2.00	0.43
2:B:446:LEU:O	2:B:447:ALA:CB	2.66	0.43
1:A:1157:ASP:O	1:A:1159:ARG:N	2.51	0.43
2:B:825:VAL:CG2	2:B:1010:LEU:HD23	2.48	0.43
1:A:377:PRO:HD3	1:A:493:GLN:OE1	2.18	0.43
2:B:1063:GLY:O	3:C:202:PRO:HG2	2.18	0.43
1:A:943:LEU:C	1:A:945:GLU:H	2.20	0.43
2:B:865:LYS:HE3	2:B:961:LEU:CD2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:144:ILE:CG2	8:H:145:ARG:N	2.81	0.43
8:H:24:CYS:HB2	8:H:44:VAL:CG2	2.46	0.43
3:C:77:ILE:C	3:C:79:GLN:N	2.72	0.43
6:F:119:ARG:HG3	6:F:119:ARG:NH1	2.33	0.43
2:B:1084:GLN:OE1	3:C:189:THR:HG22	2.18	0.43
2:B:827:ILE:O	2:B:1085:ILE:CG2	2.66	0.43
1:A:353:ILE:HD13	1:A:487:MET:CE	2.45	0.43
11:K:22:ASP:O	11:K:31:VAL:HG13	2.18	0.43
2:B:843:GLN:NE2	2:B:847:ASP:OD1	2.43	0.43
4:D:9:GLN:HE22	4:D:31:GLN:HG2	1.83	0.43
1:A:106:VAL:C	1:A:114:LEU:HD21	2.38	0.43
9:I:7:CYS:HB2	9:I:34:TYR:CD2	2.53	0.43
2:B:46:GLN:CG	2:B:47:GLN:H	2.31	0.43
2:B:1116:ARG:HD2	2:B:1198:TYR:CD1	2.53	0.43
1:A:481:ASP:OD1	1:A:485:ASP:OD2	2.37	0.43
1:A:1005:GLU:O	1:A:1009:ASN:HB2	2.18	0.43
2:B:1040:ASN:O	2:B:1041:GLU:C	2.57	0.43
2:B:38:PHE:O	2:B:39:ARG:C	2.56	0.43
12:L:52:GLY:O	12:L:54:ARG:N	2.51	0.43
3:C:66:ARG:NH1	3:C:144:ILE:O	2.51	0.43
5:E:93:MET:HG3	5:E:94:LYS:N	2.33	0.43
8:H:109:LYS:HD2	8:H:111:LEU:CD1	2.45	0.43
1:A:17:VAL:HG23	1:A:1421:CYS:SG	2.58	0.43
1:A:1258:HIS:O	1:A:1262:LYS:HG3	2.18	0.43
2:B:890:TYR:CZ	2:B:910:VAL:HG21	2.54	0.43
1:A:1308:THR:CG2	1:A:1310:GLY:O	2.65	0.43
1:A:1011:GLN:HE21	1:A:1015:VAL:HG21	1.82	0.43
1:A:877:HIS:O	1:A:878:ILE:HG12	2.17	0.43
1:A:877:HIS:O	1:A:878:ILE:CG1	2.66	0.43
2:B:1106:ARG:HD2	2:B:1125:ASP:O	2.17	0.43
2:B:1150:ARG:NH1	2:B:1150:ARG:CG	2.70	0.43
4:D:52:LEU:N	4:D:182:SER:HB3	2.34	0.43
8:H:15:VAL:HG22	8:H:26:ILE:HG21	1.99	0.43
2:B:766:ARG:NH1	2:B:769:TYR:HE2	2.16	0.43
2:B:766:ARG:HD2	2:B:984:HIS:O	2.18	0.43
2:B:510:LYS:CB	2:B:511:PRO:CD	2.96	0.43
1:A:1450:LEU:CD1	6:F:108:PHE:CZ	3.01	0.43
2:B:660:LYS:C	2:B:679:TYR:HD2	2.22	0.43
1:A:777:PHE:C	1:A:779:PHE:N	2.71	0.43
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.37	0.43
2:B:23:ALA:O	2:B:654:ARG:HD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:658:ILE:HG22	2:B:659:ALA:N	2.33	0.43
2:B:705:MET:HA	2:B:705:MET:CE	2.49	0.43
1:A:573:SER:O	1:A:574:GLY:C	2.57	0.43
3:C:143:LEU:HD21	3:C:146:LYS:CE	2.48	0.43
7:G:122:ASN:HB3	7:G:129:SER:OG	2.18	0.43
1:A:1105:LEU:CD2	1:A:1384:VAL:HG21	2.48	0.43
1:A:299:HIS:HA	1:A:302:THR:HG22	2.00	0.43
1:A:999:VAL:HG12	1:A:1000:LEU:HG	1.99	0.43
1:A:353:ILE:HG13	1:A:353:ILE:O	2.17	0.43
1:A:1225:PHE:O	1:A:1240:CYS:CB	2.67	0.43
1:A:1124:HIS:ND1	1:A:1124:HIS:N	2.51	0.43
2:B:526:GLU:CD	2:B:752:ALA:HB3	2.39	0.43
2:B:595:ARG:NH1	2:B:595:ARG:HG3	2.33	0.43
1:A:715:GLU:OE2	1:A:774:ARG:NH1	2.51	0.43
4:D:138:ASN:ND2	7:G:35:GLU:HB3	2.33	0.43
7:G:51:TYR:O	7:G:51:TYR:CD2	2.71	0.43
9:I:7:CYS:CB	9:I:14:LEU:HD21	2.41	0.43
2:B:1174:LYS:O	2:B:1175:LEU:C	2.56	0.43
1:A:885:THR:O	1:A:885:THR:CG2	2.60	0.43
9:I:2:THR:CG2	9:I:3:THR:N	2.80	0.43
2:B:846:ILE:CG2	2:B:974:PRO:HG2	2.49	0.43
4:D:202:ILE:HD11	4:D:206:GLU:OE1	2.19	0.43
1:A:783:THR:HB	1:A:787:PHE:HD1	1.84	0.43
14:N:10:DG:H2"	14:N:11:DC:OP2	2.18	0.43
1:A:923:LEU:O	1:A:927:VAL:HG23	2.18	0.43
2:B:800:GLN:HB2	2:B:821:GLN:HA	2.01	0.43
1:A:49:LYS:CD	1:A:55:ASP:HB3	2.48	0.43
2:B:192:LEU:C	2:B:194:GLU:H	2.22	0.43
2:B:785:TYR:HD2	2:B:785:TYR:H	1.66	0.43
7:G:111:THR:HG22	7:G:112:LYS:N	2.33	0.43
7:G:119:LEU:HD11	7:G:137:ILE:HD11	2.00	0.43
1:A:1223:ASP:HA	1:A:1243:VAL:CG1	2.47	0.43
3:C:186:LEU:O	3:C:187:LYS:HB2	2.19	0.43
12:L:48:CYS:O	12:L:50:ASP:N	2.44	0.43
9:I:111:THR:HG22	9:I:113:ASP:N	2.32	0.43
1:A:1154:TYR:CE2	1:A:1156:PRO:HD3	2.53	0.43
1:A:115:LEU:CD1	1:A:141:LEU:HB3	2.49	0.43
2:B:867:GLY:O	2:B:869:SER:N	2.46	0.43
1:A:172:PRO:HB2	1:A:183:GLY:HA3	2.00	0.43
2:B:1116:ARG:HG3	2:B:1198:TYR:CD2	2.54	0.43
1:A:125:ALA:C	1:A:127:ALA:N	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:909:ASP:C	1:A:911:SER:H	2.21	0.43
5:E:73:PRO:HB2	5:E:74:ASP:H	1.66	0.43
3:C:41:ILE:CG2	3:C:172:PRO:HG3	2.49	0.43
1:A:961:ARG:HG3	1:A:961:ARG:NH1	2.34	0.43
3:C:55:THR:HG22	3:C:55:THR:O	2.17	0.43
2:B:29:ASP:OD1	2:B:658:ILE:HD13	2.17	0.43
2:B:37:PHE:CZ	2:B:41:LYS:HG3	2.54	0.43
2:B:23:ALA:O	2:B:654:ARG:HB3	2.18	0.43
1:A:66:LYS:O	1:A:67:CYS:HB2	2.19	0.43
3:C:148:ARG:CG	3:C:149:LYS:H	2.31	0.43
3:C:146:LYS:HD2	10:J:57:ILE:HD13	2.00	0.43
6:F:113:GLY:O	6:F:114:GLU:C	2.57	0.43
12:L:39:SER:OG	12:L:40:LEU:N	2.51	0.43
2:B:261:ARG:NH1	2:B:261:ARG:HG3	2.33	0.43
2:B:328:GLU:C	2:B:330:ALA:N	2.71	0.43
9:I:55:THR:HG1	9:I:100:PHE:HD2	1.62	0.43
6:F:106:PRO:HG2	7:G:18:PHE:C	2.38	0.43
7:G:18:PHE:HA	7:G:22:MET:HE2	2.00	0.43
8:H:36:CYS:HB2	8:H:130:ARG:NH2	2.33	0.43
1:A:1425:SER:O	1:A:1426:GLU:C	2.57	0.43
2:B:996:ARG:HH21	3:C:175:ALA:HA	1.84	0.43
1:A:1037:LEU:HD12	1:A:1042:PHE:CA	2.48	0.43
1:A:966:ASN:O	1:A:967:ALA:C	2.57	0.43
2:B:100:PRO:CD	2:B:180:TYR:HE1	2.31	0.43
2:B:99:LYS:HA	2:B:178:ASN:ND2	2.32	0.43
1:A:289:ILE:C	1:A:291:GLU:N	2.71	0.43
1:A:725:ALA:O	1:A:726:ARG:C	2.56	0.43
10:J:35:ALA:O	10:J:39:LEU:CD1	2.67	0.43
2:B:784:ASN:ND2	2:B:788:ARG:HD2	2.33	0.43
1:A:342:GLY:O	2:B:1129:ARG:NH1	2.52	0.43
1:A:779:PHE:HD1	1:A:784:LEU:HA	1.82	0.43
2:B:340:ALA:C	2:B:342:GLY:H	2.21	0.43
1:A:1418:LEU:HD23	2:B:1222:ARG:HD2	2.01	0.43
1:A:1029:ARG:HG3	1:A:1029:ARG:NH1	2.34	0.43
5:E:135:PHE:HD2	5:E:140:LEU:HD21	1.83	0.43
2:B:277:LYS:HE3	2:B:338:GLY:O	2.18	0.43
2:B:290:GLY:CA	2:B:327:ARG:HD2	2.48	0.43
2:B:361:LEU:HD21	2:B:364:ILE:HD12	1.99	0.43
2:B:872:GLU:HA	2:B:917:PRO:HD3	2.00	0.43
5:E:161:LYS:O	5:E:164:LEU:N	2.52	0.43
1:A:541:ILE:HG21	1:A:549:MET:HE1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:952:VAL:HG12	2:B:953:LEU:H	1.83	0.43
1:A:332:LYS:C	1:A:333:GLU:HG2	2.39	0.43
2:B:1197:PRO:C	2:B:1199:ALA:N	2.71	0.43
2:B:642:ASP:C	2:B:644:GLU:H	2.22	0.43
1:A:1279:ILE:O	1:A:1280:GLU:HG3	2.19	0.43
1:A:458:HIS:CE1	1:A:507:VAL:HG21	2.53	0.43
5:E:85:GLU:C	5:E:87:SER:N	2.71	0.43
1:A:435:HIS:O	1:A:437:MET:HG3	2.19	0.43
1:A:997:LEU:HD13	1:A:1018:PHE:HE2	1.82	0.43
1:A:875:ALA:HA	1:A:878:ILE:HD12	2.01	0.43
2:B:1178:ASN:HD22	2:B:1178:ASN:N	2.15	0.43
1:A:774:ARG:NH2	1:A:797:LYS:HB2	2.33	0.43
1:A:855:THR:HG23	1:A:857:ARG:HG3	2.00	0.43
1:A:101:LYS:HE2	1:A:139:TRP:CZ2	2.54	0.43
2:B:1167:GLY:HA3	2:B:1216:LEU:N	2.32	0.43
8:H:4:THR:HA	8:H:60:ALA:CB	2.49	0.43
2:B:1122:ARG:HB3	13:T:22:DC:OP1	2.18	0.43
11:K:17:SER:O	11:K:18:LYS:C	2.56	0.43
1:A:1213:GLY:O	1:A:1216:ILE:N	2.51	0.43
2:B:492:LEU:O	2:B:495:LEU:N	2.51	0.43
2:B:355:ILE:H	2:B:355:ILE:HG13	1.68	0.43
2:B:186:GLU:HB3	2:B:187:SER:H	1.49	0.43
1:A:825:ILE:HA	1:A:825:ILE:HD12	1.70	0.43
8:H:40:LEU:HD13	8:H:123:MET:HE3	2.00	0.43
7:G:114:LEU:HA	7:G:114:LEU:HD12	1.89	0.43
5:E:137:GLU:C	5:E:139:ALA:N	2.72	0.43
5:E:15:ALA:HA	5:E:140:LEU:O	2.18	0.43
1:A:1330:ASN:OD1	1:A:1331:SER:N	2.52	0.43
1:A:626:ASN:O	1:A:631:HIS:CD2	2.72	0.43
5:E:204:THR:CG2	5:E:205:SER:H	2.28	0.43
2:B:1177:HIS:HB3	2:B:1179:GLN:HE21	1.83	0.43
4:D:64:VAL:HG22	4:D:129:LEU:CD2	2.49	0.43
1:A:700:ASN:C	1:A:701:LEU:HD23	2.39	0.43
1:A:279:LEU:O	1:A:289:ILE:HD11	2.19	0.43
1:A:1343:ALA:HB2	5:E:150:VAL:CG2	2.41	0.43
2:B:476:ARG:O	2:B:477:ALA:C	2.57	0.43
2:B:660:LYS:HB3	2:B:679:TYR:CD2	2.54	0.43
2:B:681:TRP:O	2:B:684:LEU:N	2.52	0.43
1:A:409:SER:O	1:A:410:GLY:C	2.56	0.43
2:B:402:GLY:CA	2:B:695:ALA:HB3	2.49	0.43
1:A:1299:VAL:CG1	1:A:1300:LYS:N	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:426:LYS:H	2:B:426:LYS:HG2	1.51	0.43
2:B:651:LEU:C	2:B:653:VAL:N	2.71	0.43
2:B:708:GLU:O	2:B:709:ASP:C	2.57	0.43
13:T:15:DC:C6	13:T:16:DT:H72	2.53	0.43
2:B:879:ARG:HA	2:B:879:ARG:HD3	1.46	0.43
1:A:826:ASP:O	1:A:830:LYS:N	2.37	0.43
1:A:526:ASP:HB2	2:B:835:GLN:OE1	2.18	0.43
2:B:619:ILE:O	2:B:622:LYS:HG3	2.19	0.43
1:A:899:VAL:O	1:A:929:LEU:HD12	2.19	0.43
1:A:350:ARG:HB2	1:A:488:ASN:OD1	2.18	0.43
6:F:105:ALA:HB1	6:F:106:PRO:CD	2.49	0.43
5:E:94:LYS:HE2	5:E:98:ILE:HD11	2.01	0.43
3:C:136:ASP:OD1	3:C:137:LYS:N	2.52	0.43
3:C:35:ARG:HH11	11:K:41:THR:HA	1.83	0.43
2:B:165:VAL:CG1	2:B:166:PHE:N	2.82	0.43
1:A:142:CYS:C	1:A:144:THR:H	2.22	0.43
9:I:13:MET:HE3	9:I:14:LEU:H	1.84	0.43
1:A:275:SER:O	1:A:279:LEU:HG	2.18	0.43
1:A:286:HIS:O	1:A:288:ALA:N	2.52	0.43
3:C:17:ASN:H	3:C:240:VAL:HG21	1.84	0.43
1:A:515:GLN:HB2	1:A:1071:SER:HB3	2.00	0.43
3:C:3:GLU:HG3	11:K:104:ASN:ND2	2.34	0.43
11:K:18:LYS:NZ	11:K:37:LYS:O	2.51	0.43
1:A:645:LEU:HG	1:A:649:ILE:CD1	2.48	0.43
7:G:44:TYR:HE1	7:G:157:ILE:N	2.16	0.43
4:D:214:LEU:O	4:D:216:ASN:N	2.51	0.43
2:B:484:ASN:O	2:B:485:ARG:HD2	2.19	0.43
2:B:1050:ILE:HG22	2:B:1051:THR:N	2.34	0.43
4:D:13:ARG:O	4:D:13:ARG:CD	2.67	0.43
2:B:637:LEU:CD1	2:B:703:ILE:HD13	2.48	0.42
1:A:536:LEU:O	1:A:537:ARG:C	2.58	0.42
10:J:2:ILE:HG12	10:J:57:ILE:CD1	2.48	0.42
7:G:116:PRO:HB2	7:G:118:ASP:OD1	2.19	0.42
2:B:282:ILE:CD1	2:B:382:ILE:HD13	2.48	0.42
1:A:1451:VAL:O	1:A:1454:MET:HG2	2.19	0.42
1:A:596:THR:C	1:A:597:LEU:HD12	2.38	0.42
2:B:871:THR:CG2	2:B:872:GLU:N	2.81	0.42
12:L:36:SER:O	12:L:37:LYS:O	2.37	0.42
4:D:39:ASN:HB3	4:D:43:GLU:O	2.19	0.42
2:B:860:MET:HG2	2:B:861:ASP:N	2.33	0.42
1:A:869:GLY:O	1:A:870:GLU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1146:PHE:CE1	2:B:1150:ARG:HD3	2.54	0.42
1:A:460:VAL:HG12	1:A:461:LYS:N	2.34	0.42
7:G:84:GLY:N	7:G:147:ILE:O	2.47	0.42
4:D:52:LEU:H	4:D:182:SER:HB3	1.84	0.42
2:B:65:GLU:CG	2:B:66:ASP:H	2.25	0.42
1:A:728:LYS:HA	1:A:731:ARG:HE	1.84	0.42
2:B:1020:ARG:HG3	2:B:1020:ARG:NH1	2.32	0.42
2:B:773:MET:HE2	2:B:985:GLY:HA2	2.00	0.42
6:F:85:MET:CE	6:F:93:ILE:HD12	2.49	0.42
1:A:998:LEU:H	1:A:998:LEU:CD1	2.29	0.42
1:A:555:ASP:O	1:A:556:TRP:C	2.56	0.42
2:B:61:ASP:O	2:B:64:CYS:O	2.36	0.42
2:B:27:ALA:O	2:B:29:ASP:N	2.52	0.42
8:H:41:ASP:HB2	8:H:121:LEU:HB3	1.99	0.42
2:B:284:ILE:HD13	2:B:333:PHE:HD2	1.82	0.42
9:I:54:GLU:HB3	9:I:100:PHE:CE2	2.54	0.42
8:H:63:LEU:CD1	8:H:64:ASN:H	2.32	0.42
1:A:681:GLU:O	1:A:685:GLU:HG3	2.18	0.42
12:L:27:LEU:CB	12:L:37:LYS:HB3	2.48	0.42
1:A:15:LYS:O	1:A:1421:CYS:HB2	2.19	0.42
1:A:831:THR:CG2	1:A:832:ALA:N	2.82	0.42
2:B:831:SER:CB	2:B:994:TYR:OH	2.67	0.42
1:A:522:GLY:HA2	1:A:646:PHE:HE2	1.84	0.42
1:A:384:ASN:O	1:A:386:ASP:N	2.52	0.42
1:A:387:ARG:HH11	1:A:437:MET:HE1	1.84	0.42
1:A:910:PRO:HB3	1:A:917:SER:H	1.84	0.42
2:B:465:ASN:HD22	2:B:465:ASN:N	2.13	0.42
1:A:185:TRP:CH2	1:A:200:ARG:HB3	2.54	0.42
1:A:882:SER:H	1:A:1025:ARG:HH21	1.67	0.42
1:A:103:CYS:HB3	1:A:174:ILE:CD1	2.49	0.42
1:A:556:TRP:C	1:A:558:GLY:N	2.73	0.42
5:E:31:THR:CG2	5:E:34:GLU:HB2	2.49	0.42
2:B:589:VAL:CG1	2:B:590:HIS:N	2.80	0.42
2:B:744:HIS:CD2	2:B:746:SER:OG	2.67	0.42
1:A:69:THR:O	1:A:70:CYS:C	2.58	0.42
2:B:186:GLU:HG3	10:J:62:ARG:HH12	1.84	0.42
1:A:600:PRO:HG2	1:A:601:LYS:HG3	2.00	0.42
8:H:79:TRP:O	8:H:80:ARG:C	2.57	0.42
1:A:1242:VAL:CG1	1:A:1243:VAL:H	2.13	0.42
6:F:103:MET:HE3	7:G:66:GLY:N	2.33	0.42
1:A:262:LEU:CD2	1:A:303:TYR:HE1	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:27:LEU:H	12:L:27:LEU:CD2	2.14	0.42
1:A:1424:VAL:O	1:A:1428:VAL:HG23	2.18	0.42
1:A:894:GLU:O	1:A:896:ARG:N	2.52	0.42
2:B:170:LEU:HG	2:B:170:LEU:O	2.20	0.42
1:A:711:ARG:NH2	9:I:87:GLN:OE1	2.51	0.42
2:B:1162:ILE:HG22	2:B:1163:CYS:O	2.19	0.42
6:F:75:PRO:C	6:F:77:ASP:N	2.70	0.42
1:A:728:LYS:CB	1:A:731:ARG:HH21	2.32	0.42
1:A:733:ALA:O	1:A:736:ASN:HB3	2.19	0.42
3:C:50:GLU:HB3	3:C:156:THR:HB	2.01	0.42
2:B:714:GLU:N	2:B:714:GLU:OE1	2.52	0.42
1:A:117:GLU:N	1:A:117:GLU:CD	2.69	0.42
9:I:61:ASP:HB3	9:I:64:SER:OG	2.19	0.42
6:F:108:PHE:HE1	6:F:131:PRO:HG3	1.85	0.42
1:A:1450:LEU:HD11	6:F:108:PHE:HZ	1.84	0.42
4:D:116:SER:O	4:D:117:GLU:C	2.57	0.42
1:A:108:MET:O	1:A:109:HIS:HB2	2.19	0.42
8:H:9:ILE:HG21	8:H:54:SER:HB2	2.01	0.42
2:B:711:GLU:CB	2:B:712:PRO:CD	2.98	0.42
1:A:352:VAL:HG23	1:A:467:THR:HG22	1.99	0.42
4:D:186:ASP:O	4:D:211:LEU:HD13	2.18	0.42
2:B:69:LEU:O	2:B:70:ILE:CG1	2.58	0.42
2:B:822:ASN:HD21	10:J:52:THR:CG2	2.30	0.42
2:B:348:ARG:O	2:B:351:TYR:HB3	2.19	0.42
2:B:120:ARG:HH12	12:L:54:ARG:NH1	2.16	0.42
1:A:475:THR:HG23	1:A:476:SER:H	1.79	0.42
1:A:537:ARG:NH1	8:H:120:GLY:O	2.52	0.42
3:C:91:HIS:HD2	3:C:91:HIS:O	2.02	0.42
1:A:926:GLN:O	1:A:930:ASP:HB2	2.19	0.42
2:B:1029:CYS:HB3	2:B:1086:PHE:CE2	2.55	0.42
2:B:278:GLN:CG	2:B:279:ASP:N	2.80	0.42
2:B:327:ARG:HG2	2:B:327:ARG:O	2.19	0.42
2:B:388:CYS:C	2:B:390:LEU:N	2.72	0.42
1:A:591:PHE:HD2	1:A:595:THR:HB	1.84	0.42
1:A:383:TYR:N	1:A:383:TYR:CD2	2.87	0.42
5:E:195:VAL:CG1	5:E:196:VAL:H	2.27	0.42
5:E:12:LEU:HD22	5:E:55:ARG:CZ	2.49	0.42
1:A:1423:GLY:O	1:A:1424:VAL:C	2.57	0.42
2:B:952:VAL:O	12:L:57:LEU:HD22	2.20	0.42
2:B:847:ASP:OD2	3:C:167:HIS:HA	2.20	0.42
2:B:572:HIS:O	2:B:573:GLN:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:ASN:HA	2:B:207:GLY:CA	2.41	0.42
7:G:1:MET:O	7:G:2:PHE:C	2.58	0.42
7:G:62:LEU:HB3	7:G:63:PRO:CD	2.42	0.42
4:D:63:LEU:CD1	4:D:133:THR:OG1	2.65	0.42
4:D:141:LEU:O	4:D:145:MET:HG2	2.19	0.42
1:A:167:CYS:HB2	1:A:169:ASN:HD22	1.84	0.42
1:A:107:CYS:HB2	1:A:171:GLN:HE22	1.83	0.42
1:A:726:ARG:NH2	1:A:727:ASP:OD1	2.51	0.42
1:A:1215:ARG:NH1	1:A:1272:THR:O	2.52	0.42
1:A:207:ILE:O	1:A:208:LEU:C	2.58	0.42
4:D:196:PRO:O	4:D:197:SER:C	2.57	0.42
1:A:579:SER:HB3	1:A:611:GLN:HA	2.00	0.42
2:B:436:VAL:O	2:B:436:VAL:HG12	2.18	0.42
1:A:786:HIS:CE1	2:B:519:TRP:CZ2	3.08	0.42
2:B:557:PHE:CE1	2:B:603:LEU:HD11	2.53	0.42
1:A:526:ASP:HB2	2:B:835:GLN:CD	2.40	0.42
1:A:601:LYS:HB2	1:A:603:ASN:OD1	2.19	0.42
1:A:568:PRO:CB	3:C:221:TYR:CZ	3.03	0.42
3:C:234:SER:OG	3:C:235:VAL:N	2.52	0.42
3:C:133:ILE:HG13	3:C:237:SER:N	2.34	0.42
3:C:187:LYS:C	3:C:189:THR:H	2.22	0.42
2:B:365:THR:O	2:B:374:LYS:HE3	2.19	0.42
7:G:14:HIS:CE1	7:G:15:PRO:HD2	2.54	0.42
11:K:20:LYS:O	11:K:33:ILE:HA	2.20	0.42
2:B:1203:LEU:O	2:B:1207:LEU:HG	2.20	0.42
1:A:392:VAL:C	1:A:394:ASN:N	2.73	0.42
2:B:1109:GLY:HA3	2:B:1110:PRO:HD2	1.75	0.42
6:F:138:LEU:O	6:F:140:ASP:N	2.53	0.42
1:A:1001:ARG:NH1	1:A:1001:ARG:CG	2.82	0.42
1:A:317:LYS:HG3	2:B:471:LYS:NZ	2.34	0.42
2:B:615:MET:HE2	2:B:615:MET:O	2.19	0.42
1:A:276:LEU:HD13	1:A:293:GLU:CA	2.47	0.42
1:A:1157:ASP:C	1:A:1159:ARG:N	2.70	0.42
1:A:1157:ASP:OD1	1:A:1159:ARG:HB2	2.19	0.42
2:B:825:VAL:HG21	2:B:1092:TYR:HE1	1.85	0.42
3:C:27:LEU:O	3:C:28:ALA:C	2.56	0.42
2:B:32:ALA:O	2:B:35:SER:HB2	2.20	0.42
2:B:604:ARG:HA	2:B:609:ILE:HG13	2.01	0.42
2:B:801:LYS:HD2	2:B:815:ARG:HB3	2.01	0.42
2:B:104:GLU:OE1	12:L:54:ARG:CZ	2.67	0.42
2:B:190:TYR:CE1	2:B:196:PRO:HG3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:46:ILE:HD13	3:C:157:CYS:SG	2.60	0.42
10:J:1:MET:O	10:J:1:MET:HG3	2.19	0.42
2:B:1071:VAL:HG12	2:B:1072:MET:N	2.33	0.42
2:B:1192:TYR:CD2	2:B:1218:THR:HG21	2.55	0.42
2:B:367:LEU:O	2:B:368:GLU:HB2	2.20	0.42
1:A:1446:ASP:HB3	1:A:1449:SER:OG	2.20	0.42
6:F:74:ILE:HG13	6:F:74:ILE:H	1.64	0.42
5:E:117:THR:HB	5:E:120:ALA:HB3	2.00	0.42
5:E:156:LEU:HD12	5:E:195:VAL:CG1	2.50	0.42
8:H:109:LYS:HB3	8:H:110:ASP:OD1	2.20	0.42
3:C:138:GLU:HB2	3:C:140:ASN:ND2	2.35	0.42
2:B:996:ARG:NH2	3:C:175:ALA:HA	2.34	0.42
1:A:1431:GLY:HA3	2:B:1197:PRO:HD3	2.00	0.42
3:C:166:GLU:HG3	11:K:10:PHE:CZ	2.46	0.42
4:D:166:LEU:O	4:D:169:SER:OG	2.38	0.42
5:E:87:SER:O	5:E:88:VAL:C	2.58	0.42
11:K:65:HIS:HD2	11:K:67:PHE:HB2	1.84	0.42
1:A:1037:LEU:HD13	1:A:1041:ALA:HB3	2.01	0.42
2:B:60:GLN:HE22	2:B:95:ILE:HG22	1.80	0.42
2:B:98:THR:O	2:B:126:SER:CB	2.64	0.42
1:A:102:VAL:O	1:A:105:CYS:HB2	2.19	0.42
1:A:90:VAL:HG11	1:A:297:GLN:HA	2.01	0.42
1:A:556:TRP:CD2	1:A:558:GLY:HA2	2.55	0.42
1:A:514:PRO:C	1:A:516:SER:N	2.72	0.42
9:I:49:ILE:HG22	9:I:49:ILE:O	2.20	0.42
2:B:806:THR:CG2	2:B:808:ALA:HB3	2.49	0.42
1:A:47:ARG:NH1	1:A:254:GLU:OE1	2.51	0.42
1:A:524:VAL:HG12	1:A:525:GLN:CG	2.50	0.42
3:C:56:THR:CG2	3:C:145:CYS:SG	3.07	0.42
3:C:73:GLN:NE2	3:C:75:MET:H	2.14	0.42
7:G:88:ASP:OD2	7:G:88:ASP:N	2.47	0.42
11:K:24:ASP:H	11:K:31:VAL:HA	1.85	0.42
8:H:32:THR:CG2	8:H:33:GLN:H	2.27	0.42
2:B:860:MET:HG3	2:B:965:LYS:HE2	2.01	0.42
2:B:859:TYR:OH	2:B:941:LEU:HD12	2.18	0.42
3:C:174:ALA:O	10:J:10:CYS:HB2	2.20	0.42
1:A:1409:LEU:O	1:A:1410:PHE:C	2.58	0.42
2:B:840:ILE:CG2	2:B:994:TYR:HD1	2.33	0.42
1:A:1329:THR:O	1:A:1329:THR:HG23	2.19	0.42
2:B:205:ILE:C	2:B:207:GLY:N	2.73	0.42
2:B:126:SER:O	2:B:169:ARG:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:701:LEU:HD21	9:I:114:GLN:HB2	2.02	0.42
1:A:584:ASN:O	1:A:586:ILE:N	2.53	0.42
1:A:802:ASN:CG	2:B:728:ARG:HB2	2.39	0.42
2:B:857:ARG:NH2	2:B:942:ARG:CZ	2.83	0.42
2:B:1115:THR:HG22	2:B:1117:GLN:CB	2.50	0.42
2:B:428:ILE:HG13	2:B:428:ILE:H	1.72	0.42
1:A:355:GLY:HA3	1:A:482:PHE:CZ	2.55	0.42
2:B:25:ILE:CD1	2:B:653:VAL:O	2.68	0.42
1:A:57:ARG:NH1	1:A:57:ARG:HG2	2.32	0.42
8:H:100:THR:HG23	8:H:138:GLU:CB	2.49	0.42
8:H:145:ARG:O	8:H:146:ARG:CB	2.68	0.42
3:C:118:LEU:HD12	3:C:132:PRO:HG3	2.02	0.42
3:C:82:TYR:CE2	3:C:161:LYS:HG2	2.55	0.42
1:A:919:ILE:HD13	1:A:983:ILE:CD1	2.49	0.42
2:B:247:GLY:O	2:B:248:SER:HB3	2.20	0.42
2:B:309:GLN:O	2:B:312:GLU:N	2.52	0.42
2:B:384:ARG:HD2	2:B:387:LEU:HD22	2.01	0.42
5:E:164:LEU:HD11	5:E:211:TYR:CD1	2.54	0.42
1:A:846:GLU:OE1	1:A:1425:SER:OG	2.34	0.42
1:A:1422:ARG:NH1	2:B:1224:PHE:HD2	2.18	0.42
11:K:41:THR:CG2	11:K:42:LEU:N	2.83	0.42
1:A:332:LYS:O	1:A:333:GLU:HG2	2.19	0.42
1:A:839:ARG:CG	1:A:840:ARG:N	2.83	0.42
2:B:1156:ASP:O	2:B:1157:ALA:C	2.58	0.42
2:B:1197:PRO:O	2:B:1199:ALA:N	2.53	0.42
1:A:1011:GLN:NE2	1:A:1015:VAL:CG2	2.82	0.42
4:D:175:PHE:CZ	7:G:85:GLU:HG3	2.55	0.42
1:A:712:GLU:O	1:A:714:PHE:N	2.53	0.42
1:A:781:ASP:O	1:A:790:ASP:N	2.52	0.42
4:D:119:ARG:CG	4:D:221:TYR:HE2	2.33	0.42
1:A:733:ALA:HA	1:A:736:ASN:HB3	2.01	0.42
1:A:1297:GLU:OE1	1:A:1297:GLU:N	2.52	0.42
1:A:637:LYS:HA	1:A:637:LYS:HD3	1.89	0.42
1:A:556:TRP:O	1:A:558:GLY:N	2.53	0.42
1:A:53:LEU:CD2	1:A:54:ASN:N	2.61	0.42
2:B:505:ASP:O	2:B:506:GLY:C	2.57	0.42
3:C:88:CYS:SG	3:C:91:HIS:HA	2.60	0.42
1:A:1449:SER:C	1:A:1451:VAL:H	2.23	0.42
1:A:690:VAL:O	1:A:691:LEU:C	2.59	0.42
6:F:70:LYS:O	6:F:72:LYS:N	2.43	0.42
2:B:1002:THR:O	2:B:1004:GLU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:789:MET:CE	2:B:967:ARG:HB2	2.50	0.42
7:G:45:ILE:HD13	7:G:78:VAL:HG11	2.01	0.42
2:B:843:GLN:O	2:B:844:SER:C	2.57	0.42
2:B:995:ARG:HH11	3:C:165:LYS:HA	1.84	0.42
1:A:1138:ILE:CA	1:A:1275:GLY:HA2	2.50	0.42
9:I:82:GLU:CB	9:I:104:LEU:HD12	2.40	0.42
4:D:47:LEU:CD1	7:G:3:PHE:HD2	2.31	0.42
1:A:818:MET:HA	2:B:514:LEU:HB3	2.01	0.42
4:D:64:VAL:CG2	4:D:129:LEU:HD21	2.50	0.42
2:B:529:GLU:OE1	2:B:769:TYR:CE1	2.72	0.42
4:D:26:THR:O	4:D:26:THR:HG22	2.20	0.42
1:A:1059:HIS:ND1	6:F:86:THR:HA	2.35	0.42
2:B:661:LEU:HD23	2:B:679:TYR:O	2.20	0.42
1:A:120:GLU:O	1:A:121:LEU:C	2.58	0.42
1:A:1150:SER:HA	1:A:1195:LEU:HA	2.01	0.42
2:B:36:ALA:O	2:B:39:ARG:HB2	2.20	0.42
2:B:195:CYS:SG	2:B:196:PRO:HD2	2.60	0.42
1:A:826:ASP:O	1:A:827:THR:C	2.57	0.42
3:C:100:THR:HG22	3:C:102:GLN:NE2	2.35	0.42
3:C:73:GLN:CG	3:C:74:SER:N	2.82	0.42
5:E:105:PHE:O	5:E:106:GLN:HB2	2.18	0.42
2:B:566:LEU:O	2:B:567:GLU:C	2.58	0.42
1:A:595:THR:O	1:A:596:THR:HG23	2.20	0.42
1:A:597:LEU:HD12	1:A:597:LEU:N	2.35	0.42
1:A:1100:ARG:HH12	1:A:1111:MET:HE1	1.85	0.42
1:A:1277:GLU:HA	1:A:1277:GLU:OE1	2.19	0.42
1:A:965:GLN:O	1:A:968:GLN:HB2	2.20	0.42
1:A:179:LEU:HD23	1:A:179:LEU:N	2.35	0.42
1:A:728:LYS:O	1:A:729:ALA:C	2.58	0.42
6:F:125:LEU:HB2	6:F:130:ILE:HD11	2.02	0.42
1:A:452:LYS:HE3	2:B:1141:HIS:CE1	2.55	0.42
1:A:752:LYS:HD3	1:A:752:LYS:HA	1.87	0.42
2:B:654:ARG:C	2:B:656:GLY:H	2.23	0.41
2:B:810:GLU:HB3	2:B:811:TYR:CD1	2.54	0.41
1:A:41:MET:HE3	1:A:41:MET:H	1.85	0.41
1:A:52:GLY:O	1:A:56:PRO:HG2	2.20	0.41
1:A:65:LEU:O	1:A:71:GLN:HA	2.20	0.41
2:B:879:ARG:NH1	2:B:883:LEU:CD2	2.81	0.41
2:B:287:ARG:NH1	2:B:324:ILE:O	2.52	0.41
6:F:127:GLU:O	6:F:129:LYS:N	2.53	0.41
1:A:1425:SER:HA	1:A:1428:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1192:LEU:HD13	1:A:1239:ARG:NH1	2.35	0.41
2:B:830:TYR:HB3	2:B:831:SER:H	1.68	0.41
4:D:168:LYS:O	4:D:169:SER:HB3	2.20	0.41
1:A:877:HIS:C	1:A:878:ILE:CG1	2.89	0.41
2:B:210:LYS:HE2	2:B:462:ALA:HA	2.01	0.41
2:B:818:PRO:HB2	2:B:1091:TYR:OH	2.20	0.41
1:A:790:ASP:OD2	9:I:87:GLN:HG3	2.20	0.41
11:K:30:ALA:HB2	11:K:76:GLN:CG	2.41	0.41
3:C:11:ARG:H	3:C:20:PHE:HA	1.85	0.41
1:A:1230:GLU:O	1:A:1232:ASN:N	2.53	0.41
2:B:601:ARG:HH11	2:B:605:ARG:HH22	1.66	0.41
1:A:562:THR:HA	1:A:563:PRO:HD3	1.87	0.41
1:A:602:ASP:C	1:A:603:ASN:O	2.57	0.41
8:H:55:LEU:HB3	8:H:144:ILE:CG2	2.48	0.41
10:J:18:TRP:CH2	10:J:22:LEU:HD11	2.55	0.41
2:B:236:HIS:N	2:B:236:HIS:CD2	2.87	0.41
2:B:503:GLY:CA	2:B:507:LYS:HE2	2.31	0.41
1:A:685:GLU:OE2	1:A:686:ALA:HB2	2.20	0.41
5:E:91:LYS:C	5:E:93:MET:N	2.72	0.41
1:A:1101:LEU:CD1	1:A:1105:LEU:HD11	2.46	0.41
2:B:831:SER:HB3	2:B:994:TYR:OH	2.20	0.41
3:C:47:ASP:HA	3:C:169:LYS:NZ	2.35	0.41
1:A:767:GLN:NE2	1:A:774:ARG:CB	2.83	0.41
2:B:467:GLY:O	2:B:468:GLU:C	2.58	0.41
1:A:733:ALA:O	1:A:737:LEU:HG	2.20	0.41
4:D:205:ASP:O	4:D:209:ARG:HG3	2.20	0.41
1:A:164:ARG:CG	1:A:165:GLY:N	2.82	0.41
1:A:841:LEU:HD22	1:A:1371:LEU:HD13	2.01	0.41
4:D:178:ALA:O	4:D:181:GLY:N	2.53	0.41
1:A:1400:CYS:O	1:A:1405:THR:HA	2.20	0.41
1:A:705:LYS:O	1:A:706:HIS:C	2.58	0.41
2:B:435:THR:C	2:B:437:GLU:H	2.22	0.41
1:A:54:ASN:HD21	1:A:61:ILE:HD11	1.85	0.41
2:B:879:ARG:O	2:B:934:LYS:CE	2.69	0.41
7:G:137:ILE:HG21	7:G:143:ILE:HD11	2.03	0.41
2:B:828:ALA:HB2	2:B:1085:ILE:HG23	2.02	0.41
2:B:261:ARG:HG3	2:B:261:ARG:HH11	1.85	0.41
2:B:373:ARG:HD2	2:B:567:GLU:OE2	2.19	0.41
9:I:50:THR:CG2	9:I:51:ASN:N	2.83	0.41
8:H:64:ASN:ND2	8:H:88:SER:CB	2.68	0.41
6:F:135:ARG:NH2	6:F:145:ASP:OD2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:89:GLY:C	5:E:91:LYS:N	2.72	0.41
1:A:1425:SER:HA	1:A:1428:VAL:HG21	2.02	0.41
1:A:1239:ARG:C	1:A:1240:CYS:SG	2.98	0.41
2:B:416:LEU:O	2:B:420:LEU:HG	2.20	0.41
1:A:958:VAL:HG13	1:A:1052:GLN:HB3	2.02	0.41
1:A:469:ARG:NH2	2:B:991:GLY:O	2.46	0.41
1:A:1038:THR:OG1	1:A:1039:LYS:N	2.54	0.41
2:B:1162:ILE:HG22	2:B:1163:CYS:N	2.35	0.41
13:T:7:DC:H2"	13:T:8:DT:C6	2.54	0.41
1:A:1305:VAL:HG12	1:A:1306:LEU:N	2.34	0.41
2:B:529:GLU:OE2	2:B:769:TYR:HE1	2.03	0.41
1:A:451:HIS:NE2	1:A:1074:GLU:HG3	2.35	0.41
3:C:176:ILE:HG22	3:C:177:GLU:O	2.20	0.41
1:A:108:MET:O	1:A:109:HIS:CB	2.69	0.41
1:A:516:SER:O	1:A:517:ASN:C	2.58	0.41
1:A:789:LYS:HE3	9:I:67:THR:OG1	2.21	0.41
1:A:360:GLU:O	1:A:361:LEU:C	2.59	0.41
3:C:254:LYS:O	3:C:256:ALA:N	2.53	0.41
2:B:1214:PRO:HG2	2:B:1214:PRO:O	2.19	0.41
2:B:736:THR:O	2:B:736:THR:HG22	2.21	0.41
2:B:687:GLU:O	2:B:689:LEU:HD23	2.20	0.41
1:A:50:ILE:C	1:A:52:GLY:N	2.73	0.41
2:B:186:GLU:HG2	10:J:62:ARG:HH22	1.85	0.41
1:A:567:LYS:HG2	1:A:568:PRO:CD	2.49	0.41
2:B:311:LEU:O	2:B:314:LEU:N	2.53	0.41
2:B:312:GLU:O	2:B:315:LYS:N	2.45	0.41
7:G:15:PRO:HG3	7:G:66:GLY:C	2.40	0.41
1:A:598:LEU:HA	8:H:122:LEU:HD13	2.03	0.41
1:A:269:ILE:CD1	1:A:300:VAL:HA	2.49	0.41
10:J:44:TYR:HD2	10:J:44:TYR:N	2.05	0.41
2:B:834:ASN:ND2	2:B:1013:ASN:CA	2.83	0.41
1:A:1390:ASN:OD1	1:A:1399:ARG:HA	2.20	0.41
2:B:593:PRO:CG	2:B:617:ARG:CZ	2.91	0.41
1:A:23:SER:CA	1:A:233:TRP:NE1	2.76	0.41
1:A:24:PRO:O	1:A:27:VAL:HB	2.20	0.41
1:A:1002:GLY:HA3	1:A:1007:ILE:CG2	2.42	0.41
2:B:424:LEU:HD23	2:B:453:ILE:HD11	2.03	0.41
2:B:597:MET:O	2:B:598:GLU:C	2.58	0.41
2:B:555:ILE:HG22	2:B:556:THR:N	2.35	0.41
2:B:577:ALA:HB1	2:B:589:VAL:CG1	2.18	0.41
2:B:610:ASN:C	2:B:612:GLU:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:637:LEU:CD2	2:B:742:GLU:HA	2.51	0.41
2:B:184:ALA:HB1	2:B:188:ASP:HB2	2.03	0.41
1:A:563:PRO:HG2	8:H:79:TRP:CZ2	2.55	0.41
2:B:969:ARG:CD	3:C:61:GLU:OE2	2.69	0.41
3:C:66:ARG:NH1	10:J:2:ILE:HG23	2.35	0.41
7:G:122:ASN:HB2	7:G:131:GLN:NE2	2.17	0.41
7:G:145:VAL:CG1	7:G:146:LYS:N	2.83	0.41
2:B:361:LEU:CD2	2:B:364:ILE:HD12	2.51	0.41
1:A:590:ARG:O	1:A:591:PHE:CB	2.69	0.41
1:A:1104:ILE:HD12	1:A:1355:VAL:HG21	2.02	0.41
1:A:1384:VAL:C	1:A:1385:THR:CG2	2.89	0.41
2:B:864:LYS:HD2	2:B:872:GLU:CD	2.40	0.41
5:E:45:LYS:HD3	5:E:46:TYR:CE1	2.55	0.41
1:A:309:ALA:O	1:A:311:GLN:N	2.49	0.41
4:D:39:ASN:C	4:D:41:GLN:H	2.23	0.41
1:A:860:LEU:O	2:B:1224:PHE:CE2	2.70	0.41
1:A:1146:VAL:HG11	1:A:1207:LEU:HD12	2.02	0.41
1:A:1151:GLU:HB2	1:A:1153:TYR:HE1	1.86	0.41
2:B:1001:PHE:CD1	2:B:1001:PHE:C	2.93	0.41
5:E:52:ARG:CB	5:E:53:PRO:HD2	2.45	0.41
2:B:620:ARG:H	2:B:620:ARG:HG3	1.70	0.41
9:I:68:LEU:HB3	9:I:84:VAL:CG2	2.50	0.41
5:E:114:ASN:HD22	5:E:114:ASN:HA	1.58	0.41
1:A:102:VAL:HG11	1:A:211:PHE:CE2	2.55	0.41
1:A:211:PHE:HA	1:A:214:ILE:HG13	2.01	0.41
1:A:1176:LEU:C	1:A:1176:LEU:HD23	2.41	0.41
6:F:90:ARG:HG3	6:F:91:ALA:N	2.34	0.41
1:A:939:ASP:O	1:A:940:ARG:C	2.59	0.41
1:A:1072:ILE:HD11	1:A:1368:MET:HA	2.01	0.41
1:A:1142:THR:CA	1:A:1273:LEU:HD13	2.48	0.41
2:B:582:VAL:HG23	2:B:626:ILE:HD12	2.02	0.41
10:J:14:VAL:HG12	10:J:50:ILE:HD11	2.01	0.41
6:F:148:VAL:HG23	6:F:149:GLU:N	2.34	0.41
2:B:825:VAL:HG22	2:B:1010:LEU:HB3	2.02	0.41
10:J:32:GLU:CD	10:J:32:GLU:H	2.24	0.41
2:B:22:SER:HA	2:B:654:ARG:HB2	2.01	0.41
2:B:654:ARG:HG3	2:B:654:ARG:HH11	1.84	0.41
2:B:344:LYS:O	2:B:347:LYS:HG2	2.20	0.41
1:A:38:PRO:CG	1:A:39:GLU:N	2.83	0.41
2:B:190:TYR:CE2	10:J:62:ARG:HD3	2.55	0.41
1:A:531:ILE:HD13	1:A:653:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:83:GLN:C	8:H:85:GLY:H	2.23	0.41
2:B:799:PRO:HD3	10:J:1:MET:HG2	2.02	0.41
3:C:77:ILE:CA	3:C:129:ILE:HD11	2.50	0.41
10:J:1:MET:H3	10:J:56:LEU:N	2.18	0.41
10:J:57:ILE:HG23	10:J:58:GLU:N	2.35	0.41
7:G:121:PHE:HA	7:G:130:TYR:HA	2.02	0.41
6:F:109:VAL:CG2	6:F:124:GLU:HA	2.51	0.41
12:L:49:LYS:O	12:L:50:ASP:CB	2.69	0.41
5:E:64:PRO:O	5:E:65:THR:C	2.59	0.41
2:B:390:LEU:O	2:B:391:ASP:C	2.58	0.41
1:A:1449:SER:O	1:A:1453:TYR:CD1	2.73	0.41
1:A:1451:VAL:C	1:A:1453:TYR:N	2.73	0.41
6:F:70:LYS:HA	6:F:72:LYS:HZ1	1.85	0.41
6:F:72:LYS:HB3	6:F:73:ALA:H	1.64	0.41
5:E:13:TRP:O	5:E:16:PHE:HB3	2.21	0.41
1:A:1409:LEU:O	1:A:1412:ALA:N	2.51	0.41
2:B:900:ALA:HA	2:B:901:PRO:HD3	1.90	0.41
1:A:346:ASP:OD1	2:B:1108:ARG:HA	2.20	0.41
1:A:440:ASP:O	1:A:460:VAL:HG23	2.20	0.41
1:A:964:ILE:O	1:A:967:ALA:HB3	2.21	0.41
4:D:52:LEU:HA	4:D:148:LEU:HD21	2.03	0.41
1:A:1074:GLU:N	1:A:1075:PRO:HD2	2.35	0.41
1:A:841:LEU:HA	1:A:841:LEU:HD23	1.93	0.41
2:B:435:THR:C	2:B:437:GLU:N	2.73	0.41
2:B:43:LEU:HA	2:B:43:LEU:HD23	1.90	0.41
1:A:779:PHE:HD2	1:A:779:PHE:HA	1.71	0.41
2:B:865:LYS:CD	2:B:961:LEU:HD21	2.51	0.41
1:A:532:ARG:HG2	1:A:532:ARG:HH11	1.86	0.41
3:C:43:THR:CG2	3:C:44:LEU:N	2.57	0.41
2:B:798:TYR:CE2	3:C:62:PHE:CE2	3.07	0.41
10:J:1:MET:H2	10:J:57:ILE:H	1.65	0.41
7:G:125:SER:HB2	7:G:127:PRO:O	2.21	0.41
3:C:183:TRP:CH2	3:C:203:GLN:NE2	2.88	0.41
2:B:324:ILE:HG12	2:B:329:THR:HB	2.03	0.41
2:B:287:ARG:O	2:B:327:ARG:HA	2.21	0.41
8:H:64:ASN:CG	8:H:90:ALA:H	2.14	0.41
6:F:70:LYS:HA	6:F:72:LYS:NZ	2.35	0.41
7:G:8:SER:O	7:G:9:LEU:CB	2.68	0.41
1:A:456:MET:HE2	1:A:507:VAL:HG22	2.02	0.41
5:E:2:ASP:O	5:E:3:GLN:C	2.59	0.41
2:B:1106:ARG:HD3	2:B:1126:GLY:C	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:710:LEU:HD12	1:A:710:LEU:H	1.84	0.41
1:A:722:LEU:HD23	1:A:799:PHE:CG	2.55	0.41
2:B:981:ALA:HB3	2:B:1095:LEU:HD11	2.03	0.41
1:A:101:LYS:HE2	1:A:139:TRP:CH2	2.55	0.41
9:I:35:VAL:O	9:I:36:GLU:HB3	2.21	0.41
11:K:55:LYS:HB3	11:K:81:TYR:CE1	2.55	0.41
1:A:947:PHE:CE2	1:A:954:TRP:CD2	3.09	0.41
1:A:947:PHE:C	1:A:949:ASP:N	2.74	0.41
1:A:637:LYS:HB3	1:A:641:VAL:CG2	2.47	0.41
2:B:1055:ILE:C	2:B:1057:LYS:N	2.74	0.41
4:D:153:ARG:CZ	4:D:184:ALA:HA	2.50	0.41
3:C:42:PRO:HA	3:C:163:ILE:HG22	2.02	0.41
6:F:96:THR:O	6:F:100:GLN:HG3	2.20	0.41
2:B:605:ARG:HB3	2:B:688:GLY:HA3	2.02	0.41
2:B:693:ILE:HD13	2:B:701:ILE:CD1	2.50	0.41
1:A:37:PHE:H	1:A:37:PHE:HD1	1.63	0.41
8:H:118:PHE:C	8:H:120:GLY:N	2.67	0.41
3:C:104:PHE:HD2	3:C:105:GLY:H	1.68	0.41
3:C:131:HIS:O	3:C:133:ILE:N	2.53	0.41
3:C:77:ILE:HA	3:C:77:ILE:HD13	1.89	0.41
1:A:683:ILE:HG22	1:A:684:ALA:N	2.35	0.41
5:E:93:MET:O	5:E:94:LYS:C	2.59	0.41
1:A:1227:ILE:CG2	1:A:1228:TRP:H	2.20	0.41
2:B:859:TYR:CD1	2:B:859:TYR:N	2.88	0.41
2:B:996:ARG:HH12	3:C:38:ILE:HG23	1.86	0.41
4:D:3:VAL:CG1	4:D:4:SER:N	2.83	0.41
1:A:630:ILE:CG2	1:A:631:HIS:H	2.34	0.41
2:B:63:ILE:HD12	2:B:63:ILE:HA	1.89	0.41
7:G:26:LEU:O	7:G:27:LYS:C	2.59	0.41
2:B:581:PHE:O	2:B:626:ILE:N	2.53	0.41
2:B:487:THR:CG2	2:B:488:TYR:H	2.33	0.41
9:I:2:THR:O	9:I:3:THR:C	2.59	0.41
1:A:1141:THR:CA	1:A:1205:LYS:HZ3	2.32	0.41
2:B:275:TYR:HB3	2:B:351:TYR:OH	2.21	0.41
1:A:16:GLU:HB3	1:A:1418:LEU:HD11	2.03	0.41
1:A:34:LYS:HG2	1:A:34:LYS:HZ3	1.77	0.41
1:A:38:PRO:HG2	1:A:39:GLU:H	1.86	0.41
2:B:186:GLU:HG3	10:J:62:ARG:CZ	2.51	0.41
1:A:1098:VAL:HB	1:A:1099:PRO:HD3	2.03	0.41
8:H:100:THR:N	8:H:117:SER:O	2.45	0.41
8:H:82:PRO:O	8:H:84:ALA:N	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:102:GLN:HA	3:C:153:LEU:O	2.21	0.41
3:C:82:TYR:CD2	3:C:161:LYS:HG2	2.56	0.41
3:C:56:THR:HG22	3:C:58:LEU:HD23	2.02	0.41
3:C:77:ILE:CG2	3:C:78:GLU:N	2.76	0.41
10:J:3:VAL:HA	10:J:4:PRO:HD3	1.87	0.41
3:C:183:TRP:O	3:C:184:ASN:CB	2.69	0.41
1:A:12:ARG:HD2	2:B:1218:THR:CB	2.43	0.41
2:B:368:GLU:O	2:B:371:GLU:OE1	2.38	0.41
9:I:55:THR:O	9:I:56:ALA:C	2.59	0.41
2:B:265:SER:C	2:B:267:ARG:N	2.74	0.41
2:B:273:LEU:HD12	2:B:280:ILE:HD12	2.03	0.41
1:A:265:LYS:HG3	1:A:265:LYS:O	2.21	0.41
1:A:445:ASN:ND2	1:A:446:ARG:N	2.68	0.41
1:A:1144:LYS:HD2	1:A:1269:GLU:HG3	2.02	0.41
1:A:15:LYS:HB2	2:B:1219:ASP:O	2.21	0.41
1:A:1239:ARG:HH11	1:A:1239:ARG:HB3	1.86	0.41
1:A:868:TYR:CZ	1:A:1366:ARG:HD3	2.56	0.41
2:B:1110:PRO:O	2:B:1119:VAL:HG22	2.21	0.41
1:A:1037:LEU:HD12	1:A:1042:PHE:N	2.36	0.41
2:B:457:LEU:O	2:B:458:LYS:C	2.58	0.41
4:D:175:PHE:O	4:D:179:GLN:HG2	2.21	0.41
4:D:60:LYS:HE2	4:D:126:ILE:HD11	2.03	0.41
4:D:155:ARG:O	4:D:156:ASP:HB2	2.20	0.41
1:A:746:MET:HE1	2:B:1018:PRO:HG2	2.03	0.41
1:A:1343:ALA:CB	5:E:150:VAL:HG22	2.43	0.41
1:A:800:VAL:HG13	1:A:812:GLU:OE2	2.21	0.41
2:B:112:LEU:HD12	2:B:113:TYR:N	2.32	0.41
1:A:376:TYR:HB3	1:A:434:ARG:NH1	2.36	0.41
1:A:244:PRO:HG2	1:A:245:PRO:CD	2.50	0.41
2:B:227:LYS:HB2	2:B:395:GLN:OE1	2.21	0.41
3:C:254:LYS:C	3:C:256:ALA:N	2.74	0.41
11:K:14:GLU:O	11:K:15:GLY:O	2.39	0.41
2:B:133:LYS:CG	2:B:135:ARG:HE	2.34	0.41
2:B:601:ARG:HD3	2:B:605:ARG:HH21	1.85	0.41
2:B:343:ILE:CG2	2:B:347:LYS:HE2	2.42	0.41
1:A:49:LYS:NZ	1:A:61:ILE:CG1	2.72	0.41
2:B:187:SER:O	2:B:191:LYS:HG3	2.21	0.41
12:L:52:GLY:O	12:L:53:HIS:C	2.59	0.41
1:A:568:PRO:HB2	3:C:221:TYR:CZ	2.56	0.41
3:C:204:SER:N	3:C:207:CYS:HG	2.17	0.41
5:E:145:THR:HG21	5:E:187:TYR:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:79:ARG:HH11	6:F:79:ARG:CB	2.29	0.41
5:E:116:ILE:CG2	5:E:117:THR:H	2.34	0.41
5:E:89:GLY:O	5:E:91:LYS:N	2.54	0.41
1:A:866:PHE:HB2	5:E:208:TYR:OH	2.21	0.41
1:A:1143:LEU:CD2	1:A:1267:MET:HB3	2.48	0.41
2:B:413:LEU:O	2:B:416:LEU:HB2	2.21	0.41
1:A:1308:THR:HG23	1:A:1310:GLY:N	2.28	0.41
1:A:390:GLN:O	1:A:394:ASN:N	2.54	0.41
1:A:966:ASN:C	1:A:968:GLN:N	2.73	0.41
4:D:33:PHE:CE1	7:G:80:LYS:HD3	2.56	0.41
4:D:67:ARG:HH21	4:D:129:LEU:HD13	1.86	0.41
2:B:1017:ILE:CB	2:B:1018:PRO:CD	2.99	0.41
2:B:488:TYR:CE2	2:B:813:LYS:HB2	2.55	0.41
1:A:152:VAL:HG12	1:A:153:PRO:CD	2.51	0.41
3:C:192:TRP:CZ3	3:C:194:GLU:HG3	2.56	0.41
1:A:553:VAL:HA	1:A:554:PRO:HD2	1.89	0.41
7:G:164:LYS:O	7:G:164:LYS:HG2	2.21	0.41
8:H:31:THR:O	8:H:31:THR:HG22	2.20	0.41
1:A:814:PHE:O	1:A:814:PHE:CD2	2.74	0.40
2:B:610:ASN:HA	2:B:611:PRO:HD3	1.89	0.40
1:A:568:PRO:HB3	3:C:221:TYR:OH	2.21	0.40
1:A:472:LEU:CD1	2:B:835:GLN:NE2	2.84	0.40
3:C:252:GLN:CG	11:K:95:ILE:HG23	2.50	0.40
7:G:127:PRO:CG	7:G:139:ILE:HG13	2.50	0.40
9:I:99:LEU:C	9:I:100:PHE:HD1	2.24	0.40
1:A:595:THR:O	1:A:596:THR:CG2	2.68	0.40
5:E:124:VAL:HB	5:E:125:PRO:HD3	2.03	0.40
3:C:116:LYS:HD3	3:C:140:ASN:HA	2.02	0.40
10:J:47:ARG:HG2	10:J:47:ARG:NH1	2.35	0.40
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.20	0.40
6:F:82:THR:HG22	6:F:84:TYR:N	2.35	0.40
2:B:980:PHE:CE2	2:B:1094:ARG:HB2	2.56	0.40
1:A:714:PHE:O	1:A:715:GLU:C	2.60	0.40
1:A:767:GLN:HE21	1:A:774:ARG:HB3	1.87	0.40
4:D:60:LYS:NZ	4:D:122:GLU:OE2	2.53	0.40
4:D:51:ASN:C	4:D:52:LEU:O	2.57	0.40
1:A:106:VAL:CG1	1:A:107:CYS:N	2.82	0.40
1:A:731:ARG:O	1:A:732:LEU:C	2.59	0.40
6:F:90:ARG:CG	6:F:91:ALA:N	2.84	0.40
1:A:1356:ILE:O	1:A:1356:ILE:HG22	2.21	0.40
8:H:4:THR:CG2	8:H:5:LEU:N	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:197:LYS:HG2	5:E:199:ILE:CG1	2.50	0.40
9:I:94:ASP:O	9:I:95:THR:O	2.40	0.40
1:A:569:LYS:O	1:A:571:LEU:HD13	2.20	0.40
7:G:53:ASN:HD22	7:G:53:ASN:N	2.18	0.40
1:A:779:PHE:CD1	1:A:784:LEU:HA	2.56	0.40
2:B:26:THR:O	2:B:29:ASP:HB2	2.22	0.40
2:B:605:ARG:HB3	2:B:688:GLY:HA2	2.03	0.40
1:A:49:LYS:HZ1	1:A:61:ILE:CB	2.34	0.40
3:C:249:ASP:O	3:C:252:GLN:HB3	2.21	0.40
7:G:88:ASP:HB3	7:G:144:ARG:CB	2.51	0.40
2:B:1033:LYS:NZ	2:B:1070:GLU:OE1	2.45	0.40
3:C:191:TYR:HD2	3:C:201:TRP:CD1	2.39	0.40
5:E:28:TYR:CE2	5:E:78:LEU:HB2	2.56	0.40
2:B:259:TYR:N	2:B:259:TYR:CD1	2.89	0.40
2:B:287:ARG:NH1	2:B:325:GLN:HA	2.36	0.40
1:A:1425:SER:O	1:A:1428:VAL:HG23	2.22	0.40
2:B:894:ASP:HB2	12:L:58:LYS:HZ1	1.85	0.40
2:B:980:PHE:CD2	2:B:1094:ARG:HA	2.56	0.40
7:G:1:MET:CE	7:G:3:PHE:CE1	3.05	0.40
4:D:138:ASN:OD1	4:D:141:LEU:HB2	2.21	0.40
1:A:26:GLU:O	1:A:27:VAL:C	2.58	0.40
13:T:9:DC:H2"	13:T:10:DA:H8	1.78	0.40
1:A:606:LEU:HD11	1:A:608:ILE:HG13	2.03	0.40
1:A:1342:GLU:OE2	5:E:212:ARG:NH1	2.53	0.40
2:B:856:PHE:N	2:B:856:PHE:CD1	2.89	0.40
1:A:1219:THR:HG21	1:A:1271:ILE:CD1	2.45	0.40
1:A:253:ASN:ND2	1:A:256:GLN:NE2	2.67	0.40
2:B:661:LEU:C	2:B:663:ALA:H	2.22	0.40
9:I:95:THR:CG2	9:I:96:SER:N	2.84	0.40
1:A:100:LYS:O	1:A:104:GLU:HG3	2.20	0.40
1:A:1354:ASN:HA	1:A:1357:ALA:HB3	2.03	0.40
1:A:1026:LEU:HD23	1:A:1026:LEU:HA	1.89	0.40
2:B:658:ILE:HG22	2:B:662:MET:CE	2.51	0.40
1:A:241:VAL:O	1:A:242:PRO:C	2.58	0.40
2:B:878:GLN:O	2:B:934:LYS:HE2	2.21	0.40
1:A:524:VAL:HG12	1:A:525:GLN:HG3	2.02	0.40
1:A:600:PRO:HA	8:H:25:ARG:CZ	2.51	0.40
8:H:87:ARG:O	8:H:89:LEU:HG	2.21	0.40
7:G:144:ARG:O	7:G:168:LEU:HD22	2.22	0.40
2:B:324:ILE:HD13	2:B:330:ALA:HA	2.03	0.40
2:B:289:LEU:O	2:B:371:GLU:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:LYS:HZ3	1:A:302:THR:HG21	1.86	0.40
6:F:70:LYS:C	6:F:72:LYS:HZ2	2.22	0.40
1:A:1165:GLU:OE1	1:A:1194:ARG:NH2	2.54	0.40
2:B:906:SER:HA	2:B:946:ASN:CB	2.44	0.40
3:C:259:LEU:O	3:C:262:LEU:N	2.53	0.40
11:K:11:LEU:N	11:K:11:LEU:CD2	2.82	0.40
1:A:1019:CYS:O	1:A:1020:CYS:C	2.59	0.40
2:B:172:ILE:HG22	2:B:173:MET:N	2.36	0.40
7:G:26:LEU:O	7:G:29:LYS:N	2.54	0.40
2:B:465:ASN:O	2:B:467:GLY:N	2.54	0.40
1:A:1072:ILE:O	1:A:1075:PRO:HD2	2.21	0.40
4:D:205:ASP:O	4:D:208:GLU:HB3	2.21	0.40
2:B:222:ILE:N	2:B:240:ILE:HG13	2.36	0.40
1:A:474:VAL:CG2	1:A:474:VAL:O	2.68	0.40
11:K:83:PRO:O	11:K:84:LYS:C	2.60	0.40
4:D:218:GLU:O	4:D:219:THR:C	2.60	0.40
2:B:790:ASP:N	2:B:790:ASP:OD2	2.52	0.40
1:A:359:LEU:HD23	1:A:359:LEU:HA	1.87	0.40
2:B:530:GLY:C	2:B:531:GLN:HG2	2.41	0.40
1:A:525:GLN:O	1:A:526:ASP:C	2.60	0.40
7:G:113:HIS:O	7:G:114:LEU:HB2	2.21	0.40
2:B:383:ASN:CG	2:B:387:LEU:HD11	2.42	0.40
2:B:391:ASP:CB	9:I:92:ARG:HG3	2.52	0.40
5:E:117:THR:C	5:E:119:SER:N	2.75	0.40
5:E:117:THR:CG2	5:E:120:ALA:H	2.34	0.40
1:A:265:LYS:HE3	1:A:265:LYS:HA	2.03	0.40
5:E:164:LEU:HD21	5:E:211:TYR:CG	2.57	0.40
12:L:27:LEU:HD13	12:L:37:LYS:HG2	2.03	0.40
4:D:39:ASN:HD21	4:D:41:GLN:HB2	1.79	0.40
1:A:1437:GLY:C	1:A:1439:GLY:N	2.75	0.40
7:G:9:LEU:C	7:G:9:LEU:HD12	2.41	0.40
2:B:901:PRO:HD2	12:L:59:ALA:O	2.22	0.40
12:L:58:LYS:O	12:L:59:ALA:O	2.39	0.40
11:K:67:PHE:C	11:K:68:PHE:CD2	2.87	0.40
1:A:975:HIS:HA	1:A:1036:ARG:HG3	2.02	0.40
4:D:175:PHE:HZ	7:G:85:GLU:HG3	1.87	0.40
1:A:215:SER:HB3	1:A:218:ASP:HB2	2.03	0.40
9:I:4:PHE:HD1	9:I:4:PHE:O	2.05	0.40
9:I:5:ARG:NE	9:I:36:GLU:OE2	2.55	0.40
6:F:75:PRO:O	6:F:77:ASP:N	2.54	0.40
4:D:139:LYS:HG3	4:D:143:ASN:HD22	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:LYS:O	1:A:130:ASP:CB	2.66	0.40
1:A:1006:ILE:HD12	5:E:163:GLU:HG3	2.00	0.40
1:A:1076:ALA:HA	1:A:1079:MET:CE	2.51	0.40
2:B:102:VAL:HB	2:B:110:HIS:H	1.86	0.40
1:A:447:GLN:HA	1:A:448:PRO:C	2.41	0.40
9:I:2:THR:CG2	9:I:3:THR:H	2.31	0.40
2:B:737:THR:HG22	9:I:66:PRO:HA	2.02	0.40
1:A:703:THR:C	1:A:705:LYS:H	2.24	0.40
2:B:814:PHE:C	2:B:816:GLU:H	2.24	0.40
1:A:1126:ALA:O	1:A:1128:GLN:N	2.55	0.40
1:A:1349:TYR:CD2	1:A:1349:TYR:C	2.94	0.40
2:B:1045:SER:O	2:B:1046:PRO:O	2.39	0.40
2:B:31:TRP:HE3	2:B:31:TRP:HA	1.85	0.40
2:B:351:TYR:CE2	2:B:355:ILE:HD11	2.55	0.40
7:G:14:HIS:C	7:G:16:SER:N	2.75	0.40
7:G:12:THR:HA	7:G:68:ALA:O	2.22	0.40
1:A:681:GLU:C	1:A:683:ILE:H	2.24	0.40
8:H:128:ASN:N	8:H:130:ARG:HH11	2.10	0.40
1:A:1208:THR:HG22	1:A:1210:GLY:H	1.85	0.40
11:K:42:LEU:HD23	11:K:42:LEU:C	2.42	0.40
2:B:1152:MET:C	2:B:1157:ALA:HB2	2.42	0.40
1:A:767:GLN:NE2	1:A:774:ARG:HB3	2.37	0.40
6:F:138:LEU:HA	6:F:138:LEU:HD23	1.99	0.40
1:A:110:CYS:SG	1:A:111:GLY:N	2.94	0.40
2:B:293:PRO:CG	2:B:296:GLU:OE1	2.70	0.40
13:T:12:DG:N2	14:N:6:DT:O2	2.55	0.40
2:B:469:GLN:CG	2:B:470:LYS:N	2.84	0.40
5:E:176:PRO:O	5:E:212:ARG:HA	2.21	0.40
2:B:766:ARG:HH21	15:P:11:U:H3	1.70	0.40
1:A:947:PHE:HE2	1:A:954:TRP:CD1	2.40	0.40
6:F:89:GLU:HB3	6:F:134:ILE:HD11	2.03	0.40
2:B:816:GLU:OE1	2:B:816:GLU:N	2.55	0.40
2:B:228:LYS:HD3	2:B:228:LYS:HA	1.94	0.40

There are no symmetry-related clashes.

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	1421/1733 (82%)	909 (64%)	310 (22%)	202 (14%)	0	6
2	B	1111/1224 (91%)	694 (62%)	257 (23%)	160 (14%)	0	6
3	C	268/324 (83%)	164 (61%)	66 (25%)	38 (14%)	0	6
4	D	183/221 (83%)	108 (59%)	49 (27%)	26 (14%)	0	6
5	E	212/215 (99%)	134 (63%)	49 (23%)	29 (14%)	0	6
6	F	86/155 (56%)	60 (70%)	20 (23%)	6 (7%)	1	22
7	G	169/171 (99%)	127 (75%)	32 (19%)	10 (6%)	2	27
8	H	133/146 (91%)	72 (54%)	37 (28%)	24 (18%)	0	3
9	I	114/122 (93%)	73 (64%)	26 (23%)	15 (13%)	0	6
10	J	63/70 (90%)	34 (54%)	13 (21%)	16 (25%)	0	1
11	K	114/120 (95%)	79 (69%)	26 (23%)	9 (8%)	1	18
12	L	45/70 (64%)	19 (42%)	11 (24%)	15 (33%)	0	0
All	All	3919/4571 (86%)	2473 (63%)	896 (23%)	550 (14%)	0	6

All (550) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	41	MET
1	A	43	GLU
1	A	48	ALA
1	A	58	LEU
1	A	63	ARG
1	A	67	CYS
1	A	70	CYS
1	A	74	MET
1	A	76	GLU
1	A	93	VAL
1	A	130	ASP

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Mol	Chain	Res	Type
1	A	154	SER
1	A	167	CYS
1	A	259	GLU
1	A	311	GLN
1	A	312	PRO
1	A	317	LYS
1	A	318	SER
1	A	399	HIS
1	A	409	SER
1	A	410	GLY
1	A	535	THR
1	A	536	LEU
1	A	543	LEU
1	A	544	ASP
1	A	556	TRP
1	A	567	LYS
1	A	583	PRO
1	A	619	LYS
1	A	666	ILE
1	A	705	LYS
1	A	846	GLU
1	A	871	ASP
1	A	885	THR
1	A	968	GLN
1	A	986	ILE
1	A	1002	GLY
1	A	1016	THR
1	A	1110	ASN
1	A	1114	PRO
1	A	1115	SER
1	A	1116	LEU
1	A	1122	PRO
1	A	1124	HIS
1	A	1177	LEU
1	A	1178	ASP
1	A	1206	ASP
1	A	1212	VAL
1	A	1244	ARG
1	A	1255	GLU
1	A	1314	SER
1	A	1341	ILE
1	A	1393	ASN

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Mol	Chain	Res	Type
1	A	1448	GLU
2	B	21	GLU
2	B	41	LYS
2	B	65	GLU
2	B	108	VAL
2	B	124	TYR
2	B	134	LYS
2	B	184	ALA
2	B	206	ASN
2	B	259	TYR
2	B	262	GLU
2	B	265	SER
2	B	266	ALA
2	B	278	GLN
2	B	282	ILE
2	B	295	GLY
2	B	343	ILE
2	B	344	LYS
2	B	345	LYS
2	B	346	GLU
2	B	365	THR
2	B	367	LEU
2	B	391	ASP
2	B	409	ALA
2	B	450	ALA
2	B	468	GLU
2	B	469	GLN
2	B	509	ALA
2	B	511	PRO
2	B	512	ARG
2	B	577	ALA
2	B	705	MET
2	B	708	GLU
2	B	709	ASP
2	B	751	VAL
2	B	878	GLN
2	B	879	ARG
2	B	892	LYS
2	B	958	GLN
2	B	987	LYS
2	B	1045	SER
2	B	1046	PRO

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Mol	Chain	Res	Type
2	B	1069	PHE
2	B	1097	HIS
2	B	1099	VAL
2	B	1143	ALA
2	B	1144	ALA
2	B	1157	ALA
2	B	1175	LEU
2	B	1183	LYS
3	C	4	GLU
3	C	56	THR
3	C	60	ASP
3	C	74	SER
3	C	90	ASP
3	C	141	GLY
3	C	149	LYS
3	C	161	LYS
3	C	213	PRO
3	C	214	ASN
3	C	237	SER
4	D	19	GLU
4	D	21	GLU
4	D	52	LEU
4	D	114	MET
4	D	131	GLU
4	D	169	SER
4	D	198	LEU
4	D	218	GLU
5	E	45	LYS
5	E	88	VAL
5	E	93	MET
5	E	97	VAL
5	E	106	GLN
5	E	115	ASN
5	E	129	PRO
5	E	174	GLN
6	F	72	LYS
6	F	81	THR
6	F	114	GLU
7	G	2	PHE
7	G	63	PRO
7	G	114	LEU
7	G	120	THR

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Mol	Chain	Res	Type
7	G	139	ILE
7	G	141	SER
7	G	154	VAL
8	H	78	SER
8	H	81	PRO
8	H	82	PRO
8	H	87	ARG
8	H	109	LYS
8	H	128	ASN
8	H	131	ASN
8	H	140	ALA
9	I	32	CYS
9	I	79	HIS
9	I	95	THR
9	I	106	CYS
10	J	2	ILE
10	J	64	ASN
11	K	8	GLU
12	L	40	LEU
12	L	42	ARG
12	L	50	ASP
12	L	55	ILE
12	L	59	ALA
12	L	60	ARG
1	A	5	GLN
1	A	8	SER
1	A	42	ASP
1	A	57	ARG
1	A	84	ILE
1	A	96	ILE
1	A	126	LEU
1	A	131	SER
1	A	148	CYS
1	A	283	GLY
1	A	287	HIS
1	A	392	VAL
1	A	439	ASN
1	A	516	SER
1	A	517	ASN
1	A	591	PHE
1	A	604	GLY
1	A	625	SER

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Mol	Chain	Res	Type
1	A	706	HIS
1	A	726	ARG
1	A	775	ILE
1	A	852	TYR
1	A	872	GLY
1	A	958	VAL
1	A	969	GLN
1	A	1036	ARG
1	A	1054	LEU
1	A	1095	THR
1	A	1097	GLY
1	A	1123	GLY
1	A	1127	ASP
1	A	1133	LEU
1	A	1140	HIS
1	A	1167	GLU
1	A	1176	LEU
1	A	1221	LYS
1	A	1229	SER
1	A	1233	ASP
1	A	1278	ASN
1	A	1316	VAL
1	A	1331	SER
1	A	1365	TYR
1	A	1390	ASN
1	A	1405	THR
1	A	1438	THR
1	A	1450	LEU
1	A	1454	MET
2	B	46	GLN
2	B	115	GLN
2	B	168	GLY
2	B	229	ALA
2	B	257	LYS
2	B	258	LEU
2	B	260	GLY
2	B	277	LYS
2	B	294	ASP
2	B	308	TRP
2	B	312	GLU
2	B	327	ARG
2	B	368	GLU

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Mol	Chain	Res	Type
2	B	466	TRP
2	B	480	SER
2	B	483	LEU
2	B	506	GLY
2	B	575	PRO
2	B	598	GLU
2	B	629	ASP
2	B	655	LYS
2	B	711	GLU
2	B	712	PRO
2	B	728	ARG
2	B	735	ALA
2	B	752	ALA
2	B	882	THR
2	B	907	GLY
2	B	943	SER
2	B	951	GLN
2	B	1003	ALA
2	B	1006	ILE
2	B	1041	GLU
2	B	1075	GLY
2	B	1103	ILE
2	B	1108	ARG
2	B	1112	GLN
2	B	1155	SER
2	B	1167	GLY
2	B	1171	VAL
2	B	1176	ASN
2	B	1181	GLU
2	B	1186	ASP
3	C	17	ASN
3	C	78	GLU
3	C	89	GLU
3	C	110	THR
3	C	132	PRO
3	C	175	ALA
4	D	12	ARG
4	D	16	LYS
4	D	20	GLU
4	D	112	ASP
4	D	117	GLU
4	D	168	LYS

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Mol	Chain	Res	Type
4	D	201	LYS
4	D	220	LEU
5	E	3	GLN
5	E	43	LYS
5	E	66	GLU
5	E	70	SER
5	E	73	PRO
5	E	76	GLY
5	E	94	LYS
5	E	130	ALA
6	F	128	LYS
7	G	9	LEU
8	H	2	SER
8	H	6	PHE
8	H	84	ALA
8	H	92	ASP
8	H	110	ASP
8	H	119	GLY
8	H	137	GLN
9	I	3	THR
9	I	56	ALA
10	J	6	ARG
10	J	17	LYS
10	J	24	LEU
10	J	42	LYS
11	K	15	GLY
12	L	37	LYS
12	L	45	ALA
12	L	53	HIS
12	L	56	LEU
1	A	54	ASN
1	A	187	LYS
1	A	194	ALA
1	A	219	PHE
1	A	222	LEU
1	A	257	ARG
1	A	286	HIS
1	A	331	GLY
1	A	332	LYS
1	A	382	PRO
1	A	419	LYS
1	A	465	TYR

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Mol	Chain	Res	Type
1	A	483	ASP
1	A	510	GLN
1	A	538	ASP
1	A	557	ASP
1	A	568	PRO
1	A	597	LEU
1	A	600	PRO
1	A	731	ARG
1	A	734	GLU
1	A	789	LYS
1	A	875	ALA
1	A	895	LYS
1	A	910	PRO
1	A	979	SER
1	A	1098	VAL
1	A	1168	GLU
1	A	1211	GLN
1	A	1223	ASP
1	A	1270	ASN
1	A	1388	GLY
1	A	1416	ALA
1	A	1435	PRO
2	B	28	GLU
2	B	48	LEU
2	B	100	PRO
2	B	135	ARG
2	B	186	GLU
2	B	197	PHE
2	B	267	ARG
2	B	305	VAL
2	B	384	ARG
2	B	385	LEU
2	B	394	ASP
2	B	510	LYS
2	B	543	SER
2	B	591	ARG
2	B	707	PRO
2	B	746	SER
2	B	793	ALA
2	B	797	TYR
2	B	848	ARG
2	B	942	ARG

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Mol	Chain	Res	Type
2	B	957	ASN
2	B	1017	ILE
2	B	1056	SER
2	B	1074	ASN
2	B	1082	MET
3	C	9	LYS
3	C	10	ILE
3	C	25	VAL
3	C	109	SER
3	C	127	ARG
3	C	128	ASN
3	C	191	TYR
3	C	209	TYR
3	C	218	PRO
3	C	240	VAL
3	C	269	LYS
4	D	4	SER
4	D	47	LEU
4	D	61	GLU
4	D	156	ASP
4	D	192	LYS
5	E	36	GLU
5	E	64	PRO
5	E	74	ASP
5	E	86	PRO
5	E	148	GLU
6	F	71	GLU
8	H	14	GLU
8	H	32	THR
8	H	63	LEU
8	H	90	ALA
9	I	8	ARG
9	I	57	GLY
9	I	62	ILE
10	J	14	VAL
10	J	28	ASP
10	J	57	ILE
11	K	29	ASN
12	L	28	LYS
1	A	35	ILE
1	A	51	GLY
1	A	71	GLN

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Mol	Chain	Res	Type
1	A	169	ASN
1	A	186	LYS
1	A	232	GLU
1	A	253	ASN
1	A	281	HIS
1	A	418	SER
1	A	424	ILE
1	A	684	ALA
1	A	692	ASP
1	A	830	LYS
1	A	847	ASP
1	A	891	ALA
1	A	972	HIS
1	A	973	ILE
1	A	1067	LEU
1	A	1111	MET
1	A	1165	GLU
1	A	1242	VAL
1	A	1403	GLU
2	B	24	PRO
2	B	45	SER
2	B	114	PRO
2	B	309	GLN
2	B	341	LEU
2	B	369	GLY
2	B	456	GLY
2	B	559	SER
2	B	761	HIS
2	B	828	ALA
2	B	867	GLY
2	B	868	MET
2	B	881	ASN
2	B	901	PRO
2	B	937	ALA
2	B	1035	ALA
2	B	1203	LEU
3	C	125	MET
3	C	133	ILE
3	C	169	LYS
3	C	184	ASN
3	C	216	GLY
4	D	15	LEU

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Mol	Chain	Res	Type
4	D	157	GLN
4	D	203	SER
5	E	6	GLU
5	E	90	VAL
5	E	122	LYS
5	E	187	TYR
8	H	17	PRO
8	H	52	GLN
8	H	108	SER
9	I	9	ASP
9	I	34	TYR
9	I	58	VAL
10	J	9	SER
10	J	29	GLU
10	J	55	ASP
11	K	14	GLU
12	L	35	SER
12	L	39	SER
1	A	44	THR
1	A	155	GLU
1	A	164	ARG
1	A	196	GLU
1	A	234	MET
1	A	322	VAL
1	A	700	ASN
1	A	713	SER
1	A	718	VAL
1	A	1014	ALA
1	A	1108	ALA
1	A	1378	GLN
2	B	30	SER
2	B	37	PHE
2	B	325	GLN
2	B	334	ILE
2	B	353	LYS
2	B	467	GLY
2	B	566	LEU
2	B	613	VAL
2	B	687	GLU
2	B	792	MET
2	B	946	ASN
2	B	1178	ASN

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Mol	Chain	Res	Type
2	B	1214	PRO
3	C	3	GLU
3	C	108	GLU
3	C	142	VAL
4	D	40	HIS
5	E	12	LEU
5	E	59	SER
5	E	121	MET
6	F	139	PRO
8	H	105	GLU
9	I	65	ASP
9	I	107	SER
11	K	53	ASP
11	K	90	ALA
12	L	25	ALA
1	A	52	GLY
1	A	73	GLY
1	A	197	PRO
1	A	313	GLN
1	A	400	PRO
1	A	603	ASN
1	A	650	GLN
1	A	673	GLY
1	A	780	VAL
1	A	987	VAL
1	A	1164	PRO
2	B	187	SER
2	B	435	THR
2	B	540	SER
2	B	620	ARG
2	B	780	VAL
2	B	1131	GLY
4	D	191	ALA
9	I	11	ASN
10	J	13	VAL
10	J	32	GLU
11	K	79	GLU
12	L	46	VAL
1	A	59	GLY
1	A	138	ILE
1	A	250	ILE
1	A	623	GLY

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Mol	Chain	Res	Type
1	A	1437	GLY
3	C	126	GLY
7	G	20	PRO
11	K	43	GLY
1	A	77	CYS
1	A	223	GLY
1	A	245	PRO
1	A	258	GLY
1	A	719	VAL
1	A	765	VAL
1	A	1263	ILE
2	B	283	VAL
2	B	501	PRO
8	H	120	GLY
10	J	33	GLY
1	A	158	PRO
1	A	207	ILE
1	A	244	PRO
1	A	585	GLY
1	A	693	VAL
1	A	888	GLY
1	A	1428	VAL
2	B	284	ILE
2	B	355	ILE
2	B	562	GLY
2	B	729	ILE
3	C	182	PRO
10	J	4	PRO
11	K	66	PRO
1	A	385	ILE
2	B	592	ASN
7	G	92	VAL
1	A	948	VAL
5	E	154	ILE

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	1249/1520 (82%)	1135 (91%)	114 (9%)	12	49
2	B	974/1061 (92%)	879 (90%)	95 (10%)	10	45
3	C	238/280 (85%)	215 (90%)	23 (10%)	10	46
4	D	167/200 (84%)	145 (87%)	22 (13%)	5	31
5	E	196/197 (100%)	179 (91%)	17 (9%)	13	51
6	F	78/137 (57%)	69 (88%)	9 (12%)	7	37
7	G	152/152 (100%)	138 (91%)	14 (9%)	11	49
8	H	121/128 (94%)	112 (93%)	9 (7%)	17	58
9	I	110/116 (95%)	98 (89%)	12 (11%)	8	40
10	J	60/65 (92%)	55 (92%)	5 (8%)	14	53
11	K	99/102 (97%)	87 (88%)	12 (12%)	6	34
12	L	41/57 (72%)	35 (85%)	6 (15%)	4	27
All	All	3485/4015 (87%)	3147 (90%)	338 (10%)	10	46

All (338) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	18	GLN
1	A	32	VAL
1	A	34	LYS
1	A	37	PHE
1	A	41	MET
1	A	57	ARG
1	A	58	LEU
1	A	68	GLN
1	A	83	HIS
1	A	93	VAL
1	A	103	CYS
1	A	108	MET
1	A	174	ILE
1	A	179	LEU
1	A	185	TRP
1	A	196	GLU
1	A	204	THR
1	A	236	LEU
1	A	245	PRO
1	A	281	HIS
1	A	307	ASP

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Mol	Chain	Res	Type
1	A	312	PRO
1	A	320	ARG
1	A	322	VAL
1	A	326	ARG
1	A	332	LYS
1	A	333	GLU
1	A	335	ARG
1	A	337	ARG
1	A	345	VAL
1	A	351	THR
1	A	379	VAL
1	A	385	ILE
1	A	393	ARG
1	A	408	ASP
1	A	425	GLN
1	A	428	TYR
1	A	438	ASP
1	A	442	VAL
1	A	443	LEU
1	A	445	ASN
1	A	447	GLN
1	A	450	LEU
1	A	451	HIS
1	A	453	MET
1	A	466	SER
1	A	469	ARG
1	A	479	ASN
1	A	481	ASP
1	A	489	LEU
1	A	493	GLN
1	A	518	LYS
1	A	590	ARG
1	A	618	GLU
1	A	635	ARG
1	A	701	LEU
1	A	711	ARG
1	A	758	ILE
1	A	774	ARG
1	A	779	PHE
1	A	821	ARG
1	A	833	GLU
1	A	839	ARG

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Mol	Chain	Res	Type
1	A	858	ASN
1	A	903	ASN
1	A	906	HIS
1	A	923	LEU
1	A	929	LEU
1	A	930	ASP
1	A	942	PHE
1	A	961	ARG
1	A	969	GLN
1	A	998	LEU
1	A	1001	ARG
1	A	1009	ASN
1	A	1029	ARG
1	A	1035	TYR
1	A	1037	LEU
1	A	1038	THR
1	A	1058	VAL
1	A	1101	LEU
1	A	1120	LEU
1	A	1122	PRO
1	A	1124	HIS
1	A	1146	VAL
1	A	1152	ILE
1	A	1174	PHE
1	A	1178	ASP
1	A	1191	TRP
1	A	1193	LEU
1	A	1195	LEU
1	A	1214	GLU
1	A	1223	ASP
1	A	1240	CYS
1	A	1245	PRO
1	A	1255	GLU
1	A	1259	MET
1	A	1260	LEU
1	A	1264	GLU
1	A	1271	ILE
1	A	1295	THR
1	A	1297	GLU
1	A	1308	THR
1	A	1333	ILE
1	A	1364	ASN

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Mol	Chain	Res	Type
1	A	1371	LEU
1	A	1372	VAL
1	A	1393	ASN
1	A	1400	CYS
1	A	1408	ILE
1	A	1444	MET
1	A	1445	ILE
1	A	1449	SER
2	B	20	ASP
2	B	30	SER
2	B	44	VAL
2	B	46	GLN
2	B	57	TYR
2	B	61	ASP
2	B	100	PRO
2	B	164	LYS
2	B	167	ILE
2	B	170	LEU
2	B	175	ARG
2	B	194	GLU
2	B	203	PHE
2	B	213	ILE
2	B	217	ARG
2	B	272	THR
2	B	332	ASP
2	B	365	THR
2	B	371	GLU
2	B	376	PHE
2	B	378	LEU
2	B	393	LYS
2	B	396	ASP
2	B	426	LYS
2	B	429	PHE
2	B	455	SER
2	B	465	ASN
2	B	466	TRP
2	B	468	GLU
2	B	482	VAL
2	B	485	ARG
2	B	502	ILE
2	B	510	LYS
2	B	516	ASN

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Mol	Chain	Res	Type
2	B	557	PHE
2	B	563	MET
2	B	570	VAL
2	B	582	VAL
2	B	591	ARG
2	B	597	MET
2	B	601	ARG
2	B	602	THR
2	B	603	LEU
2	B	615	MET
2	B	616	ILE
2	B	635	ARG
2	B	636	PRO
2	B	680	THR
2	B	685	LEU
2	B	714	GLU
2	B	737	THR
2	B	748	ILE
2	B	766	ARG
2	B	785	TYR
2	B	798	TYR
2	B	811	TYR
2	B	815	ARG
2	B	830	TYR
2	B	839	MET
2	B	844	SER
2	B	855	PHE
2	B	859	TYR
2	B	878	GLN
2	B	895	ASP
2	B	909	ASP
2	B	933	SER
2	B	944	THR
2	B	951	GLN
2	B	955	THR
2	B	959	ASP
2	B	978	ASP
2	B	999	MET
2	B	1002	THR
2	B	1006	ILE
2	B	1022	THR
2	B	1048	THR

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Mol	Chain	Res	Type
2	B	1049	ASP
2	B	1069	PHE
2	B	1077	THR
2	B	1082	MET
2	B	1084	GLN
2	B	1095	LEU
2	B	1097	HIS
2	B	1098	MET
2	B	1133	MET
2	B	1137	CYS
2	B	1150	ARG
2	B	1156	ASP
2	B	1159	ARG
2	B	1163	CYS
2	B	1170	THR
2	B	1178	ASN
2	B	1182	CYS
2	B	1214	PRO
2	B	1218	THR
3	C	1	MET
3	C	29	MET
3	C	56	THR
3	C	58	LEU
3	C	62	PHE
3	C	77	ILE
3	C	91	HIS
3	C	104	PHE
3	C	106	GLU
3	C	124	LEU
3	C	145	CYS
3	C	147	LEU
3	C	166	GLU
3	C	190	ASP
3	C	193	TYR
3	C	197	SER
3	C	209	TYR
3	C	217	ASP
3	C	229	TYR
3	C	233	GLU
3	C	235	VAL
3	C	238	ILE
3	C	245	VAL

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Mol	Chain	Res	Type
4	D	13	ARG
4	D	15	LEU
4	D	21	GLU
4	D	22	GLU
4	D	28	GLN
4	D	40	HIS
4	D	43	GLU
4	D	47	LEU
4	D	61	GLU
4	D	63	LEU
4	D	70	PHE
4	D	115	HIS
4	D	137	ASN
4	D	149	THR
4	D	156	ASP
4	D	170	THR
4	D	187	THR
4	D	200	ASN
4	D	206	GLU
4	D	213	GLU
4	D	220	LEU
4	D	221	TYR
5	E	17	ARG
5	E	31	THR
5	E	59	SER
5	E	60	PHE
5	E	65	THR
5	E	70	SER
5	E	74	ASP
5	E	82	PHE
5	E	104	ASN
5	E	114	ASN
5	E	132	ILE
5	E	134	THR
5	E	169	ARG
5	E	172	GLU
5	E	190	LEU
5	E	207	ARG
5	E	212	ARG
6	F	71	GLU
6	F	72	LYS
6	F	79	ARG

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Mol	Chain	Res	Type
6	F	82	THR
6	F	90	ARG
6	F	111	LEU
6	F	115	THR
6	F	116	ASP
6	F	153	VAL
7	G	1	MET
7	G	13	LEU
7	G	17	PHE
7	G	30	LEU
7	G	39	THR
7	G	51	TYR
7	G	73	LYS
7	G	74	TYR
7	G	113	HIS
7	G	117	GLN
7	G	137	ILE
7	G	141	SER
7	G	165	GLU
7	G	171	ILE
8	H	8	ASP
8	H	10	PHE
8	H	17	PRO
8	H	63	LEU
8	H	64	ASN
8	H	86	ASP
8	H	91	ASP
8	H	95	TYR
8	H	102	TYR
9	I	4	PHE
9	I	6	PHE
9	I	7	CYS
9	I	8	ARG
9	I	15	TYR
9	I	37	GLU
9	I	44	TYR
9	I	85	PHE
9	I	86	PHE
9	I	94	ASP
9	I	100	PHE
9	I	101	PHE
10	J	2	ILE

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Mol	Chain	Res	Type
10	J	38	ARG
10	J	43	ARG
10	J	44	TYR
10	J	48	ARG
11	K	5	ASP
11	K	6	ARG
11	K	10	PHE
11	K	21	ILE
11	K	25	THR
11	K	41	THR
11	K	47	ARG
11	K	50	LEU
11	K	61	TYR
11	K	81	TYR
11	K	91	CYS
11	K	114	LEU
12	L	27	LEU
12	L	34	CYS
12	L	55	ILE
12	L	65	VAL
12	L	68	GLU
12	L	70	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (130) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	68	GLN
1	A	75	ASN
1	A	83	HIS
1	A	92	HIS
1	A	109	HIS
1	A	118	HIS
1	A	169	ASN
1	A	171	GLN
1	A	213	HIS
1	A	225	ASN
1	A	256	GLN
1	A	282	ASN
1	A	299	HIS
1	A	306	ASN
1	A	339	ASN

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Mol	Chain	Res	Type
1	A	358	ASN
1	A	390	GLN
1	A	394	ASN
1	A	435	HIS
1	A	439	ASN
1	A	445	ASN
1	A	447	GLN
1	A	493	GLN
1	A	517	ASN
1	A	611	GLN
1	A	654	ASN
1	A	659	HIS
1	A	700	ASN
1	A	736	ASN
1	A	741	ASN
1	A	757	ASN
1	A	767	GLN
1	A	786	HIS
1	A	802	ASN
1	A	858	ASN
1	A	877	HIS
1	A	903	ASN
1	A	926	GLN
1	A	935	GLN
1	A	968	GLN
1	A	975	HIS
1	A	1106	ASN
1	A	1130	GLN
1	A	1140	HIS
1	A	1188	GLN
1	A	1203	ASN
1	A	1278	ASN
1	A	1354	ASN
1	A	1364	ASN
1	A	1393	ASN
1	A	1427	ASN
1	A	1432	GLN
2	B	52	ASN
2	B	60	GLN
2	B	178	ASN
2	B	215	GLN
2	B	236	HIS

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Mol	Chain	Res	Type
2	B	357	GLN
2	B	366	GLN
2	B	383	ASN
2	B	465	ASN
2	B	484	ASN
2	B	513	GLN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	538	ASN
2	B	573	GLN
2	B	587	HIS
2	B	744	HIS
2	B	763	GLN
2	B	821	GLN
2	B	834	ASN
2	B	835	GLN
2	B	842	ASN
2	B	951	GLN
2	B	957	ASN
2	B	975	GLN
2	B	1065	GLN
2	B	1076	HIS
2	B	1084	GLN
2	B	1117	GLN
2	B	1141	HIS
2	B	1161	HIS
2	B	1178	ASN
2	B	1179	GLN
2	B	1193	GLN
2	B	1195	HIS
3	C	24	ASN
3	C	65	HIS
3	C	73	GLN
3	C	79	GLN
3	C	102	GLN
3	C	112	ASN
3	C	123	ASN
3	C	135	GLN
3	C	203	GLN
4	D	9	GLN
4	D	39	ASN

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Mol	Chain	Res	Type
4	D	40	HIS
4	D	115	HIS
4	D	137	ASN
4	D	138	ASN
4	D	143	ASN
4	D	179	GLN
5	E	54	GLN
5	E	101	GLN
5	E	104	ASN
5	E	114	ASN
5	E	147	HIS
7	G	53	ASN
7	G	126	ASN
7	G	131	GLN
7	G	158	HIS
8	H	33	GLN
8	H	35	GLN
8	H	131	ASN
8	H	137	GLN
8	H	139	ASN
9	I	89	GLN
9	I	90	GLN
9	I	108	HIS
9	I	114	GLN
10	J	53	HIS
10	J	64	ASN
11	K	44	ASN
11	K	52	ASN
11	K	65	HIS
11	K	76	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	9/16 (56%)	1 (11%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	11	U

There are no RNA pucker outliers to report.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
13	8OG	T	19	13,15	16,25,26	1.31	2 (12%)	21,37,40	2.69	4 (19%)
13	BRU	T	23	13,15	13,21,22	4.58	4 (30%)	16,30,33	4.31	3 (18%)

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
13	8OG	T	19	13,15	-	0/3/21/22	0/3/3/3
13	BRU	T	23	13,15	-	0/3/21/22	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	T	23	BRU	BR-C5	-15.18	1.49	1.90
13	T	19	8OG	C8-N7	-2.70	1.31	1.34
13	T	23	BRU	C6-N1	2.18	1.38	1.35
13	T	23	BRU	C4-N3	2.41	1.37	1.33
13	T	19	8OG	C6-N1	3.57	1.39	1.33
13	T	23	BRU	C4-C5	5.40	1.45	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	T	19	8OG	C5-C6-N1	-8.75	111.62	123.59
13	T	23	BRU	C5-C4-N3	-8.30	115.14	124.00
13	T	23	BRU	O3'-C3'-C2'	-2.33	103.03	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	T	19	8OG	N3-C2-N1	-2.28	123.98	127.44
13	T	19	8OG	C2'-C1'-N9	3.43	119.27	115.83
13	T	19	8OG	C6-N1-C2	6.44	124.88	115.94
13	T	23	BRU	C4-N3-C2	14.59	127.86	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	T	23	BRU	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95th 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 ²)	Q<0.9
1	A	1429/1733 (82%)	-0.29	1 (0%) 95 94	15, 73, 135, 195	0
2	B	1125/1224 (91%)	-0.12	15 (1%) 79 66	11, 88, 154, 194	0
3	C	270/324 (83%)	-0.27	1 (0%) 93 88	34, 73, 131, 174	0
4	D	187/221 (84%)	-0.12	4 (2%) 67 52	58, 98, 152, 197	0
5	E	214/215 (99%)	-0.24	2 (0%) 85 75	42, 112, 155, 161	0
6	F	88/155 (56%)	-0.44	0 100 100	24, 48, 91, 122	0
7	G	171/171 (100%)	-0.21	0 100 100	48, 74, 117, 128	0
8	H	137/146 (93%)	0.17	3 (2%) 65 50	91, 125, 152, 157	0
9	I	116/122 (95%)	-0.09	2 (1%) 73 58	65, 121, 152, 153	0
10	J	65/70 (92%)	-0.39	0 100 100	48, 67, 106, 121	0
11	K	116/120 (96%)	-0.29	2 (1%) 73 58	32, 79, 108, 160	0
12	L	47/70 (67%)	-0.03	1 (2%) 67 52	73, 124, 147, 159	0
13	T	19/26 (73%)	0.46	0 100 100	128, 194, 200, 200	0
14	N	11/12 (91%)	0.93	1 (9%) 11 7	186, 198, 200, 200	0
15	P	10/16 (62%)	0.33	1 (10%) 9 6	177, 193, 199, 200	0
All	All	4005/4625 (86%)	-0.20	33 (0%) 87 77	11, 83, 152, 200	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	471	LYS	6.2
2	B	883	LEU	3.7
2	B	722	ASP	3.4
11	K	116	ALA	3.2
2	B	504	ARG	3.2
11	K	115	ALA	3.2
5	E	126	SER	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	339	THR	2.8
4	D	111	ASP	2.7
2	B	472	ALA	2.6
2	B	507	LYS	2.6
8	H	146	ARG	2.5
9	I	102	VAL	2.4
4	D	112	ASP	2.4
2	B	468	GLU	2.3
2	B	723	VAL	2.3
14	N	8	DG	2.3
2	B	713	ALA	2.3
15	P	2	U	2.3
12	L	26	THR	2.3
4	D	76	LYS	2.3
8	H	83	GLN	2.2
8	H	142	LEU	2.2
2	B	470	LYS	2.1
2	B	714	GLU	2.1
2	B	248	SER	2.1
9	I	84	VAL	2.1
2	B	341	LEU	2.1
1	A	251	SER	2.1
2	B	505	ASP	2.1
3	C	270	VAL	2.1
4	D	1	MET	2.1
5	E	82	PHE	2.0

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

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, 95th 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(Å ²)	Q<0.9
13	8OG	T	19	23/24	0.89	0.17	-	131,141,154,155	0
13	BRU	T	23	20/21	0.68	0.27	-	153,162,167,170	0

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, 95th 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(\AA^2)	Q<0.9
17	ZN	I	1121	1/1	0.99	0.12	-0.71	70,70,70,70	0
17	ZN	C	1269	1/1	1.00	0.12	-0.72	39,39,39,39	0
17	ZN	A	2457	1/1	1.00	0.14	-1.17	38,38,38,38	0
17	ZN	I	1122	1/1	0.91	0.04	-1.72	134,134,134,134	0
17	ZN	L	1071	1/1	0.97	0.06	-2.00	111,111,111,111	0
17	ZN	J	1066	1/1	0.99	0.23	-2.36	47,47,47,47	0
17	ZN	A	2456	1/1	0.96	0.07	-2.64	96,96,96,96	0
16	MG	A	2458	1/1	0.95	0.09	-3.37	69,69,69,69	0
17	ZN	B	2225	1/1	0.99	0.21	-	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.