



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:57 PM GMT

PDB ID : 1R9S
Title : RNA POLYMERASE II STRAND SEPARATED ELONGATION COM-
PLEX, MATCHED NUCLEOTIDE
Authors : Westover, K.D.; Bushnell, D.A.; Kornberg, R.D.
Deposited on : 2003-10-30
Resolution : 4.25 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

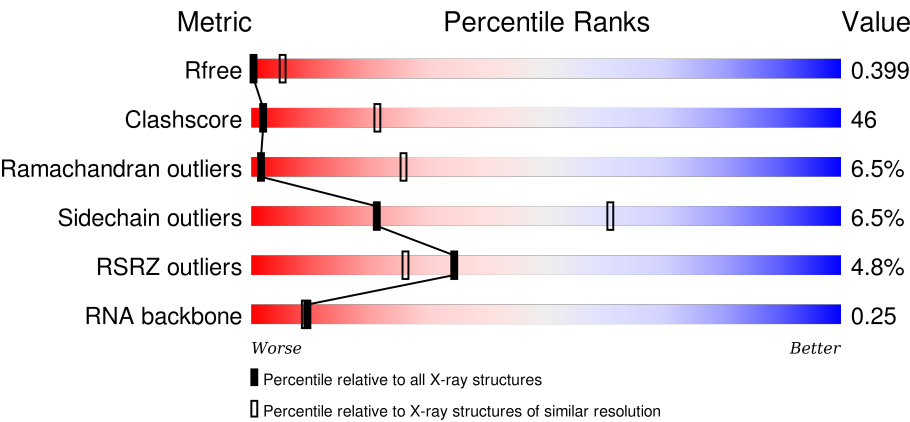
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.25 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.



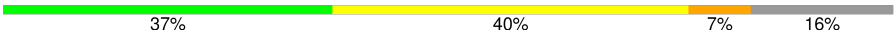



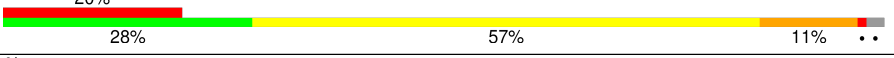
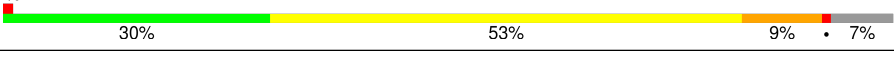
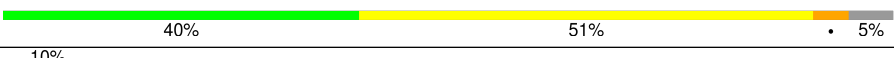

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1043 (4.92-3.60)
Clashscore	102246	1145 (4.92-3.60)
Ramachandran outliers	100387	1088 (4.92-3.60)
Sidechain outliers	100360	1072 (4.92-3.60)
RSRZ outliers	91569	1047 (4.92-3.60)
RNA backbone	2183	1087 (5.60-2.80)

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	R	10	<div><div></div><div>50%50%</div></div>
2	T	14	<div><div></div><div>21%64%14%</div></div>
3	A	1733	<div><div>4%</div><div>31%41%7%20%</div><div></div></div>
4	B	1224	<div><div>4%</div><div>32%51%7%10%</div><div></div></div>

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Mol	Chain	Length	Quality of chain
5	C	318	
6	E	215	
7	F	155	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	ZN	I	204	-	-	X	-
15	UTP	R	3000	X	-	-	-

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 28491 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 RNA chain called RNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	10	Total	C	N	O	P	0	0	0
			217	98	45	65	9			

- Molecule 2 is a DNA chain called DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	14	Total	C	N	O	P	0	0	0
			279	135	48	83	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	1381	Total	C	N	O	S	0	0	0
			10857	6851	1899	2046	61			

- Molecule 4 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	1097	Total	C	N	O	S	0	0	0
			8720	5526	1523	1617	54			

- Molecule 5 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

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

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 9 is a protein called DNA-directed RNA polymerase II 14.2 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide.

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 13.6 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

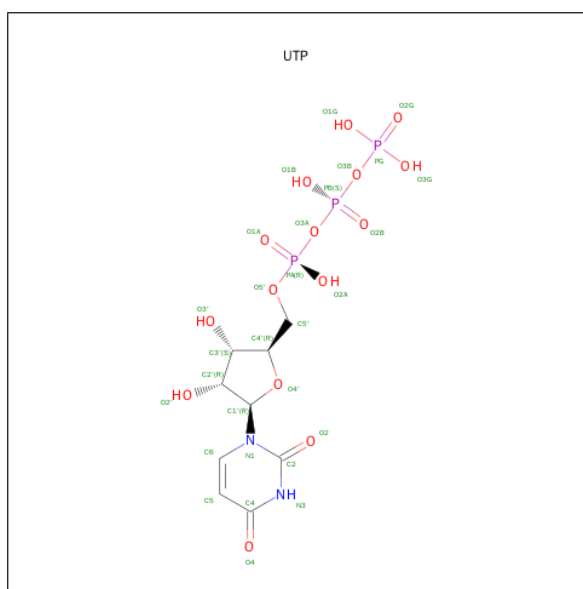
- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	J	1	Total	Zn	0	0
			1	1		
13	B	1	Total	Zn	0	0
			1	1		
13	I	2	Total	Zn	0	0
			2	2		
13	C	1	Total	Zn	0	0
			1	1		
13	A	2	Total	Zn	0	0
			2	2		
13	L	1	Total	Zn	0	0
			1	1		

- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	R	1	Total	Mg	0	0
			1	1		
14	A	1	Total	Mg	0	0
			1	1		

- Molecule 15 is URIDINE 5'-TRIPHOSPHATE (three-letter code: UTP) (formula: C₉H₁₅N₂O₁₅P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	R	1	Total	C	N	O	P	0	0
			29	9	2	15	3		

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.

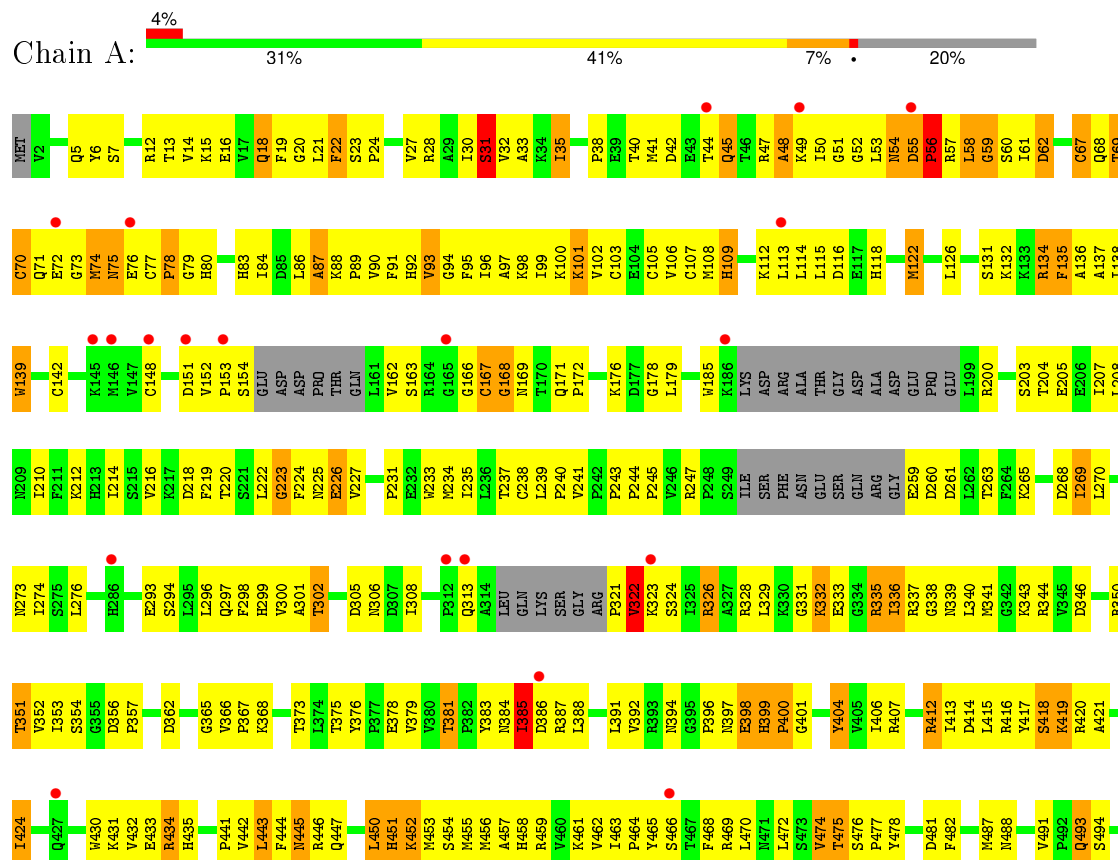
- Molecule 1: RNA strand



- Molecule 2: DNA strand

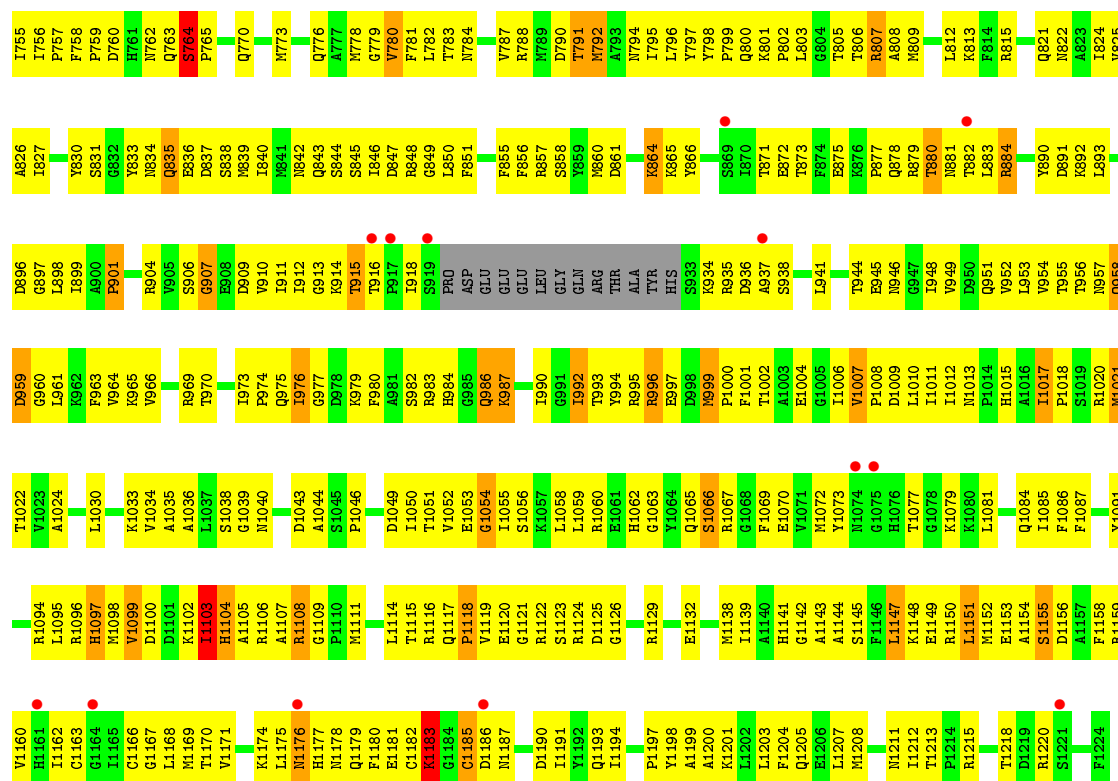


- Molecule 3: DNA-directed RNA polymerase II largest subunit



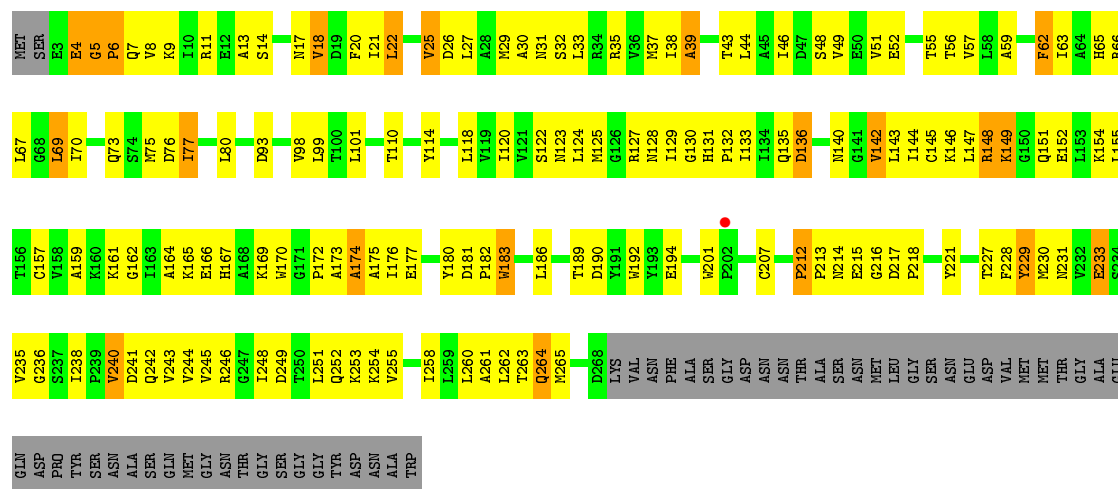
GLY	S4415	E1351	R1281	I1216	S1150	PHE	T1016	E931	V862	K789	R711	Q640	A564	T497
LEU	A1416	V1352	V1282	K1217	E1151	HIS	L1017	E932	V863	D790	E712	Q644	I565	R498
VAL	E1417	V1353	V1283	Q1218	I1152	PHE	F1018	Y933	R864	P794	E715	K644	I566	R499
ASN	L1418	I1356	M1284	T1219	I1153	ALA	C1019	L936	Q865	E795	E716	L645	K567	E500
ALA	D1419	D1359	M1285	F1220	Y1154	GLY	C1020	L936	F866	S803	D716	F646	P568	
ASP	D1420	D1360	K1286	K1221	D1155	VAL	L1021	R940	I567	S804	Y718	K648	K569	Q503
LEU	C1421	G1360		M1222	P1158	ALA	L1022		V868		Y719	K649	P570	
ASP		S1293		D1223	P1159	SER	R1023	L943	G869		K720	Q650	L571	A506
VAL	V1424	Y1362	P1294	L1224	M1159		S1024		E870		K721	Q650	M572	A507
LVS	S1425	V1363	T1295	F1225	S1160	ASP	R1025	L943	E871		F721	Q652	S573	P508
ASP		N1364	G1296	V1226	T1161		L1026	V948	G872		K722	V652	G574	
GLU	V1428	Y1365	E1297	I1227	V1162	T1095	A1027	D949	N873			V653	K575	T511
LEU	I1429	R1366	Y1298	M1228	I1163	T1096	T1028		D874		A725	K654	Q576	V512
MET	L1430	H1367	V1299		F1164	G1097	R1029	A952	A975			F655	I577	S513
PHE	Q1431	M1368	E1165	D1231	E1166	V1098	R1030	N953				M656	L578	P514
SER	G1432	A1369	N1232	M1232	E1167	P1099	Y954	N954			A728	L657	S579	Q515
PRO					E1168	R1100	Y1035	P955				L658	V580	S516
LEU	V1305	V1306	L1236	L1236	E1169	K1101	R1036	L956	Q881		N736	S663	N584	K518
VAL	D1373	E1307	I1237	I1237	T1169	K1102	L1037	P957	S882		L737	T664		P519
ASP	T1308	T1308	I1238	I1238	I1170	E1103	T1038	V958			K738	G665	H587	G520
SER	M1375	D1309	R1239	R1239	Q1171	I1104	K1039	N959	T885		D739	G666		N521
GLY	G1439	T1376	C1240	C1240	L1172	L1105	Q1040	I960	I886		L740	I666	L588	
SER	A1440	T1377	R1241	R1241	H1173	N1106	A1041	R961	G887		N741	G667	Q589	G522
ASN	Q1378	N1312	V1242	V1242	I1176	V1107	F1042	R962	G888		N742		R590	
ASP	G1379	V1243					D1043	I963	S889		K743	L670	F591	V524
ALA	G1380				LEU		W1044	I964	D890		K744	A671	D592	Q525
MET	L1444				ASP	M1111	V1045	Q965			Q745	D672		
ALA	I1445				GLU	T1113	L1046		F893		G673	G673	T595	L528
GLY	ASP				LEU	T1113	S1047	Q968	K895		G750	P674	T596	C529
GLY	GLU				ALA	S1115	N1048		K896		T675	T675	L597	G530
PHE	GLU				GLU	T1116	I1049	H972	R896		K752	V676	L588	T531
THR	SER				GLN	T1117	E1050	I973	R897		G753	R677	S599	R532
ALA	LEU				SER	V1118	A1051	H975	R898		G754	E578	M605	K533
THR	VAL				PHE	E1121	F1052		V899		T756	T682	L606	R537
GLY	GLU				ASP	P1122	Q1053	S979	L901		N757	T681	L534	T535
ALA	ASP				GLU	E1122	L1054	D980	L902		T758	T682	L607	D538
ALA	MET				E1188	A1125		L981	I903		A759	A686	I608	T539
ASP	PRO				S1189	A1126	V1057	L982	T907		Q760		F540	
THR	GLU				P1190	D1127	H1058	T982	L908		A763	K689	I612	F540
GLY	GLU				W1191	Q1128	H1059	K984	D909		C764	K689	I613	E542
LVS	G1395	T1394	M1259	L1192	L1193	E1129	P1060	D985	V842		A764	V690	I614	L543
ALA	A1396	S1331	L1260	L1193	R1194	Q1130	E1062	I986	P910			L691	G615	D544
THR	L1397	F1332	K1261	L1195	A1131	Q1131	M1063	V987	A844		Q768	L691	G615	D544
SER	M1398	I1333	K1262	L1196	K1132	K1132	V1064	L988	L845			D692	V616	Q545
PRO	R1399	D1334	I1263	E1196	L1133	I1134	G1065	Q994	E846		E771	V693	V617	V546
PHE	C1400	I1335	E1264	E1197	V1066	L1067	V1066		D847			T694	E618	L547
GLY	ASP	F1402			L1067	R1135	A1068	L998	I848		R774	K696	K619	N548
ALA	GLY				A1068		A1069		M849			E596		M549
THR	GLN				A1069			R1001	V850			V697	V622	N552
GLY	ASP				K1205	I1138			I919		G778	Q698	G623	N553
GLY	GLY				D1206	H1139	G1073	N1004	L923		F779	L701	G628	V556
ALA	T1405	E1269	E1270	L1207	L1207	H1140	E1074	E1005	D853			L702	L629	V557
PRO	V1406	I1341	I1271	T1208	T1208	T1141	P1075	N1005	N854			T703	T855	G558
THR	A1343	A1343	L1272	M1209	M1209	T1142	A1076	I1007	T856			A704	V633	V559
SER	L1408	G1344	L1273	G1210	G1210	L1143	T1077	Q1008	N927			K705		
PRO	L1409	R1345	G1211	G1211	Q1211									
THR	F1410	A1346	V1276	V1276	V1212	V1146								
GLY	A1347	A1347	E1277	E1277	G1213	T1147	L1081		L928				K637	T562
ASN	L1348	L1348	M1278	M1278	E1214	T1148	ASN	A1014	I929		F787	T709	G638	P563
GLY	G1413	G1413	E1280	E1280	R1215	A1149	THR	V1015	D930		S788	L710	P639	





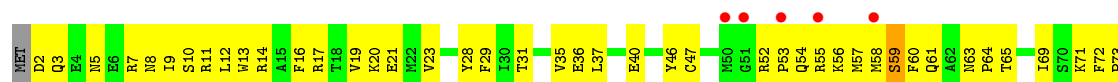
• Molecule 5: DNA-directed RNA polymerase II 45 kDa polypeptide

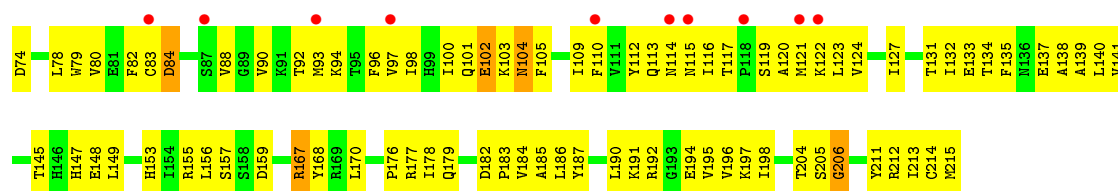
Chain C: 37% 40% 7% 16%



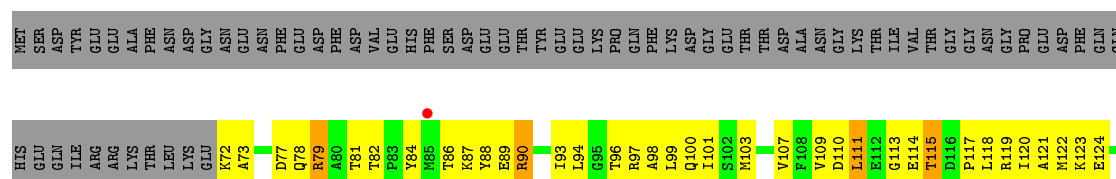
• Molecule 6: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide

Chain E: 7% 40% 56%

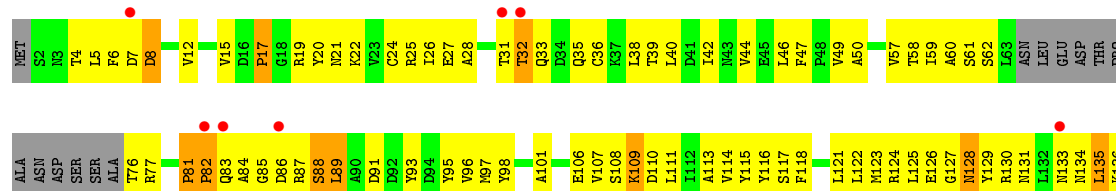




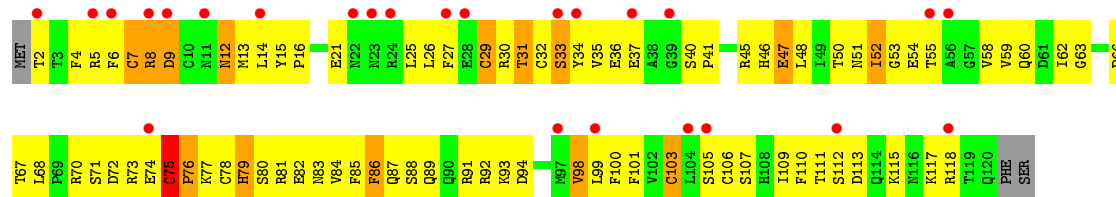
- Molecule 7: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide



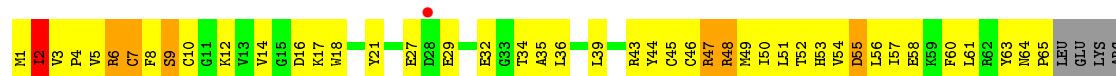
- Molecule 8: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide



- Molecule 9: DNA-directed RNA polymerase II 14.2 kDa polypeptide

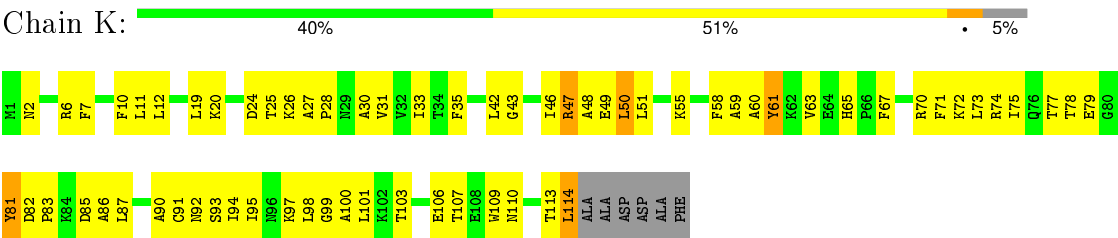


- Molecule 10: DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide

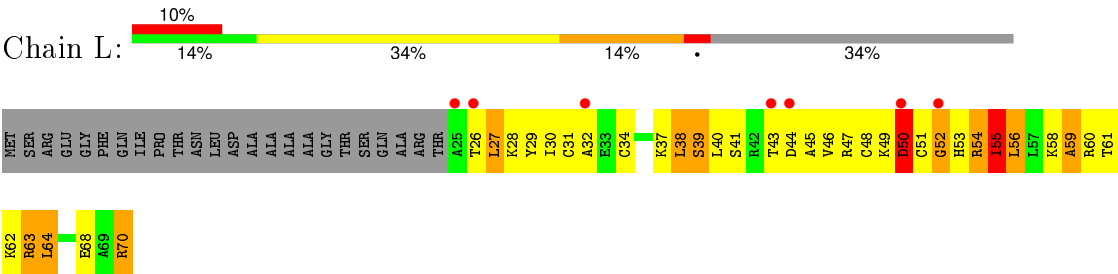


ASP

- Molecule 11: DNA-directed RNA polymerase II 13.6 kDa polypeptide



- Molecule 12: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	169.65Å 222.34Å 194.32Å 90.00° 101.67° 90.00°	Depositor
Resolution (Å)	40.00 – 4.25 39.94 – 4.20	Depositor EDS
% Data completeness (in resolution range)	95.8 (40.00-4.25) 84.6 (39.94-4.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 4.13Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.349 , 0.398 0.345 , 0.399	Depositor DCC
R_{free} test set	4227 reflections (10.08%)	DCC
Wilson B-factor (Å ²)	96.8	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 104.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 51407 reflections	Xtriage
F_o, F_c correlation	0.71	EDS
Total number of atoms	28491	wwPDB-VP
Average B, all atoms (Å ²)	130.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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: UTP, MG, ZN

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	R	3.97	33/244 (13.5%)	3.92	44/380 (11.6%)
2	T	4.38	37/311 (11.9%)	3.99	55/477 (11.5%)
3	A	0.41	0/11048	0.71	5/14936 (0.0%)
4	B	0.46	0/8890	0.72	1/11990 (0.0%)
5	C	0.48	0/2133	0.76	2/2891 (0.1%)
6	E	0.36	0/1788	0.65	0/2406
7	F	0.40	0/691	0.64	0/933
8	H	0.40	0/1086	0.73	0/1470
9	I	0.48	0/989	0.76	1/1331 (0.1%)
10	J	0.53	0/541	0.78	0/727
11	K	0.46	0/937	0.68	0/1265
12	L	0.48	0/365	0.78	0/485
All	All	0.72	70/29023 (0.2%)	0.92	108/39291 (0.3%)

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	R	0	1
2	T	1	2
All	All	1	3

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	3	DG	O3'-P	-35.59	1.18	1.61
2	T	4	DA	O3'-P	-30.26	1.24	1.61
1	R	10	A	P-OP1	-23.82	1.08	1.49
1	R	5	A	O3'-P	-22.75	1.33	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	3	DG	C3'-O3'	-20.45	1.17	1.44
1	R	10	A	P-O5'	18.42	1.78	1.59
2	T	7	DC	O3'-P	-17.97	1.39	1.61
2	T	7	DC	O5'-C5'	14.34	1.78	1.42
1	R	5	A	P-O5'	13.14	1.72	1.59
2	T	2	DC	C3'-O3'	13.04	1.60	1.44
1	R	7	A	C5'-C4'	-12.56	1.36	1.51
1	R	4	G	P-OP1	12.19	1.69	1.49
1	R	1	A	O3'-P	-11.94	1.46	1.61
2	T	9	DC	C4'-O4'	-11.93	1.33	1.45
2	T	6	DC	C3'-O3'	-11.70	1.28	1.44
2	T	3	DG	P-OP1	11.43	1.68	1.49
1	R	8	G	C3'-O3'	11.15	1.57	1.42
2	T	8	DT	P-OP2	11.14	1.67	1.49
1	R	10	A	C5'-C4'	-11.06	1.38	1.51
1	R	4	G	O3'-P	10.78	1.74	1.61
1	R	9	G	O3'-P	10.10	1.73	1.61
2	T	9	DC	C3'-O3'	-9.95	1.31	1.44
2	T	9	DC	C4'-C3'	-9.74	1.42	1.52
1	R	4	G	C3'-O3'	9.40	1.55	1.42
2	T	9	DC	N1-C2	-9.31	1.30	1.40
1	R	6	G	P-OP2	9.08	1.64	1.49
1	R	2	U	P-OP2	8.68	1.63	1.49
2	T	7	DC	C3'-O3'	-8.68	1.32	1.44
2	T	9	DC	P-O5'	8.46	1.68	1.59
2	T	9	DC	O3'-P	-7.94	1.51	1.61
2	T	7	DC	C3'-C2'	-7.88	1.42	1.52
2	T	5	DT	C3'-O3'	-7.87	1.33	1.44
2	T	7	DC	P-O5'	7.87	1.67	1.59
1	R	10	A	P-OP2	-7.69	1.35	1.49
2	T	4	DA	P-O5'	-7.69	1.52	1.59
1	R	2	U	C3'-O3'	-7.51	1.31	1.42
2	T	1	DA	C3'-O3'	7.48	1.53	1.44
2	T	10	DT	P-OP1	-6.76	1.37	1.49
1	R	9	G	C4'-C3'	-6.73	1.45	1.53
1	R	3	C	C3'-O3'	6.64	1.51	1.42
2	T	3	DG	C4'-C3'	-6.41	1.46	1.52
2	T	7	DC	N1-C2	-6.37	1.33	1.40
1	R	9	G	P-OP1	-6.30	1.38	1.49
1	R	1	A	C3'-O3'	6.26	1.50	1.42
2	T	11	DC	N1-C6	6.25	1.40	1.37
2	T	5	DT	P-OP2	6.13	1.59	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	7	A	P-O5'	-5.96	1.53	1.59
2	T	11	DC	N1-C2	-5.86	1.34	1.40
2	T	5	DT	O3'-P	5.80	1.68	1.61
2	T	6	DC	C4'-C3'	-5.79	1.46	1.52
2	T	5	DT	C4'-C3'	-5.79	1.46	1.52
1	R	6	G	N9-C4	5.78	1.42	1.38
1	R	7	A	O3'-P	-5.69	1.54	1.61
2	T	13	DA	C3'-O3'	-5.66	1.36	1.44
2	T	7	DC	C2'-C1'	-5.58	1.46	1.52
1	R	4	G	C3'-C2'	-5.54	1.46	1.52
1	R	6	G	C5-C4	5.45	1.42	1.38
1	R	8	G	O3'-P	-5.45	1.54	1.61
2	T	9	DC	C2-N3	-5.37	1.31	1.35
2	T	9	DC	N1-C6	5.33	1.40	1.37
2	T	4	DA	C3'-O3'	-5.27	1.37	1.44
1	R	5	A	C3'-O3'	5.25	1.49	1.42
1	R	6	G	O3'-P	-5.25	1.54	1.61
1	R	9	G	C3'-O3'	-5.24	1.34	1.42
2	T	11	DC	C5-C6	5.22	1.38	1.34
1	R	9	G	C5'-C4'	5.20	1.57	1.51
1	R	8	G	P-OP1	-5.19	1.40	1.49
2	T	9	DC	C2'-C1'	-5.13	1.47	1.52
1	R	6	G	O4'-C1'	5.06	1.48	1.41
1	R	6	G	C8-N7	5.05	1.33	1.30

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	3	DG	O3'-P-O5'	-28.04	50.72	104.00
1	R	9	G	P-O3'-C3'	28.01	153.31	119.70
1	R	4	G	OP2-P-O3'	-25.63	48.80	105.20
2	T	3	DG	P-O3'-C3'	-25.44	89.17	119.70
2	T	7	DC	O5'-P-OP1	25.27	141.02	110.70
2	T	6	DC	OP1-P-O3'	-22.05	56.68	105.20
2	T	13	DA	OP1-P-O3'	-21.51	57.88	105.20
1	R	8	G	OP1-P-O3'	-16.21	69.53	105.20
1	R	3	C	O3'-P-O5'	-15.99	73.63	104.00
2	T	7	DC	O4'-C4'-C3'	-14.92	97.05	106.00
1	R	8	G	OP2-P-O3'	14.83	137.82	105.20
1	R	4	G	O3'-P-O5'	13.83	130.28	104.00
1	R	3	C	OP1-P-O3'	13.81	135.59	105.20
2	T	7	DC	C4'-C3'-C2'	13.53	115.28	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	7	DC	C5'-C4'-C3'	13.28	138.00	114.10
2	T	6	DC	OP2-P-O3'	12.92	133.62	105.20
2	T	13	DA	OP2-P-O3'	12.62	132.96	105.20
1	R	4	G	O5'-P-OP1	-12.45	94.49	105.70
1	R	6	G	OP1-P-OP2	-12.30	101.14	119.60
2	T	3	DG	C4'-C3'-C2'	11.85	113.76	103.10
2	T	9	DC	C4'-C3'-O3'	11.67	138.88	109.70
1	R	9	G	O5'-P-OP1	11.23	124.18	110.70
2	T	9	DC	O5'-P-OP2	-10.82	95.96	105.70
1	R	4	G	P-O3'-C3'	10.69	132.53	119.70
1	R	7	A	O5'-P-OP2	-10.66	96.11	105.70
2	T	3	DG	O4'-C4'-C3'	-10.54	99.68	106.00
2	T	7	DC	C4'-C3'-O3'	10.46	135.85	109.70
2	T	3	DG	O5'-P-OP1	-9.93	96.76	105.70
2	T	9	DC	O5'-P-OP1	9.92	122.61	110.70
1	R	1	A	C2'-C3'-O3'	9.87	131.21	109.50
1	R	9	G	OP1-P-O3'	9.77	126.69	105.20
1	R	5	A	O5'-P-OP2	-9.66	97.00	105.70
1	R	7	A	P-O5'-C5'	-9.38	105.88	120.90
1	R	10	A	O5'-P-OP1	-9.38	97.26	105.70
1	R	5	A	C5'-C4'-C3'	9.34	130.95	116.00
1	R	9	G	O3'-P-O5'	-9.22	86.48	104.00
1	R	4	G	OP1-P-O3'	9.12	125.26	105.20
1	R	5	A	C2'-C3'-O3'	9.01	129.31	109.50
1	R	5	A	OP2-P-O3'	8.82	124.61	105.20
2	T	9	DC	O4'-C1'-N1	8.76	114.13	108.00
1	R	9	G	OP1-P-OP2	-8.66	106.61	119.60
1	R	10	A	O5'-P-OP2	8.35	120.72	110.70
1	R	2	U	OP1-P-OP2	-8.30	107.15	119.60
1	R	1	A	OP2-P-O3'	8.22	123.30	105.20
2	T	2	DC	OP1-P-O3'	8.21	123.27	105.20
2	T	3	DG	OP1-P-OP2	-8.19	107.32	119.60
1	R	10	A	C5'-C4'-C3'	8.09	128.95	116.00
2	T	11	DC	O4'-C1'-N1	8.09	113.66	108.00
1	R	10	A	O5'-C5'-C4'	-8.00	96.51	111.70
2	T	5	DT	O5'-P-OP1	7.97	120.27	110.70
1	R	5	A	OP1-P-O3'	7.96	122.72	105.20
2	T	5	DT	OP1-P-OP2	-7.89	107.76	119.60
2	T	9	DC	C4'-C3'-C2'	7.82	110.14	103.10
1	R	6	G	O5'-P-OP2	-7.79	98.69	105.70
1	R	2	U	O5'-P-OP2	-7.61	98.85	105.70
2	T	9	DC	C2-N1-C1'	-7.46	110.60	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	4	DA	OP1-P-O3'	-7.42	88.88	105.20
2	T	8	DT	O5'-P-OP2	-7.35	99.09	105.70
2	T	9	DC	C5'-C4'-O4'	7.04	122.67	109.30
2	T	11	DC	O4'-C1'-C2'	6.99	111.50	105.90
2	T	6	DC	C4'-C3'-O3'	6.90	126.96	109.70
1	R	10	A	OP1-P-OP2	-6.90	109.25	119.60
2	T	7	DC	OP2-P-O3'	6.86	120.30	105.20
2	T	6	DC	O4'-C4'-C3'	-6.79	101.78	104.50
2	T	10	DT	C6-N1-C1'	6.79	130.58	120.40
2	T	7	DC	O4'-C1'-C2'	6.73	111.28	105.90
1	R	6	G	C5'-C4'-O4'	6.73	117.17	109.10
2	T	5	DT	OP2-P-O3'	-6.70	90.47	105.20
1	R	1	A	P-O3'-C3'	6.58	127.59	119.70
2	T	3	DG	OP1-P-O3'	6.52	119.54	105.20
1	R	6	G	P-O5'-C5'	-6.47	110.54	120.90
2	T	6	DC	C4'-C3'-C2'	6.37	108.83	103.10
3	A	1392	SER	N-CA-C	6.30	128.02	111.00
1	R	7	A	C4'-C3'-O3'	6.29	125.58	113.00
2	T	8	DT	O5'-P-OP1	6.21	118.16	110.70
2	T	9	DC	N1-C2-O2	-6.21	115.18	118.90
1	R	9	G	O5'-P-OP2	6.19	118.13	110.70
5	C	39	ALA	N-CA-C	6.05	127.34	111.00
2	T	10	DT	C2-N1-C1'	-5.96	108.66	118.20
1	R	10	A	N9-C1'-C2'	5.91	121.68	114.00
1	R	6	G	N3-C4-N9	5.86	129.52	126.00
2	T	8	DT	O3'-P-O5'	-5.85	92.89	104.00
1	R	5	A	P-O3'-C3'	5.83	126.70	119.70
3	A	398	GLU	N-CA-C	-5.78	95.41	111.00
1	R	4	G	OP1-P-OP2	-5.75	110.98	119.60
1	R	6	G	OP1-P-O3'	5.74	117.82	105.20
1	R	10	A	P-O5'-C5'	5.72	130.05	120.90
2	T	5	DT	P-O5'-C5'	-5.72	111.75	120.90
5	C	183	TRP	N-CA-C	-5.62	95.84	111.00
2	T	3	DG	C4'-C3'-O3'	5.61	123.71	109.70
2	T	10	DT	O4'-C1'-N1	5.60	111.92	108.00
1	R	1	A	OP1-P-O3'	5.60	117.52	105.20
2	T	13	DA	O3'-P-O5'	5.53	114.50	104.00
2	T	7	DC	N1-C2-O2	-5.48	115.61	118.90
2	T	9	DC	C6-N1-C1'	5.48	127.37	120.80
2	T	3	DG	OP2-P-O3'	5.37	117.01	105.20
2	T	14	DT	N1-C1'-C2'	5.34	122.75	112.60
4	B	647	GLY	N-CA-C	5.22	126.15	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	2	DC	OP1-P-OP2	-5.21	111.79	119.60
3	A	750	GLY	N-CA-C	-5.21	100.08	113.10
2	T	8	DT	OP1-P-OP2	-5.20	111.80	119.60
3	A	1403	GLU	N-CA-C	5.20	125.05	111.00
2	T	9	DC	C5-C6-N1	-5.16	118.42	121.00
9	I	75	CYS	N-CA-C	-5.16	97.06	111.00
2	T	7	DC	C1'-O4'-C4'	5.08	115.18	110.10
3	A	452	LYS	N-CA-C	-5.07	97.32	111.00
2	T	1	DA	OP1-P-O3'	5.05	116.31	105.20
2	T	4	DA	C4'-C3'-C2'	5.03	107.63	103.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	T	7	DC	C3'

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	R	10	A	Sidechain
2	T	7	DC	Sidechain
2	T	9	DC	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	217	0	110	48	0
2	T	279	0	160	69	0
3	A	10857	0	10959	1037	18
4	B	8720	0	8746	901	13
5	C	2095	0	2052	164	0
6	E	1752	0	1776	133	0
7	F	679	0	701	67	0
8	H	1068	0	1040	134	0
9	I	971	0	933	105	59
10	J	532	0	544	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	919	0	929	85	0
12	L	363	0	388	55	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	I	2	0	0	2	0
13	J	1	0	0	1	0
13	L	1	0	0	0	0
14	A	1	0	0	0	0
14	R	1	0	0	0	0
15	R	29	0	8	8	0
All	All	28491	0	28346	2619	59

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 46.

All (2619) 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)
1:R:10:A:OP1	1:R:10:A:P	1.08	1.47
2:T:6:DC:H2''	2:T:7:DC:C5'	1.54	1.36
2:T:7:DC:C5'	2:T:7:DC:O5'	1.78	1.30
3:A:567:LYS:HB2	3:A:568:PRO:HD2	1.18	1.17
2:T:6:DC:C2'	2:T:7:DC:H5'	1.75	1.15
9:I:111:THR:HG22	9:I:113:ASP:H	1.05	1.15
4:B:345:LYS:HA	4:B:348:ARG:HE	1.11	1.15
3:A:666:ILE:HD11	4:B:1030:LEU:HD13	1.27	1.12
12:L:60:ARG:HG3	12:L:61:THR:H	1.05	1.12
3:A:1329:THR:HG22	3:A:1331:SER:H	1.16	1.11
3:A:855:THR:HG21	3:A:857:ARG:HE	1.12	1.11
6:E:124:VAL:HG13	6:E:132:ILE:HB	1.33	1.10
4:B:1051:THR:HG22	4:B:1053:GLU:H	1.00	1.09
3:A:1364:ASN:ND2	3:A:1366:ARG:HG2	1.65	1.09
4:B:570:VAL:HB	4:B:573:GLN:HB3	1.36	1.08
1:R:8:G:O2'	1:R:9:G:H5'	1.55	1.06
4:B:512:ARG:HH21	4:B:535:LEU:HD11	1.17	1.06
3:A:1161:THR:HG22	3:A:1163:ILE:H	1.18	1.06
3:A:704:ALA:HB2	3:A:710:LEU:HG	1.34	1.06
2:T:1:DA:H2''	2:T:2:DC:O5'	1.46	1.05
2:T:1:DA:C2	2:T:2:DC:H5	1.74	1.05
4:B:708:GLU:HG3	4:B:709:ASP:H	1.17	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:287:ARG:HG2	4:B:292:ILE:HA	1.38	1.04
3:A:93:VAL:HG13	3:A:301:ALA:HB1	1.33	1.03
5:C:80:LEU:HD22	5:C:129:ILE:HD11	1.41	1.03
4:B:1159:ARG:HE	4:B:1193:GLN:NE2	1.56	1.03
7:F:81:THR:HG21	7:F:136:ARG:HD3	1.38	1.03
4:B:977:GLY:HA3	4:B:1099:VAL:HG21	1.41	1.03
12:L:32:ALA:HB3	12:L:55:ILE:HD12	1.39	1.02
3:A:567:LYS:CB	3:A:568:PRO:HD2	1.91	1.01
4:B:1159:ARG:NE	4:B:1193:GLN:HE21	1.57	1.00
5:C:57:VAL:HG11	10:J:60:PHE:HB3	1.44	1.00
3:A:902:LEU:HG	3:A:926:GLN:HG3	1.40	1.00
4:B:1002:THR:HG22	4:B:1006:ILE:H	1.22	0.99
11:K:113:THR:O	11:K:114:LEU:HB2	1.60	0.99
4:B:120:ARG:HG2	4:B:955:THR:HG21	1.40	0.99
3:A:913:LEU:HD12	3:A:914:GLU:H	1.25	0.99
5:C:56:THR:HG22	5:C:57:VAL:H	1.28	0.98
6:E:135:PHE:HB3	6:E:140:LEU:HD11	1.45	0.98
4:B:842:ASN:ND2	4:B:845:SER:H	1.62	0.97
3:A:567:LYS:HB3	8:H:96:VAL:H	1.26	0.97
4:B:174:LEU:O	4:B:175:ARG:HB2	1.64	0.97
2:T:1:DA:C2	2:T:2:DC:C5	2.53	0.97
4:B:1100:ASP:HA	4:B:1103:ILE:HD11	1.46	0.97
1:R:5:A:C2	1:R:6:G:C5	2.52	0.96
5:C:167:HIS:CD2	5:C:169:LYS:H	1.83	0.96
4:B:1051:THR:HG22	4:B:1053:GLU:N	1.81	0.96
4:B:200:GLY:HA2	4:B:202:TYR:CE2	2.02	0.95
4:B:392:ARG:HH21	9:I:52:ILE:HD11	1.30	0.95
4:B:639:ILE:HD11	4:B:691:GLU:HG3	1.47	0.94
4:B:737:THR:HG21	9:I:66:PRO:O	1.68	0.94
3:A:1116:LEU:HD12	3:A:1329:THR:OG1	1.67	0.94
3:A:244:PRO:HG2	3:A:245:PRO:HD3	1.46	0.94
3:A:338:GLY:HA2	4:B:1129:ARG:HH22	1.33	0.94
3:A:783:THR:HG22	3:A:784:LEU:HG	1.48	0.93
4:B:824:ILE:HG12	10:J:48:ARG:HH12	1.32	0.93
4:B:1159:ARG:HD3	4:B:1193:GLN:HG3	1.47	0.93
9:I:7:CYS:HB2	9:I:14:LEU:HD21	1.47	0.92
4:B:955:THR:HG22	4:B:956:THR:H	1.31	0.92
3:A:1435:PRO:HA	3:A:1439:GLY:O	1.69	0.92
3:A:1281:ARG:HD2	3:A:1309:ASP:OD2	1.68	0.92
12:L:60:ARG:HG3	12:L:61:THR:N	1.85	0.92
1:R:9:G:C6	1:R:10:A:N6	2.37	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:46:CYS:HG	13:J:101:ZN:ZN	0.78	0.91
5:C:73:GLN:HE21	5:C:75:MET:H	1.14	0.91
3:A:15:LYS:HB3	4:B:1220:ARG:HG2	1.51	0.91
3:A:381:THR:HG22	3:A:383:TYR:H	1.35	0.91
3:A:1399:ARG:HB3	3:A:1408:ILE:HD13	1.50	0.91
3:A:1194:ARG:NH2	3:A:1237:ILE:HD13	1.87	0.90
4:B:1002:THR:HG22	4:B:1006:ILE:N	1.84	0.90
4:B:956:THR:HA	4:B:961:LEU:O	1.71	0.90
4:B:842:ASN:HD22	4:B:845:SER:H	1.17	0.90
5:C:22:LEU:HD22	5:C:25:VAL:HG21	1.53	0.90
3:A:1105:LEU:HD22	3:A:1384:VAL:HG21	1.53	0.90
3:A:590:ARG:NH1	3:A:590:ARG:HG3	1.86	0.90
4:B:955:THR:HG22	4:B:956:THR:N	1.85	0.90
9:I:75:CYS:HG	13:I:204:ZN:ZN	0.68	0.90
7:F:93:ILE:HD11	7:F:134:ILE:HD11	1.54	0.90
3:A:351:THR:HG23	4:B:1103:ILE:HA	1.53	0.90
9:I:111:THR:HG22	9:I:113:ASP:N	1.86	0.89
4:B:1159:ARG:HE	4:B:1193:GLN:HE21	0.93	0.89
3:A:868:TYR:HD2	3:A:1058:VAL:HG21	1.38	0.89
3:A:1410:PHE:CD2	4:B:1212:ILE:HD11	2.08	0.89
2:T:2:DC:H2'	2:T:3:DG:C8	2.07	0.89
6:E:5:ASN:HD21	6:E:52:ARG:HG2	1.35	0.89
4:B:800:GLN:HB3	10:J:52:THR:HG21	1.54	0.89
3:A:567:LYS:HB2	3:A:568:PRO:CD	2.02	0.88
4:B:1077:THR:HG22	4:B:1079:LYS:H	1.35	0.88
3:A:549:MET:SD	3:A:577:ILE:HD12	2.12	0.88
4:B:955:THR:CG2	4:B:956:THR:H	1.87	0.88
1:R:9:G:O6	1:R:10:A:N6	2.07	0.88
3:A:666:ILE:CD1	4:B:1030:LEU:HD13	2.04	0.87
4:B:512:ARG:HH21	4:B:535:LEU:CD1	1.88	0.87
3:A:886:ILE:HD11	3:A:943:LEU:HB3	1.56	0.87
3:A:567:LYS:NZ	8:H:46:LEU:HB2	1.87	0.87
4:B:1065:GLN:HE21	4:B:1067:ARG:N	1.73	0.87
5:C:57:VAL:HG11	10:J:60:PHE:CB	2.03	0.87
3:A:590:ARG:HH11	3:A:590:ARG:HG3	1.37	0.87
2:T:8:DT:H2''	2:T:9:DC:O5'	1.74	0.87
4:B:345:LYS:CA	4:B:348:ARG:HE	1.87	0.87
3:A:61:ILE:HG22	3:A:62:ASP:H	1.37	0.87
4:B:1072:MET:HE3	4:B:1085:ILE:HB	1.56	0.87
4:B:744:HIS:HD2	4:B:746:SER:H	1.22	0.87
3:A:1192:LEU:HD11	3:A:1239:ARG:HB3	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:667:GLY:HA2	3:A:670:ILE:HD12	1.56	0.87
3:A:337:ARG:NH1	3:A:839:ARG:HH12	1.72	0.87
5:C:44:LEU:HB2	5:C:77:ILE:HD11	1.55	0.87
3:A:962:ARG:HA	3:A:965:GLN:HE21	1.38	0.86
2:T:3:DG:H5'	3:A:836:TYR:CD1	2.09	0.86
4:B:130:VAL:HG21	4:B:167:ILE:HD12	1.56	0.86
4:B:977:GLY:HA3	4:B:1099:VAL:CG2	2.04	0.86
3:A:605:MET:HE3	3:A:614:PHE:O	1.75	0.86
2:T:11:DC:H2''	2:T:12:DG:H5'	1.56	0.86
3:A:1242:VAL:HG12	3:A:1243:VAL:H	1.40	0.86
4:B:1106:ARG:HH21	4:B:1109:GLY:H	1.24	0.86
4:B:801:LYS:O	10:J:52:THR:HG23	1.75	0.86
4:B:912:ILE:O	4:B:938:SER:HB2	1.76	0.86
5:C:167:HIS:HD2	5:C:169:LYS:H	0.90	0.85
3:A:269:ILE:HD11	3:A:300:VAL:HA	1.57	0.85
11:K:10:PHE:CD1	11:K:11:LEU:HD13	2.11	0.85
4:B:345:LYS:HA	4:B:348:ARG:NE	1.91	0.85
3:A:417:TYR:O	3:A:418:SER:HB2	1.75	0.85
2:T:6:DC:H4'	3:A:447:GLN:NE2	1.91	0.85
3:A:1348:LEU:HD23	3:A:1372:VAL:HG13	1.59	0.85
3:A:1039:LYS:O	3:A:1043:ASP:HB2	1.76	0.85
1:R:5:A:N1	1:R:6:G:C6	2.44	0.84
4:B:1106:ARG:NH1	4:B:1118:PRO:HB3	1.91	0.84
3:A:709:THR:HG21	9:I:93:LYS:O	1.78	0.84
8:H:125:LEU:HG	8:H:130:ARG:NH1	1.92	0.84
6:E:177:ARG:HD3	6:E:215:MET:SD	2.18	0.84
2:T:9:DC:OP1	4:B:1123:SER:HB3	1.77	0.84
3:A:1390:ASN:ND2	3:A:1399:ARG:HA	1.93	0.84
3:A:1118:VAL:CG2	3:A:1306:LEU:HB2	2.08	0.84
11:K:12:LEU:H	11:K:12:LEU:HD12	1.42	0.84
4:B:228:LYS:HD3	4:B:234:ILE:HD13	1.57	0.84
2:T:6:DC:H4'	3:A:447:GLN:HE22	1.42	0.83
7:F:147:SER:OG	7:F:150:GLU:HG3	1.78	0.83
4:B:1002:THR:CG2	4:B:1006:ILE:H	1.91	0.83
4:B:200:GLY:HA2	4:B:202:TYR:HE2	1.43	0.83
4:B:637:LEU:HD12	4:B:693:ILE:HD12	1.60	0.83
4:B:519:TRP:HZ2	4:B:705:MET:HE1	1.42	0.83
5:C:11:ARG:NH2	5:C:229:TYR:HD2	1.77	0.82
3:A:535:THR:HG21	3:A:617:VAL:H	1.43	0.82
3:A:565:ILE:HG23	3:A:567:LYS:HG2	1.62	0.82
4:B:269:ILE:HD11	4:B:386:LEU:HD21	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:108:VAL:HG12	4:B:109:THR:H	1.42	0.82
3:A:885:THR:HG23	3:A:893:PHE:HE1	1.43	0.82
6:E:2:ASP:O	6:E:3:GLN:HG2	1.78	0.82
3:A:683:ILE:HD11	3:A:764:CYS:HB2	1.61	0.82
4:B:999:MET:HG3	4:B:1000:PRO:HD2	1.61	0.82
4:B:763:GLN:HG2	4:B:765:PRO:HD2	1.61	0.82
3:A:563:PRO:HG3	3:A:572:TRP:CZ2	2.14	0.81
8:H:81:PRO:HB2	8:H:82:PRO:HD3	1.62	0.81
8:H:93:TYR:HB3	8:H:144:ILE:O	1.80	0.81
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.61	0.81
3:A:1017:LEU:HB2	6:E:206:GLY:H	1.45	0.81
4:B:1106:ARG:HE	4:B:1109:GLY:N	1.79	0.81
4:B:800:GLN:HB3	10:J:52:THR:CG2	2.11	0.81
3:A:208:LEU:HD22	3:A:212:LYS:HE3	1.62	0.81
4:B:1106:ARG:HE	4:B:1109:GLY:H	1.29	0.81
3:A:742:ASN:HA	3:A:745:GLN:HB2	1.63	0.81
5:C:37:MET:HG2	5:C:243:VAL:HG12	1.62	0.81
9:I:50:THR:CG2	9:I:52:ILE:HG23	2.11	0.81
4:B:121:ASN:HD22	4:B:121:ASN:N	1.79	0.81
8:H:81:PRO:HB2	8:H:82:PRO:CD	2.11	0.81
3:A:472:LEU:O	3:A:475:THR:HB	1.81	0.81
4:B:899:ILE:HD11	4:B:911:ILE:HA	1.62	0.80
3:A:337:ARG:NH1	3:A:839:ARG:NH1	2.29	0.80
4:B:244:LEU:O	4:B:249:ARG:HG2	1.81	0.80
5:C:148:ARG:NH1	10:J:64:ASN:HA	1.96	0.80
3:A:406:ILE:HB	3:A:431:LYS:HB2	1.61	0.80
9:I:75:CYS:SG	9:I:78:CYS:SG	2.80	0.80
3:A:868:TYR:CE1	3:A:1064:VAL:HG11	2.17	0.80
4:B:1106:ARG:HH21	4:B:1109:GLY:N	1.78	0.80
4:B:796:LEU:HB3	4:B:799:PRO:HG3	1.63	0.80
2:T:6:DC:C2'	2:T:7:DC:C5'	2.45	0.80
4:B:1100:ASP:HA	4:B:1103:ILE:CD1	2.12	0.80
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.12	0.80
3:A:523:ILE:HD12	3:A:622:VAL:CG2	2.12	0.80
4:B:519:TRP:CZ2	4:B:705:MET:HE1	2.16	0.79
3:A:1118:VAL:HG22	3:A:1306:LEU:HB2	1.64	0.79
1:R:5:A:H2'	1:R:6:G:C8	2.18	0.79
3:A:93:VAL:CG1	3:A:301:ALA:HB1	2.11	0.79
4:B:313:MET:HE3	4:B:386:LEU:HD22	1.62	0.79
2:T:3:DG:H5'	3:A:836:TYR:CE1	2.18	0.79
4:B:293:PRO:HG2	4:B:296:GLU:CB	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:40:THR:HG22	3:A:41:MET:HG3	1.64	0.79
4:B:487:THR:HG22	4:B:489:SER:H	1.48	0.79
4:B:1065:GLN:HE21	4:B:1067:ARG:H	1.29	0.79
3:A:32:VAL:HG21	3:A:68:GLN:NE2	1.97	0.79
5:C:56:THR:HG22	5:C:57:VAL:N	1.97	0.79
4:B:1106:ARG:NH2	4:B:1109:GLY:H	1.79	0.79
3:A:298:PHE:O	3:A:302:THR:HB	1.83	0.79
3:A:913:LEU:HD12	3:A:914:GLU:N	1.98	0.79
3:A:768:GLN:CG	3:A:816:HIS:HA	2.13	0.79
4:B:834:ASN:HB3	4:B:840:ILE:HG13	1.63	0.78
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.63	0.78
3:A:1299:VAL:HG12	3:A:1300:LYS:H	1.47	0.78
3:A:666:ILE:HD13	4:B:1030:LEU:HD22	1.65	0.78
3:A:1281:ARG:O	3:A:1282:VAL:HG23	1.83	0.78
8:H:5:LEU:HD11	8:H:135:LEU:HG	1.63	0.78
8:H:40:LEU:HD23	8:H:42:ILE:HD11	1.66	0.78
3:A:58:LEU:HD22	3:A:80:HIS:O	1.83	0.78
3:A:353:ILE:HD13	3:A:487:MET:CE	2.14	0.78
3:A:313:GLN:HB2	3:A:322:VAL:CG2	2.14	0.78
4:B:102:VAL:HG23	4:B:112:LEU:HB2	1.65	0.78
3:A:783:THR:HG21	3:A:815:PHE:CZ	2.19	0.78
4:B:855:PHE:HZ	4:B:857:ARG:NH1	1.81	0.78
3:A:70:CYS:O	3:A:72:GLU:HG2	1.84	0.78
4:B:392:ARG:NH2	9:I:52:ILE:HD11	1.98	0.78
4:B:583:ASN:HD21	4:B:628:THR:HB	1.49	0.78
3:A:679:ILE:HG23	3:A:729:ALA:HB1	1.63	0.78
5:C:165:LYS:O	11:K:6:ARG:NH1	2.17	0.77
4:B:496:ARG:NH1	4:B:539:LEU:HB2	1.99	0.77
3:A:313:GLN:HB2	3:A:322:VAL:HG23	1.64	0.77
8:H:123:MET:HE3	8:H:142:LEU:HD22	1.66	0.77
3:A:901:LEU:H	3:A:926:GLN:NE2	1.82	0.77
4:B:1100:ASP:OD1	4:B:1103:ILE:HD11	1.84	0.77
4:B:102:VAL:CG2	4:B:112:LEU:HB2	2.13	0.77
4:B:842:ASN:ND2	4:B:845:SER:N	2.31	0.77
11:K:47:ARG:HH11	11:K:47:ARG:HB3	1.49	0.77
4:B:1166:CYS:O	4:B:1168:LEU:N	2.18	0.77
10:J:12:LYS:O	10:J:14:VAL:HG23	1.85	0.77
3:A:855:THR:HG21	3:A:857:ARG:NE	1.95	0.77
4:B:232:SER:OG	4:B:234:ILE:HD12	1.84	0.77
10:J:10:CYS:SG	10:J:46:CYS:SG	2.83	0.77
3:A:1438:THR:HB	4:B:1144:ALA:HB3	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:31:SER:CB	3:A:83:HIS:HB2	2.15	0.77
3:A:23:SER:HB3	3:A:233:TRP:CZ2	2.19	0.77
3:A:1345:ARG:HD2	3:A:1373:ASP:OD1	1.84	0.77
3:A:24:PRO:HB3	3:A:237:THR:HB	1.67	0.76
4:B:708:GLU:HG3	4:B:709:ASP:N	1.98	0.76
3:A:567:LYS:HZ1	8:H:46:LEU:HB2	1.49	0.76
4:B:707:PRO:HG2	4:B:708:GLU:H	1.49	0.76
3:A:326:ARG:HG2	3:A:1406:VAL:HG21	1.67	0.76
3:A:896:ARG:HD3	3:A:897:TYR:CE1	2.21	0.76
4:B:1096:ARG:O	4:B:1097:HIS:HB2	1.85	0.76
3:A:549:MET:HE1	3:A:656:TRP:HD1	1.49	0.76
4:B:899:ILE:CD1	4:B:911:ILE:HA	2.16	0.76
6:E:69:ILE:HG23	6:E:73:PRO:HA	1.68	0.76
2:T:6:DC:H2''	2:T:7:DC:H5'	0.79	0.76
3:A:353:ILE:HD13	3:A:487:MET:HE3	1.67	0.76
3:A:399:HIS:O	3:A:401:GLY:N	2.17	0.76
5:C:57:VAL:CG1	10:J:60:PHE:HB3	2.15	0.76
4:B:842:ASN:HD22	4:B:845:SER:N	1.83	0.76
5:C:166:GLU:HG3	11:K:10:PHE:HZ	1.51	0.76
3:A:223:GLY:O	3:A:1415:SER:HA	1.86	0.76
3:A:1094:VAL:HG13	3:A:1113:THR:HG21	1.66	0.76
4:B:996:ARG:NH2	5:C:174:ALA:O	2.19	0.76
3:A:336:ILE:HD12	3:A:1405:THR:HG21	1.68	0.75
8:H:93:TYR:HA	8:H:145:ARG:HB3	1.68	0.75
5:C:124:LEU:O	5:C:127:ARG:HG2	1.85	0.75
3:A:469:ARG:HH21	4:B:976:ILE:HD13	1.50	0.75
4:B:882:THR:HG22	4:B:884:ARG:H	1.50	0.75
4:B:211:VAL:HG21	4:B:483:LEU:HD13	1.67	0.75
4:B:711:GLU:N	4:B:712:PRO:HD3	2.01	0.75
4:B:118:ARG:HG3	4:B:204:ILE:HD13	1.68	0.75
3:A:1323:ASP:OD1	3:A:1325:THR:HB	1.85	0.75
3:A:41:MET:HA	3:A:49:LYS:HA	1.68	0.75
11:K:55:LYS:HB3	11:K:81:TYR:HD1	1.50	0.75
7:F:111:LEU:N	7:F:111:LEU:HD12	2.02	0.75
10:J:48:ARG:HH21	10:J:49:MET:HE1	1.52	0.75
3:A:265:LYS:NZ	3:A:323:LYS:H	1.84	0.74
3:A:1436:ILE:HG22	3:A:1437:GLY:H	1.52	0.74
12:L:38:LEU:O	12:L:39:SER:HB3	1.85	0.74
4:B:62:ILE:HG23	4:B:418:LYS:HG2	1.69	0.74
4:B:118:ARG:HH22	4:B:194:GLU:CD	1.90	0.74
2:T:2:DC:OP1	3:A:1403:GLU:O	2.04	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:458:HIS:CE1	3:A:507:VAL:HG21	2.22	0.74
3:A:1146:VAL:HG11	3:A:1202:MET:SD	2.27	0.74
4:B:708:GLU:CG	4:B:709:ASP:H	1.97	0.74
3:A:575:LYS:HB3	3:A:612:ILE:CG2	2.17	0.74
3:A:535:THR:CG2	3:A:616:VAL:HA	2.17	0.74
3:A:1436:ILE:HG22	3:A:1437:GLY:N	2.03	0.74
3:A:693:VAL:HG21	3:A:721:PHE:HE1	1.51	0.74
6:E:61:GLN:HE21	6:E:105:PHE:HE2	1.34	0.74
3:A:853:ASP:OD1	3:A:855:THR:HB	1.88	0.74
3:A:95:PHE:O	3:A:99:ILE:HG13	1.85	0.74
4:B:521:LEU:HD22	4:B:633:VAL:HG12	1.69	0.74
4:B:46:GLN:HG3	4:B:47:GLN:N	2.03	0.74
4:B:423:LYS:HA	4:B:426:LYS:HE2	1.68	0.74
3:A:443:LEU:HD21	3:A:455:MET:HB3	1.70	0.74
4:B:770:GLN:HG2	4:B:983:ARG:O	1.86	0.74
3:A:710:LEU:H	3:A:710:LEU:HD12	1.52	0.74
3:A:1436:ILE:CG2	4:B:1142:GLY:HA2	2.17	0.74
3:A:154:SER:HB3	3:A:162:VAL:CG2	2.17	0.74
5:C:167:HIS:HD2	5:C:169:LYS:N	1.76	0.74
8:H:5:LEU:HB3	8:H:133:ASN:O	1.88	0.74
3:A:1299:VAL:HG12	3:A:1300:LYS:N	2.02	0.74
11:K:65:HIS:CD2	11:K:67:PHE:H	2.06	0.74
3:A:541:ILE:HG21	3:A:549:MET:HE3	1.68	0.73
4:B:363:HIS:O	4:B:364:ILE:HB	1.88	0.73
4:B:172:ILE:HD13	4:B:178:ASN:HB3	1.70	0.73
11:K:65:HIS:HD2	11:K:67:PHE:H	1.35	0.73
3:A:500:GLU:OE2	4:B:1145:SER:HB2	1.88	0.73
4:B:542:MET:HE3	4:B:747:MET:HG3	1.67	0.73
2:T:1:DA:N3	2:T:1:DA:H2'	2.03	0.73
4:B:651:LEU:HD11	4:B:707:PRO:HB3	1.69	0.73
3:A:828:ALA:HB2	4:B:530:GLY:HA2	1.70	0.73
3:A:857:ARG:HD3	3:A:861:GLY:O	1.88	0.73
6:E:124:VAL:HA	6:E:132:ILE:HD12	1.70	0.73
3:A:1441:PHE:CZ	7:F:89:GLU:HA	2.23	0.73
3:A:417:TYR:O	3:A:418:SER:CB	2.36	0.73
3:A:321:PRO:O	3:A:322:VAL:HB	1.87	0.73
6:E:61:GLN:NE2	6:E:105:PHE:HE2	1.86	0.73
3:A:268:ASP:HB3	3:A:299:HIS:CE1	2.23	0.73
3:A:341:MET:HE1	3:A:1401:SER:HB2	1.70	0.73
3:A:32:VAL:HB	3:A:57:ARG:HD2	1.71	0.73
4:B:1106:ARG:NE	4:B:1109:GLY:H	1.85	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:10:A:OP1	1:R:10:A:OP2	1.99	0.73
3:A:534:LEU:O	3:A:574:GLY:HA3	1.88	0.73
8:H:35:GLN:HB3	8:H:111:LEU:HD21	1.70	0.73
3:A:567:LYS:HB3	8:H:96:VAL:N	2.02	0.73
3:A:691:LEU:HD11	3:A:695:LYS:HE3	1.71	0.73
1:R:9:G:N1	1:R:10:A:N6	2.36	0.73
3:A:75:ASN:O	3:A:76:GLU:HB3	1.88	0.73
4:B:234:ILE:H	4:B:234:ILE:HD12	1.54	0.73
4:B:313:MET:CE	4:B:386:LEU:HD22	2.19	0.73
4:B:708:GLU:O	4:B:710:LEU:N	2.22	0.73
4:B:980:PHE:CE2	4:B:1094:ARG:HG3	2.23	0.73
3:A:1152:ILE:HG23	3:A:1260:LEU:HD23	1.71	0.73
4:B:570:VAL:HG21	4:B:573:GLN:NE2	2.04	0.72
4:B:542:MET:HG3	4:B:747:MET:HE3	1.69	0.72
3:A:868:TYR:CD2	3:A:1058:VAL:HG21	2.23	0.72
3:A:445:ASN:HB2	3:A:455:MET:HG2	1.70	0.72
4:B:542:MET:HE1	4:B:743:ILE:HG21	1.70	0.72
8:H:89:LEU:C	8:H:91:ASP:H	1.90	0.72
3:A:899:VAL:HB	3:A:929:LEU:HD12	1.71	0.72
4:B:193:LYS:HD3	4:B:787:VAL:HG11	1.70	0.72
4:B:570:VAL:HB	4:B:573:GLN:CB	2.18	0.72
3:A:1399:ARG:HB2	3:A:1408:ILE:HG21	1.70	0.72
3:A:598:LEU:HD22	8:H:25:ARG:NH1	2.05	0.72
3:A:337:ARG:NE	3:A:839:ARG:HH22	1.88	0.72
8:H:89:LEU:HB3	8:H:91:ASP:OD1	1.88	0.72
3:A:925:LEU:O	3:A:929:LEU:HD23	1.88	0.72
1:R:4:G:H1	2:T:11:DC:H42	1.37	0.72
11:K:55:LYS:HD3	11:K:78:THR:CB	2.20	0.72
3:A:1258:HIS:ND1	3:A:1262:LYS:HE3	2.04	0.72
3:A:48:ALA:O	3:A:49:LYS:HG3	1.89	0.72
3:A:901:LEU:HG	3:A:926:GLN:HE21	1.55	0.72
4:B:879:ARG:HB3	4:B:883:LEU:HD23	1.70	0.72
2:T:2:DC:H2'	2:T:3:DG:H8	1.55	0.72
4:B:58:THR:O	4:B:62:ILE:HG13	1.89	0.72
3:A:1209:MET:SD	3:A:1236:LEU:HB3	2.30	0.72
4:B:429:PHE:HA	4:B:432:MET:HE2	1.71	0.72
3:A:399:HIS:HB3	3:A:400:PRO:HD3	1.70	0.72
3:A:445:ASN:CB	3:A:455:MET:HG2	2.19	0.72
4:B:745:PRO:O	4:B:748:ILE:HG12	1.88	0.72
3:A:567:LYS:HD3	8:H:95:TYR:CD1	2.25	0.72
3:A:1397:LEU:O	3:A:1400:CYS:HB2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:309:GLN:HG3	9:I:52:ILE:HD13	1.72	0.71
3:A:340:LEU:HD21	4:B:1200:ALA:HB2	1.72	0.71
5:C:18:VAL:HG23	5:C:240:VAL:HG11	1.72	0.71
4:B:1007:VAL:HG22	4:B:1008:PRO:HD2	1.71	0.71
6:E:168:TYR:HB3	6:E:170:LEU:HD21	1.72	0.71
4:B:737:THR:HG23	9:I:66:PRO:CB	2.20	0.71
4:B:637:LEU:CD1	4:B:693:ILE:HD12	2.20	0.71
9:I:74:GLU:HB3	9:I:79:HIS:HA	1.70	0.71
11:K:7:PHE:HB2	11:K:11:LEU:HD22	1.71	0.71
15:R:3000:UTP:O2	2:T:4:DA:C2	2.44	0.71
3:A:567:LYS:HE3	8:H:46:LEU:HD12	1.72	0.71
4:B:1066:SER:O	4:B:1067:ARG:HD3	1.90	0.71
3:A:575:LYS:HB3	3:A:612:ILE:HG23	1.71	0.71
4:B:108:VAL:HG12	4:B:109:THR:N	2.06	0.71
4:B:281:PRO:HG2	4:B:284:ILE:HD12	1.73	0.71
4:B:792:MET:HA	4:B:856:PHE:O	1.91	0.71
3:A:675:THR:HG21	3:A:736:ASN:ND2	2.06	0.71
3:A:672:ASP:HB2	3:A:736:ASN:OD1	1.90	0.71
3:A:855:THR:HG23	3:A:857:ARG:HG3	1.72	0.70
4:B:555:ILE:HD13	4:B:587:HIS:CE1	2.26	0.70
3:A:900:ASP:OD2	3:A:903:ASN:HB2	1.90	0.70
3:A:1015:VAL:HG12	3:A:1019:CYS:SG	2.31	0.70
4:B:1056:SER:HB3	4:B:1066:SER:HB2	1.73	0.70
1:R:5:A:C2	1:R:6:G:C6	2.79	0.70
3:A:225:ASN:O	3:A:227:VAL:N	2.21	0.70
4:B:839:MET:HE3	4:B:1010:LEU:HD11	1.72	0.70
3:A:451:HIS:NE2	3:A:1074:GLU:HG3	2.07	0.70
3:A:343:LYS:HE3	4:B:1151:LEU:O	1.92	0.70
3:A:367:PRO:HB3	3:A:466:SER:HA	1.73	0.70
3:A:675:THR:CB	3:A:736:ASN:HD21	2.04	0.70
8:H:49:VAL:HG12	8:H:50:ALA:N	2.07	0.70
4:B:957:ASN:HD22	4:B:961:LEU:HD12	1.57	0.70
4:B:636:PRO:O	4:B:637:LEU:HG	1.90	0.70
3:A:994:GLN:HE22	3:A:1023:ARG:HE	1.38	0.70
6:E:56:LYS:HG3	6:E:84:ASP:HB2	1.73	0.70
4:B:955:THR:HG23	12:L:54:ARG:O	1.91	0.70
3:A:44:THR:O	3:A:45:GLN:HB2	1.91	0.70
4:B:65:GLU:HG3	4:B:66:ASP:H	1.56	0.70
3:A:351:THR:HG21	4:B:1103:ILE:HG23	1.72	0.70
3:A:463:ILE:HB	3:A:464:PRO:HD2	1.74	0.70
4:B:638:PHE:CE1	4:B:743:ILE:HA	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:503:GLN:HE21	7:F:90:ARG:NH2	1.88	0.70
12:L:60:ARG:CG	12:L:61:THR:H	1.94	0.69
3:A:1095:THR:HG22	3:A:1100:ARG:HB2	1.74	0.69
11:K:55:LYS:HD3	11:K:78:THR:HB	1.72	0.69
2:T:8:DT:C2'	2:T:9:DC:O5'	2.39	0.69
3:A:1208:THR:HB	3:A:1211:GLN:HG3	1.74	0.69
12:L:47:ARG:HG2	12:L:52:GLY:HA2	1.72	0.69
3:A:472:LEU:HD11	4:B:835:GLN:NE2	2.07	0.69
4:B:378:LEU:O	4:B:382:ILE:HG13	1.92	0.69
4:B:130:VAL:HG12	4:B:131:ASP:N	2.07	0.69
3:A:335:ARG:HA	3:A:339:ASN:HD22	1.56	0.69
4:B:293:PRO:HG2	4:B:296:GLU:HB3	1.74	0.69
3:A:383:TYR:HB3	7:F:115:THR:HG22	1.73	0.69
5:C:80:LEU:HD22	5:C:129:ILE:CD1	2.21	0.69
4:B:54:PHE:HA	4:B:58:THR:HB	1.74	0.69
3:A:567:LYS:HE3	8:H:46:LEU:CD1	2.22	0.69
8:H:36:CYS:SG	8:H:130:ARG:NH2	2.65	0.69
4:B:463:THR:CG2	4:B:465:ASN:HD22	2.05	0.69
2:T:1:DA:N1	2:T:2:DC:C5	2.61	0.69
7:F:81:THR:HG21	7:F:136:ARG:CD	2.20	0.69
3:A:392:VAL:HG13	3:A:415:LEU:HD11	1.74	0.69
3:A:414:ASP:OD1	3:A:416:ARG:HG2	1.93	0.69
3:A:1332:PHE:H	3:A:1332:PHE:HD2	1.38	0.69
3:A:763:ALA:O	3:A:803:SER:HB3	1.92	0.69
3:A:786:HIS:HE1	4:B:742:GLU:OE1	1.76	0.69
3:A:768:GLN:HG2	3:A:816:HIS:HA	1.75	0.69
4:B:314:LEU:O	4:B:317:CYS:HB2	1.92	0.69
4:B:884:ARG:O	4:B:936:ASP:HB3	1.93	0.69
3:A:443:LEU:HD22	3:A:455:MET:HE2	1.73	0.69
3:A:340:LEU:HD13	3:A:1429:ILE:HG23	1.74	0.69
5:C:39:ALA:HA	5:C:164:ALA:HB3	1.75	0.68
6:E:83:CYS:SG	6:E:88:VAL:HG22	2.32	0.68
3:A:1111:MET:HE1	3:A:1114:PRO:HA	1.74	0.68
3:A:391:LEU:HD22	3:A:400:PRO:O	1.93	0.68
4:B:288:ALA:HB1	4:B:331:LEU:HD12	1.75	0.68
3:A:1390:ASN:HD22	3:A:1399:ARG:HA	1.57	0.68
3:A:584:ASN:O	3:A:637:LYS:HE3	1.92	0.68
4:B:22:SER:O	4:B:654:ARG:HD2	1.94	0.68
4:B:46:GLN:HG3	4:B:47:GLN:H	1.59	0.68
4:B:542:MET:CE	4:B:747:MET:HG3	2.22	0.68
3:A:72:GLU:OE2	4:B:1175:LEU:HD12	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:954:VAL:O	12:L:55:ILE:O	2.11	0.68
3:A:693:VAL:CG2	3:A:721:PHE:HE1	2.07	0.68
4:B:280:ILE:CD1	4:B:334:ILE:HG12	2.23	0.68
3:A:599:SER:HB2	3:A:603:ASN:H	1.58	0.68
5:C:51:VAL:HG22	5:C:155:LEU:HD22	1.76	0.68
3:A:563:PRO:HB2	3:A:565:ILE:O	1.94	0.68
11:K:47:ARG:NH1	11:K:47:ARG:HB3	2.09	0.68
4:B:562:GLY:HA3	4:B:590:HIS:CE1	2.29	0.68
8:H:7:ASP:O	8:H:8:ASP:HB2	1.92	0.68
3:A:858:ASN:HD22	3:A:858:ASN:C	1.95	0.68
4:B:709:ASP:O	4:B:710:LEU:HD23	1.94	0.68
3:A:535:THR:HG21	3:A:617:VAL:N	2.08	0.68
4:B:986:GLN:OE1	4:B:986:GLN:HA	1.92	0.68
3:A:590:ARG:CG	3:A:590:ARG:HH11	2.06	0.68
5:C:254:LYS:HB3	11:K:42:LEU:HD11	1.75	0.68
2:T:1:DA:C6	2:T:2:DC:C5	2.81	0.67
4:B:280:ILE:HG22	4:B:285:ILE:HG13	1.76	0.67
4:B:842:ASN:ND2	4:B:844:SER:HB2	2.09	0.67
3:A:994:GLN:HE21	3:A:1019:CYS:HB3	1.59	0.67
5:C:166:GLU:HG3	11:K:10:PHE:CZ	2.29	0.67
4:B:514:LEU:HD12	4:B:515:HIS:N	2.09	0.67
4:B:121:ASN:HA	4:B:207:GLY:HA3	1.77	0.67
7:F:109:VAL:HG12	7:F:110:ASP:N	2.10	0.67
12:L:46:VAL:HG13	12:L:56:LEU:HD12	1.76	0.67
5:C:5:GLY:O	5:C:7:GLN:HG3	1.95	0.67
9:I:75:CYS:SG	9:I:103:CYS:SG	2.92	0.67
9:I:53:GLY:O	9:I:89:GLN:HB2	1.94	0.67
3:A:351:THR:CG2	4:B:1103:ILE:HG23	2.24	0.67
3:A:535:THR:HG21	3:A:616:VAL:HA	1.75	0.67
5:C:8:VAL:HG12	5:C:9:LYS:N	2.09	0.67
3:A:814:PHE:O	3:A:817:ALA:HB3	1.95	0.67
4:B:976:ILE:O	4:B:990:ILE:HB	1.94	0.67
4:B:1147:LEU:HD22	4:B:1151:LEU:HD22	1.77	0.67
2:T:1:DA:C1'	3:A:1386:ARG:HH12	2.08	0.67
4:B:711:GLU:N	4:B:712:PRO:CD	2.57	0.67
4:B:864:LYS:HB3	4:B:872:GLU:H	1.59	0.67
2:T:1:DA:C4	2:T:2:DC:C5	2.83	0.67
5:C:93:ASP:O	5:C:127:ARG:NH2	2.27	0.67
3:A:450:LEU:HD13	3:A:1074:GLU:HG2	1.77	0.67
3:A:694:THR:O	3:A:698:GLN:HG3	1.94	0.67
3:A:16:GLU:HB3	3:A:1418:LEU:HD11	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:260:LEU:O	5:C:264:GLN:HG3	1.95	0.67
4:B:566:LEU:HD13	4:B:588:GLY:HA2	1.77	0.67
8:H:26:ILE:HD12	8:H:42:ILE:HD12	1.77	0.66
4:B:1039:GLY:HA2	10:J:51:LEU:HD21	1.77	0.66
3:A:1342:GLU:OE2	6:E:212:ARG:NH1	2.28	0.66
4:B:882:THR:HG21	4:B:935:ARG:HA	1.75	0.66
4:B:711:GLU:H	4:B:712:PRO:HD3	1.60	0.66
3:A:828:ALA:CB	4:B:530:GLY:HA2	2.25	0.66
3:A:1267:MET:HA	3:A:1271:ILE:HD12	1.77	0.66
8:H:115:TYR:CE2	8:H:124:ARG:HG3	2.30	0.66
3:A:305:ASP:HB3	3:A:308:ILE:HD11	1.77	0.66
4:B:957:ASN:O	4:B:959:ASP:N	2.29	0.66
3:A:525:GLN:CB	4:B:835:GLN:HG2	2.25	0.66
3:A:897:TYR:CD2	3:A:936:LEU:HD13	2.30	0.66
8:H:95:TYR:CE2	8:H:97:MET:HG3	2.31	0.66
3:A:1348:LEU:HD21	3:A:1375:MET:SD	2.35	0.66
4:B:986:GLN:HE22	4:B:1020:ARG:CZ	2.08	0.66
9:I:55:THR:HG23	9:I:58:VAL:HG21	1.76	0.66
3:A:453:MET:HB3	3:A:477:PRO:HB3	1.76	0.66
3:A:446:ARG:HH11	3:A:446:ARG:HG2	1.59	0.66
6:E:127:ILE:O	6:E:127:ILE:HG13	1.93	0.66
3:A:1364:ASN:ND2	3:A:1365:TYR:N	2.43	0.66
4:B:1002:THR:HG23	4:B:1004:GLU:N	2.10	0.66
3:A:590:ARG:HB3	3:A:605:MET:N	2.10	0.66
8:H:38:LEU:HD13	8:H:125:LEU:HD13	1.77	0.66
3:A:1333:ILE:O	3:A:1336:MET:HB3	1.96	0.66
5:C:98:VAL:C	5:C:99:LEU:HD23	2.16	0.66
4:B:1051:THR:CG2	4:B:1053:GLU:H	1.93	0.66
4:B:287:ARG:NH2	4:B:294:ASP:OD2	2.28	0.66
3:A:76:GLU:OE2	4:B:1159:ARG:NH1	2.28	0.66
3:A:1042:PHE:CE2	3:A:1046:LEU:HD11	2.31	0.66
8:H:97:MET:HE2	8:H:142:LEU:HD23	1.76	0.66
12:L:45:ALA:O	12:L:46:VAL:HG23	1.95	0.66
5:C:56:THR:HG21	5:C:145:CYS:SG	2.35	0.66
3:A:90:VAL:CG1	3:A:297:GLN:HA	2.26	0.66
6:E:93:MET:HE2	6:E:120:ALA:HB1	1.77	0.66
3:A:381:THR:HG22	3:A:383:TYR:N	2.09	0.66
4:B:363:HIS:O	4:B:364:ILE:CB	2.44	0.66
2:T:6:DC:C4	2:T:7:DC:C5	2.84	0.66
4:B:1106:ARG:CZ	4:B:1109:GLY:H	2.07	0.66
10:J:58:GLU:HA	10:J:61:LEU:HD12	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:311:LEU:HB3	9:I:4:PHE:CZ	2.31	0.66
4:B:349:ILE:O	4:B:352:ALA:HB3	1.96	0.66
3:A:741:ASN:HD22	3:A:741:ASN:C	1.99	0.66
9:I:32:CYS:SG	9:I:33:SER:N	2.69	0.66
4:B:751:VAL:O	4:B:754:SER:HB2	1.95	0.66
6:E:176:PRO:O	6:E:212:ARG:HA	1.95	0.66
5:C:11:ARG:HH21	5:C:229:TYR:HD2	1.44	0.66
3:A:306:ASN:HD21	3:A:324:SER:H	1.43	0.66
3:A:1193:LEU:HB2	3:A:1260:LEU:HD11	1.78	0.66
4:B:1001:PHE:CZ	4:B:1073:TYR:HB2	2.30	0.66
3:A:751:SER:O	3:A:752:LYS:HG2	1.95	0.65
3:A:914:GLU:HB2	3:A:979:SER:O	1.95	0.65
3:A:95:PHE:HE2	3:A:1414:ALA:HB2	1.62	0.65
4:B:128:LEU:HB3	4:B:167:ILE:O	1.95	0.65
4:B:211:VAL:HG23	4:B:483:LEU:HB2	1.78	0.65
7:F:111:LEU:H	7:F:111:LEU:HD12	1.62	0.65
4:B:603:LEU:HB3	4:B:609:ILE:HG13	1.76	0.65
3:A:715:GLU:O	3:A:719:VAL:HG23	1.96	0.65
12:L:51:CYS:O	12:L:53:HIS:N	2.28	0.65
5:C:8:VAL:HG12	5:C:9:LYS:H	1.60	0.65
1:R:8:G:N2	2:T:8:DT:N3	2.45	0.65
4:B:293:PRO:HG2	4:B:296:GLU:HB2	1.79	0.65
3:A:816:HIS:CE1	4:B:764:SER:HB2	2.30	0.65
3:A:329:LEU:HD23	3:A:335:ARG:HG3	1.78	0.65
3:A:994:GLN:HE22	3:A:1023:ARG:NE	1.95	0.65
9:I:111:THR:HG21	9:I:113:ASP:HB2	1.78	0.65
5:C:22:LEU:HD22	5:C:25:VAL:CG2	2.25	0.65
3:A:1242:VAL:HG12	3:A:1243:VAL:N	2.12	0.65
4:B:911:ILE:CG2	4:B:966:VAL:HG11	2.26	0.65
8:H:24:CYS:HB2	8:H:44:VAL:CG2	2.27	0.65
4:B:1197:PRO:HG2	4:B:1200:ALA:HB2	1.79	0.65
3:A:1319:VAL:HG13	3:A:1320:PRO:HD2	1.79	0.65
12:L:48:CYS:SG	12:L:49:LYS:N	2.70	0.65
4:B:805:THR:HG21	4:B:815:ARG:HE	1.62	0.65
15:R:3000:UTP:O2	2:T:4:DA:H2	1.80	0.65
4:B:512:ARG:NH2	4:B:535:LEU:HD11	2.02	0.65
4:B:120:ARG:CG	4:B:955:THR:HG21	2.23	0.65
3:A:381:THR:HG21	3:A:383:TYR:CD1	2.31	0.65
4:B:1162:ILE:HD11	4:B:1194:ILE:HD13	1.77	0.65
4:B:824:ILE:CG1	10:J:48:ARG:HH12	2.08	0.64
10:J:9:SER:OG	10:J:48:ARG:NH2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:109:VAL:HG21	7:F:124:GLU:HA	1.79	0.64
7:F:96:THR:O	7:F:100:GLN:HG3	1.97	0.64
8:H:12:VAL:HA	8:H:28:ALA:CB	2.28	0.64
2:T:1:DA:N1	2:T:2:DC:H5	1.94	0.64
6:E:96:PHE:CZ	6:E:100:ILE:HD11	2.32	0.64
5:C:241:ASP:HB3	11:K:109:TRP:CE2	2.32	0.64
3:A:1444:MET:HE1	7:F:135:ARG:NE	2.12	0.64
4:B:1170:THR:O	4:B:1170:THR:HG22	1.97	0.64
3:A:475:THR:HG22	3:A:476:SER:N	2.12	0.64
3:A:512:VAL:HA	3:A:519:PRO:HA	1.79	0.64
3:A:87:ALA:HB3	3:A:276:LEU:HD23	1.79	0.64
4:B:879:ARG:HB3	4:B:883:LEU:CD2	2.27	0.64
4:B:788:ARG:NH1	4:B:790:ASP:OD1	2.31	0.64
4:B:649:LYS:HE2	4:B:738:PHE:O	1.96	0.64
8:H:107:VAL:HG21	8:H:126:GLU:HG3	1.79	0.64
4:B:46:GLN:HE22	4:B:496:ARG:HA	1.62	0.64
3:A:1035:TYR:O	3:A:1037:LEU:N	2.30	0.64
3:A:1224:LEU:HD12	3:A:1241:ARG:O	1.97	0.64
3:A:1115:SER:HA	3:A:1308:THR:HG22	1.77	0.64
4:B:25:ILE:HG22	4:B:29:ASP:HB2	1.79	0.64
3:A:901:LEU:HA	3:A:907:THR:HG23	1.80	0.64
4:B:1001:PHE:CE1	4:B:1073:TYR:HB2	2.33	0.64
5:C:114:TYR:CD2	5:C:140:ASN:HB3	2.32	0.64
3:A:1394:THR:CG2	3:A:1395:GLY:N	2.61	0.64
2:T:4:DA:H2''	2:T:5:DT:H5'	1.80	0.64
4:B:446:LEU:O	4:B:447:ALA:HB3	1.97	0.64
6:E:124:VAL:HG22	6:E:132:ILE:HG21	1.78	0.64
3:A:244:PRO:CG	3:A:245:PRO:HD3	2.27	0.64
4:B:842:ASN:HD21	4:B:844:SER:HB2	1.63	0.64
3:A:381:THR:CG2	3:A:383:TYR:H	2.09	0.64
3:A:84:ILE:HG23	3:A:239:LEU:HB3	1.80	0.64
12:L:40:LEU:HD13	12:L:44:ASP:CG	2.19	0.64
1:R:5:A:H2'	1:R:6:G:O4'	1.98	0.63
3:A:225:ASN:O	3:A:226:GLU:HG2	1.99	0.63
4:B:1034:VAL:HG23	4:B:1059:LEU:HB2	1.80	0.63
4:B:515:HIS:HD2	4:B:517:THR:OG1	1.81	0.63
3:A:778:GLY:HA3	4:B:516:ASN:HB2	1.80	0.63
3:A:1402:PHE:CD2	3:A:1403:GLU:HG3	2.33	0.63
4:B:114:PRO:HG3	4:B:181:LEU:HD11	1.79	0.63
3:A:1436:ILE:HB	4:B:1144:ALA:HB2	1.80	0.63
4:B:1201:LYS:O	4:B:1205:GLN:HG3	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:577:ALA:HB1	4:B:589:VAL:CG1	2.27	0.63
8:H:101:ALA:HB2	8:H:116:TYR:CE2	2.33	0.63
4:B:525:ALA:O	4:B:527:THR:HG22	1.98	0.63
8:H:31:THR:O	8:H:32:THR:CB	2.47	0.63
3:A:108:MET:O	3:A:109:HIS:HB2	1.99	0.63
4:B:604:ARG:HG2	4:B:604:ARG:O	1.98	0.63
4:B:1104:HIS:HB2	4:B:1122:ARG:HD2	1.80	0.63
3:A:709:THR:HB	3:A:712:GLU:H	1.64	0.63
3:A:579:SER:OG	3:A:612:ILE:HG22	1.97	0.63
6:E:100:ILE:HG23	6:E:105:PHE:HB2	1.80	0.63
7:F:86:THR:OG1	7:F:89:GLU:HG3	1.98	0.63
3:A:523:ILE:HD12	3:A:622:VAL:HG22	1.79	0.63
2:T:1:DA:H1'	3:A:1386:ARG:HH12	1.64	0.63
4:B:914:LYS:HB3	4:B:937:ALA:O	1.98	0.63
4:B:1187:ASN:OD1	4:B:1190:ASP:HB3	1.99	0.63
15:R:3000:UTP:N3	2:T:4:DA:N1	2.46	0.63
1:R:5:A:C4	1:R:6:G:N7	2.67	0.63
3:A:871:ASP:OD2	6:E:204:THR:HG23	1.99	0.63
4:B:913:GLY:HA2	4:B:938:SER:HB3	1.81	0.63
6:E:96:PHE:O	6:E:100:ILE:HG13	1.99	0.63
6:E:156:LEU:HD12	6:E:195:VAL:HG12	1.81	0.63
2:T:11:DC:H2'	2:T:12:DG:C8	2.34	0.62
9:I:7:CYS:HB2	9:I:29:CYS:HB2	1.81	0.62
4:B:496:ARG:HH11	4:B:539:LEU:HB2	1.62	0.62
12:L:55:ILE:HG13	12:L:56:LEU:H	1.63	0.62
3:A:871:ASP:HB3	6:E:204:THR:HG22	1.82	0.62
4:B:780:VAL:HG21	10:J:56:LEU:CD1	2.29	0.62
5:C:173:ALA:O	5:C:174:ALA:HB3	2.00	0.62
4:B:1106:ARG:HD2	4:B:1126:GLY:O	1.99	0.62
3:A:629:LEU:HD13	3:A:645:LEU:HD21	1.79	0.62
4:B:39:ARG:HE	4:B:665:GLU:HG2	1.64	0.62
3:A:73:GLY:O	3:A:75:ASN:N	2.32	0.62
5:C:166:GLU:HA	11:K:6:ARG:HB3	1.82	0.62
3:A:418:SER:O	3:A:420:ARG:N	2.32	0.62
3:A:523:ILE:HD12	3:A:622:VAL:HG21	1.80	0.62
3:A:1074:GLU:HB3	3:A:1075:PRO:CD	2.29	0.62
7:F:97:ARG:O	7:F:101:ILE:HG13	1.99	0.62
3:A:982:THR:HG22	3:A:984:LYS:H	1.64	0.62
5:C:235:VAL:HG21	10:J:6:ARG:HH21	1.65	0.62
4:B:1002:THR:HG23	4:B:1004:GLU:H	1.64	0.62
3:A:871:ASP:HB3	6:E:204:THR:CG2	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1212:VAL:O	3:A:1216:ILE:HG13	1.99	0.62
3:A:33:ALA:O	3:A:83:HIS:HB3	1.99	0.62
6:E:78:LEU:C	6:E:78:LEU:HD23	2.20	0.62
3:A:268:ASP:HB3	3:A:299:HIS:ND1	2.14	0.62
4:B:373:ARG:NE	4:B:567:GLU:OE2	2.29	0.62
4:B:208:SER:OG	4:B:210:LYS:HD3	1.99	0.62
2:T:11:DC:H2''	2:T:12:DG:C5'	2.29	0.62
12:L:34:CYS:SG	12:L:51:CYS:SG	2.98	0.62
4:B:549:THR:HB	4:B:628:THR:CG2	2.30	0.62
3:A:672:ASP:OD1	3:A:674:PRO:HD2	2.00	0.62
7:F:135:ARG:HG2	7:F:137:TYR:CE1	2.34	0.62
4:B:195:CYS:HB3	4:B:782:LEU:HD22	1.81	0.62
4:B:616:ILE:N	4:B:616:ILE:HD12	2.15	0.62
4:B:25:ILE:HG22	4:B:26:THR:H	1.65	0.62
4:B:1072:MET:CE	4:B:1085:ILE:HB	2.28	0.62
10:J:3:VAL:HG21	10:J:18:TRP:CG	2.34	0.62
7:F:111:LEU:H	7:F:111:LEU:CD1	2.13	0.62
6:E:93:MET:O	6:E:97:VAL:HG23	2.00	0.62
8:H:49:VAL:HG12	8:H:50:ALA:H	1.62	0.61
3:A:338:GLY:HA2	4:B:1129:ARG:NH2	2.10	0.61
3:A:590:ARG:HB3	3:A:605:MET:H	1.63	0.61
3:A:328:ARG:O	3:A:335:ARG:HG2	1.99	0.61
7:F:109:VAL:HG23	7:F:124:GLU:HG2	1.82	0.61
4:B:446:LEU:O	4:B:447:ALA:CB	2.48	0.61
4:B:221:ASN:OD1	4:B:242:SER:HA	1.98	0.61
11:K:63:VAL:O	11:K:63:VAL:CG2	2.48	0.61
3:A:855:THR:CG2	3:A:857:ARG:HG3	2.30	0.61
4:B:29:ASP:HB3	4:B:658:ILE:CD1	2.30	0.61
4:B:211:VAL:O	4:B:480:SER:HA	2.01	0.61
3:A:689:LYS:O	3:A:693:VAL:HG23	1.99	0.61
3:A:898:ARG:HB2	3:A:933:TYR:CE1	2.34	0.61
3:A:1054:LEU:O	3:A:1057:VAL:HG23	1.99	0.61
1:R:9:G:OP1	4:B:776:GLN:NE2	2.33	0.61
3:A:549:MET:SD	3:A:577:ILE:CD1	2.87	0.61
3:A:961:ARG:O	3:A:965:GLN:HG3	2.00	0.61
10:J:64:ASN:HB3	10:J:65:PRO:CD	2.29	0.61
3:A:354:SER:HA	3:A:482:PHE:CD2	2.34	0.61
3:A:88:LYS:HD2	3:A:293:GLU:CD	2.20	0.61
6:E:5:ASN:ND2	6:E:52:ARG:HG2	2.12	0.61
3:A:709:THR:OG1	3:A:712:GLU:HG3	2.00	0.61
4:B:839:MET:HE3	4:B:1010:LEU:CD1	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:178:ILE:HG23	6:E:214:CYS:HA	1.81	0.61
9:I:8:ARG:HG3	9:I:9:ASP:N	2.16	0.61
4:B:803:LEU:H	4:B:822:ASN:HD21	1.48	0.61
3:A:1021:LEU:O	3:A:1025:ARG:HG2	2.00	0.61
3:A:1437:GLY:HA3	7:F:88:TYR:CD2	2.36	0.61
3:A:789:LYS:HG3	9:I:67:THR:HB	1.83	0.61
5:C:49:VAL:HG21	5:C:67:LEU:HD12	1.82	0.61
3:A:821:ARG:HG3	3:A:825:ILE:HD11	1.82	0.61
3:A:1364:ASN:HD22	3:A:1364:ASN:C	2.04	0.61
3:A:915:SER:O	3:A:919:ILE:HG13	2.00	0.61
4:B:582:VAL:HG22	4:B:626:ILE:HB	1.82	0.61
3:A:1111:MET:HE1	3:A:1330:ASN:OD1	2.00	0.61
12:L:51:CYS:HB2	12:L:53:HIS:CD2	2.35	0.61
3:A:148:CYS:O	3:A:168:GLY:HA2	1.99	0.61
10:J:48:ARG:HE	10:J:49:MET:HE2	1.66	0.61
9:I:103:CYS:SG	9:I:106:CYS:SG	2.99	0.61
3:A:1192:LEU:HD22	3:A:1239:ARG:NH2	2.16	0.61
3:A:506:ALA:HB1	3:A:508:PRO:HD2	1.83	0.61
4:B:185:THR:HG23	4:B:188:ASP:OD2	2.01	0.61
7:F:138:LEU:HB3	7:F:139:PRO:HD2	1.83	0.61
3:A:565:ILE:CG2	3:A:567:LYS:HG2	2.31	0.61
4:B:1102:LYS:O	4:B:1104:HIS:N	2.32	0.61
4:B:57:TYR:CD1	4:B:57:TYR:N	2.68	0.61
3:A:736:ASN:O	3:A:737:LEU:C	2.38	0.61
5:C:123:ASN:HD22	5:C:125:MET:HG2	1.66	0.61
5:C:46:ILE:HA	5:C:159:ALA:HA	1.82	0.61
3:A:1317:MET:HA	3:A:1322:ILE:HD11	1.81	0.61
8:H:15:VAL:HG22	8:H:26:ILE:HG12	1.83	0.60
4:B:1039:GLY:HA2	10:J:51:LEU:CD2	2.31	0.60
3:A:337:ARG:CZ	3:A:839:ARG:NH1	2.64	0.60
3:A:824:LEU:O	3:A:827:THR:HB	2.00	0.60
3:A:306:ASN:OD1	3:A:324:SER:HB3	2.01	0.60
4:B:995:ARG:NH1	4:B:995:ARG:HB2	2.16	0.60
3:A:445:ASN:HB2	3:A:454:SER:O	2.00	0.60
3:A:511:ILE:HA	3:A:521:MET:HE3	1.83	0.60
8:H:106:GLU:C	8:H:108:SER:H	2.02	0.60
3:A:219:PHE:O	3:A:222:LEU:N	2.33	0.60
3:A:1132:LYS:O	3:A:1135:ARG:HB3	2.01	0.60
3:A:528:LEU:O	3:A:531:ILE:HG22	2.01	0.60
3:A:1293:SER:OG	3:A:1294:PRO:HD2	2.01	0.60
4:B:913:GLY:HA2	4:B:938:SER:CB	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:322:VAL:O	3:A:323:LYS:HG3	2.01	0.60
6:E:78:LEU:HD23	6:E:79:TRP:N	2.16	0.60
3:A:1158:PRO:HB3	3:A:1241:ARG:NH1	2.17	0.60
9:I:5:ARG:HD3	9:I:36:GLU:OE2	2.01	0.60
3:A:567:LYS:O	3:A:569:LYS:N	2.35	0.60
4:B:114:PRO:HB3	4:B:174:LEU:HD11	1.82	0.60
3:A:1208:THR:O	3:A:1212:VAL:HG23	2.01	0.60
3:A:86:LEU:HA	3:A:273:ASN:OD1	2.02	0.60
11:K:90:ALA:O	11:K:94:ILE:HG13	2.01	0.60
2:T:1:DA:C6	2:T:2:DC:C4	2.90	0.60
3:A:896:ARG:NH2	3:A:1030:ARG:HH21	2.00	0.60
7:F:101:ILE:HD12	7:F:121:ALA:HB2	1.82	0.60
6:E:47:CYS:HA	6:E:53:PRO:HA	1.83	0.60
10:J:1:MET:N	10:J:56:LEU:HB2	2.17	0.60
3:A:1223:ASP:HA	3:A:1243:VAL:CG1	2.32	0.60
3:A:1115:SER:O	3:A:1329:THR:HG23	2.02	0.60
4:B:778:MET:CE	4:B:1094:ARG:HD3	2.32	0.60
4:B:787:VAL:O	4:B:787:VAL:HG12	2.00	0.60
4:B:1169:MET:HE1	4:B:1201:LYS:O	2.01	0.60
4:B:299:GLU:OE1	4:B:571:PRO:HG2	2.01	0.60
3:A:567:LYS:CG	3:A:568:PRO:HD2	2.31	0.60
9:I:85:PHE:CD1	9:I:99:LEU:HD22	2.37	0.60
3:A:31:SER:OG	3:A:83:HIS:HB2	2.02	0.60
3:A:779:PHE:CZ	4:B:517:THR:HA	2.37	0.60
3:A:231:PRO:HA	3:A:234:MET:HE2	1.83	0.60
4:B:686:ASN:C	4:B:688:GLY:H	2.04	0.60
2:T:1:DA:C6	2:T:2:DC:N4	2.70	0.59
4:B:479:VAL:HG12	4:B:480:SER:N	2.17	0.59
3:A:503:GLN:HE21	7:F:90:ARG:HH21	1.47	0.59
4:B:198:ASP:OD1	4:B:485:ARG:NH2	2.34	0.59
5:C:244:VAL:O	5:C:248:ILE:HG13	2.03	0.59
4:B:1174:LYS:HB2	4:B:1179:GLN:O	2.02	0.59
3:A:1402:PHE:CE2	3:A:1403:GLU:HG3	2.37	0.59
3:A:68:GLN:HE22	3:A:80:HIS:HB3	1.67	0.59
2:T:11:DC:H2'	2:T:12:DG:H8	1.66	0.59
8:H:89:LEU:C	8:H:91:ASP:N	2.55	0.59
9:I:15:TYR:O	9:I:27:PHE:HA	2.02	0.59
3:A:76:GLU:O	3:A:76:GLU:HG3	2.02	0.59
10:J:1:MET:H2	10:J:56:LEU:HB2	1.68	0.59
4:B:975:GLN:HG2	4:B:976:ILE:H	1.67	0.59
3:A:239:LEU:HD12	3:A:240:PRO:HD2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:567:LYS:CB	3:A:568:PRO:CD	2.67	0.59
3:A:44:THR:HG22	3:A:44:THR:O	2.02	0.59
4:B:463:THR:HG22	4:B:465:ASN:HD22	1.66	0.59
8:H:84:ALA:HA	8:H:87:ARG:CG	2.32	0.59
2:T:1:DA:C2'	2:T:2:DC:O5'	2.38	0.59
9:I:106:CYS:HG	13:I:204:ZN:ZN	1.16	0.59
3:A:469:ARG:NH2	4:B:976:ILE:HD13	2.17	0.59
4:B:512:ARG:NH2	4:B:535:LEU:CD1	2.61	0.59
3:A:68:GLN:HE22	3:A:80:HIS:CB	2.15	0.59
5:C:56:THR:CG2	5:C:57:VAL:H	2.09	0.59
5:C:166:GLU:CG	11:K:10:PHE:HZ	2.14	0.59
3:A:151:ASP:HA	3:A:162:VAL:O	2.02	0.59
8:H:24:CYS:HB2	8:H:44:VAL:HG21	1.84	0.59
4:B:217:ARG:NH1	4:B:407:ASP:OD1	2.35	0.59
12:L:26:THR:O	12:L:27:LEU:HB3	2.01	0.59
3:A:704:ALA:HB2	3:A:710:LEU:CG	2.23	0.59
4:B:642:ASP:O	4:B:644:GLU:N	2.36	0.59
3:A:57:ARG:O	3:A:68:GLN:HG3	2.03	0.59
4:B:912:ILE:HD11	4:B:966:VAL:HG23	1.84	0.59
4:B:211:VAL:CG2	4:B:483:LEU:HD13	2.32	0.59
4:B:90:ILE:HD12	4:B:432:MET:SD	2.42	0.59
8:H:139:ASN:O	8:H:140:ALA:HB2	2.02	0.59
12:L:70:ARG:HG2	12:L:70:ARG:HH11	1.66	0.59
3:A:1385:THR:HG22	3:A:1386:ARG:H	1.68	0.59
3:A:93:VAL:HG11	3:A:308:ILE:CD1	2.33	0.59
3:A:1018:PHE:O	3:A:1021:LEU:HB3	2.03	0.59
3:A:1336:MET:CE	3:A:1381:LEU:HG	2.33	0.59
6:E:29:PHE:HB2	6:E:65:THR:HG22	1.83	0.59
8:H:109:LYS:NZ	8:H:109:LYS:HB2	2.18	0.59
4:B:642:ASP:HB3	4:B:649:LYS:HD2	1.85	0.59
4:B:848:ARG:NH1	10:J:8:PHE:O	2.35	0.59
3:A:596:THR:O	3:A:598:LEU:N	2.36	0.59
4:B:46:GLN:O	4:B:408:LEU:HD23	2.03	0.59
11:K:55:LYS:HB3	11:K:81:TYR:CD1	2.35	0.59
4:B:1117:GLN:HG3	4:B:1156:ASP:OD1	2.02	0.59
3:A:1394:THR:HG22	3:A:1395:GLY:N	2.17	0.59
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.33	0.59
11:K:49:GLU:HG3	11:K:94:ILE:HG12	1.83	0.59
3:A:1004:ASN:ND2	6:E:167:ARG:HD2	2.18	0.59
4:B:519:TRP:C	4:B:519:TRP:CD1	2.76	0.59
4:B:1159:ARG:CD	4:B:1193:GLN:HE21	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:896:ARG:HD3	3:A:897:TYR:HE1	1.67	0.59
6:E:61:GLN:HB2	6:E:79:TRP:CE3	2.38	0.59
5:C:18:VAL:HG23	5:C:240:VAL:CG1	2.33	0.59
4:B:1171:VAL:CG1	4:B:1191:ILE:HD13	2.32	0.59
9:I:111:THR:CG2	9:I:113:ASP:HB2	2.33	0.58
3:A:840:ARG:HB3	3:A:1384:VAL:HG12	1.85	0.58
3:A:385:ILE:HG22	3:A:386:ASP:N	2.18	0.58
3:A:90:VAL:HG11	3:A:297:GLN:HA	1.84	0.58
6:E:156:LEU:HD12	6:E:195:VAL:CG1	2.33	0.58
3:A:482:PHE:CD1	4:B:836:GLU:HB2	2.38	0.58
8:H:123:MET:HE3	8:H:142:LEU:CD2	2.33	0.58
3:A:901:LEU:H	3:A:926:GLN:HE21	1.50	0.58
4:B:860:MET:HG2	4:B:861:ASP:N	2.18	0.58
3:A:756:ILE:HG22	3:A:757:ASN:N	2.17	0.58
4:B:958:GLN:O	4:B:960:GLY:N	2.33	0.58
4:B:1106:ARG:HH12	4:B:1118:PRO:HB3	1.67	0.58
3:A:1325:THR:O	6:E:148:GLU:HB2	2.04	0.58
3:A:444:PHE:HB3	3:A:458:HIS:HD2	1.68	0.58
4:B:806:THR:HB	4:B:809:MET:HG3	1.85	0.58
3:A:107:CYS:HB2	3:A:114:LEU:CD2	2.32	0.58
3:A:1308:THR:HG21	3:A:1310:GLY:O	2.04	0.58
4:B:666:TYR:C	4:B:668:ASP:H	2.06	0.58
4:B:405:ARG:NH1	4:B:632:ARG:HG2	2.17	0.58
3:A:97:ALA:HA	3:A:100:LYS:HE3	1.84	0.58
3:A:663:SER:OG	3:A:664:THR:N	2.34	0.58
8:H:12:VAL:HA	8:H:28:ALA:HB2	1.85	0.58
3:A:1161:THR:HG22	3:A:1163:ILE:N	2.03	0.58
4:B:287:ARG:NH1	4:B:324:ILE:O	2.37	0.58
10:J:48:ARG:HE	10:J:49:MET:CE	2.16	0.58
4:B:779:GLY:HA2	4:B:796:LEU:HB2	1.85	0.58
11:K:47:ARG:HD3	11:K:59:ALA:O	2.04	0.58
6:E:46:TYR:HA	6:E:57:MET:SD	2.43	0.58
3:A:1364:ASN:ND2	3:A:1364:ASN:C	2.56	0.58
3:A:1155:ASP:OD2	3:A:1161:THR:HG23	2.04	0.58
7:F:81:THR:HG22	7:F:82:THR:N	2.18	0.58
4:B:744:HIS:CD2	4:B:746:SER:H	2.13	0.58
3:A:742:ASN:CA	3:A:745:GLN:HB2	2.33	0.58
12:L:49:LYS:O	12:L:50:ASP:HB2	2.03	0.58
4:B:205:ILE:HD12	4:B:205:ILE:N	2.19	0.58
9:I:16:PRO:HB3	9:I:27:PHE:CE2	2.38	0.58
3:A:260:ASP:OD1	3:A:261:ASP:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1201:LYS:HE2	4:B:1205:GLN:NE2	2.18	0.58
3:A:225:ASN:ND2	3:A:227:VAL:HB	2.18	0.58
4:B:589:VAL:HG12	4:B:590:HIS:N	2.18	0.58
3:A:849:MET:HE1	3:A:1061:GLY:HA2	1.86	0.58
4:B:955:THR:OG1	12:L:55:ILE:HA	2.04	0.58
3:A:1149:ALA:HB2	9:I:47:GLU:HA	1.84	0.58
9:I:47:GLU:OE1	9:I:50:THR:HG23	2.04	0.58
3:A:28:ARG:HG2	3:A:83:HIS:CE1	2.39	0.58
7:F:111:LEU:C	7:F:113:GLY:H	2.07	0.58
3:A:1074:GLU:O	3:A:1076:ALA:N	2.37	0.58
7:F:127:GLU:O	7:F:129:LYS:HG3	2.03	0.58
3:A:1042:PHE:HE2	3:A:1046:LEU:HD11	1.66	0.58
4:B:101:MET:HB2	4:B:169:ARG:HH12	1.69	0.58
4:B:1077:THR:HG22	4:B:1079:LYS:N	2.13	0.58
4:B:93:GLY:N	4:B:131:ASP:O	2.37	0.58
3:A:418:SER:O	3:A:419:LYS:C	2.39	0.58
3:A:524:VAL:HG12	3:A:525:GLN:H	1.69	0.58
5:C:148:ARG:HG3	10:J:61:LEU:O	2.03	0.58
4:B:980:PHE:CE1	4:B:990:ILE:HD11	2.39	0.58
8:H:81:PRO:CB	8:H:82:PRO:CD	2.81	0.57
11:K:65:HIS:CD2	11:K:67:PHE:HB2	2.39	0.57
3:A:1420:ASP:O	3:A:1421:CYS:HB2	2.04	0.57
4:B:973:ILE:HG23	4:B:974:PRO:HD2	1.86	0.57
1:R:9:G:N1	1:R:10:A:C6	2.71	0.57
4:B:803:LEU:N	4:B:822:ASN:HD21	2.02	0.57
4:B:855:PHE:HZ	4:B:857:ARG:HH11	1.52	0.57
3:A:1143:LEU:HD23	3:A:1267:MET:HB3	1.86	0.57
3:A:225:ASN:HD22	3:A:227:VAL:HB	1.69	0.57
6:E:213:ILE:O	6:E:213:ILE:HG23	2.04	0.57
5:C:175:ALA:HB3	10:J:43:ARG:NH2	2.20	0.57
4:B:25:ILE:HG22	4:B:29:ASP:CB	2.34	0.57
4:B:653:VAL:HG22	4:B:689:LEU:HB3	1.85	0.57
3:A:41:MET:HB3	3:A:48:ALA:O	2.04	0.57
3:A:1400:CYS:SG	3:A:1409:LEU:HG	2.44	0.57
4:B:1147:LEU:HD22	4:B:1151:LEU:CD2	2.34	0.57
4:B:701:ILE:HD11	4:B:703:ILE:HD11	1.86	0.57
11:K:33:ILE:HD13	11:K:87:LEU:HD22	1.85	0.57
2:T:1:DA:C4	2:T:2:DC:C6	2.92	0.57
3:A:1399:ARG:CB	3:A:1408:ILE:HD13	2.28	0.57
9:I:78:CYS:SG	9:I:106:CYS:SG	3.02	0.57
3:A:353:ILE:HG22	3:A:468:PHE:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:61:GLN:HB2	6:E:79:TRP:HE3	1.69	0.57
4:B:23:ALA:O	4:B:654:ARG:HB3	2.04	0.57
4:B:1079:LYS:HA	5:C:27:LEU:HD21	1.87	0.57
4:B:1077:THR:CG2	4:B:1079:LYS:HB2	2.34	0.57
3:A:337:ARG:CD	3:A:839:ARG:HH22	2.17	0.57
3:A:399:HIS:O	3:A:435:HIS:HD2	1.87	0.57
7:F:111:LEU:N	7:F:111:LEU:CD1	2.67	0.57
11:K:65:HIS:HD2	11:K:67:PHE:N	2.02	0.57
3:A:92:HIS:HD2	3:A:94:GLY:H	1.53	0.57
3:A:1111:MET:CE	3:A:1114:PRO:HA	2.35	0.57
2:T:1:DA:C5	2:T:2:DC:C5	2.93	0.57
3:A:76:GLU:O	3:A:76:GLU:CG	2.53	0.57
3:A:901:LEU:N	3:A:926:GLN:NE2	2.50	0.57
5:C:251:LEU:O	5:C:255:VAL:HG23	2.04	0.57
4:B:801:LYS:O	10:J:52:THR:CG2	2.52	0.57
4:B:1116:ARG:HD2	4:B:1198:TYR:CG	2.40	0.57
3:A:1332:PHE:CD2	3:A:1332:PHE:N	2.72	0.57
5:C:258:ILE:O	5:C:261:ALA:HB3	2.04	0.57
7:F:97:ARG:NE	7:F:124:GLU:OE1	2.31	0.57
6:E:157:SER:C	6:E:159:ASP:H	2.07	0.57
4:B:979:LYS:HG2	4:B:1095:LEU:HD12	1.87	0.57
11:K:46:ILE:HG22	11:K:50:LEU:HD12	1.86	0.57
9:I:111:THR:HG22	9:I:112:SER:N	2.19	0.57
3:A:1329:THR:HG22	3:A:1331:SER:N	2.01	0.57
2:T:1:DA:N3	2:T:2:DC:C5	2.71	0.57
3:A:1281:ARG:HB2	3:A:1309:ASP:HB2	1.86	0.57
3:A:879:GLU:OE2	3:A:962:ARG:NH2	2.37	0.57
3:A:1342:GLU:HG2	6:E:212:ARG:NH1	2.20	0.57
5:C:37:MET:HG2	5:C:243:VAL:CG1	2.34	0.57
4:B:806:THR:OG1	4:B:809:MET:HE3	2.04	0.57
3:A:1295:THR:HG23	3:A:1297:GLU:OE1	2.03	0.57
4:B:756:ILE:O	4:B:759:PRO:HD3	2.04	0.57
3:A:537:ARG:HB2	8:H:20:TYR:CE2	2.39	0.57
3:A:1315:GLU:O	3:A:1318:THR:HG23	2.04	0.57
3:A:710:LEU:N	3:A:710:LEU:HD12	2.20	0.57
1:R:5:A:C4	1:R:6:G:C8	2.93	0.57
3:A:414:ASP:O	3:A:417:TYR:O	2.22	0.57
3:A:69:THR:HB	4:B:1174:LYS:HE2	1.87	0.57
11:K:50:LEU:CD1	11:K:73:LEU:HD21	2.35	0.57
3:A:101:LYS:O	3:A:105:CYS:HB2	2.04	0.57
3:A:882:SER:HA	3:A:952:ALA:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:6:DC:C5	2:T:7:DC:C5	2.93	0.57
3:A:93:VAL:HG22	3:A:301:ALA:HA	1.85	0.57
8:H:6:PHE:HE1	8:H:130:ARG:HE	1.53	0.57
4:B:57:TYR:HD1	4:B:57:TYR:N	2.03	0.57
8:H:89:LEU:HD22	8:H:91:ASP:OD2	2.05	0.57
3:A:166:GLY:O	3:A:167:CYS:HB3	2.03	0.57
1:R:10:A:H61	2:T:6:DC:N4	2.03	0.56
3:A:1364:ASN:ND2	3:A:1366:ARG:N	2.53	0.56
3:A:886:ILE:CD1	3:A:943:LEU:HB3	2.31	0.56
4:B:130:VAL:HG12	4:B:131:ASP:H	1.67	0.56
3:A:1342:GLU:HG3	6:E:198:ILE:HG21	1.86	0.56
7:F:87:LYS:HE2	7:F:88:TYR:CZ	2.39	0.56
3:A:672:ASP:HB3	3:A:675:THR:OG1	2.05	0.56
4:B:1051:THR:HG22	4:B:1052:VAL:N	2.17	0.56
3:A:40:THR:HG21	3:A:259:GLU:OE2	2.04	0.56
3:A:577:ILE:O	3:A:580:VAL:HG23	2.04	0.56
3:A:98:LYS:O	3:A:102:VAL:HG23	2.05	0.56
3:A:974:ASP:HB2	8:H:136:LYS:NZ	2.20	0.56
8:H:97:MET:CE	8:H:142:LEU:HD23	2.35	0.56
3:A:1389:PHE:O	3:A:1392:SER:HB3	2.05	0.56
4:B:23:ALA:HB1	4:B:24:PRO:HD2	1.85	0.56
4:B:704:ALA:HB1	4:B:710:LEU:HD12	1.87	0.56
4:B:955:THR:HG1	12:L:55:ILE:HA	1.71	0.56
10:J:1:MET:HG3	10:J:60:PHE:HE2	1.69	0.56
1:R:5:A:C2	1:R:6:G:C4	2.93	0.56
9:I:7:CYS:O	9:I:8:ARG:O	2.24	0.56
5:C:242:GLN:HE21	5:C:246:ARG:HE	1.54	0.56
8:H:5:LEU:CD1	8:H:135:LEU:HG	2.34	0.56
5:C:229:TYR:N	5:C:229:TYR:CD1	2.74	0.56
8:H:82:PRO:O	8:H:83:GLN:HB2	2.04	0.56
3:A:401:GLY:O	3:A:435:HIS:CD2	2.58	0.56
6:E:46:TYR:CE2	6:E:58:MET:HA	2.40	0.56
4:B:429:PHE:HA	4:B:432:MET:CE	2.35	0.56
4:B:311:LEU:HB3	9:I:4:PHE:CE2	2.40	0.56
4:B:522:VAL:HG11	4:B:537:LYS:HB3	1.86	0.56
4:B:243:ALA:HA	4:B:250:PHE:O	2.05	0.56
3:A:452:LYS:HB3	4:B:1141:HIS:CE1	2.40	0.56
5:C:145:CYS:SG	5:C:146:LYS:N	2.79	0.56
3:A:665:GLY:HA3	4:B:1086:PHE:CD1	2.41	0.56
8:H:89:LEU:HD22	8:H:91:ASP:CG	2.25	0.56
3:A:885:THR:O	3:A:885:THR:HG22	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:24:CYS:SG	8:H:44:VAL:HG21	2.44	0.56
5:C:131:HIS:O	5:C:132:PRO:C	2.43	0.56
4:B:984:HIS:HB3	4:B:1022:THR:OG1	2.05	0.56
5:C:99:LEU:HD23	5:C:99:LEU:N	2.20	0.56
3:A:875:ALA:HB2	3:A:1366:ARG:HD2	1.88	0.56
3:A:1300:LYS:NZ	3:A:1300:LYS:HB3	2.20	0.56
11:K:51:LEU:HD13	11:K:59:ALA:HB3	1.86	0.56
4:B:864:LYS:HD3	4:B:871:THR:OG1	2.05	0.56
3:A:547:LEU:HD22	11:K:58:PHE:CD1	2.41	0.56
3:A:35:ILE:HG12	3:A:52:GLY:O	2.06	0.56
3:A:567:LYS:HZ2	8:H:46:LEU:HB2	1.70	0.56
5:C:242:GLN:NE2	5:C:246:ARG:HE	2.02	0.56
4:B:839:MET:CE	4:B:980:PHE:HB2	2.35	0.56
3:A:401:GLY:C	3:A:435:HIS:CD2	2.79	0.56
5:C:248:ILE:CD1	11:K:101:LEU:HD22	2.35	0.56
3:A:185:TRP:CZ3	3:A:200:ARG:HG2	2.40	0.56
9:I:111:THR:CG2	9:I:112:SER:N	2.69	0.56
3:A:1328:TYR:CG	3:A:1329:THR:N	2.74	0.56
3:A:1365:TYR:O	3:A:1366:ARG:C	2.43	0.56
4:B:983:ARG:HD2	4:B:1091:TYR:HB3	1.86	0.56
4:B:361:LEU:N	4:B:362:PRO:CD	2.69	0.56
4:B:566:LEU:HD22	4:B:586:TRP:O	2.06	0.56
4:B:1180:PHE:O	4:B:1181:GLU:HB2	2.05	0.56
8:H:59:ILE:HG22	8:H:60:ALA:N	2.20	0.56
7:F:99:LEU:HD12	7:F:99:LEU:O	2.06	0.56
1:R:8:G:N2	2:T:8:DT:C4	2.74	0.56
3:A:825:ILE:HD12	4:B:513:GLN:NE2	2.21	0.56
4:B:1171:VAL:HG11	4:B:1191:ILE:HD13	1.88	0.56
4:B:1022:THR:HG23	4:B:1022:THR:O	2.05	0.56
3:A:1261:LYS:HA	3:A:1264:GLU:HB3	1.88	0.56
3:A:1017:LEU:HD23	6:E:204:THR:O	2.06	0.55
6:E:61:GLN:NE2	6:E:105:PHE:CE2	2.71	0.55
4:B:515:HIS:H	4:B:518:HIS:CD2	2.24	0.55
4:B:120:ARG:NH1	12:L:54:ARG:NH1	2.54	0.55
3:A:1436:ILE:HG22	4:B:1142:GLY:HA2	1.87	0.55
4:B:34:ILE:O	4:B:37:PHE:HB3	2.06	0.55
3:A:50:ILE:C	3:A:52:GLY:H	2.09	0.55
4:B:980:PHE:HE1	4:B:990:ILE:HD11	1.70	0.55
4:B:566:LEU:HD13	4:B:588:GLY:CA	2.37	0.55
8:H:106:GLU:C	8:H:108:SER:N	2.57	0.55
4:B:63:ILE:HA	4:B:421:PHE:CE2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:556:THR:HG22	4:B:557:PHE:N	2.20	0.55
3:A:843:LYS:HG3	3:A:1402:PHE:HD1	1.72	0.55
9:I:7:CYS:C	9:I:8:ARG:O	2.43	0.55
3:A:216:VAL:O	3:A:219:PHE:HB2	2.06	0.55
3:A:849:MET:CE	3:A:1061:GLY:HA2	2.36	0.55
4:B:898:LEU:HD22	4:B:964:VAL:HG11	1.89	0.55
5:C:162:GLY:HA3	5:C:170:TRP:CE2	2.41	0.55
10:J:21:TYR:HA	10:J:39:LEU:HD11	1.89	0.55
3:A:548:ASN:HA	11:K:60:ALA:HB1	1.87	0.55
4:B:120:ARG:HE	4:B:955:THR:CG2	2.20	0.55
4:B:121:ASN:ND2	4:B:121:ASN:N	2.50	0.55
4:B:864:LYS:N	4:B:872:GLU:OE1	2.39	0.55
6:E:195:VAL:HG22	6:E:213:ILE:CB	2.37	0.55
4:B:794:ASN:C	4:B:795:ILE:HD12	2.26	0.55
3:A:1339:LEU:HD13	6:E:147:HIS:CD2	2.41	0.55
12:L:26:THR:HG22	12:L:27:LEU:N	2.21	0.55
3:A:1096:SER:O	3:A:1099:PRO:HG2	2.06	0.55
5:C:238:ILE:HG23	5:C:242:GLN:HB2	1.89	0.55
3:A:963:ILE:HD12	3:A:1049:ILE:HG12	1.88	0.55
3:A:463:ILE:HD11	3:A:469:ARG:HG3	1.89	0.55
3:A:556:TRP:CE3	3:A:558:GLY:HA2	2.40	0.55
3:A:838:GLN:O	3:A:842:VAL:HG23	2.06	0.55
3:A:1364:ASN:HD21	3:A:1366:ARG:HG2	1.67	0.55
5:C:57:VAL:HG11	10:J:60:PHE:HB2	1.88	0.55
8:H:89:LEU:O	8:H:91:ASP:N	2.37	0.55
5:C:55:THR:HB	5:C:152:GLU:H	1.70	0.55
5:C:70:ILE:HD11	5:C:144:ILE:HG12	1.88	0.55
12:L:63:ARG:O	12:L:64:LEU:O	2.25	0.55
4:B:25:ILE:HD11	4:B:653:VAL:HB	1.89	0.55
4:B:864:LYS:HG3	4:B:865:LYS:N	2.21	0.55
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.47	0.55
3:A:556:TRP:CD2	3:A:558:GLY:HA2	2.42	0.55
11:K:61:TYR:HA	11:K:72:LYS:O	2.06	0.55
3:A:23:SER:HB3	3:A:233:TRP:CE2	2.41	0.55
10:J:32:GLU:O	10:J:36:LEU:HG	2.07	0.55
3:A:517:ASN:ND2	3:A:1362:TYR:HE2	2.05	0.55
3:A:710:LEU:H	3:A:710:LEU:CD1	2.19	0.55
3:A:89:PRO:O	3:A:204:THR:HG21	2.07	0.55
3:A:451:HIS:CE1	3:A:1074:GLU:HG3	2.42	0.55
6:E:195:VAL:HG22	6:E:213:ILE:HB	1.88	0.55
4:B:308:TRP:CH2	9:I:45:ARG:HG2	2.43	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1308:THR:CG2	3:A:1310:GLY:O	2.54	0.54
3:A:533:LYS:O	3:A:535:THR:N	2.40	0.54
3:A:885:THR:O	3:A:940:ARG:HG3	2.07	0.54
3:A:399:HIS:O	3:A:435:HIS:CD2	2.60	0.54
3:A:356:ASP:OD2	11:K:65:HIS:HE1	1.90	0.54
4:B:195:CYS:CB	4:B:782:LEU:HD22	2.37	0.54
3:A:1116:LEU:O	3:A:1308:THR:HB	2.07	0.54
4:B:780:VAL:HG21	10:J:56:LEU:HD13	1.88	0.54
3:A:902:LEU:HD21	3:A:923:LEU:HD23	1.90	0.54
3:A:337:ARG:NE	3:A:839:ARG:NH2	2.55	0.54
4:B:911:ILE:HD11	4:B:941:LEU:CD1	2.37	0.54
3:A:233:TRP:C	3:A:235:ILE:N	2.60	0.54
6:E:46:TYR:CD2	6:E:58:MET:HG2	2.42	0.54
3:A:1193:LEU:HD21	3:A:1267:MET:HE2	1.88	0.54
8:H:84:ALA:HA	8:H:87:ARG:HG3	1.88	0.54
4:B:756:ILE:HG21	4:B:759:PRO:HB3	1.90	0.54
3:A:974:ASP:HB2	8:H:136:LYS:HZ1	1.73	0.54
4:B:1051:THR:CG2	4:B:1052:VAL:N	2.70	0.54
3:A:515:GLN:HG3	3:A:516:SER:N	2.22	0.54
3:A:443:LEU:HD13	3:A:455:MET:HE1	1.90	0.54
4:B:542:MET:HE2	4:B:747:MET:HE2	1.89	0.54
6:E:168:TYR:HB3	6:E:170:LEU:CD2	2.36	0.54
3:A:741:ASN:ND2	3:A:743:VAL:H	2.05	0.54
5:C:101:LEU:HD13	5:C:118:LEU:HD23	1.88	0.54
3:A:350:ARG:HB2	3:A:488:ASN:OD1	2.08	0.54
7:F:118:LEU:O	7:F:122:MET:HG3	2.08	0.54
5:C:183:TRP:CZ2	5:C:207:CYS:HB3	2.42	0.54
1:R:9:G:H1	1:R:10:A:N6	2.04	0.54
3:A:563:PRO:HG3	3:A:572:TRP:CE2	2.42	0.54
2:T:1:DA:H1'	3:A:1386:ARG:NH1	2.22	0.54
5:C:13:ALA:O	11:K:114:LEU:HD13	2.08	0.54
4:B:179:CYS:SG	4:B:181:LEU:HB2	2.47	0.54
6:E:197:LYS:HG3	6:E:211:TYR:CE2	2.42	0.54
4:B:1034:VAL:HG12	4:B:1035:ALA:N	2.23	0.54
12:L:27:LEU:HD13	12:L:37:LYS:HB3	1.90	0.54
2:T:3:DG:C5'	3:A:836:TYR:CD1	2.87	0.54
3:A:1375:MET:HG2	3:A:1382:THR:O	2.08	0.54
4:B:102:VAL:HG22	4:B:112:LEU:HD22	1.88	0.54
3:A:898:ARG:HD2	3:A:899:VAL:H	1.73	0.54
12:L:70:ARG:HG2	12:L:70:ARG:NH1	2.22	0.54
3:A:619:LYS:O	3:A:623:GLY:N	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:809:THR:O	3:A:810:PRO:C	2.46	0.54
3:A:1341:ILE:HD12	3:A:1379:GLY:O	2.07	0.54
6:E:153:HIS:CE1	6:E:184:VAL:HG11	2.43	0.54
3:A:1116:LEU:H	3:A:1308:THR:HG22	1.72	0.54
3:A:154:SER:HB3	3:A:162:VAL:HG23	1.89	0.54
4:B:172:ILE:HD13	4:B:178:ASN:CB	2.37	0.54
3:A:821:ARG:O	3:A:822:GLU:C	2.46	0.54
3:A:92:HIS:CD2	3:A:94:GLY:H	2.26	0.54
3:A:38:PRO:N	3:A:270:LEU:HD23	2.22	0.54
3:A:852:TYR:CE2	7:F:136:ARG:HG2	2.42	0.54
4:B:783:THR:HA	10:J:60:PHE:HE1	1.72	0.54
3:A:15:LYS:HD2	4:B:1220:ARG:HE	1.72	0.54
11:K:10:PHE:HD1	11:K:11:LEU:HD13	1.67	0.54
6:E:176:PRO:HD2	6:E:211:TYR:O	2.07	0.54
4:B:837:ASP:OD1	4:B:1020:ARG:NH2	2.41	0.54
7:F:109:VAL:HG13	7:F:127:GLU:OE1	2.07	0.54
4:B:784:ASN:ND2	4:B:788:ARG:HD2	2.23	0.54
4:B:758:PHE:C	4:B:760:ASP:H	2.11	0.54
1:R:9:G:C4	1:R:10:A:N7	2.76	0.54
3:A:367:PRO:HB3	3:A:465:TYR:O	2.08	0.54
7:F:72:LYS:N	7:F:142:SER:HA	2.22	0.54
1:R:8:G:C2'	1:R:9:G:H5'	2.36	0.54
3:A:590:ARG:O	3:A:591:PHE:HB2	2.08	0.54
12:L:51:CYS:C	12:L:53:HIS:H	2.12	0.54
3:A:226:GLU:HG2	3:A:227:VAL:HG23	1.90	0.54
4:B:680:THR:HG22	4:B:681:TRP:H	1.72	0.54
4:B:406:LEU:HD12	4:B:545:ILE:HD11	1.89	0.54
3:A:646:PHE:O	3:A:650:GLN:HG3	2.08	0.54
3:A:867:ILE:HG22	3:A:872:GLY:N	2.22	0.54
3:A:1366:ARG:O	3:A:1369:ALA:HB3	2.08	0.54
4:B:549:THR:HB	4:B:628:THR:HG23	1.89	0.54
4:B:28:GLU:CD	4:B:807:ARG:HH22	2.10	0.54
4:B:288:ALA:HB1	4:B:331:LEU:CD1	2.38	0.54
7:F:107:VAL:HG12	7:F:109:VAL:H	1.72	0.54
8:H:32:THR:HG22	8:H:33:GLN:HG3	1.90	0.54
5:C:248:ILE:HD13	11:K:101:LEU:HD22	1.89	0.54
9:I:2:THR:HG22	9:I:2:THR:O	2.07	0.54
3:A:567:LYS:NZ	8:H:95:TYR:CE1	2.71	0.53
3:A:1222:ASN:O	3:A:1223:ASP:HB3	2.06	0.53
6:E:23:VAL:HG12	6:E:28:TYR:HB2	1.89	0.53
3:A:1073:GLY:O	3:A:1076:ALA:HB3	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:225:ASN:C	3:A:227:VAL:H	2.10	0.53
4:B:515:HIS:H	4:B:518:HIS:HD2	1.55	0.53
3:A:738:LYS:HB2	3:A:740:LEU:HG	1.89	0.53
3:A:845:LEU:N	3:A:845:LEU:HD23	2.22	0.53
10:J:52:THR:O	10:J:52:THR:HG22	2.08	0.53
3:A:353:ILE:HD13	3:A:487:MET:HE2	1.88	0.53
6:E:78:LEU:HD21	6:E:109:ILE:HD12	1.90	0.53
7:F:94:LEU:HD21	7:F:122:MET:HA	1.89	0.53
3:A:1341:ILE:HD12	3:A:1379:GLY:C	2.28	0.53
3:A:608:ILE:HD12	3:A:613:ILE:CD1	2.39	0.53
3:A:122:MET:O	3:A:126:LEU:HG	2.07	0.53
4:B:644:GLU:HG3	4:B:654:ARG:HH22	1.74	0.53
4:B:842:ASN:HD22	4:B:845:SER:CB	2.21	0.53
9:I:46:HIS:CD2	9:I:48:LEU:HD21	2.44	0.53
3:A:90:VAL:HG13	3:A:297:GLN:HA	1.90	0.53
5:C:46:ILE:HD13	5:C:157:CYS:CB	2.38	0.53
3:A:114:LEU:HD22	3:A:171:GLN:NE2	2.23	0.53
4:B:235:SER:OG	4:B:236:HIS:HD2	1.91	0.53
4:B:755:ILE:O	4:B:755:ILE:CG2	2.55	0.53
4:B:292:ILE:H	4:B:293:PRO:HD2	1.73	0.53
3:A:741:ASN:ND2	3:A:741:ASN:C	2.62	0.53
11:K:63:VAL:HG23	11:K:63:VAL:O	2.08	0.53
3:A:557:ASP:OD2	3:A:559:VAL:HB	2.08	0.53
3:A:852:TYR:CZ	7:F:136:ARG:HG2	2.44	0.53
9:I:29:CYS:O	9:I:29:CYS:SG	2.66	0.53
3:A:399:HIS:C	3:A:401:GLY:H	2.10	0.53
3:A:1205:LYS:O	3:A:1207:LEU:N	2.41	0.53
3:A:738:LYS:HZ1	5:C:194:GLU:C	2.11	0.53
4:B:1069:PHE:HA	4:B:1085:ILE:O	2.08	0.53
3:A:768:GLN:HG2	3:A:816:HIS:CA	2.38	0.53
4:B:479:VAL:HG12	4:B:480:SER:H	1.72	0.53
4:B:1177:HIS:HB3	4:B:1179:GLN:HE21	1.74	0.53
4:B:405:ARG:HA	4:B:631:GLY:O	2.09	0.53
5:C:189:THR:HG22	5:C:190:ASP:N	2.24	0.53
1:R:10:A:O5'	1:R:10:A:OP1	2.19	0.53
3:A:1365:TYR:O	3:A:1367:HIS:N	2.42	0.53
3:A:1161:THR:HG22	3:A:1162:VAL:N	2.24	0.53
4:B:120:ARG:HB2	4:B:122:LEU:HG	1.91	0.53
5:C:241:ASP:O	5:C:245:VAL:HG23	2.08	0.53
4:B:205:ILE:HD11	4:B:461:LEU:HD23	1.90	0.53
3:A:134:ARG:HH12	3:A:220:THR:HG22	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1094:VAL:HG13	3:A:1113:THR:CG2	2.37	0.53
4:B:956:THR:CG2	4:B:960:GLY:HA2	2.38	0.53
3:A:384:ASN:OD1	3:A:385:ILE:N	2.42	0.53
3:A:1220:PHE:O	3:A:1222:ASN:N	2.42	0.53
3:A:387:ARG:O	3:A:391:LEU:HG	2.09	0.53
6:E:28:TYR:CE1	6:E:78:LEU:HD12	2.44	0.53
3:A:339:ASN:O	3:A:343:LYS:HG2	2.07	0.53
3:A:1225:PHE:CE2	3:A:1227:ILE:HD11	2.43	0.53
4:B:875:GLU:O	4:B:877:PRO:HD3	2.09	0.53
3:A:552:TRP:NE1	3:A:655:PHE:CD1	2.77	0.53
4:B:916:THR:HG22	4:B:918:ILE:HG13	1.90	0.53
9:I:29:CYS:C	9:I:31:THR:H	2.13	0.53
8:H:38:LEU:CD1	8:H:125:LEU:HD13	2.38	0.53
4:B:234:ILE:HG21	4:B:257:LYS:HB3	1.91	0.53
12:L:38:LEU:O	12:L:39:SER:CB	2.56	0.53
6:E:17:ARG:O	6:E:21:GLU:HG3	2.09	0.53
9:I:62:ILE:HG23	9:I:63:GLY:N	2.22	0.53
4:B:484:ASN:ND2	4:B:486:TYR:CD1	2.76	0.53
3:A:407:ARG:HD2	3:A:413:ILE:HD11	1.91	0.53
3:A:1111:MET:CE	3:A:1330:ASN:OD1	2.57	0.53
2:T:3:DG:H5'	3:A:836:TYR:HD1	1.70	0.53
4:B:287:ARG:HA	4:B:291:ILE:O	2.09	0.53
3:A:442:VAL:O	3:A:457:ALA:HA	2.09	0.53
3:A:444:PHE:HB3	3:A:458:HIS:CD2	2.43	0.53
3:A:928:LEU:O	3:A:931:GLU:N	2.43	0.53
3:A:696:GLU:OE2	3:A:702:LEU:HD23	2.08	0.53
4:B:43:LEU:HD13	4:B:812:LEU:CD2	2.38	0.53
1:R:9:G:C5	1:R:10:A:N7	2.76	0.52
3:A:337:ARG:CZ	3:A:839:ARG:HH12	2.22	0.52
8:H:6:PHE:O	8:H:58:THR:HA	2.08	0.52
5:C:93:ASP:OD1	5:C:122:SER:HB2	2.09	0.52
4:B:463:THR:HG21	4:B:465:ASN:HD22	1.74	0.52
4:B:898:LEU:CD2	4:B:964:VAL:HG11	2.38	0.52
4:B:547:VAL:H	4:B:612:GLU:CD	2.12	0.52
4:B:120:ARG:NH2	12:L:54:ARG:HD2	2.24	0.52
4:B:911:ILE:HD11	4:B:941:LEU:HD12	1.91	0.52
4:B:248:SER:O	4:B:249:ARG:HB2	2.09	0.52
3:A:1299:VAL:CG1	3:A:1300:LYS:H	2.20	0.52
3:A:507:VAL:N	3:A:508:PRO:CD	2.72	0.52
3:A:167:CYS:HB2	3:A:169:ASN:ND2	2.24	0.52
11:K:46:ILE:O	11:K:50:LEU:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:36:LEU:HD12	10:J:47:ARG:NH1	2.23	0.52
4:B:43:LEU:HD13	4:B:812:LEU:HD23	1.90	0.52
7:F:114:GLU:OE1	7:F:119:ARG:HG3	2.08	0.52
4:B:707:PRO:CG	4:B:708:GLU:H	2.21	0.52
1:R:5:A:H2'	1:R:6:G:H8	1.70	0.52
5:C:164:ALA:HA	5:C:167:HIS:O	2.10	0.52
4:B:999:MET:HE2	4:B:1011:ILE:HD11	1.91	0.52
8:H:95:TYR:HE2	8:H:97:MET:HG3	1.73	0.52
6:E:124:VAL:HG22	6:E:132:ILE:CG2	2.39	0.52
4:B:287:ARG:HG2	4:B:292:ILE:CA	2.27	0.52
3:A:907:THR:HG22	3:A:908:LEU:N	2.25	0.52
4:B:899:ILE:HD11	4:B:910:VAL:O	2.09	0.52
3:A:261:ASP:OD2	3:A:323:LYS:HD2	2.10	0.52
3:A:675:THR:CG2	3:A:736:ASN:HD21	2.22	0.52
4:B:484:ASN:ND2	4:B:486:TYR:CE1	2.77	0.52
4:B:98:THR:OG1	4:B:127:GLY:HA3	2.09	0.52
7:F:132:LEU:O	7:F:148:VAL:HG23	2.09	0.52
6:E:12:LEU:HD22	6:E:55:ARG:CZ	2.39	0.52
4:B:1065:GLN:NE2	4:B:1067:ARG:HG2	2.24	0.52
4:B:271:ALA:HB3	4:B:285:ILE:CD1	2.40	0.52
4:B:293:PRO:HA	9:I:12:ASN:HD21	1.75	0.52
3:A:529:CYS:HB2	4:B:1015:HIS:CE1	2.43	0.52
4:B:857:ARG:HD2	4:B:945:GLU:OE1	2.08	0.52
3:A:451:HIS:CD2	3:A:1074:GLU:HG3	2.45	0.52
1:R:10:A:N6	2:T:6:DC:H42	2.06	0.52
3:A:670:ILE:HD13	4:B:1067:ARG:CZ	2.39	0.52
4:B:284:ILE:HD13	4:B:324:ILE:HD12	1.91	0.52
4:B:118:ARG:NH2	4:B:194:GLU:CD	2.60	0.52
4:B:100:PRO:HG3	4:B:172:ILE:HD12	1.92	0.52
4:B:31:TRP:CD1	4:B:807:ARG:NH1	2.78	0.52
4:B:542:MET:HE1	4:B:743:ILE:CG2	2.39	0.52
4:B:90:ILE:CD1	4:B:432:MET:SD	2.97	0.52
3:A:225:ASN:O	3:A:227:VAL:HG23	2.09	0.52
8:H:84:ALA:C	8:H:86:ASP:H	2.13	0.52
6:E:35:VAL:C	6:E:37:LEU:H	2.12	0.52
4:B:428:ILE:O	4:B:431:TYR:HB3	2.10	0.52
3:A:1147:THR:HA	3:A:1197:LEU:HD23	1.90	0.52
3:A:901:LEU:HD23	3:A:907:THR:HG23	1.92	0.52
3:A:470:LEU:HD21	3:A:487:MET:HE3	1.92	0.52
4:B:59:LEU:HD11	4:B:417:PHE:CZ	2.44	0.52
4:B:559:SER:HA	4:B:563:MET:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1319:VAL:CG1	3:A:1320:PRO:HD2	2.39	0.52
11:K:49:GLU:OE2	11:K:97:LYS:HE3	2.10	0.52
3:A:1359:ASP:C	3:A:1361:SER:H	2.13	0.52
4:B:25:ILE:HG22	4:B:26:THR:N	2.24	0.52
3:A:596:THR:O	3:A:597:LEU:C	2.47	0.52
3:A:1299:VAL:CG1	3:A:1300:LYS:N	2.72	0.52
3:A:443:LEU:HD11	4:B:1138:MET:SD	2.50	0.52
3:A:91:PHE:HB2	3:A:297:GLN:OE1	2.09	0.52
3:A:821:ARG:HG3	3:A:825:ILE:CD1	2.40	0.52
4:B:614:SER:OG	4:B:627:PHE:HB2	2.09	0.52
3:A:134:ARG:NH1	3:A:220:THR:O	2.42	0.52
9:I:73:ARG:O	9:I:81:ARG:HA	2.09	0.52
4:B:1084:GLN:HG2	5:C:201:TRP:CZ2	2.45	0.52
3:A:1029:ARG:HG3	3:A:1029:ARG:HH11	1.74	0.52
3:A:1116:LEU:N	3:A:1308:THR:HG22	2.25	0.52
4:B:648:HIS:NE2	4:B:650:GLU:OE1	2.43	0.52
4:B:287:ARG:CG	4:B:292:ILE:HA	2.26	0.52
3:A:817:ALA:HA	4:B:764:SER:OG	2.10	0.52
4:B:542:MET:HG3	4:B:747:MET:CE	2.38	0.52
3:A:1152:ILE:CG2	3:A:1260:LEU:HD23	2.38	0.52
4:B:806:THR:C	4:B:808:ALA:H	2.12	0.52
4:B:552:MET:N	4:B:553:PRO:HD2	2.24	0.52
3:A:49:LYS:HB3	3:A:55:ASP:HB2	1.92	0.52
7:F:77:ASP:O	7:F:78:GLN:HB2	2.09	0.52
4:B:825:VAL:HG12	4:B:826:ALA:N	2.24	0.52
1:R:9:G:C6	1:R:10:A:N7	2.78	0.51
3:A:836:TYR:CE2	3:A:840:ARG:HD2	2.45	0.51
2:T:1:DA:N6	2:T:2:DC:N4	2.58	0.51
4:B:25:ILE:CG2	4:B:29:ASP:HB3	2.40	0.51
4:B:640:VAL:O	4:B:641:GLU:C	2.46	0.51
3:A:326:ARG:HG2	3:A:1406:VAL:CG2	2.39	0.51
3:A:365:GLY:HA3	3:A:469:ARG:HB2	1.91	0.51
4:B:46:GLN:NE2	4:B:496:ARG:HA	2.25	0.51
12:L:38:LEU:HG	12:L:39:SER:N	2.25	0.51
4:B:864:LYS:HD3	4:B:871:THR:HA	1.91	0.51
3:A:1214:GLU:O	3:A:1218:GLN:HG2	2.10	0.51
3:A:568:PRO:HB2	5:C:221:TYR:CE1	2.45	0.51
8:H:40:LEU:CD2	8:H:42:ILE:HD11	2.39	0.51
3:A:1392:SER:O	3:A:1393:ASN:CB	2.58	0.51
3:A:13:THR:HG23	3:A:1432:GLN:NE2	2.24	0.51
8:H:84:ALA:C	8:H:86:ASP:N	2.64	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:50:ILE:HG22	3:A:51:GLY:N	2.24	0.51
4:B:827:ILE:HG12	4:B:1012:ILE:HD11	1.93	0.51
6:E:155:ARG:HD2	6:E:194:GLU:OE2	2.09	0.51
4:B:240:ILE:HG23	4:B:240:ILE:O	2.09	0.51
3:A:41:MET:HG2	3:A:49:LYS:HG2	1.92	0.51
1:R:5:A:N1	1:R:6:G:C5	2.74	0.51
3:A:384:ASN:OD1	3:A:388:LEU:HD12	2.10	0.51
4:B:834:ASN:O	4:B:1013:ASN:HB2	2.10	0.51
3:A:1269:GLU:OE2	4:B:263:GLY:HA3	2.10	0.51
10:J:9:SER:CB	10:J:45:CYS:HB2	2.40	0.51
3:A:737:LEU:HD11	3:A:758:ILE:HG21	1.92	0.51
7:F:109:VAL:CG1	7:F:110:ASP:N	2.73	0.51
3:A:1336:MET:HE1	3:A:1381:LEU:HG	1.92	0.51
6:E:121:MET:C	6:E:123:LEU:H	2.13	0.51
1:R:9:G:C2	1:R:10:A:N7	2.79	0.51
4:B:737:THR:CG2	9:I:66:PRO:HB2	2.40	0.51
3:A:1436:ILE:CG2	3:A:1437:GLY:N	2.72	0.51
11:K:65:HIS:HD2	11:K:67:PHE:HB2	1.74	0.51
3:A:341:MET:CE	3:A:1401:SER:HB2	2.41	0.51
3:A:847:ASP:OD2	3:A:858:ASN:HB2	2.10	0.51
3:A:219:PHE:O	3:A:222:LEU:O	2.28	0.51
4:B:846:ILE:HD13	4:B:974:PRO:HG2	1.91	0.51
3:A:357:PRO:HG2	4:B:833:TYR:CE1	2.45	0.51
3:A:61:ILE:HG22	3:A:62:ASP:N	2.16	0.51
9:I:50:THR:HG22	9:I:52:ILE:H	1.75	0.51
9:I:75:CYS:O	9:I:77:LYS:N	2.44	0.51
3:A:1410:PHE:CE2	4:B:1212:ILE:HD11	2.45	0.51
4:B:1106:ARG:HH12	4:B:1118:PRO:CB	2.24	0.51
3:A:535:THR:HG23	3:A:575:LYS:HE2	1.93	0.51
3:A:898:ARG:HD2	3:A:899:VAL:N	2.26	0.51
4:B:864:LYS:HG2	4:B:871:THR:HG23	1.93	0.51
3:A:511:ILE:HG12	3:A:521:MET:HE3	1.93	0.51
4:B:751:VAL:HG12	4:B:752:ALA:N	2.26	0.51
4:B:1084:GLN:CD	4:B:1084:GLN:H	2.14	0.51
3:A:722:LEU:HD11	3:A:794:PRO:HB3	1.91	0.51
1:R:9:G:N1	1:R:10:A:C5	2.79	0.51
3:A:567:LYS:HD2	3:A:568:PRO:HD2	1.92	0.51
3:A:1312:ASN:O	3:A:1316:VAL:HG23	2.11	0.51
3:A:1376:THR:HG23	6:E:212:ARG:NH2	2.26	0.51
6:E:23:VAL:HG13	6:E:28:TYR:CD1	2.45	0.51
3:A:929:LEU:H	3:A:929:LEU:CD2	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:340:LEU:HD21	4:B:1200:ALA:CB	2.40	0.51
7:F:101:ILE:HD13	7:F:120:ILE:HG22	1.92	0.51
3:A:810:PRO:O	3:A:813:PHE:HB3	2.11	0.51
12:L:32:ALA:HB3	12:L:55:ILE:CD1	2.26	0.51
10:J:7:CYS:SG	10:J:9:SER:HB2	2.50	0.51
4:B:130:VAL:CG2	4:B:167:ILE:HD12	2.33	0.51
3:A:751:SER:O	3:A:752:LYS:CG	2.59	0.51
4:B:563:MET:HG3	4:B:563:MET:O	2.10	0.51
3:A:715:GLU:OE2	3:A:774:ARG:NH1	2.43	0.51
12:L:40:LEU:HD13	12:L:44:ASP:OD1	2.11	0.51
3:A:649:ILE:O	3:A:653:VAL:HG23	2.11	0.51
3:A:753:GLY:HA2	3:A:757:ASN:HD22	1.74	0.51
3:A:96:ILE:O	3:A:100:LYS:HG3	2.10	0.51
10:J:54:VAL:O	10:J:56:LEU:N	2.43	0.51
5:C:33:LEU:HG	5:C:37:MET:CE	2.41	0.51
10:J:14:VAL:HG12	10:J:50:ILE:HD11	1.92	0.51
3:A:329:LEU:HD22	4:B:1203:LEU:CD1	2.41	0.51
4:B:1163:CYS:SG	4:B:1182:CYS:SG	3.08	0.51
11:K:91:CYS:O	11:K:95:ILE:HG13	2.11	0.51
11:K:101:LEU:HD23	11:K:101:LEU:O	2.11	0.51
12:L:27:LEU:HD13	12:L:37:LYS:CG	2.41	0.51
4:B:755:ILE:O	4:B:755:ILE:HG22	2.09	0.51
3:A:1351:GLU:O	3:A:1352:VAL:C	2.49	0.51
5:C:177:GLU:HG3	5:C:231:ASN:HB3	1.93	0.51
4:B:283:VAL:HG13	4:B:297:ILE:CD1	2.41	0.51
2:T:8:DT:H73	2:T:8:DT:OP2	2.10	0.51
3:A:1384:VAL:HG12	3:A:1384:VAL:O	2.11	0.51
4:B:271:ALA:O	4:B:279:ASP:HA	2.11	0.51
3:A:233:TRP:C	3:A:235:ILE:H	2.13	0.51
6:E:46:TYR:HE2	6:E:58:MET:HA	1.76	0.51
3:A:675:THR:HG21	3:A:736:ASN:HD21	1.76	0.51
7:F:109:VAL:CG2	7:F:124:GLU:HG2	2.40	0.51
4:B:195:CYS:SG	4:B:197:PHE:HB2	2.51	0.51
9:I:25:LEU:HD12	9:I:26:LEU:H	1.76	0.51
10:J:36:LEU:HD13	10:J:47:ARG:HG2	1.92	0.51
3:A:795:GLU:HG2	4:B:731:VAL:HG21	1.93	0.51
3:A:1364:ASN:ND2	3:A:1366:ARG:HH11	2.09	0.50
10:J:48:ARG:NE	10:J:49:MET:HE2	2.26	0.50
4:B:130:VAL:CG1	4:B:131:ASP:N	2.74	0.50
4:B:1119:VAL:O	4:B:1126:GLY:HA3	2.11	0.50
4:B:234:ILE:H	4:B:234:ILE:CD1	2.16	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:24:ASP:HB3	11:K:30:ALA:HB3	1.93	0.50
4:B:1197:PRO:HG2	4:B:1200:ALA:CB	2.40	0.50
4:B:1035:ALA:HB1	4:B:1040:ASN:O	2.10	0.50
3:A:587:HIS:HA	3:A:607:ILE:O	2.11	0.50
4:B:642:ASP:HB3	4:B:649:LYS:CD	2.41	0.50
4:B:292:ILE:N	4:B:293:PRO:HD2	2.25	0.50
12:L:47:ARG:HG2	12:L:52:GLY:CA	2.39	0.50
1:R:5:A:C2'	1:R:6:G:O4'	2.60	0.50
3:A:1376:THR:HG23	3:A:1376:THR:O	2.12	0.50
4:B:975:GLN:O	4:B:990:ILE:HD12	2.12	0.50
4:B:1096:ARG:O	4:B:1097:HIS:CB	2.59	0.50
3:A:107:CYS:HB2	3:A:114:LEU:HD23	1.93	0.50
4:B:756:ILE:CG2	4:B:759:PRO:HB3	2.42	0.50
3:A:346:ASP:CG	4:B:1108:ARG:HA	2.31	0.50
3:A:1362:TYR:OH	3:A:1364:ASN:HA	2.11	0.50
9:I:75:CYS:C	9:I:77:LYS:N	2.59	0.50
6:E:5:ASN:O	6:E:9:ILE:HG13	2.11	0.50
3:A:444:PHE:CB	3:A:458:HIS:HD2	2.24	0.50
3:A:105:CYS:SG	3:A:138:ILE:HG22	2.52	0.50
10:J:16:ASP:OD1	10:J:17:LYS:HE3	2.12	0.50
3:A:754:SER:O	3:A:755:PHE:C	2.48	0.50
3:A:829:VAL:C	3:A:831:THR:H	2.15	0.50
3:A:32:VAL:HG21	3:A:68:GLN:HE22	1.74	0.50
3:A:384:ASN:O	3:A:385:ILE:C	2.48	0.50
4:B:577:ALA:HB1	4:B:589:VAL:HG11	1.91	0.50
5:C:254:LYS:HE2	11:K:42:LEU:HD13	1.94	0.50
4:B:514:LEU:HD12	4:B:515:HIS:H	1.74	0.50
4:B:185:THR:O	4:B:189:LEU:HG	2.11	0.50
3:A:1349:TYR:CD2	3:A:1349:TYR:C	2.84	0.50
5:C:66:ARG:NH2	10:J:2:ILE:CG2	2.74	0.50
4:B:911:ILE:HD11	4:B:941:LEU:HB2	1.94	0.50
3:A:893:PHE:CE1	3:A:940:ARG:HD2	2.46	0.50
6:E:168:TYR:HB3	6:E:170:LEU:CG	2.41	0.50
3:A:27:VAL:HG13	3:A:240:PRO:HB3	1.92	0.50
8:H:31:THR:O	8:H:32:THR:HB	2.11	0.50
3:A:167:CYS:O	3:A:169:ASN:N	2.45	0.50
3:A:738:LYS:NZ	5:C:194:GLU:HA	2.26	0.50
4:B:581:PHE:HB2	4:B:625:LYS:HG2	1.93	0.50
4:B:653:VAL:CG2	4:B:689:LEU:HB3	2.42	0.50
4:B:977:GLY:CA	4:B:1099:VAL:CG2	2.86	0.50
4:B:858:SER:HA	4:B:966:VAL:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:683:ILE:HD11	3:A:764:CYS:CB	2.36	0.50
3:A:500:GLU:OE1	4:B:1143:ALA:HB1	2.11	0.50
4:B:542:MET:CG	4:B:747:MET:HE3	2.38	0.50
9:I:101:PHE:O	9:I:109:ILE:HA	2.12	0.50
3:A:1142:THR:O	3:A:1273:LEU:HD22	2.12	0.50
9:I:68:LEU:HB3	9:I:84:VAL:HG22	1.94	0.50
4:B:35:SER:O	4:B:36:ALA:C	2.50	0.50
8:H:47:PHE:HB2	8:H:95:TYR:HD1	1.76	0.50
4:B:271:ALA:HB3	4:B:285:ILE:HD11	1.93	0.50
5:C:77:ILE:HG23	5:C:161:LYS:HE3	1.94	0.50
3:A:306:ASN:HD21	3:A:324:SER:N	2.08	0.50
4:B:1177:HIS:CB	4:B:1179:GLN:HE21	2.24	0.50
6:E:157:SER:C	6:E:159:ASP:N	2.64	0.50
3:A:1134:ILE:O	3:A:1138:ILE:HG13	2.12	0.50
1:R:10:A:C3'	15:R:3000:UTP:O1A	2.60	0.50
1:R:8:G:C2	2:T:8:DT:N3	2.79	0.50
9:I:99:LEU:HB2	9:I:112:SER:HB3	1.94	0.50
4:B:800:GLN:OE1	4:B:822:ASN:HB2	2.12	0.50
8:H:83:GLN:C	8:H:85:GLY:H	2.14	0.50
3:A:100:LYS:NZ	3:A:176:LYS:HD2	2.27	0.50
8:H:128:ASN:O	8:H:131:ASN:ND2	2.45	0.50
4:B:365:THR:HG23	4:B:367:LEU:HG	1.93	0.50
3:A:573:SER:O	3:A:576:GLN:HB2	2.11	0.50
4:B:1159:ARG:CD	4:B:1193:GLN:HG3	2.31	0.50
3:A:709:THR:CB	3:A:712:GLU:HG3	2.41	0.50
5:C:11:ARG:NH2	5:C:229:TYR:CD2	2.68	0.50
3:A:612:ILE:O	3:A:612:ILE:HG23	2.12	0.50
3:A:888:GLY:O	3:A:940:ARG:NH2	2.44	0.50
6:E:54:GLN:O	6:E:57:MET:HB3	2.11	0.50
3:A:135:PHE:HD1	3:A:222:LEU:HD22	1.76	0.50
4:B:260:GLY:O	4:B:267:ARG:HD3	2.12	0.50
3:A:376:TYR:OH	3:A:498:ARG:HD2	2.11	0.50
12:L:62:LYS:C	12:L:64:LEU:H	2.13	0.49
7:F:82:THR:HG22	7:F:84:TYR:N	2.27	0.49
4:B:737:THR:CG2	9:I:66:PRO:CB	2.89	0.49
8:H:6:PHE:HE1	8:H:130:ARG:NE	2.10	0.49
6:E:177:ARG:O	6:E:212:ARG:HD3	2.11	0.49
6:E:80:VAL:HG22	6:E:109:ILE:HD12	1.94	0.49
5:C:18:VAL:HG12	5:C:20:PHE:HD2	1.76	0.49
9:I:15:TYR:CD1	9:I:15:TYR:N	2.79	0.49
3:A:115:LEU:HB2	3:A:122:MET:CE	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:808:LEU:O	4:B:728:ARG:NH1	2.43	0.49
6:E:98:ILE:O	6:E:102:GLU:HG3	2.12	0.49
12:L:62:LYS:O	12:L:64:LEU:HG	2.11	0.49
3:A:1189:SER:OG	3:A:1190:PRO:HD2	2.12	0.49
4:B:844:SER:OG	4:B:996:ARG:N	2.33	0.49
4:B:873:THR:O	4:B:914:LYS:HA	2.13	0.49
7:F:133:VAL:HG22	7:F:147:SER:HA	1.95	0.49
4:B:269:ILE:CD1	4:B:386:LEU:HD21	2.39	0.49
3:A:394:ASN:OD1	3:A:398:GLU:OE1	2.30	0.49
4:B:579:ARG:HB2	4:B:586:TRP:NE1	2.27	0.49
4:B:240:ILE:O	4:B:253:THR:HG23	2.11	0.49
4:B:896:ASP:OD2	12:L:58:LYS:HE3	2.13	0.49
3:A:567:LYS:NZ	8:H:46:LEU:CB	2.67	0.49
8:H:123:MET:HE1	8:H:142:LEU:CD1	2.42	0.49
4:B:25:ILE:CG2	4:B:29:ASP:CB	2.90	0.49
3:A:74:MET:O	3:A:75:ASN:HB2	2.13	0.49
3:A:1410:PHE:HD2	4:B:1212:ILE:HD11	1.70	0.49
3:A:332:LYS:HG3	3:A:333:GLU:HG2	1.94	0.49
5:C:43:THR:CG2	5:C:44:LEU:N	2.75	0.49
3:A:1150:SER:HB2	3:A:1195:LEU:HD23	1.92	0.49
8:H:88:SER:O	8:H:89:LEU:HG	2.12	0.49
3:A:741:ASN:ND2	3:A:743:VAL:N	2.61	0.49
11:K:97:LYS:O	11:K:100:ALA:HB3	2.12	0.49
3:A:185:TRP:HZ3	3:A:200:ARG:HG2	1.74	0.49
4:B:1053:GLU:O	4:B:1054:GLY:C	2.50	0.49
12:L:52:GLY:O	12:L:54:ARG:HG3	2.12	0.49
3:A:15:LYS:CB	4:B:1220:ARG:HG2	2.33	0.49
3:A:1284:MET:HG2	3:A:1306:LEU:CD2	2.43	0.49
4:B:283:VAL:O	4:B:286:PHE:HB2	2.11	0.49
4:B:660:LYS:O	4:B:663:ALA:HB3	2.13	0.49
3:A:538:ASP:OD1	8:H:22:LYS:HB2	2.13	0.49
3:A:545:GLN:O	3:A:548:ASN:N	2.44	0.49
4:B:635:ARG:NH1	4:B:742:GLU:OE2	2.46	0.49
3:A:783:THR:HG21	3:A:815:PHE:CE2	2.48	0.49
3:A:589:GLN:OE1	3:A:591:PHE:HE1	1.96	0.49
3:A:606:LEU:HB2	3:A:614:PHE:CE2	2.48	0.49
3:A:418:SER:HB3	3:A:421:ALA:HB2	1.94	0.49
3:A:466:SER:HB3	11:K:2:ASN:ND2	2.27	0.49
3:A:834:THR:HG21	3:A:1077:THR:CA	2.43	0.49
8:H:76:THR:HG22	8:H:76:THR:O	2.11	0.49
8:H:49:VAL:CG1	8:H:50:ALA:N	2.74	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:734:HIS:O	4:B:735:ALA:HB2	2.12	0.49
4:B:108:VAL:CG1	4:B:109:THR:N	2.76	0.49
3:A:391:LEU:O	3:A:394:ASN:N	2.46	0.49
9:I:55:THR:HG21	9:I:109:ILE:HD13	1.93	0.49
4:B:485:ARG:NH2	4:B:782:LEU:HD11	2.27	0.49
3:A:857:ARG:HG2	3:A:863:VAL:HA	1.94	0.49
7:F:82:THR:HG22	7:F:84:TYR:H	1.77	0.49
4:B:906:SER:O	4:B:907:GLY:C	2.50	0.49
3:A:31:SER:HB2	3:A:83:HIS:HB2	1.91	0.49
3:A:511:ILE:HG12	3:A:521:MET:CE	2.42	0.49
3:A:69:THR:HG22	3:A:69:THR:O	2.12	0.49
8:H:84:ALA:HB1	8:H:87:ARG:HB2	1.94	0.49
4:B:1043:ASP:O	4:B:1050:ILE:HD12	2.13	0.49
3:A:474:VAL:HG13	3:A:478:TYR:CE1	2.48	0.49
3:A:491:VAL:O	3:A:493:GLN:NE2	2.46	0.49
3:A:1001:ARG:HG2	3:A:1001:ARG:HH11	1.77	0.49
3:A:1153:TYR:HA	9:I:41:PRO:O	2.12	0.49
2:T:5:DT:H2"	2:T:6:DC:H5'	1.95	0.49
3:A:1364:ASN:HD21	3:A:1366:ARG:HH11	1.61	0.49
3:A:54:ASN:HA	3:A:58:LEU:HD12	1.95	0.49
3:A:61:ILE:HA	3:A:74:MET:SD	2.53	0.49
10:J:7:CYS:O	10:J:8:PHE:C	2.50	0.49
4:B:1208:MET:HA	4:B:1212:ILE:O	2.12	0.49
5:C:4:GLU:O	5:C:5:GLY:O	2.31	0.49
4:B:821:GLN:OE1	4:B:850:LEU:HD12	2.13	0.49
5:C:142:VAL:H	10:J:16:ASP:HB3	1.77	0.49
6:E:102:GLU:O	6:E:104:ASN:N	2.46	0.49
4:B:653:VAL:HG12	4:B:654:ARG:N	2.28	0.49
4:B:351:TYR:O	4:B:355:ILE:HG13	2.13	0.49
2:T:10:DT:H2"	2:T:11:DC:H5'	1.93	0.49
4:B:1077:THR:HG22	4:B:1079:LYS:HB2	1.94	0.49
4:B:1118:PRO:HD3	4:B:1155:SER:HA	1.95	0.49
5:C:67:LEU:HD11	5:C:155:LEU:HD13	1.95	0.49
8:H:59:ILE:O	8:H:60:ALA:HB3	2.12	0.49
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.94	0.49
4:B:890:TYR:O	4:B:892:LYS:N	2.46	0.49
1:R:2:U:C4	1:R:3:C:C4	3.01	0.49
4:B:726:ALA:HB1	4:B:1051:THR:HG21	1.95	0.49
4:B:1106:ARG:HH21	4:B:1109:GLY:C	2.16	0.49
3:A:418:SER:C	3:A:420:ARG:N	2.63	0.49
7:F:87:LYS:HE2	7:F:88:TYR:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:819:GLY:O	3:A:820:GLY:C	2.49	0.49
8:H:118:PHE:HB2	8:H:121:LEU:HB2	1.95	0.49
3:A:666:ILE:CD1	4:B:1030:LEU:HD22	2.41	0.48
3:A:1100:ARG:NH2	3:A:1330:ASN:HB2	2.28	0.48
4:B:726:ALA:HB1	4:B:1051:THR:CG2	2.43	0.48
3:A:1392:SER:O	3:A:1393:ASN:CG	2.51	0.48
1:R:5:A:N1	2:T:10:DT:O4	2.46	0.48
3:A:1406:VAL:CG1	3:A:1410:PHE:HE1	2.26	0.48
3:A:89:PRO:C	3:A:204:THR:HG21	2.33	0.48
4:B:1160:VAL:HG11	4:B:1169:MET:SD	2.53	0.48
3:A:1326:ARG:O	3:A:1327:ILE:C	2.49	0.48
3:A:563:PRO:HG3	3:A:572:TRP:CH2	2.48	0.48
3:A:567:LYS:HZ2	8:H:46:LEU:CB	2.27	0.48
9:I:85:PHE:O	9:I:86:PHE:HB3	2.13	0.48
4:B:1054:GLY:O	4:B:1058:LEU:HG	2.13	0.48
4:B:284:ILE:CD1	4:B:324:ILE:HD12	2.43	0.48
7:F:81:THR:HG22	7:F:82:THR:H	1.78	0.48
9:I:29:CYS:SG	9:I:31:THR:HG22	2.52	0.48
3:A:332:LYS:H	3:A:337:ARG:HD2	1.76	0.48
8:H:36:CYS:HA	8:H:126:GLU:O	2.13	0.48
3:A:1099:PRO:O	3:A:1102:LYS:HB3	2.13	0.48
3:A:1066:VAL:O	3:A:1068:ALA:N	2.46	0.48
4:B:291:ILE:HD13	4:B:300:HIS:CD2	2.48	0.48
1:R:5:A:N3	1:R:6:G:C8	2.81	0.48
3:A:674:PRO:O	3:A:677:ARG:HB3	2.14	0.48
8:H:44:VAL:O	8:H:44:VAL:HG12	2.12	0.48
1:R:10:A:H2'	15:R:3000:UTP:O4'	2.13	0.48
4:B:1053:GLU:O	4:B:1055:ILE:N	2.46	0.48
4:B:570:VAL:HG11	4:B:573:GLN:OE1	2.13	0.48
4:B:1106:ARG:NH2	4:B:1109:GLY:C	2.67	0.48
6:E:78:LEU:HD21	6:E:80:VAL:HG22	1.95	0.48
4:B:1156:ASP:HB3	4:B:1197:PRO:HA	1.95	0.48
3:A:994:GLN:NE2	3:A:1019:CYS:HB3	2.27	0.48
5:C:254:LYS:O	5:C:258:ILE:HD13	2.13	0.48
4:B:864:LYS:HB3	4:B:871:THR:HA	1.96	0.48
4:B:781:PHE:O	4:B:782:LEU:HG	2.12	0.48
4:B:225:VAL:HG11	4:B:388:CYS:HB3	1.95	0.48
3:A:890:ASP:H	3:A:1296:GLY:HA3	1.77	0.48
6:E:191:LYS:O	6:E:192:ARG:C	2.50	0.48
3:A:68:GLN:NE2	3:A:80:HIS:CB	2.76	0.48
4:B:488:TYR:CE2	4:B:813:LYS:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:994:GLN:HE21	3:A:1019:CYS:CB	2.26	0.48
4:B:1162:ILE:HD11	4:B:1194:ILE:CD1	2.41	0.48
8:H:33:GLN:OE1	8:H:129:TYR:CE2	2.67	0.48
3:A:821:ARG:CG	3:A:825:ILE:HD11	2.41	0.48
11:K:83:PRO:HA	11:K:86:ALA:HB3	1.95	0.48
4:B:825:VAL:CG1	4:B:826:ALA:N	2.76	0.48
3:A:18:GLN:O	4:B:1215:ARG:CG	2.62	0.48
4:B:227:LYS:HB2	4:B:395:GLN:OE1	2.14	0.48
3:A:918:GLU:HG3	3:A:918:GLU:O	2.12	0.48
3:A:913:LEU:HD11	3:A:981:LEU:O	2.13	0.48
5:C:75:MET:HG3	5:C:246:ARG:NH2	2.28	0.48
3:A:549:MET:HE1	3:A:656:TRP:CD1	2.39	0.48
10:J:57:ILE:HG12	10:J:61:LEU:HD11	1.94	0.48
3:A:226:GLU:CG	3:A:227:VAL:N	2.75	0.48
4:B:1182:CYS:O	4:B:1183:LYS:O	2.31	0.48
4:B:101:MET:HE2	4:B:169:ARG:HH12	1.78	0.48
5:C:212:PRO:HB3	5:C:213:PRO:HD2	1.95	0.48
3:A:178:GLY:O	3:A:179:LEU:HD23	2.13	0.48
4:B:171:PRO:HD2	4:B:457:LEU:CD1	2.43	0.48
4:B:380:TYR:CE1	4:B:384:ARG:HD3	2.48	0.48
3:A:1386:ARG:HE	3:A:1387:HIS:CE1	2.32	0.48
5:C:62:PHE:O	5:C:66:ARG:HG3	2.13	0.48
1:R:5:A:N1	1:R:6:G:O6	2.46	0.48
3:A:874:ASP:HA	3:A:1058:VAL:HG22	1.95	0.48
6:E:7:ARG:C	6:E:9:ILE:H	2.17	0.48
12:L:31:CYS:SG	12:L:34:CYS:SG	3.11	0.48
9:I:74:GLU:OE1	9:I:79:HIS:ND1	2.47	0.48
4:B:806:THR:HG22	4:B:808:ALA:H	1.79	0.48
11:K:27:ALA:HB1	11:K:28:PRO:HD2	1.95	0.48
11:K:43:GLY:HA2	11:K:71:PHE:CZ	2.49	0.48
3:A:244:PRO:HG2	3:A:245:PRO:CD	2.33	0.48
3:A:5:GLN:O	4:B:1159:ARG:NH2	2.47	0.48
4:B:956:THR:HG21	4:B:960:GLY:HA2	1.96	0.48
3:A:378:GLU:HG2	3:A:388:LEU:HD11	1.94	0.48
11:K:10:PHE:CE1	11:K:11:LEU:HD13	2.49	0.48
4:B:108:VAL:CG1	4:B:109:THR:H	2.19	0.48
4:B:55:VAL:HG12	4:B:56:ASP:N	2.27	0.48
3:A:929:LEU:HD21	3:A:983:ILE:HG21	1.94	0.48
3:A:376:TYR:CD2	3:A:376:TYR:C	2.87	0.48
4:B:798:TYR:CD2	10:J:4:PRO:HG3	2.49	0.48
2:T:9:DC:O2	2:T:9:DC:C2'	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1412:ALA:HA	3:A:1417:GLU:OE2	2.14	0.48
8:H:125:LEU:HG	8:H:130:ARG:CZ	2.43	0.48
3:A:89:PRO:HG3	3:A:208:LEU:CD1	2.44	0.48
3:A:365:GLY:O	3:A:468:PHE:HA	2.14	0.48
4:B:123:THR:O	4:B:125:SER:N	2.47	0.48
3:A:1195:LEU:HD11	3:A:1267:MET:HE3	1.94	0.48
4:B:236:HIS:CE1	4:B:389:ALA:HA	2.49	0.48
1:R:10:A:H61	2:T:6:DC:H42	1.60	0.48
3:A:515:GLN:HA	3:A:1367:HIS:NE2	2.29	0.48
4:B:845:SER:HB2	10:J:8:PHE:HB3	1.96	0.48
3:A:817:ALA:HA	4:B:764:SER:HG	1.78	0.48
3:A:742:ASN:O	3:A:745:GLN:HB2	2.13	0.48
4:B:46:GLN:HE21	4:B:496:ARG:HG2	1.78	0.48
3:A:1436:ILE:CG2	3:A:1437:GLY:H	2.22	0.48
5:C:258:ILE:HG23	11:K:19:LEU:HD11	1.96	0.48
3:A:738:LYS:HB3	8:H:19:ARG:HH22	1.79	0.48
3:A:1356:ILE:HD12	3:A:1368:MET:SD	2.54	0.48
3:A:116:ASP:HB2	3:A:118:HIS:CD2	2.49	0.48
4:B:708:GLU:C	4:B:710:LEU:H	2.16	0.47
6:E:135:PHE:HD2	6:E:140:LEU:HD21	1.79	0.47
4:B:174:LEU:O	4:B:175:ARG:CB	2.48	0.47
3:A:351:THR:CG2	4:B:1103:ILE:HA	2.36	0.47
9:I:50:THR:HG22	9:I:51:ASN:N	2.28	0.47
5:C:43:THR:HG22	5:C:44:LEU:N	2.29	0.47
3:A:265:LYS:HZ1	3:A:323:LYS:H	1.62	0.47
9:I:54:GLU:O	9:I:89:GLN:HG2	2.14	0.47
4:B:1124:ARG:O	4:B:1125:ASP:HB3	2.14	0.47
3:A:954:TRP:O	3:A:956:LEU:HG	2.14	0.47
8:H:47:PHE:CD1	8:H:95:TYR:HB2	2.49	0.47
3:A:1017:LEU:O	3:A:1018:PHE:C	2.53	0.47
3:A:869:GLY:O	6:E:204:THR:HG21	2.14	0.47
3:A:226:GLU:HG2	3:A:227:VAL:N	2.29	0.47
7:F:98:ALA:O	7:F:117:PRO:HB2	2.14	0.47
4:B:773:MET:SD	4:B:987:LYS:HD2	2.54	0.47
8:H:39:THR:O	8:H:123:MET:HA	2.14	0.47
8:H:49:VAL:CG1	8:H:50:ALA:H	2.27	0.47
3:A:1392:SER:O	3:A:1393:ASN:ND2	2.48	0.47
5:C:66:ARG:CZ	10:J:2:ILE:HG21	2.44	0.47
3:A:783:THR:CG2	3:A:815:PHE:CE2	2.97	0.47
3:A:475:THR:CG2	3:A:476:SER:N	2.76	0.47
4:B:51:PHE:CD2	4:B:173:MET:HB3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1134:ILE:HD11	3:A:1321:GLY:HA3	1.96	0.47
3:A:332:LYS:N	3:A:337:ARG:HD2	2.29	0.47
3:A:1074:GLU:C	3:A:1076:ALA:N	2.67	0.47
6:E:56:LYS:HG3	6:E:84:ASP:CB	2.42	0.47
7:F:101:ILE:HD13	7:F:120:ILE:CG2	2.45	0.47
9:I:62:ILE:CG2	9:I:63:GLY:N	2.77	0.47
5:C:75:MET:HG3	5:C:246:ARG:HH22	1.77	0.47
3:A:14:VAL:H	3:A:1432:GLN:HE22	1.61	0.47
3:A:897:TYR:HD2	3:A:936:LEU:HD13	1.78	0.47
6:E:100:ILE:CG2	6:E:105:PHE:HB2	2.42	0.47
3:A:222:LEU:O	3:A:224:PHE:N	2.46	0.47
12:L:30:ILE:CD1	12:L:59:ALA:HA	2.44	0.47
3:A:12:ARG:HD3	4:B:1218:THR:HB	1.97	0.47
4:B:294:ASP:H	9:I:12:ASN:ND2	2.12	0.47
11:K:59:ALA:HA	11:K:74:ARG:O	2.15	0.47
3:A:1074:GLU:C	3:A:1076:ALA:H	2.18	0.47
3:A:443:LEU:CD2	3:A:455:MET:HB3	2.42	0.47
4:B:363:HIS:CD2	4:B:585:VAL:HG22	2.49	0.47
4:B:1169:MET:SD	4:B:1201:LYS:HG2	2.54	0.47
4:B:750:GLY:O	4:B:751:VAL:C	2.52	0.47
4:B:210:LYS:HE2	4:B:461:LEU:O	2.14	0.47
4:B:1177:HIS:C	4:B:1179:GLN:N	2.68	0.47
5:C:142:VAL:H	10:J:16:ASP:CB	2.26	0.47
3:A:890:ASP:N	3:A:1296:GLY:HA3	2.30	0.47
7:F:79:ARG:HG2	7:F:146:TRP:CZ2	2.49	0.47
3:A:568:PRO:HB2	5:C:221:TYR:CZ	2.50	0.47
3:A:666:ILE:O	3:A:667:GLY:C	2.53	0.47
4:B:1065:GLN:HE22	4:B:1067:ARG:HG2	1.79	0.47
4:B:726:ALA:CB	4:B:1051:THR:HG21	2.45	0.47
3:A:923:LEU:O	3:A:927:VAL:HG23	2.14	0.47
4:B:1104:HIS:HB2	4:B:1122:ARG:CD	2.44	0.47
9:I:7:CYS:CB	9:I:14:LEU:HD21	2.32	0.47
3:A:1237:ILE:CG2	3:A:1238:ILE:N	2.78	0.47
4:B:800:GLN:HB3	10:J:52:THR:HG22	1.96	0.47
4:B:230:ALA:C	4:B:232:SER:H	2.17	0.47
3:A:531:ILE:CD1	3:A:617:VAL:HG11	2.44	0.47
4:B:1013:ASN:OD1	4:B:1015:HIS:HB2	2.15	0.47
4:B:763:GLN:CG	4:B:765:PRO:HD2	2.40	0.47
3:A:1074:GLU:HB3	3:A:1075:PRO:HD3	1.97	0.47
3:A:154:SER:HB3	3:A:162:VAL:HG21	1.92	0.47
4:B:1158:PHE:HE2	4:B:1201:LYS:HE3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1117:GLN:NE2	4:B:1156:ASP:OD2	2.48	0.47
3:A:804:TYR:HE1	4:B:1021:MET:CE	2.28	0.47
4:B:566:LEU:CD1	4:B:588:GLY:HA2	2.43	0.47
3:A:90:VAL:HG21	3:A:296:LEU:HG	1.96	0.47
3:A:112:LYS:HG2	3:A:113:LEU:H	1.79	0.47
3:A:22:PHE:HB2	4:B:1211:ASN:CG	2.35	0.47
5:C:38:ILE:HG13	5:C:176:ILE:HD12	1.97	0.47
5:C:35:ARG:O	5:C:38:ILE:N	2.47	0.47
4:B:332:ASP:C	4:B:334:ILE:H	2.17	0.47
4:B:284:ILE:HD13	4:B:333:PHE:CD2	2.49	0.47
4:B:1098:MET:O	4:B:1099:VAL:C	2.53	0.47
4:B:802:PRO:HA	4:B:822:ASN:HD21	1.79	0.47
7:F:147:SER:HG	7:F:150:GLU:HG3	1.77	0.47
6:E:58:MET:O	6:E:59:SER:C	2.53	0.47
7:F:101:ILE:HD11	7:F:124:GLU:OE1	2.15	0.47
3:A:1327:ILE:O	6:E:147:HIS:HE1	1.98	0.47
4:B:640:VAL:HG23	4:B:740:HIS:HA	1.97	0.47
4:B:280:ILE:HD13	4:B:334:ILE:HG12	1.95	0.47
3:A:1410:PHE:C	3:A:1412:ALA:N	2.68	0.47
4:B:487:THR:HG22	4:B:489:SER:N	2.24	0.47
4:B:100:PRO:O	4:B:180:TYR:OH	2.31	0.47
4:B:100:PRO:HD2	4:B:180:TYR:CE1	2.50	0.47
5:C:258:ILE:N	5:C:258:ILE:HD12	2.30	0.47
9:I:2:THR:OG1	9:I:45:ARG:HB3	2.15	0.47
4:B:321:GLY:C	4:B:323:VAL:H	2.17	0.47
5:C:263:THR:C	5:C:265:MET:H	2.18	0.47
4:B:291:ILE:HD13	4:B:300:HIS:NE2	2.30	0.47
4:B:780:VAL:HG21	10:J:56:LEU:HD11	1.97	0.47
10:J:1:MET:O	10:J:2:ILE:O	2.33	0.47
3:A:1237:ILE:HG22	3:A:1238:ILE:N	2.29	0.47
4:B:1116:ARG:NH1	4:B:1198:TYR:CD1	2.83	0.47
3:A:964:ILE:HD13	3:A:1035:TYR:CZ	2.50	0.47
3:A:294:SER:HA	3:A:297:GLN:HB3	1.96	0.47
3:A:1227:ILE:HG22	3:A:1228:TRP:N	2.30	0.47
11:K:83:PRO:O	11:K:87:LEU:N	2.46	0.47
6:E:179:GLN:OE1	6:E:179:GLN:HA	2.16	0.47
4:B:324:ILE:HG23	4:B:329:THR:HB	1.96	0.46
9:I:75:CYS:HG	9:I:106:CYS:HG	1.62	0.46
3:A:1192:LEU:HD11	3:A:1239:ARG:CB	2.37	0.46
5:C:18:VAL:O	5:C:18:VAL:HG12	2.15	0.46
7:F:109:VAL:HG11	7:F:123:LYS:HG2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:851:PHE:O	4:B:974:PRO:HD3	2.15	0.46
4:B:96:TYR:CD1	4:B:96:TYR:N	2.83	0.46
3:A:829:VAL:O	3:A:831:THR:N	2.48	0.46
1:R:8:G:C2	2:T:8:DT:C4	3.04	0.46
5:C:62:PHE:C	5:C:62:PHE:CD2	2.89	0.46
4:B:1106:ARG:CD	4:B:1126:GLY:O	2.62	0.46
3:A:530:GLY:O	3:A:531:ILE:C	2.54	0.46
3:A:693:VAL:HG21	3:A:721:PHE:CE1	2.38	0.46
3:A:1173:HIS:CD2	3:A:1227:ILE:HG23	2.51	0.46
4:B:298:LEU:N	4:B:298:LEU:HD23	2.29	0.46
4:B:821:GLN:HB2	4:B:851:PHE:CE2	2.49	0.46
3:A:881:GLN:OE1	3:A:959:ASN:HA	2.15	0.46
4:B:300:HIS:ND1	4:B:376:PHE:CD2	2.81	0.46
4:B:1072:MET:O	4:B:1081:LEU:HB2	2.15	0.46
4:B:842:ASN:HD22	4:B:845:SER:HB3	1.80	0.46
4:B:906:SER:CB	4:B:946:ASN:HB2	2.46	0.46
4:B:315:LYS:O	4:B:318:VAL:N	2.46	0.46
3:A:893:PHE:CD1	3:A:940:ARG:HD2	2.51	0.46
3:A:352:VAL:HG12	3:A:353:ILE:N	2.29	0.46
3:A:679:ILE:HG23	3:A:729:ALA:CB	2.39	0.46
6:E:96:PHE:CE1	6:E:100:ILE:HD11	2.50	0.46
4:B:871:THR:HG22	4:B:872:GLU:O	2.14	0.46
4:B:1182:CYS:O	4:B:1183:LYS:HD2	2.15	0.46
3:A:975:HIS:ND1	3:A:1036:ARG:HG3	2.30	0.46
9:I:34:TYR:O	9:I:35:VAL:HG23	2.16	0.46
4:B:1051:THR:HG21	4:B:1053:GLU:HB2	1.97	0.46
3:A:517:ASN:ND2	3:A:1362:TYR:CE2	2.83	0.46
4:B:653:VAL:C	4:B:654:ARG:HG2	2.36	0.46
3:A:381:THR:CG2	3:A:383:TYR:CD1	2.98	0.46
3:A:1166:ASP:CG	3:A:1194:ARG:HH21	2.19	0.46
4:B:167:ILE:HG22	4:B:167:ILE:O	2.14	0.46
3:A:709:THR:C	3:A:711:ARG:N	2.67	0.46
4:B:830:TYR:CE2	4:B:1000:PRO:HD3	2.50	0.46
12:L:34:CYS:HG	12:L:51:CYS:HG	1.62	0.46
5:C:5:GLY:O	5:C:6:PRO:C	2.54	0.46
3:A:1394:THR:HG21	3:A:1398:MET:SD	2.56	0.46
3:A:848:ILE:CD1	3:A:1374:VAL:HG21	2.45	0.46
3:A:112:LYS:HG2	3:A:113:LEU:N	2.31	0.46
6:E:102:GLU:C	6:E:104:ASN:N	2.67	0.46
3:A:20:GLY:HA2	3:A:1413:GLY:O	2.14	0.46
3:A:1140:HIS:HB2	3:A:1276:VAL:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:180:TYR:O	5:C:181:ASP:HB3	2.15	0.46
4:B:640:VAL:HG12	4:B:640:VAL:O	2.15	0.46
4:B:332:ASP:C	4:B:334:ILE:N	2.68	0.46
3:A:1209:MET:CG	3:A:1236:LEU:HD22	2.45	0.46
3:A:1037:LEU:HD13	3:A:1042:PHE:HA	1.98	0.46
3:A:849:MET:HB2	3:A:1063:MET:SD	2.55	0.46
4:B:282:ILE:HG13	4:B:283:VAL:N	2.31	0.46
3:A:1277:GLU:O	3:A:1278:ASN:HB2	2.14	0.46
3:A:567:LYS:CD	3:A:568:PRO:HD2	2.45	0.46
3:A:666:ILE:H	3:A:666:ILE:HG13	1.33	0.46
3:A:535:THR:HG22	3:A:616:VAL:HA	1.97	0.46
4:B:314:LEU:O	4:B:315:LYS:C	2.53	0.46
6:E:96:PHE:CE2	6:E:110:PHE:HB2	2.50	0.46
4:B:31:TRP:CE3	4:B:34:ILE:HD12	2.50	0.46
4:B:574:SER:HB3	4:B:577:ALA:HB2	1.98	0.46
3:A:446:ARG:HG2	3:A:446:ARG:NH1	2.28	0.46
3:A:50:ILE:HG22	3:A:51:GLY:H	1.81	0.46
4:B:50:SER:O	4:B:53:GLN:HB3	2.16	0.46
8:H:26:ILE:HD13	8:H:49:VAL:HG11	1.97	0.46
4:B:519:TRP:HE1	4:B:635:ARG:HH22	1.64	0.46
10:J:5:VAL:O	10:J:6:ARG:HB2	2.15	0.46
4:B:737:THR:HG23	9:I:66:PRO:HB2	1.94	0.46
6:E:205:SER:O	6:E:206:GLY:C	2.54	0.46
8:H:113:ALA:HA	8:H:125:LEU:O	2.15	0.46
3:A:658:LEU:HD13	4:B:831:SER:HA	1.98	0.46
4:B:1013:ASN:OD1	4:B:1015:HIS:N	2.44	0.46
3:A:223:GLY:HA3	3:A:1415:SER:HB3	1.98	0.46
4:B:62:ILE:HG21	4:B:417:PHE:HD2	1.80	0.46
3:A:1208:THR:HG22	3:A:1210:GLY:H	1.81	0.46
3:A:87:ALA:HB3	3:A:276:LEU:CD2	2.45	0.46
3:A:738:LYS:NZ	5:C:194:GLU:CA	2.79	0.46
3:A:573:SER:OG	3:A:576:GLN:HG3	2.15	0.46
4:B:260:GLY:HA3	4:B:267:ARG:HG2	1.98	0.46
4:B:890:TYR:C	4:B:892:LYS:H	2.19	0.46
5:C:262:LEU:O	5:C:265:MET:HB3	2.15	0.46
4:B:704:ALA:HB2	4:B:738:PHE:CE1	2.51	0.46
4:B:605:ARG:CZ	4:B:639:ILE:HD13	2.46	0.46
4:B:800:GLN:CB	10:J:52:THR:CG2	2.89	0.46
3:A:1242:VAL:CG1	3:A:1243:VAL:H	2.22	0.46
4:B:316:PRO:HA	4:B:319:GLU:HG2	1.98	0.46
3:A:83:HIS:CE1	3:A:238:CYS:SG	3.08	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:858:ASN:ND2	3:A:858:ASN:C	2.68	0.46
8:H:138:GLU:O	8:H:139:ASN:C	2.53	0.46
3:A:167:CYS:C	3:A:169:ASN:H	2.18	0.46
5:C:252:GLN:CG	11:K:95:ILE:HG23	2.46	0.46
4:B:295:GLY:O	4:B:299:GLU:HG3	2.16	0.46
3:A:47:ARG:O	3:A:48:ALA:HB2	2.16	0.46
4:B:1085:ILE:CG2	4:B:1086:PHE:N	2.78	0.46
4:B:702:LEU:HD21	4:B:735:ALA:HB1	1.98	0.46
3:A:540:PHE:C	3:A:541:ILE:HD12	2.35	0.46
11:K:12:LEU:CD1	11:K:12:LEU:H	2.23	0.46
4:B:230:ALA:N	4:B:231:PRO:HD2	2.31	0.46
3:A:35:ILE:HD12	3:A:241:VAL:HG21	1.98	0.46
3:A:53:LEU:HD13	3:A:263:THR:HG23	1.97	0.46
11:K:61:TYR:CD1	11:K:61:TYR:C	2.89	0.46
6:E:94:LYS:O	6:E:98:ILE:HG13	2.16	0.46
4:B:1017:ILE:HB	4:B:1018:PRO:HD3	1.98	0.46
4:B:893:LEU:HD22	4:B:897:GLY:O	2.16	0.46
3:A:1041:ALA:O	3:A:1044:TRP:HB3	2.15	0.46
8:H:40:LEU:HG	8:H:42:ILE:HG13	1.98	0.46
3:A:1116:LEU:HD12	3:A:1329:THR:HG1	1.76	0.46
4:B:300:HIS:ND1	4:B:376:PHE:CE2	2.83	0.46
5:C:80:LEU:CD2	5:C:129:ILE:HD11	2.28	0.46
12:L:45:ALA:O	12:L:46:VAL:CG2	2.64	0.46
4:B:1154:ALA:O	4:B:1155:SER:CB	2.64	0.46
4:B:914:LYS:H	4:B:938:SER:HB3	1.81	0.46
5:C:166:GLU:CG	11:K:10:PHE:CZ	2.96	0.46
8:H:81:PRO:HD2	8:H:82:PRO:HD2	1.98	0.46
4:B:860:MET:HB2	4:B:965:LYS:HG2	1.97	0.46
4:B:515:HIS:CD2	4:B:517:THR:OG1	2.66	0.46
7:F:117:PRO:O	7:F:120:ILE:HB	2.16	0.46
4:B:864:LYS:H	4:B:872:GLU:CG	2.28	0.46
8:H:114:VAL:O	8:H:124:ARG:HA	2.16	0.46
3:A:645:LEU:O	3:A:649:ILE:HG13	2.15	0.46
4:B:758:PHE:C	4:B:760:ASP:N	2.68	0.46
3:A:1208:THR:HG22	3:A:1210:GLY:N	2.32	0.45
3:A:477:PRO:HG2	3:A:521:MET:HG2	1.97	0.45
11:K:73:LEU:CD2	11:K:75:ILE:HD11	2.46	0.45
3:A:556:TRP:CZ3	3:A:558:GLY:HA2	2.51	0.45
3:A:848:ILE:HD13	3:A:864:ILE:HD13	1.98	0.45
3:A:573:SER:H	3:A:576:GLN:HG3	1.81	0.45
4:B:1120:GLU:HG2	4:B:1121:GLY:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:100:PHE:HZ	9:I:118:ARG:HH12	1.62	0.45
8:H:26:ILE:CD1	8:H:49:VAL:HG11	2.46	0.45
4:B:345:LYS:O	4:B:347:LYS:N	2.49	0.45
5:C:73:GLN:NE2	5:C:75:MET:H	1.97	0.45
9:I:75:CYS:O	9:I:76:PRO:C	2.52	0.45
4:B:839:MET:HE2	4:B:980:PHE:CD1	2.51	0.45
4:B:1200:ALA:O	4:B:1201:LYS:C	2.54	0.45
3:A:1225:PHE:O	3:A:1240:CYS:HA	2.14	0.45
8:H:116:TYR:HE2	8:H:140:ALA:CB	2.30	0.45
11:K:91:CYS:O	11:K:94:ILE:HB	2.16	0.45
6:E:112:TYR:CE2	6:E:134:THR:HB	2.51	0.45
6:E:10:SER:O	6:E:14:ARG:HG3	2.16	0.45
2:T:4:DA:H2'	2:T:5:DT:H72	1.98	0.45
3:A:567:LYS:NZ	8:H:95:TYR:CD1	2.80	0.45
4:B:977:GLY:C	4:B:1099:VAL:HG23	2.37	0.45
4:B:824:ILE:CG2	4:B:1087:PHE:CE2	3.00	0.45
10:J:48:ARG:HH21	10:J:49:MET:CE	2.24	0.45
4:B:201:GLY:H	4:B:202:TYR:HD2	1.63	0.45
3:A:388:LEU:O	3:A:392:VAL:HG23	2.17	0.45
11:K:55:LYS:CD	11:K:78:THR:HB	2.41	0.45
4:B:361:LEU:N	4:B:362:PRO:HD2	2.31	0.45
4:B:589:VAL:HG12	4:B:590:HIS:H	1.81	0.45
3:A:889:SER:HB3	3:A:1297:GLU:HG3	1.97	0.45
3:A:152:VAL:CG1	3:A:153:PRO:HD2	2.45	0.45
3:A:103:CYS:O	3:A:106:VAL:O	2.35	0.45
8:H:40:LEU:HD13	8:H:123:MET:HB2	1.99	0.45
3:A:571:LEU:HD22	8:H:46:LEU:HD11	1.99	0.45
3:A:1155:ASP:OD1	3:A:1162:VAL:HG23	2.17	0.45
3:A:786:HIS:CE1	4:B:742:GLU:OE1	2.64	0.45
3:A:1149:ALA:CB	9:I:47:GLU:HA	2.45	0.45
9:I:8:ARG:HG3	9:I:9:ASP:CG	2.37	0.45
5:C:242:GLN:OE1	5:C:242:GLN:HA	2.16	0.45
4:B:1106:ARG:HG2	4:B:1107:ALA:N	2.31	0.45
3:A:418:SER:O	3:A:421:ALA:N	2.49	0.45
4:B:100:PRO:HA	4:B:125:SER:O	2.17	0.45
3:A:644:LYS:O	3:A:645:LEU:C	2.55	0.45
4:B:215:GLN:HB2	4:B:407:ASP:HB2	1.98	0.45
8:H:109:LYS:HZ2	8:H:109:LYS:HB2	1.82	0.45
5:C:17:ASN:OD1	5:C:233:GLU:HG2	2.16	0.45
1:R:9:G:C2	1:R:10:A:C5	3.05	0.45
15:R:3000:UTP:C6	15:R:3000:UTP:C3'	3.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:542:GLU:C	3:A:546:VAL:HG23	2.36	0.45
5:C:62:PHE:C	5:C:62:PHE:HD2	2.20	0.45
9:I:75:CYS:C	9:I:77:LYS:H	2.20	0.45
3:A:1209:MET:CE	3:A:1236:LEU:HB3	2.47	0.45
4:B:1020:ARG:H	4:B:1020:ARG:HG2	1.51	0.45
3:A:1046:LEU:O	3:A:1047:SER:C	2.55	0.45
9:I:34:TYR:O	9:I:35:VAL:CG2	2.65	0.45
3:A:1114:PRO:O	3:A:1330:ASN:OD1	2.35	0.45
4:B:247:GLY:O	4:B:248:SER:HB3	2.17	0.45
4:B:549:THR:H	4:B:628:THR:HG22	1.81	0.45
4:B:1158:PHE:CD2	4:B:1198:TYR:HD1	2.35	0.45
8:H:101:ALA:HB2	8:H:116:TYR:CD2	2.51	0.45
4:B:25:ILE:HD11	4:B:653:VAL:CB	2.46	0.45
4:B:332:ASP:O	4:B:334:ILE:N	2.50	0.45
3:A:55:ASP:HB3	3:A:56:PRO:HD3	1.98	0.45
3:A:592:ASP:N	3:A:595:THR:OG1	2.48	0.45
3:A:1410:PHE:C	3:A:1412:ALA:H	2.19	0.45
3:A:420:ARG:O	3:A:424:ILE:HG13	2.16	0.45
4:B:56:ASP:HB3	4:B:57:TYR:CD1	2.52	0.45
4:B:185:THR:H	4:B:188:ASP:HB2	1.81	0.45
6:E:102:GLU:C	6:E:104:ASN:H	2.20	0.45
3:A:210:ILE:O	3:A:214:ILE:HG13	2.17	0.45
4:B:322:PHE:O	4:B:322:PHE:CG	2.69	0.45
2:T:1:DA:N3	2:T:1:DA:C2'	2.77	0.45
12:L:55:ILE:H	12:L:55:ILE:HG12	1.53	0.45
4:B:1100:ASP:HA	4:B:1103:ILE:CG1	2.46	0.45
4:B:702:LEU:HA	4:B:702:LEU:HD12	1.76	0.45
9:I:29:CYS:O	9:I:31:THR:N	2.49	0.45
3:A:1405:THR:O	3:A:1406:VAL:C	2.54	0.45
4:B:744:HIS:CD2	4:B:746:SER:OG	2.70	0.45
4:B:963:PHE:HE2	4:B:965:LYS:HE3	1.81	0.45
4:B:980:PHE:HE1	4:B:990:ILE:CD1	2.30	0.45
3:A:69:THR:O	4:B:1174:LYS:HG2	2.17	0.45
3:A:958:VAL:HG22	3:A:1052:GLN:HB3	1.98	0.45
4:B:371:GLU:N	4:B:371:GLU:OE1	2.49	0.45
4:B:276:ILE:HD13	4:B:334:ILE:CG2	2.47	0.45
3:A:80:HIS:O	3:A:243:PRO:HB3	2.17	0.45
4:B:839:MET:HE1	4:B:980:PHE:HB2	1.98	0.45
11:K:24:ASP:HB3	11:K:30:ALA:CB	2.47	0.45
8:H:111:LEU:HA	8:H:127:GLY:O	2.17	0.45
3:A:329:LEU:HA	3:A:335:ARG:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:109:VAL:HG12	7:F:110:ASP:H	1.82	0.45
5:C:249:ASP:O	5:C:252:GLN:HB3	2.16	0.45
4:B:686:ASN:C	4:B:688:GLY:N	2.70	0.45
3:A:974:ASP:CB	8:H:136:LYS:NZ	2.80	0.45
4:B:680:THR:O	4:B:683:SER:OG	2.34	0.45
4:B:377:PHE:C	4:B:379:GLY:N	2.68	0.45
3:A:517:ASN:OD1	3:A:517:ASN:O	2.34	0.45
5:C:39:ALA:HA	5:C:164:ALA:CB	2.46	0.45
9:I:92:ARG:CG	9:I:93:LYS:H	2.30	0.45
11:K:78:THR:O	11:K:79:GLU:C	2.56	0.45
4:B:986:GLN:OE1	4:B:986:GLN:CA	2.64	0.45
4:B:515:HIS:O	4:B:516:ASN:C	2.54	0.45
3:A:219:PHE:CE2	3:A:231:PRO:HD2	2.52	0.45
1:R:2:U:C5	1:R:3:C:C4	3.05	0.45
5:C:120:ILE:HD11	5:C:130:GLY:O	2.17	0.45
4:B:238:ALA:HB3	4:B:256:VAL:HB	1.98	0.45
4:B:426:LYS:O	4:B:430:ARG:HG3	2.17	0.44
4:B:1169:MET:HE3	4:B:1205:GLN:HG2	2.00	0.44
3:A:1207:LEU:HA	3:A:1211:GLN:OE1	2.17	0.44
4:B:864:LYS:HD3	4:B:871:THR:CA	2.47	0.44
3:A:1336:MET:SD	3:A:1381:LEU:HG	2.56	0.44
8:H:24:CYS:CB	8:H:44:VAL:HG21	2.47	0.44
6:E:147:HIS:CD2	6:E:149:LEU:H	2.35	0.44
8:H:84:ALA:HA	8:H:87:ARG:HB2	1.98	0.44
4:B:1038:SER:HB3	4:B:1062:HIS:NE2	2.33	0.44
9:I:99:LEU:HB2	9:I:112:SER:CB	2.46	0.44
12:L:62:LYS:O	12:L:64:LEU:N	2.37	0.44
3:A:1155:ASP:CG	3:A:1162:VAL:HG23	2.37	0.44
4:B:957:ASN:O	4:B:958:GLN:C	2.55	0.44
4:B:200:GLY:HA2	4:B:202:TYR:CD2	2.50	0.44
9:I:7:CYS:HB2	9:I:14:LEU:CD2	2.34	0.44
8:H:5:LEU:O	8:H:133:ASN:HB3	2.17	0.44
4:B:229:ALA:HB1	4:B:231:PRO:HD2	1.98	0.44
3:A:340:LEU:HD21	4:B:1200:ALA:CA	2.47	0.44
5:C:9:LYS:HB2	5:C:21:ILE:HB	1.98	0.44
3:A:152:VAL:HG13	3:A:153:PRO:HD2	1.99	0.44
6:E:190:LEU:HD11	6:E:196:VAL:HG11	1.98	0.44
4:B:1085:ILE:HG22	4:B:1086:PHE:N	2.31	0.44
4:B:800:GLN:CB	10:J:52:THR:HG22	2.47	0.44
3:A:541:ILE:HG12	3:A:549:MET:HE3	1.99	0.44
4:B:130:VAL:CG1	4:B:131:ASP:H	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:825:ILE:C	3:A:827:THR:N	2.70	0.44
5:C:31:ASN:O	5:C:35:ARG:HG3	2.17	0.44
3:A:701:LEU:HA	9:I:115:LYS:HE3	1.98	0.44
3:A:67:CYS:SG	3:A:77:CYS:SG	3.11	0.44
2:T:6:DC:H4'	3:A:447:GLN:CD	2.37	0.44
4:B:707:PRO:O	4:B:708:GLU:O	2.35	0.44
4:B:276:ILE:HD13	4:B:334:ILE:HG23	1.99	0.44
3:A:78:PRO:O	3:A:79:GLY:C	2.56	0.44
4:B:958:GLN:C	4:B:960:GLY:H	2.20	0.44
4:B:1033:LYS:NZ	4:B:1070:GLU:OE1	2.46	0.44
3:A:13:THR:HG23	3:A:1432:GLN:CD	2.38	0.44
3:A:1441:PHE:HB2	7:F:134:ILE:CG2	2.47	0.44
4:B:408:LEU:HA	4:B:408:LEU:HD12	1.71	0.44
3:A:1415:SER:O	3:A:1416:ALA:C	2.55	0.44
3:A:21:LEU:HD21	3:A:95:PHE:CZ	2.53	0.44
4:B:288:ALA:HA	4:B:331:LEU:HD13	1.99	0.44
4:B:446:LEU:HD23	4:B:446:LEU:N	2.33	0.44
4:B:781:PHE:CE2	4:B:795:ILE:HD11	2.53	0.44
3:A:756:ILE:CG2	3:A:757:ASN:N	2.80	0.44
4:B:216:GLU:OE1	4:B:537:LYS:CE	2.66	0.44
4:B:365:THR:CG2	4:B:367:LEU:H	2.30	0.44
3:A:456:MET:HB2	3:A:478:TYR:OH	2.17	0.44
8:H:98:TYR:O	8:H:118:PHE:HD2	1.99	0.44
3:A:1068:ALA:O	3:A:1069:ALA:C	2.55	0.44
4:B:915:THR:HG21	4:B:934:LYS:HG2	1.99	0.44
5:C:69:LEU:HA	5:C:69:LEU:HD12	1.76	0.44
4:B:664:THR:HG1	4:B:678:GLU:N	2.15	0.44
4:B:709:ASP:C	4:B:710:LEU:HD23	2.38	0.44
4:B:1002:THR:CG2	4:B:1004:GLU:HB2	2.47	0.44
6:E:138:ALA:C	6:E:140:LEU:H	2.21	0.44
3:A:815:PHE:O	3:A:818:MET:N	2.50	0.44
8:H:93:TYR:HA	8:H:145:ARG:CB	2.41	0.44
3:A:525:GLN:HB2	4:B:835:GLN:HG2	2.00	0.44
11:K:24:ASP:OD1	11:K:26:LYS:N	2.51	0.44
3:A:233:TRP:O	3:A:235:ILE:N	2.50	0.44
6:E:28:TYR:CE2	6:E:64:PRO:HG3	2.53	0.44
4:B:361:LEU:O	4:B:363:HIS:O	2.35	0.44
3:A:741:ASN:HD22	3:A:743:VAL:N	2.16	0.44
4:B:526:GLU:CD	4:B:752:ALA:HB3	2.38	0.44
4:B:995:ARG:NH1	4:B:997:GLU:OE1	2.49	0.44
3:A:50:ILE:C	3:A:52:GLY:N	2.69	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:32:GLU:CD	10:J:32:GLU:H	2.19	0.44
3:A:1066:VAL:O	3:A:1067:LEU:C	2.56	0.44
4:B:1060:ARG:O	4:B:1063:GLY:N	2.45	0.44
3:A:829:VAL:C	3:A:831:THR:N	2.70	0.44
3:A:1384:VAL:O	3:A:1389:PHE:HE2	2.01	0.44
4:B:640:VAL:HG23	4:B:740:HIS:CA	2.48	0.44
3:A:243:PRO:HB2	3:A:245:PRO:HD2	1.99	0.44
5:C:236:GLY:C	5:C:238:ILE:N	2.69	0.44
3:A:388:LEU:HA	3:A:388:LEU:HD23	1.88	0.44
3:A:591:PHE:HD2	3:A:595:THR:HB	1.83	0.44
3:A:595:THR:HG22	3:A:596:THR:N	2.33	0.44
4:B:168:GLY:H	4:B:450:ALA:HB1	1.82	0.44
4:B:214:ALA:HB2	4:B:408:LEU:CD1	2.48	0.44
4:B:65:GLU:HG3	4:B:66:ASP:N	2.27	0.44
3:A:760:GLN:OE1	4:B:1021:MET:HE2	2.16	0.44
4:B:864:LYS:HD3	4:B:871:THR:CB	2.47	0.44
4:B:805:THR:HA	4:B:809:MET:HE1	2.00	0.44
4:B:995:ARG:HH11	4:B:995:ARG:HB2	1.81	0.44
6:E:185:ALA:CB	6:E:190:LEU:HD12	2.47	0.44
6:E:138:ALA:O	6:E:140:LEU:N	2.50	0.44
3:A:960:ILE:HD12	3:A:1021:LEU:HD21	1.99	0.44
4:B:487:THR:O	4:B:488:TYR:C	2.56	0.44
3:A:679:ILE:O	3:A:682:THR:HB	2.18	0.44
12:L:38:LEU:HG	12:L:39:SER:H	1.82	0.44
4:B:56:ASP:HB3	4:B:57:TYR:CE1	2.53	0.44
4:B:973:ILE:CG2	4:B:974:PRO:HD2	2.47	0.44
3:A:494:SER:HB2	3:A:497:THR:OG1	2.18	0.44
9:I:50:THR:HG22	9:I:52:ILE:N	2.33	0.44
3:A:381:THR:O	3:A:384:ASN:N	2.41	0.44
4:B:912:ILE:O	4:B:938:SER:CB	2.59	0.44
3:A:1118:VAL:O	3:A:1305:VAL:HG13	2.17	0.44
4:B:102:VAL:HG21	4:B:112:LEU:HD13	1.99	0.44
3:A:458:HIS:ND1	3:A:507:VAL:HG21	2.33	0.44
3:A:845:LEU:O	3:A:848:ILE:HG13	2.17	0.44
4:B:370:PHE:N	4:B:371:GLU:OE1	2.50	0.44
4:B:847:ASP:O	5:C:65:HIS:HE1	2.01	0.44
3:A:567:LYS:HZ3	8:H:95:TYR:HE1	1.52	0.44
3:A:1094:VAL:HG12	3:A:1095:THR:N	2.32	0.44
3:A:1364:ASN:HD22	3:A:1365:TYR:N	2.13	0.44
5:C:143:LEU:HD21	5:C:146:LYS:HE3	1.99	0.44
6:E:137:GLU:O	6:E:140:LEU:N	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:778:MET:HE1	4:B:1094:ARG:HD3	1.98	0.44
11:K:24:ASP:OD2	11:K:74:ARG:NH1	2.51	0.44
3:A:366:VAL:HA	3:A:367:PRO:HD2	1.81	0.44
5:C:8:VAL:CG1	5:C:9:LYS:N	2.80	0.44
4:B:1185:CYS:O	4:B:1186:ASP:HB2	2.17	0.44
3:A:84:ILE:CG2	3:A:239:LEU:HB3	2.48	0.44
4:B:205:ILE:HG12	4:B:461:LEU:HB3	1.99	0.44
10:J:16:ASP:OD1	10:J:17:LYS:HG3	2.17	0.44
3:A:1121:GLU:O	3:A:1122:PRO:C	2.56	0.44
4:B:203:PHE:HE1	4:B:212:LEU:CD1	2.31	0.44
3:A:562:THR:HA	3:A:563:PRO:HD3	1.92	0.43
9:I:98:VAL:CG1	9:I:99:LEU:N	2.81	0.43
3:A:1364:ASN:HD22	3:A:1366:ARG:N	2.16	0.43
4:B:650:GLU:HG2	4:B:654:ARG:NH1	2.33	0.43
3:A:54:ASN:O	3:A:55:ASP:HB2	2.18	0.43
4:B:690:VAL:HG12	4:B:691:GLU:N	2.33	0.43
3:A:614:PHE:C	3:A:614:PHE:CD1	2.92	0.43
3:A:1441:PHE:HB2	7:F:134:ILE:HG23	2.00	0.43
3:A:326:ARG:HE	3:A:1406:VAL:HG11	1.82	0.43
5:C:77:ILE:CG2	5:C:161:LYS:HE3	2.48	0.43
8:H:5:LEU:O	8:H:6:PHE:HB2	2.18	0.43
4:B:310:MET:O	4:B:313:MET:HB2	2.18	0.43
11:K:55:LYS:HD3	11:K:78:THR:OG1	2.18	0.43
4:B:745:PRO:C	4:B:747:MET:N	2.70	0.43
5:C:46:ILE:HG23	5:C:157:CYS:HB3	2.00	0.43
3:A:404:TYR:HA	3:A:413:ILE:O	2.18	0.43
3:A:1349:TYR:O	3:A:1350:LYS:C	2.56	0.43
5:C:135:GLN:C	5:C:136:ASP:O	2.56	0.43
9:I:91:ARG:HD3	9:I:91:ARG:HA	1.75	0.43
12:L:61:THR:HG22	12:L:62:LYS:N	2.33	0.43
4:B:1002:THR:HG21	4:B:1006:ILE:HB	2.00	0.43
6:E:133:GLU:HB3	6:E:135:PHE:HE1	1.83	0.43
3:A:533:LYS:C	3:A:535:THR:N	2.72	0.43
3:A:535:THR:HG21	3:A:616:VAL:CA	2.43	0.43
4:B:315:LYS:N	4:B:316:PRO:HD2	2.32	0.43
3:A:742:ASN:C	3:A:745:GLN:HB2	2.38	0.43
4:B:34:ILE:HG12	4:B:542:MET:HE1	2.00	0.43
3:A:1015:VAL:O	3:A:1015:VAL:HG12	2.18	0.43
8:H:84:ALA:CA	8:H:87:ARG:HB2	2.48	0.43
8:H:84:ALA:CB	8:H:87:ARG:HB2	2.49	0.43
1:R:2:U:H3'	1:R:3:C:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:82:PHE:N	6:E:82:PHE:CD1	2.85	0.43
2:T:8:DT:H2'	2:T:9:DC:C6	2.53	0.43
6:E:113:GLN:HG2	6:E:137:GLU:OE1	2.19	0.43
5:C:173:ALA:O	5:C:174:ALA:CB	2.64	0.43
6:E:7:ARG:C	6:E:9:ILE:N	2.71	0.43
3:A:1049:ILE:O	3:A:1050:GLU:C	2.56	0.43
3:A:367:PRO:CB	3:A:466:SER:HA	2.47	0.43
3:A:42:ASP:OD1	3:A:45:GLN:O	2.36	0.43
4:B:562:GLY:O	4:B:563:MET:C	2.56	0.43
3:A:629:LEU:CD1	3:A:645:LEU:HD21	2.48	0.43
4:B:781:PHE:HE2	4:B:795:ILE:HD11	1.83	0.43
4:B:189:LEU:O	4:B:190:TYR:C	2.57	0.43
11:K:92:ASN:O	11:K:93:SER:C	2.56	0.43
4:B:850:LEU:CD2	4:B:1009:ASP:HB3	2.48	0.43
9:I:84:VAL:CG1	9:I:84:VAL:O	2.65	0.43
4:B:1060:ARG:C	4:B:1062:HIS:N	2.69	0.43
4:B:212:LEU:HD13	4:B:409:ALA:HA	2.00	0.43
4:B:358:LYS:O	4:B:359:GLU:OE1	2.36	0.43
3:A:850:VAL:O	3:A:1060:PRO:HA	2.18	0.43
3:A:1385:THR:HG22	3:A:1386:ARG:N	2.33	0.43
2:T:1:DA:N3	2:T:2:DC:C6	2.86	0.43
5:C:56:THR:CG2	5:C:57:VAL:N	2.69	0.43
8:H:57:VAL:HG12	8:H:58:THR:N	2.32	0.43
3:A:399:HIS:C	3:A:401:GLY:N	2.71	0.43
3:A:778:GLY:HA3	4:B:516:ASN:CB	2.46	0.43
5:C:264:GLN:H	5:C:264:GLN:HG3	1.61	0.43
4:B:806:THR:C	4:B:808:ALA:N	2.70	0.43
4:B:784:ASN:HB3	10:J:63:TYR:OH	2.18	0.43
5:C:123:ASN:ND2	5:C:125:MET:HG2	2.31	0.43
5:C:251:LEU:HG	11:K:98:LEU:HD11	2.01	0.43
12:L:27:LEU:HD13	12:L:37:LYS:CB	2.48	0.43
3:A:412:ARG:CZ	4:B:1108:ARG:NH2	2.81	0.43
4:B:366:GLN:O	4:B:367:LEU:O	2.36	0.43
5:C:31:ASN:O	5:C:32:SER:C	2.56	0.43
5:C:52:GLU:HB3	5:C:154:LYS:HB3	1.99	0.43
3:A:1148:ILE:HD12	3:A:1196:GLU:HG2	2.01	0.43
12:L:43:THR:O	12:L:43:THR:HG22	2.18	0.43
3:A:373:THR:HG21	4:B:1105:ALA:O	2.17	0.43
3:A:901:LEU:HD13	3:A:919:ILE:CG2	2.48	0.43
4:B:202:TYR:CD2	4:B:202:TYR:N	2.87	0.43
4:B:831:SER:CB	4:B:994:TYR:OH	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:47:ARG:CB	11:K:47:ARG:HH11	2.23	0.43
4:B:194:GLU:HA	4:B:194:GLU:OE1	2.18	0.43
3:A:84:ILE:HG23	3:A:84:ILE:O	2.17	0.43
3:A:148:CYS:HB3	3:A:167:CYS:O	2.18	0.43
4:B:1171:VAL:HG13	4:B:1191:ILE:HD13	1.99	0.43
3:A:845:LEU:O	3:A:846:GLU:C	2.57	0.43
6:E:114:ASN:O	6:E:115:ASN:HB3	2.18	0.43
4:B:904:ARG:CZ	4:B:948:ILE:HD11	2.48	0.43
15:R:3000:UTP:C2	2:T:4:DA:N1	2.86	0.43
3:A:565:ILE:HD13	3:A:567:LYS:HE2	2.01	0.43
4:B:345:LYS:N	4:B:348:ARG:HE	2.15	0.43
4:B:280:ILE:CG2	4:B:285:ILE:HG13	2.47	0.43
4:B:955:THR:CG2	4:B:956:THR:N	2.49	0.43
4:B:955:THR:HA	12:L:54:ARG:O	2.19	0.43
1:R:6:G:H2'	1:R:7:A:O5'	2.19	0.43
5:C:39:ALA:CA	5:C:164:ALA:HB3	2.47	0.43
3:A:344:ARG:O	4:B:1118:PRO:HG2	2.19	0.43
3:A:751:SER:OG	4:B:1015:HIS:CE1	2.71	0.43
5:C:148:ARG:HD3	5:C:149:LYS:H	1.83	0.43
3:A:99:ILE:O	3:A:102:VAL:HB	2.19	0.43
4:B:1116:ARG:CZ	4:B:1198:TYR:CE1	3.01	0.43
3:A:968:GLN:NE2	3:A:1035:TYR:HB2	2.33	0.43
3:A:774:ARG:O	3:A:775:ILE:C	2.57	0.43
4:B:295:GLY:H	4:B:298:LEU:HG	1.84	0.43
4:B:1177:HIS:C	4:B:1179:GLN:H	2.22	0.43
4:B:758:PHE:CZ	4:B:1044:ALA:HA	2.53	0.43
3:A:1424:VAL:HG11	4:B:1139:ILE:HD13	2.00	0.43
4:B:648:HIS:HB2	4:B:649:LYS:H	1.61	0.43
4:B:1175:LEU:O	4:B:1176:ASN:CG	2.56	0.43
3:A:852:TYR:CE2	7:F:136:ARG:NE	2.86	0.43
6:E:9:ILE:C	6:E:11:ARG:N	2.71	0.43
3:A:1409:LEU:HD23	3:A:1409:LEU:HA	1.83	0.43
3:A:673:GLY:N	3:A:674:PRO:HD2	2.33	0.43
3:A:672:ASP:O	3:A:675:THR:HB	2.19	0.43
3:A:1336:MET:HE1	3:A:1381:LEU:N	2.33	0.43
12:L:40:LEU:HD23	12:L:40:LEU:HA	1.77	0.43
3:A:645:LEU:HD11	3:A:649:ILE:HD11	2.01	0.43
3:A:1097:GLY:C	3:A:1099:PRO:HD2	2.39	0.43
5:C:135:GLN:O	5:C:136:ASP:O	2.37	0.43
6:E:145:THR:HG21	6:E:187:TYR:CE2	2.53	0.43
3:A:545:GLN:O	3:A:546:VAL:C	2.55	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:47:PHE:CB	8:H:95:TYR:HD1	2.31	0.43
4:B:642:ASP:O	4:B:643:ASP:C	2.56	0.43
4:B:705:MET:H	4:B:710:LEU:CD1	2.32	0.43
3:A:1194:ARG:HH22	3:A:1237:ILE:HD13	1.73	0.43
9:I:106:CYS:O	9:I:107:SER:HB2	2.18	0.43
4:B:128:LEU:HD12	4:B:128:LEU:HA	1.82	0.43
3:A:709:THR:O	3:A:712:GLU:N	2.52	0.43
3:A:709:THR:HG23	9:I:94:ASP:HA	2.00	0.43
3:A:89:PRO:HG3	3:A:208:LEU:HD12	2.00	0.43
3:A:457:ALA:O	3:A:507:VAL:HG23	2.19	0.43
4:B:126:SER:OG	4:B:172:ILE:HD11	2.18	0.43
3:A:466:SER:HB3	11:K:2:ASN:HD22	1.83	0.43
4:B:784:ASN:HD21	4:B:788:ARG:HD2	1.84	0.43
4:B:101:MET:HE3	4:B:169:ARG:HH22	1.84	0.43
4:B:1108:ARG:O	4:B:1108:ARG:CG	2.67	0.43
4:B:1103:ILE:O	4:B:1104:HIS:C	2.56	0.43
4:B:702:LEU:HD22	4:B:737:THR:CG2	2.49	0.43
3:A:396:PRO:HG3	3:A:416:ARG:HB3	2.00	0.43
3:A:1300:LYS:HB3	3:A:1300:LYS:HZ2	1.84	0.43
6:E:69:ILE:O	6:E:73:PRO:HG3	2.19	0.43
8:H:111:LEU:HD23	8:H:127:GLY:O	2.18	0.43
3:A:1394:THR:HG22	3:A:1395:GLY:O	2.19	0.43
4:B:113:TYR:CD2	4:B:192:LEU:HD22	2.53	0.43
3:A:1004:ASN:O	3:A:1008:GLN:HB2	2.19	0.43
3:A:114:LEU:HD12	3:A:142:CYS:O	2.19	0.43
3:A:547:LEU:HD22	11:K:58:PHE:HD1	1.84	0.43
7:F:140:ASP:OD1	7:F:141:GLY:N	2.52	0.43
6:E:16:PHE:CZ	6:E:20:LYS:HE2	2.54	0.43
4:B:274:PRO:O	4:B:276:ILE:N	2.51	0.43
3:A:907:THR:HG22	3:A:908:LEU:H	1.82	0.43
9:I:46:HIS:O	9:I:47:GLU:HB2	2.18	0.43
3:A:815:PHE:C	3:A:817:ALA:N	2.72	0.43
3:A:337:ARG:CZ	3:A:839:ARG:CZ	2.97	0.43
3:A:960:ILE:O	3:A:961:ARG:C	2.57	0.43
3:A:306:ASN:OD1	3:A:313:GLN:NE2	2.51	0.43
6:E:168:TYR:O	6:E:170:LEU:HD23	2.19	0.43
5:C:249:ASP:OD1	5:C:253:LYS:HE3	2.19	0.43
9:I:59:VAL:HG12	9:I:60:GLN:N	2.34	0.43
5:C:148:ARG:H	5:C:151:GLN:HG3	1.84	0.42
4:B:34:ILE:HG12	4:B:542:MET:CE	2.49	0.42
3:A:1428:VAL:HG13	4:B:1151:LEU:HD23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:518:LYS:HB2	3:A:519:PRO:HD2	2.01	0.42
4:B:794:ASN:O	4:B:795:ILE:HD12	2.19	0.42
3:A:134:ARG:O	3:A:137:ALA:N	2.52	0.42
3:A:362:ASP:OD1	3:A:459:ARG:HD3	2.18	0.42
3:A:1366:ARG:HG2	3:A:1366:ARG:HH11	1.84	0.42
4:B:708:GLU:C	4:B:710:LEU:N	2.72	0.42
4:B:329:THR:O	4:B:332:ASP:HB3	2.19	0.42
6:E:137:GLU:O	6:E:138:ALA:C	2.57	0.42
4:B:601:ARG:O	4:B:605:ARG:HG3	2.19	0.42
3:A:86:LEU:HB3	3:A:296:LEU:HD21	2.00	0.42
4:B:806:THR:O	4:B:808:ALA:N	2.52	0.42
5:C:59:ALA:O	5:C:63:ILE:HG13	2.18	0.42
5:C:76:ASP:OD2	5:C:128:ASN:N	2.47	0.42
2:T:6:DC:C2'	2:T:7:DC:O5'	2.67	0.42
2:T:1:DA:H2''	2:T:2:DC:C5'	2.41	0.42
4:B:281:PRO:HG2	4:B:284:ILE:CD1	2.45	0.42
3:A:80:HIS:N	3:A:243:PRO:HB3	2.34	0.42
4:B:955:THR:CG2	12:L:54:ARG:O	2.65	0.42
10:J:9:SER:HB2	10:J:45:CYS:HB2	2.00	0.42
5:C:242:GLN:O	5:C:246:ARG:N	2.52	0.42
3:A:962:ARG:O	3:A:963:ILE:C	2.57	0.42
3:A:30:ILE:O	3:A:31:SER:O	2.37	0.42
3:A:1027:ALA:O	3:A:1030:ARG:HB2	2.20	0.42
3:A:451:HIS:HB2	3:A:454:SER:OG	2.19	0.42
4:B:880:THR:O	4:B:881:ASN:HB2	2.20	0.42
4:B:1148:LYS:O	4:B:1152:MET:HB2	2.19	0.42
6:E:168:TYR:CB	6:E:170:LEU:HG	2.49	0.42
5:C:8:VAL:HA	5:C:21:ILE:O	2.19	0.42
4:B:1073:TYR:N	4:B:1073:TYR:CD1	2.87	0.42
11:K:95:ILE:O	11:K:98:LEU:HB2	2.19	0.42
4:B:1177:HIS:O	4:B:1179:GLN:HG3	2.19	0.42
3:A:753:GLY:HA2	3:A:757:ASN:ND2	2.34	0.42
9:I:84:VAL:O	9:I:84:VAL:HG13	2.19	0.42
3:A:131:SER:OG	3:A:132:LYS:N	2.51	0.42
8:H:143:LEU:N	8:H:143:LEU:HD12	2.34	0.42
3:A:68:GLN:O	3:A:70:CYS:N	2.52	0.42
3:A:7:SER:OG	4:B:1193:GLN:NE2	2.51	0.42
10:J:53:HIS:CE1	10:J:55:ASP:HA	2.54	0.42
3:A:751:SER:O	3:A:752:LYS:CB	2.67	0.42
4:B:994:TYR:HD1	4:B:999:MET:HE3	1.84	0.42
3:A:223:GLY:O	3:A:1415:SER:CA	2.64	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:55:VAL:O	4:B:59:LEU:HB3	2.19	0.42
3:A:151:ASP:OD1	3:A:163:SER:HA	2.19	0.42
3:A:1152:ILE:HG23	3:A:1260:LEU:CD2	2.43	0.42
9:I:55:THR:HG21	9:I:109:ILE:CD1	2.49	0.42
3:A:166:GLY:O	3:A:167:CYS:CB	2.67	0.42
4:B:757:PRO:HG2	4:B:984:HIS:CE1	2.54	0.42
3:A:35:ILE:HD13	3:A:53:LEU:HD23	2.00	0.42
10:J:21:TYR:CA	10:J:39:LEU:HD11	2.49	0.42
4:B:969:ARG:HG2	4:B:970:THR:N	2.33	0.42
4:B:115:GLN:HG2	4:B:193:LYS:HB2	2.01	0.42
4:B:1197:PRO:O	4:B:1200:ALA:HB3	2.19	0.42
4:B:39:ARG:HG2	4:B:39:ARG:HH11	1.85	0.42
6:E:72:PHE:CD2	6:E:155:ARG:NH2	2.83	0.42
4:B:1204:PHE:O	4:B:1207:LEU:HB2	2.19	0.42
2:T:4:DA:C6	3:A:831:THR:HG21	2.54	0.42
3:A:1161:THR:OG1	3:A:1170:ILE:HD11	2.20	0.42
4:B:1106:ARG:HH12	4:B:1118:PRO:CA	2.33	0.42
4:B:234:ILE:N	4:B:234:ILE:HD12	2.30	0.42
3:A:530:GLY:O	3:A:532:ARG:N	2.53	0.42
4:B:121:ASN:HA	4:B:207:GLY:CA	2.46	0.42
6:E:59:SER:HA	6:E:80:VAL:O	2.19	0.42
4:B:28:GLU:OE1	4:B:807:ARG:NH2	2.44	0.42
3:A:984:LYS:O	3:A:988:LEU:HB2	2.19	0.42
4:B:405:ARG:CZ	4:B:632:ARG:HG2	2.49	0.42
5:C:214:ASN:CB	5:C:217:ASP:OD2	2.68	0.42
3:A:441:PRO:HG2	3:A:441:PRO:O	2.20	0.42
4:B:640:VAL:HG22	4:B:651:LEU:HD23	2.01	0.42
3:A:76:GLU:O	3:A:78:PRO:CD	2.68	0.42
3:A:1187:GLN:HA	3:A:1243:VAL:HG23	2.02	0.42
3:A:533:LYS:C	3:A:535:THR:H	2.23	0.42
4:B:834:ASN:HB2	4:B:838:SER:O	2.19	0.42
6:E:100:ILE:O	6:E:101:GLN:C	2.58	0.42
3:A:1150:SER:HB2	3:A:1195:LEU:CD2	2.49	0.42
4:B:331:LEU:HA	4:B:331:LEU:HD12	1.87	0.42
4:B:1182:CYS:SG	4:B:1185:CYS:HB2	2.60	0.42
4:B:995:ARG:CB	4:B:995:ARG:HH11	2.33	0.42
5:C:252:GLN:NE2	11:K:99:GLY:N	2.68	0.42
4:B:101:MET:HE2	4:B:169:ARG:NH1	2.35	0.42
4:B:758:PHE:CE2	4:B:1044:ALA:HA	2.53	0.42
3:A:115:LEU:HB2	3:A:122:MET:HE2	2.02	0.42
4:B:346:GLU:O	4:B:347:LYS:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:640:VAL:HG22	4:B:651:LEU:CD2	2.50	0.42
3:A:908:LEU:O	3:A:909:ASP:C	2.58	0.42
4:B:1072:MET:HE2	4:B:1087:PHE:HD1	1.85	0.42
7:F:89:GLU:HB3	7:F:134:ILE:HD13	2.00	0.42
3:A:873:MET:C	3:A:1058:VAL:HG23	2.40	0.42
3:A:683:ILE:CD1	3:A:764:CYS:HB2	2.42	0.42
3:A:401:GLY:H	3:A:435:HIS:HD2	1.66	0.42
9:I:101:PHE:HD1	9:I:110:PHE:O	2.02	0.42
4:B:666:TYR:C	4:B:668:ASP:N	2.72	0.42
3:A:113:LEU:HG	3:A:218:ASP:OD1	2.19	0.42
4:B:484:ASN:CG	4:B:486:TYR:HE1	2.23	0.42
4:B:203:PHE:HE1	4:B:212:LEU:HD12	1.85	0.42
4:B:105:SER:O	4:B:106:ASP:HB2	2.20	0.42
10:J:27:GLU:C	10:J:29:GLU:H	2.23	0.42
3:A:639:PRO:HG2	3:A:640:GLN:H	1.84	0.42
4:B:435:THR:O	4:B:435:THR:HG22	2.20	0.42
8:H:12:VAL:HG13	8:H:26:ILE:HG23	2.01	0.42
4:B:705:MET:N	4:B:710:LEU:HD12	2.34	0.42
3:A:383:TYR:HB3	7:F:115:THR:CG2	2.44	0.42
3:A:1390:ASN:HD21	3:A:1399:ARG:HA	1.78	0.42
3:A:534:LEU:HD13	3:A:656:TRP:CD1	2.54	0.42
4:B:855:PHE:HZ	4:B:857:ARG:HH12	1.64	0.42
4:B:1152:MET:SD	4:B:1197:PRO:HD3	2.59	0.42
3:A:637:LYS:HA	3:A:637:LYS:HD3	1.93	0.42
3:A:113:LEU:C	3:A:115:LEU:H	2.23	0.42
4:B:877:PRO:O	4:B:878:GLN:HG2	2.19	0.42
3:A:834:THR:HG21	3:A:1077:THR:HA	2.00	0.42
4:B:634:TYR:CD1	4:B:692:TYR:HB3	2.55	0.42
4:B:749:LEU:HD22	4:B:753:ALA:CB	2.50	0.42
3:A:1168:GLU:O	3:A:1172:LEU:HG	2.19	0.42
6:E:117:THR:C	6:E:119:SER:N	2.73	0.42
3:A:68:GLN:C	3:A:70:CYS:N	2.73	0.42
4:B:1106:ARG:HH12	4:B:1118:PRO:HA	1.85	0.42
3:A:1347:ALA:O	3:A:1348:LEU:C	2.55	0.42
3:A:1342:GLU:HG2	6:E:212:ARG:HH11	1.83	0.42
5:C:5:GLY:O	5:C:6:PRO:O	2.37	0.42
3:A:84:ILE:HG21	3:A:239:LEU:HD23	2.01	0.42
8:H:31:THR:O	8:H:32:THR:OG1	2.37	0.42
3:A:633:VAL:HG11	3:A:645:LEU:HD22	2.01	0.42
11:K:93:SER:O	11:K:97:LYS:HG3	2.20	0.42
4:B:546:SER:OG	4:B:631:GLY:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:407:ARG:HG2	3:A:430:TRP:CE2	2.54	0.42
3:A:474:VAL:HG13	3:A:474:VAL:O	2.20	0.42
3:A:725:ALA:HA	3:A:728:LYS:HE2	2.02	0.42
6:E:19:VAL:O	6:E:19:VAL:HG12	2.20	0.42
5:C:14:SER:HA	11:K:114:LEU:HD22	2.02	0.41
3:A:1406:VAL:CG1	3:A:1410:PHE:CE1	3.03	0.41
8:H:57:VAL:CG1	8:H:58:THR:N	2.83	0.41
4:B:230:ALA:O	4:B:232:SER:N	2.47	0.41
3:A:1436:ILE:O	3:A:1437:GLY:C	2.56	0.41
3:A:399:HIS:CB	3:A:400:PRO:HD3	2.45	0.41
7:F:111:LEU:C	7:F:113:GLY:N	2.71	0.41
3:A:343:LYS:NZ	4:B:1156:ASP:OD2	2.49	0.41
6:E:178:ILE:CG2	6:E:214:CYS:HA	2.48	0.41
3:A:782:ARG:NH2	9:I:67:THR:HG22	2.35	0.41
3:A:101:LYS:HG2	3:A:139:TRP:CZ2	2.55	0.41
3:A:38:PRO:CA	3:A:270:LEU:HD23	2.50	0.41
3:A:866:PHE:C	3:A:867:ILE:HG13	2.40	0.41
11:K:71:PHE:CD1	11:K:71:PHE:C	2.93	0.41
3:A:59:GLY:HA2	3:A:67:CYS:SG	2.60	0.41
3:A:1343:ALA:O	3:A:1346:ALA:HB3	2.20	0.41
3:A:1329:THR:HG22	3:A:1330:ASN:N	2.35	0.41
3:A:515:GLN:CG	3:A:516:SER:N	2.84	0.41
4:B:350:GLN:O	4:B:351:TYR:C	2.58	0.41
5:C:27:LEU:HD12	5:C:27:LEU:O	2.20	0.41
4:B:56:ASP:CB	4:B:57:TYR:HD1	2.34	0.41
6:E:79:TRP:HD1	6:E:96:PHE:HE1	1.67	0.41
8:H:139:ASN:O	8:H:140:ALA:CB	2.68	0.41
3:A:982:THR:HB	3:A:985:ASP:CG	2.40	0.41
3:A:474:VAL:HG13	3:A:478:TYR:HE1	1.85	0.41
1:R:2:U:C4	1:R:3:C:N4	2.88	0.41
4:B:368:GLU:O	4:B:371:GLU:OE1	2.37	0.41
3:A:1364:ASN:HD21	3:A:1366:ARG:NH1	2.19	0.41
10:J:53:HIS:CD2	10:J:54:VAL:N	2.88	0.41
8:H:4:THR:O	8:H:5:LEU:HD23	2.20	0.41
4:B:315:LYS:O	4:B:317:CYS:N	2.53	0.41
3:A:683:ILE:O	3:A:686:ALA:N	2.53	0.41
4:B:879:ARG:O	4:B:880:THR:HB	2.20	0.41
4:B:1114:LEU:O	4:B:1198:TYR:HE2	2.04	0.41
4:B:1162:ILE:HG22	4:B:1163:CYS:N	2.34	0.41
3:A:1173:HIS:NE2	3:A:1227:ILE:HG23	2.35	0.41
3:A:88:LYS:HD2	3:A:293:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1177:HIS:O	4:B:1179:GLN:N	2.52	0.41
9:I:25:LEU:HD12	9:I:26:LEU:N	2.35	0.41
4:B:797:TYR:HB3	4:B:798:TYR:CD1	2.55	0.41
3:A:881:GLN:NE2	3:A:958:VAL:O	2.46	0.41
3:A:1139:GLU:HG3	3:A:1280:GLU:O	2.20	0.41
11:K:35:PHE:O	11:K:70:ARG:HB2	2.21	0.41
3:A:542:GLU:OE1	3:A:569:LYS:HE2	2.20	0.41
3:A:568:PRO:CB	5:C:221:TYR:CZ	3.03	0.41
4:B:707:PRO:O	4:B:708:GLU:C	2.59	0.41
3:A:49:LYS:NZ	3:A:60:SER:HA	2.34	0.41
3:A:783:THR:CG2	3:A:815:PHE:CZ	2.98	0.41
3:A:871:ASP:CB	6:E:204:THR:CG2	2.98	0.41
12:L:41:SER:O	12:L:44:ASP:HB2	2.21	0.41
11:K:82:ASP:O	11:K:85:ASP:HB2	2.20	0.41
10:J:34:THR:O	10:J:35:ALA:C	2.58	0.41
3:A:1402:PHE:O	3:A:1404:GLU:N	2.51	0.41
4:B:1033:LYS:NZ	4:B:1087:PHE:O	2.51	0.41
3:A:383:TYR:O	7:F:115:THR:HG22	2.20	0.41
3:A:598:LEU:O	3:A:599:SER:C	2.59	0.41
3:A:885:THR:HG23	3:A:893:PHE:CE1	2.36	0.41
8:H:83:GLN:C	8:H:85:GLY:N	2.73	0.41
3:A:401:GLY:N	3:A:435:HIS:HD2	2.19	0.41
4:B:54:PHE:HA	4:B:58:THR:CB	2.47	0.41
3:A:928:LEU:O	3:A:929:LEU:C	2.59	0.41
3:A:339:ASN:HB3	4:B:1117:GLN:HE22	1.85	0.41
4:B:1020:ARG:O	4:B:1021:MET:C	2.58	0.41
3:A:1317:MET:CA	3:A:1322:ILE:HD11	2.46	0.41
3:A:172:PRO:HB3	3:A:185:TRP:CZ2	2.55	0.41
4:B:307:ASP:O	4:B:308:TRP:C	2.59	0.41
4:B:240:ILE:C	4:B:253:THR:HG23	2.41	0.41
4:B:171:PRO:HD2	4:B:457:LEU:HD12	2.03	0.41
6:E:13:TRP:O	6:E:16:PHE:HB3	2.21	0.41
4:B:499:ASN:OD1	4:B:500:THR:N	2.53	0.41
3:A:1254:ALA:O	3:A:1255:GLU:HB2	2.20	0.41
3:A:1126:ALA:O	3:A:1128:GLN:N	2.53	0.41
3:A:568:PRO:HB3	5:C:221:TYR:OH	2.21	0.41
9:I:85:PHE:HD1	9:I:99:LEU:HD22	1.83	0.41
3:A:244:PRO:O	3:A:245:PRO:C	2.59	0.41
3:A:71:GLN:HB2	3:A:72:GLU:H	1.62	0.41
4:B:167:ILE:O	4:B:168:GLY:O	2.38	0.41
4:B:92:PHE:HD2	4:B:130:VAL:HG11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:911:ILE:HD11	4:B:941:LEU:CB	2.50	0.41
3:A:980:ASP:OD2	3:A:1039:LYS:HB3	2.21	0.41
10:J:3:VAL:CG2	10:J:18:TRP:CG	3.02	0.41
5:C:252:GLN:HG3	11:K:95:ILE:HG23	2.03	0.41
5:C:175:ALA:HB3	10:J:43:ARG:CZ	2.51	0.41
9:I:63:GLY:O	9:I:70:ARG:NH2	2.53	0.41
6:E:72:PHE:CD1	6:E:72:PHE:N	2.89	0.41
6:E:116:ILE:CG2	6:E:117:THR:N	2.84	0.41
3:A:553:VAL:HG22	3:A:652:VAL:CG2	2.51	0.41
3:A:514:PRO:HB2	3:A:875:ALA:HB3	2.01	0.41
3:A:1155:ASP:O	3:A:1190:PRO:O	2.37	0.41
3:A:79:GLY:C	3:A:243:PRO:HG3	2.41	0.41
4:B:120:ARG:HH12	12:L:54:ARG:NH1	2.18	0.41
3:A:541:ILE:N	3:A:541:ILE:HD12	2.34	0.41
4:B:1106:ARG:HH11	4:B:1118:PRO:HB3	1.82	0.41
4:B:269:ILE:HB	4:B:317:CYS:SG	2.60	0.41
6:E:71:LYS:C	6:E:73:PRO:HD3	2.40	0.41
4:B:850:LEU:HD22	4:B:1009:ASP:HB3	2.02	0.41
4:B:53:GLN:HG2	4:B:547:VAL:HG13	2.02	0.41
3:A:808:LEU:HD12	3:A:808:LEU:N	2.35	0.41
6:E:131:THR:HG21	6:E:191:LYS:HE2	2.02	0.41
5:C:186:LEU:HD12	5:C:186:LEU:HA	1.86	0.41
4:B:702:LEU:CD2	4:B:735:ALA:HB1	2.51	0.41
3:A:14:VAL:HB	3:A:1430:LEU:HD13	2.02	0.41
3:A:332:LYS:H	3:A:337:ARG:CB	2.33	0.41
4:B:952:VAL:HG13	4:B:966:VAL:HG22	2.03	0.41
4:B:244:LEU:HB2	4:B:249:ARG:HA	2.03	0.41
3:A:648:ASN:O	3:A:649:ILE:C	2.59	0.41
4:B:205:ILE:HG21	4:B:462:ALA:HB2	2.03	0.41
3:A:556:TRP:CE2	3:A:558:GLY:HA2	2.56	0.41
3:A:407:ARG:HG2	3:A:430:TRP:CZ2	2.56	0.41
9:I:40:SER:HB2	9:I:41:PRO:HD2	2.03	0.41
11:K:106:GLU:O	11:K:110:ASN:ND2	2.54	0.41
4:B:387:LEU:HD23	4:B:393:LYS:HD2	2.03	0.41
3:A:1107:VAL:CG2	3:A:1383:SER:HA	2.51	0.41
3:A:481:ASP:C	3:A:481:ASP:OD1	2.58	0.41
2:T:9:DC:OP1	4:B:1123:SER:CB	2.61	0.41
9:I:99:LEU:HB2	9:I:112:SER:OG	2.21	0.41
9:I:98:VAL:HG12	9:I:99:LEU:N	2.36	0.41
3:A:1116:LEU:CD2	3:A:1316:VAL:HG21	2.51	0.41
3:A:843:LYS:HG3	3:A:1402:PHE:CD1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:5:A:C5	1:R:6:G:N7	2.89	0.41
4:B:737:THR:HG23	9:I:66:PRO:HB3	2.01	0.41
3:A:14:VAL:O	3:A:15:LYS:HD3	2.20	0.41
6:E:3:GLN:HG3	6:E:5:ASN:H	1.85	0.41
6:E:7:ARG:HG3	6:E:8:ASN:N	2.36	0.41
3:A:574:GLY:O	3:A:577:ILE:HG12	2.21	0.41
3:A:1039:LYS:NZ	3:A:1043:ASP:OD1	2.47	0.41
8:H:38:LEU:HD13	8:H:125:LEU:CD1	2.46	0.41
4:B:51:PHE:O	4:B:54:PHE:N	2.54	0.41
4:B:418:LYS:O	4:B:420:LEU:N	2.54	0.41
11:K:65:HIS:HD2	11:K:67:PHE:CB	2.33	0.41
4:B:1152:MET:O	4:B:1156:ASP:O	2.39	0.41
4:B:589:VAL:CG1	4:B:590:HIS:N	2.84	0.41
4:B:577:ALA:HB1	4:B:589:VAL:HG12	2.00	0.41
7:F:109:VAL:CG1	7:F:110:ASP:H	2.34	0.41
4:B:579:ARG:HB2	4:B:586:TRP:HE1	1.84	0.41
5:C:114:TYR:CG	5:C:140:ASN:HB3	2.56	0.41
4:B:205:ILE:CD1	4:B:205:ILE:N	2.84	0.41
4:B:188:ASP:O	4:B:192:LEU:HG	2.21	0.41
4:B:1177:HIS:HB2	4:B:1179:GLN:HG3	2.03	0.41
3:A:738:LYS:NZ	5:C:194:GLU:C	2.74	0.41
3:A:134:ARG:O	3:A:136:ALA:N	2.54	0.41
6:E:116:ILE:HG22	6:E:117:THR:N	2.36	0.41
11:K:103:THR:O	11:K:106:GLU:N	2.53	0.41
3:A:1006:ILE:HG22	3:A:1007:ILE:N	2.36	0.41
9:I:6:PHE:HD2	9:I:13:MET:HA	1.86	0.41
4:B:843:GLN:HB2	4:B:993:THR:OG1	2.20	0.41
3:A:432:VAL:O	3:A:434:ARG:N	2.54	0.41
4:B:1115:THR:CG2	4:B:1199:ALA:HB2	2.50	0.41
4:B:704:ALA:HB2	4:B:738:PHE:CD1	2.56	0.41
3:A:336:ILE:CD1	3:A:1405:THR:HG21	2.45	0.41
3:A:1017:LEU:HB3	6:E:205:SER:HA	2.03	0.41
4:B:233:PRO:HG2	4:B:234:ILE:HG13	2.03	0.41
3:A:535:THR:O	3:A:536:LEU:C	2.59	0.41
4:B:992:ILE:CD1	4:B:994:TYR:CE2	3.04	0.41
4:B:121:ASN:HD21	4:B:965:LYS:HE3	1.86	0.41
3:A:321:PRO:O	3:A:322:VAL:CB	2.63	0.41
4:B:864:LYS:CG	4:B:865:LYS:N	2.80	0.41
9:I:16:PRO:HA	9:I:26:LEU:O	2.20	0.41
9:I:26:LEU:HD23	9:I:37:GLU:HA	2.03	0.41
8:H:84:ALA:HA	8:H:87:ARG:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:846:ILE:CG2	4:B:974:PRO:HG2	2.51	0.41
4:B:321:GLY:C	4:B:323:VAL:N	2.74	0.41
4:B:1149:GLU:HG3	4:B:1153:GLU:OE1	2.20	0.41
3:A:909:ASP:OD1	3:A:910:PRO:HD2	2.22	0.40
10:J:48:ARG:HG2	10:J:48:ARG:HH11	1.86	0.40
3:A:960:ILE:HD12	3:A:1021:LEU:CD2	2.50	0.40
4:B:941:LEU:HD21	4:B:946:ASN:HA	2.02	0.40
8:H:126:GLU:N	8:H:130:ARG:HH12	2.19	0.40
3:A:530:GLY:O	3:A:533:LYS:N	2.53	0.40
3:A:205:GLU:O	3:A:208:LEU:HB2	2.22	0.40
11:K:47:ARG:HH11	11:K:48:ALA:N	2.19	0.40
6:E:63:ASN:HA	6:E:64:PRO:HD3	1.92	0.40
6:E:28:TYR:CE1	6:E:78:LEU:CD1	3.03	0.40
5:C:51:VAL:HG22	5:C:155:LEU:CD2	2.47	0.40
7:F:138:LEU:HD23	7:F:138:LEU:HA	1.83	0.40
5:C:46:ILE:CG2	5:C:157:CYS:HB3	2.51	0.40
4:B:627:PHE:O	4:B:632:ARG:NH1	2.54	0.40
3:A:650:GLN:O	3:A:651:LYS:C	2.58	0.40
3:A:1107:VAL:HG23	3:A:1383:SER:HA	2.03	0.40
4:B:578:THR:HG23	4:B:622:LYS:C	2.42	0.40
5:C:29:MET:O	5:C:30:ALA:C	2.59	0.40
2:T:7:DC:C5'	2:T:7:DC:P	3.05	0.40
8:H:123:MET:HE1	8:H:142:LEU:HD11	2.03	0.40
8:H:96:VAL:HG13	8:H:143:LEU:HG	2.02	0.40
9:I:99:LEU:O	9:I:111:THR:HG23	2.21	0.40
5:C:146:LYS:O	5:C:147:LEU:HD23	2.20	0.40
4:B:175:ARG:HH11	4:B:175:ARG:HG2	1.87	0.40
3:A:1166:ASP:OD1	3:A:1194:ARG:NH2	2.49	0.40
4:B:803:LEU:CD1	4:B:1036:ALA:HB2	2.52	0.40
4:B:911:ILE:HG21	4:B:966:VAL:HG11	2.01	0.40
3:A:399:HIS:NE2	3:A:462:VAL:HG21	2.36	0.40
4:B:1197:PRO:O	4:B:1200:ALA:N	2.52	0.40
8:H:33:GLN:OE1	8:H:129:TYR:HE2	2.05	0.40
3:A:771:GLU:H	3:A:822:GLU:CD	2.25	0.40
4:B:846:ILE:HG23	4:B:974:PRO:HG2	2.04	0.40
3:A:1102:LYS:HG2	3:A:1106:ASN:ND2	2.36	0.40
4:B:901:PRO:O	4:B:949:VAL:O	2.38	0.40
3:A:203:SER:O	3:A:207:ILE:HG12	2.21	0.40
1:R:10:A:O3'	15:R:3000:UTP:O1A	2.37	0.40
4:B:276:ILE:HD11	4:B:355:ILE:CD1	2.50	0.40
3:A:901:LEU:O	3:A:920:LEU:HD23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:913:LEU:CD1	3:A:981:LEU:O	2.69	0.40
4:B:175:ARG:CG	4:B:175:ARG:HH11	2.34	0.40
4:B:1104:HIS:HB2	4:B:1122:ARG:CB	2.51	0.40
6:E:11:ARG:NH2	6:E:141:VAL:HG21	2.37	0.40
3:A:331:GLY:O	3:A:332:LYS:O	2.39	0.40
3:A:751:SER:OG	4:B:1015:HIS:HE1	2.03	0.40
4:B:840:ILE:HB	4:B:1011:ILE:HB	2.03	0.40
3:A:463:ILE:CD1	3:A:469:ARG:HG3	2.50	0.40
3:A:679:ILE:CG2	3:A:729:ALA:HB1	2.44	0.40
3:A:445:ASN:HB3	3:A:455:MET:HG2	2.03	0.40
3:A:719:VAL:HG22	3:A:774:ARG:HD2	2.03	0.40
3:A:1224:LEU:HD11	3:A:1240:CYS:HB3	2.03	0.40
8:H:138:GLU:HG2	8:H:139:ASN:N	2.35	0.40
3:A:1322:ILE:HD12	3:A:1327:ILE:HD12	2.03	0.40
4:B:758:PHE:HB2	4:B:1024:ALA:HB1	2.03	0.40
3:A:738:LYS:HA	8:H:19:ARG:NH2	2.36	0.40
3:A:18:GLN:O	4:B:1215:ARG:HG3	2.21	0.40
4:B:380:TYR:O	4:B:384:ARG:HG2	2.21	0.40
3:A:19:PHE:HA	4:B:1213:THR:O	2.22	0.40
4:B:61:ASP:N	4:B:61:ASP:OD1	2.54	0.40
4:B:801:LYS:HE2	10:J:51:LEU:O	2.22	0.40
11:K:51:LEU:CD1	11:K:59:ALA:HB3	2.51	0.40
3:A:894:GLU:C	3:A:896:ARG:N	2.74	0.40
4:B:363:HIS:O	4:B:364:ILE:CG1	2.70	0.40
4:B:1156:ASP:HB3	4:B:1197:PRO:CA	2.52	0.40
5:C:182:PRO:HB2	5:C:207:CYS:SG	2.61	0.40
3:A:270:LEU:O	3:A:274:ILE:HG13	2.22	0.40
4:B:283:VAL:HG13	4:B:297:ILE:HD12	2.04	0.40
6:E:182:ASP:O	6:E:186:LEU:HG	2.21	0.40
12:L:28:LYS:O	12:L:29:TYR:CG	2.74	0.40
3:A:1116:LEU:H	3:A:1308:THR:CG2	2.34	0.40
3:A:48:ALA:O	3:A:49:LYS:CG	2.65	0.40
4:B:1159:ARG:NE	4:B:1193:GLN:NE2	2.33	0.40
4:B:120:ARG:HH22	12:L:54:ARG:HD2	1.86	0.40
5:C:66:ARG:HB3	10:J:5:VAL:HG21	2.04	0.40
3:A:1220:PHE:O	3:A:1221:LYS:C	2.60	0.40
9:I:92:ARG:CG	9:I:93:LYS:N	2.84	0.40
3:A:531:ILE:CG2	3:A:532:ARG:N	2.84	0.40
3:A:379:VAL:HG22	3:A:431:LYS:HG2	2.03	0.40
3:A:302:THR:O	3:A:313:GLN:NE2	2.54	0.40
4:B:1198:TYR:HE1	4:B:1201:LYS:HZ2	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:288:ALA:O	4:B:331:LEU:CD1	2.69	0.40
6:E:90:VAL:HA	6:E:120:ALA:HB2	2.04	0.40
4:B:616:ILE:HG12	4:B:696:GLU:HG3	2.03	0.40
7:F:138:LEU:HB3	7:F:139:PRO:CD	2.51	0.40
4:B:849:GLY:O	4:B:850:LEU:C	2.59	0.40
4:B:1180:PHE:O	4:B:1181:GLU:CB	2.70	0.40
4:B:484:ASN:ND2	4:B:486:TYR:HD1	2.19	0.40
4:B:1084:GLN:NE2	5:C:192:TRP:HB2	2.37	0.40
9:I:34:TYR:C	9:I:35:VAL:HG23	2.41	0.40
3:A:19:PHE:HB3	3:A:1413:GLY:HA2	2.03	0.40
4:B:1120:GLU:CG	4:B:1121:GLY:N	2.84	0.40
5:C:228:PHE:HB2	5:C:230:MET:HE2	2.02	0.40
7:F:130:ILE:HA	7:F:131:PRO:HD2	1.94	0.40
8:H:117:SER:HA	8:H:122:LEU:HD23	2.02	0.40

All (59) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:736:THR:CB	9:I:79:HIS:CD2[2_556]	0.78	1.42
4:B:736:THR:OG1	9:I:79:HIS:NE2[2_556]	0.83	1.37
9:I:81:ARG:O	9:I:81:ARG:CB[2_556]	1.01	1.19
4:B:736:THR:OG1	9:I:79:HIS:CD2[2_556]	1.02	1.18
3:A:923:LEU:CD1	9:I:35:VAL:C[4_546]	1.06	1.14
3:A:918:GLU:CB	9:I:21:GLU:OE1[4_546]	1.09	1.11
9:I:81:ARG:CA	9:I:81:ARG:O[2_556]	1.16	1.04
4:B:736:THR:OG1	9:I:79:HIS:CE1[2_556]	1.24	0.96
9:I:81:ARG:CA	9:I:81:ARG:C[2_556]	1.27	0.93
9:I:81:ARG:C	9:I:81:ARG:CB[2_556]	1.30	0.90
4:B:736:THR:CB	9:I:79:HIS:NE2[2_556]	1.35	0.85
9:I:71:SER:O	9:I:81:ARG:NE[2_556]	1.40	0.80
4:B:736:THR:OG1	9:I:79:HIS:CG[2_556]	1.42	0.78
3:A:923:LEU:CD1	9:I:36:GLU:N[4_546]	1.50	0.70
4:B:736:THR:OG1	9:I:79:HIS:ND1[2_556]	1.51	0.69
3:A:923:LEU:CD2	9:I:35:VAL:CB[4_546]	1.54	0.66
9:I:80:SER:OG	9:I:82:GLU:OE1[2_556]	1.56	0.64
9:I:81:ARG:N	9:I:81:ARG:O[2_556]	1.57	0.63
3:A:918:GLU:CB	9:I:21:GLU:CD[4_546]	1.62	0.58
9:I:81:ARG:O	9:I:81:ARG:CG[2_556]	1.66	0.54
3:A:923:LEU:CG	9:I:35:VAL:CB[4_546]	1.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:81:ARG:N	9:I:81:ARG:C[2_556]	1.73	0.47
3:A:923:LEU:CD1	9:I:35:VAL:O[4_546]	1.74	0.46
9:I:71:SER:N	9:I:81:ARG:NH2[2_556]	1.75	0.45
9:I:70:ARG:CA	9:I:81:ARG:NH2[2_556]	1.76	0.44
4:B:736:THR:CA	9:I:79:HIS:NE2[2_556]	1.77	0.43
9:I:80:SER:CB	9:I:82:GLU:CG[2_556]	1.79	0.41
9:I:70:ARG:C	9:I:81:ARG:NH2[2_556]	1.80	0.40
9:I:81:ARG:NH1	9:I:83:ASN:CB[2_556]	1.83	0.37
9:I:81:ARG:CA	9:I:81:ARG:CA[2_556]	1.83	0.37
3:A:918:GLU:CB	9:I:21:GLU:OE2[4_546]	1.85	0.35
9:I:81:ARG:NH1	9:I:83:ASN:CA[2_556]	1.89	0.31
9:I:81:ARG:NH1	9:I:83:ASN:C[2_556]	1.89	0.31
9:I:81:ARG:CA	9:I:81:ARG:CB[2_556]	1.91	0.29
9:I:81:ARG:C	9:I:81:ARG:C[2_556]	1.91	0.29
3:A:918:GLU:CA	9:I:21:GLU:OE1[4_546]	1.91	0.29
3:A:923:LEU:CD1	9:I:35:VAL:CA[4_546]	1.92	0.28
3:A:923:LEU:CD1	9:I:35:VAL:CG1[4_546]	1.92	0.28
3:A:923:LEU:CD2	9:I:35:VAL:CA[4_546]	1.93	0.27
4:B:736:THR:CG2	9:I:79:HIS:CD2[2_556]	1.96	0.24
9:I:71:SER:O	9:I:81:ARG:CD[2_556]	2.01	0.19
9:I:72:ASP:O	9:I:72:ASP:CB[2_556]	2.02	0.18
3:A:923:LEU:CD2	9:I:35:VAL:N[4_546]	2.04	0.16
3:A:923:LEU:CG	9:I:35:VAL:O[4_546]	2.07	0.13
3:A:923:LEU:CG	9:I:35:VAL:CG1[4_546]	2.07	0.13
3:A:923:LEU:CG	9:I:35:VAL:C[4_546]	2.07	0.13
3:A:923:LEU:CB	9:I:35:VAL:O[4_546]	2.09	0.11
9:I:80:SER:CB	9:I:82:GLU:CD[2_556]	2.09	0.11
9:I:81:ARG:NH1	9:I:83:ASN:O[2_556]	2.09	0.11
3:A:923:LEU:CD1	9:I:35:VAL:CB[4_546]	2.11	0.09
4:B:736:THR:CB	9:I:79:HIS:CG[2_556]	2.13	0.07
9:I:72:ASP:O	9:I:72:ASP:O[2_556]	2.15	0.05
9:I:82:GLU:OE2	9:I:105:SER:OG[2_556]	2.15	0.05
4:B:736:THR:CA	9:I:79:HIS:CD2[2_556]	2.15	0.05
4:B:736:THR:N	9:I:79:HIS:NE2[2_556]	2.15	0.05
4:B:715:ALA:CB	9:I:117:LYS:CD[2_556]	2.17	0.03
9:I:81:ARG:CD	9:I:83:ASN:ND2[2_556]	2.19	0.01
9:I:71:SER:C	9:I:81:ARG:NE[2_556]	2.19	0.01
9:I:80:SER:CB	9:I:82:GLU:OE1[2_556]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	1365/1733 (79%)	1023 (75%)	252 (18%)	90 (7%)	1	25
4	B	1077/1224 (88%)	839 (78%)	169 (16%)	69 (6%)	2	26
5	C	264/318 (83%)	208 (79%)	40 (15%)	16 (6%)	2	27
6	E	212/215 (99%)	170 (80%)	33 (16%)	9 (4%)	3	35
7	F	82/155 (53%)	64 (78%)	15 (18%)	3 (4%)	4	40
8	H	129/146 (88%)	93 (72%)	21 (16%)	15 (12%)	0	9
9	I	117/122 (96%)	93 (80%)	15 (13%)	9 (8%)	1	20
10	J	63/70 (90%)	48 (76%)	11 (18%)	4 (6%)	2	26
11	K	112/120 (93%)	96 (86%)	15 (13%)	1 (1%)	21	67
12	L	44/70 (63%)	22 (50%)	12 (27%)	10 (23%)	0	1
All	All	3465/4173 (83%)	2656 (77%)	583 (17%)	226 (6%)	1	26

All (226) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	31	SER
3	A	48	ALA
3	A	55	ASP
3	A	56	PRO
3	A	74	MET
3	A	75	ASN
3	A	167	CYS
3	A	322	VAL
3	A	404	TYR
3	A	418	SER
3	A	543	LEU
3	A	567	LYS
3	A	597	LEU
3	A	598	LEU

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Mol	Chain	Res	Type
3	A	628	GLY
3	A	752	LYS
3	A	846	GLU
3	A	998	LEU
3	A	1036	ARG
3	A	1127	ASP
3	A	1206	ASP
3	A	1221	LYS
3	A	1223	ASP
3	A	1392	SER
3	A	1393	ASN
3	A	1403	GLU
3	A	1406	VAL
3	A	1416	ALA
4	B	65	GLU
4	B	124	TYR
4	B	174	LEU
4	B	175	ARG
4	B	200	GLY
4	B	229	ALA
4	B	364	ILE
4	B	367	LEU
4	B	531	GLN
4	B	708	GLU
4	B	709	ASP
4	B	731	VAL
4	B	751	VAL
4	B	958	GLN
4	B	959	ASP
4	B	1046	PRO
4	B	1103	ILE
4	B	1167	GLY
4	B	1176	ASN
4	B	1183	LYS
5	C	4	GLU
5	C	5	GLY
5	C	6	PRO
5	C	110	THR
5	C	142	VAL
5	C	215	GLU
7	F	73	ALA
8	H	32	THR

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Mol	Chain	Res	Type
8	H	81	PRO
8	H	140	ALA
9	I	8	ARG
10	J	2	ILE
10	J	55	ASP
12	L	27	LEU
12	L	38	LEU
12	L	64	LEU
3	A	35	ILE
3	A	54	ASN
3	A	62	ASP
3	A	87	ALA
3	A	109	HIS
3	A	135	PHE
3	A	168	GLY
3	A	332	LYS
3	A	385	ILE
3	A	419	LYS
3	A	534	LEU
3	A	568	PRO
3	A	790	ASP
3	A	986	ILE
3	A	1114	PRO
3	A	1365	TYR
3	A	1366	ARG
3	A	1379	GLY
4	B	55	VAL
4	B	168	GLY
4	B	275	TYR
4	B	346	GLU
4	B	410	GLY
4	B	480	SER
4	B	641	GLU
4	B	643	ASP
4	B	792	MET
4	B	864	LYS
4	B	866	TYR
4	B	884	ARG
4	B	891	ASP
4	B	992	ILE
4	B	1066	SER
4	B	1155	SER

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Mol	Chain	Res	Type
5	C	136	ASP
7	F	142	SER
8	H	61	SER
8	H	77	ARG
8	H	88	SER
8	H	128	ASN
9	I	30	ARG
9	I	79	HIS
12	L	39	SER
12	L	52	GLY
3	A	6	TYR
3	A	45	GLN
3	A	59	GLY
3	A	67	CYS
3	A	69	THR
3	A	335	ARG
3	A	433	GLU
3	A	596	THR
3	A	737	LEU
3	A	775	ILE
3	A	830	LYS
3	A	920	LEU
4	B	28	GLU
4	B	249	ARG
4	B	277	LYS
4	B	447	ALA
4	B	629	ASP
4	B	735	ALA
4	B	807	ARG
4	B	880	THR
4	B	1017	ILE
4	B	1099	VAL
4	B	1104	HIS
4	B	1178	ASN
5	C	48	SER
5	C	149	LYS
5	C	212	PRO
5	C	227	THR
6	E	31	THR
6	E	102	GLU
6	E	103	LYS
6	E	122	LYS

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Mol	Chain	Res	Type
6	E	139	ALA
6	E	206	GLY
7	F	128	LYS
8	H	8	ASP
8	H	17	PRO
8	H	82	PRO
8	H	135	LEU
8	H	139	ASN
9	I	9	ASP
9	I	33	SER
9	I	86	PHE
10	J	9	SER
12	L	63	ARG
3	A	101	LYS
3	A	134	ARG
3	A	139	TRP
3	A	223	GLY
3	A	424	ILE
3	A	599	SER
3	A	1067	LEU
3	A	1097	GLY
3	A	1115	SER
3	A	1122	PRO
3	A	1405	THR
4	B	304	ASP
4	B	436	VAL
4	B	501	PRO
4	B	667	GLN
4	B	791	THR
4	B	1054	GLY
4	B	1097	HIS
5	C	18	VAL
5	C	174	ALA
6	E	59	SER
10	J	6	ARG
12	L	50	ASP
12	L	56	LEU
3	A	58	LEU
3	A	399	HIS
3	A	400	PRO
3	A	958	VAL
3	A	972	HIS

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Mol	Chain	Res	Type
3	A	1098	VAL
3	A	1130	GLN
3	A	1282	VAL
3	A	1351	GLU
3	A	1378	GLN
4	B	248	SER
4	B	419	THR
4	B	619	ILE
4	B	648	HIS
4	B	687	GLU
4	B	707	PRO
4	B	712	PRO
4	B	764	SER
4	B	907	GLY
4	B	982	SER
4	B	1108	ARG
6	E	36	GLU
8	H	62	SER
8	H	89	LEU
9	I	47	GLU
9	I	88	SER
3	A	226	GLU
3	A	368	LYS
3	A	531	ILE
3	A	1014	ALA
3	A	1352	VAL
4	B	27	ALA
6	E	167	ARG
8	H	138	GLU
9	I	98	VAL
11	K	107	THR
12	L	59	ALA
4	B	247	GLY
3	A	336	ILE
3	A	1104	ILE
12	L	55	ILE
3	A	810	PRO
3	A	1075	PRO
3	A	1242	VAL
5	C	172	PRO
5	C	216	GLY
3	A	78	PRO

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Mol	Chain	Res	Type
4	B	511	PRO
5	C	218	PRO

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	
3	A	1206/1520 (79%)	1128 (94%)	78 (6%)	21	61
4	B	952/1061 (90%)	886 (93%)	66 (7%)	19	59
5	C	234/274 (85%)	222 (95%)	12 (5%)	29	68
6	E	196/197 (100%)	189 (96%)	7 (4%)	42	76
7	F	74/137 (54%)	68 (92%)	6 (8%)	15	52
8	H	117/128 (91%)	112 (96%)	5 (4%)	35	72
9	I	113/116 (97%)	104 (92%)	9 (8%)	15	53
10	J	60/65 (92%)	56 (93%)	4 (7%)	20	60
11	K	99/102 (97%)	90 (91%)	9 (9%)	12	47
12	L	40/57 (70%)	35 (88%)	5 (12%)	6	32
All	All	3091/3657 (84%)	2890 (94%)	201 (6%)	21	61

All (201) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	18	GLN
3	A	22	PHE
3	A	31	SER
3	A	56	PRO
3	A	70	CYS
3	A	93	VAL
3	A	122	MET
3	A	247	ARG
3	A	269	ILE
3	A	302	THR
3	A	322	VAL

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Mol	Chain	Res	Type
3	A	326	ARG
3	A	351	THR
3	A	375	THR
3	A	381	THR
3	A	385	ILE
3	A	397	ASN
3	A	412	ARG
3	A	434	ARG
3	A	443	LEU
3	A	445	ASN
3	A	450	LEU
3	A	451	HIS
3	A	461	LYS
3	A	474	VAL
3	A	475	THR
3	A	493	GLN
3	A	503	GLN
3	A	524	VAL
3	A	538	ASP
3	A	590	ARG
3	A	596	THR
3	A	597	LEU
3	A	598	LEU
3	A	618	GLU
3	A	629	LEU
3	A	666	ILE
3	A	682	THR
3	A	740	LEU
3	A	741	ASN
3	A	745	GLN
3	A	756	ILE
3	A	768	GLN
3	A	774	ARG
3	A	821	ARG
3	A	845	LEU
3	A	849	MET
3	A	855	THR
3	A	858	ASN
3	A	920	LEU
3	A	929	LEU
3	A	948	VAL
3	A	949	ASP

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Mol	Chain	Res	Type
3	A	979	SER
3	A	1029	ARG
3	A	1035	TYR
3	A	1043	ASP
3	A	1057	VAL
3	A	1077	THR
3	A	1122	PRO
3	A	1128	GLN
3	A	1222	ASN
3	A	1232	ASN
3	A	1258	HIS
3	A	1264	GLU
3	A	1295	THR
3	A	1308	THR
3	A	1318	THR
3	A	1332	PHE
3	A	1335	ILE
3	A	1351	GLU
3	A	1359	ASP
3	A	1364	ASN
3	A	1366	ARG
3	A	1375	MET
3	A	1376	THR
3	A	1425	SER
3	A	1442	ASP
4	B	20	ASP
4	B	43	LEU
4	B	57	TYR
4	B	61	ASP
4	B	63	ILE
4	B	98	THR
4	B	109	THR
4	B	121	ASN
4	B	175	ARG
4	B	194	GLU
4	B	232	SER
4	B	234	ILE
4	B	261	ARG
4	B	268	THR
4	B	278	GLN
4	B	309	GLN
4	B	313	MET

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Mol	Chain	Res	Type
4	B	317	CYS
4	B	320	ASP
4	B	331	LEU
4	B	376	PHE
4	B	387	LEU
4	B	396	ASP
4	B	408	LEU
4	B	466	TRP
4	B	485	ARG
4	B	513	GLN
4	B	514	LEU
4	B	538	ASN
4	B	547	VAL
4	B	570	VAL
4	B	576	ASP
4	B	624	LEU
4	B	629	ASP
4	B	644	GLU
4	B	680	THR
4	B	723	VAL
4	B	732	SER
4	B	762	ASN
4	B	764	SER
4	B	780	VAL
4	B	791	THR
4	B	835	GLN
4	B	901	PRO
4	B	909	ASP
4	B	915	THR
4	B	944	THR
4	B	951	GLN
4	B	953	LEU
4	B	976	ILE
4	B	986	GLN
4	B	987	LYS
4	B	996	ARG
4	B	999	MET
4	B	1007	VAL
4	B	1021	MET
4	B	1049	ASP
4	B	1103	ILE
4	B	1111	MET

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Mol	Chain	Res	Type
4	B	1118	PRO
4	B	1132	GLU
4	B	1147	LEU
4	B	1150	ARG
4	B	1151	LEU
4	B	1183	LYS
4	B	1185	CYS
5	C	22	LEU
5	C	25	VAL
5	C	26	ASP
5	C	62	PHE
5	C	69	LEU
5	C	77	ILE
5	C	133	ILE
5	C	148	ARG
5	C	229	TYR
5	C	233	GLU
5	C	240	VAL
5	C	264	GLN
6	E	40	GLU
6	E	60	PHE
6	E	74	ASP
6	E	84	ASP
6	E	92	THR
6	E	104	ASN
6	E	183	PRO
7	F	79	ARG
7	F	90	ARG
7	F	103	MET
7	F	111	LEU
7	F	115	THR
7	F	133	VAL
8	H	21	ASN
8	H	27	GLU
8	H	109	LYS
8	H	110	ASP
8	H	134	ASN
9	I	7	CYS
9	I	12	ASN
9	I	29	CYS
9	I	31	THR
9	I	52	ILE

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Mol	Chain	Res	Type
9	I	75	CYS
9	I	76	PRO
9	I	87	GLN
9	I	103	CYS
10	J	2	ILE
10	J	7	CYS
10	J	47	ARG
10	J	48	ARG
11	K	20	LYS
11	K	25	THR
11	K	31	VAL
11	K	47	ARG
11	K	50	LEU
11	K	61	TYR
11	K	77	THR
11	K	81	TYR
11	K	114	LEU
12	L	50	ASP
12	L	54	ARG
12	L	55	ILE
12	L	68	GLU
12	L	70	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	68	GLN
3	A	92	HIS
3	A	118	HIS
3	A	169	ASN
3	A	225	ASN
3	A	339	ASN
3	A	358	ASN
3	A	435	HIS
3	A	445	ASN
3	A	447	GLN
3	A	493	GLN
3	A	503	GLN
3	A	517	ASN
3	A	631	HIS
3	A	723	ASN
3	A	736	ASN

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Mol	Chain	Res	Type
3	A	741	ASN
3	A	757	ASN
3	A	768	GLN
3	A	786	HIS
3	A	858	ASN
3	A	926	GLN
3	A	965	GLN
3	A	968	GLN
3	A	994	GLN
3	A	1364	ASN
3	A	1387	HIS
3	A	1390	ASN
3	A	1393	ASN
3	A	1432	GLN
4	B	46	GLN
4	B	53	GLN
4	B	178	ASN
4	B	215	GLN
4	B	236	HIS
4	B	325	GLN
4	B	363	HIS
4	B	465	ASN
4	B	484	ASN
4	B	513	GLN
4	B	515	HIS
4	B	516	ASN
4	B	518	HIS
4	B	538	ASN
4	B	657	HIS
4	B	744	HIS
4	B	822	ASN
4	B	842	ASN
4	B	862	GLN
4	B	957	ASN
4	B	975	GLN
4	B	1015	HIS
4	B	1065	GLN
4	B	1117	GLN
4	B	1179	GLN
4	B	1193	GLN
5	C	65	HIS
5	C	73	GLN

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Mol	Chain	Res	Type
5	C	112	ASN
5	C	123	ASN
5	C	167	HIS
5	C	242	GLN
5	C	252	GLN
6	E	5	ASN
6	E	32	GLN
6	E	101	GLN
6	E	104	ASN
6	E	114	ASN
6	E	147	HIS
8	H	33	GLN
9	I	12	ASN
10	J	53	HIS
11	K	52	ASN
11	K	65	HIS
11	K	76	GLN
11	K	110	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	10/10 (100%)	3 (30%)	3 (30%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	2	U
1	R	5	A
1	R	6	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	R	1	A
1	R	4	G
1	R	5	A

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 10 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
15	UTP	R	3000	1,14	20,30,30	2.67	7 (35%)	30,47,47	4.03	11 (36%)

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
15	UTP	R	3000	1,14	1/1/7/7	0/18/38/38	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	R	3000	UTP	C3'-C4'	-5.22	1.38	1.53
15	R	3000	UTP	O3'-C3'	-4.26	1.32	1.43
15	R	3000	UTP	O4'-C4'	-4.16	1.35	1.45
15	R	3000	UTP	PB-O1B	-2.12	1.45	1.54
15	R	3000	UTP	C4-N3	3.06	1.38	1.33
15	R	3000	UTP	C5'-C4'	5.05	1.68	1.51
15	R	3000	UTP	O2'-C2'	5.09	1.55	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	R	3000	UTP	C5'-C4'-C3'	-6.23	90.48	115.21
15	R	3000	UTP	O3'-C3'-C2'	-4.54	97.06	111.83
15	R	3000	UTP	C4'-O4'-C1'	-4.30	105.00	109.72
15	R	3000	UTP	C5-C4-N3	-3.37	114.47	123.12
15	R	3000	UTP	O2'-C2'-C3'	-2.08	105.06	111.83
15	R	3000	UTP	O3A-PA-O5'	-2.03	97.54	102.94
15	R	3000	UTP	O1B-PB-O3A	2.43	116.10	105.09
15	R	3000	UTP	O4'-C4'-C3'	4.24	113.69	105.15
15	R	3000	UTP	O5'-C5'-C4'	6.30	132.33	109.12
15	R	3000	UTP	O4'-C4'-C5'	12.07	152.51	109.32
15	R	3000	UTP	C4-N3-C2	12.92	126.94	114.14

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	R	3000	UTP	C4'

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	R	3000	UTP	8	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	R	10/10 (100%)	0.78	0	100	100	79, 137, 196, 199	0
2	T	14/14 (100%)	0.63	0	100	100	91, 150, 197, 202	0
3	A	1381/1733 (79%)	0.18	63 (4%)	36	28	12, 134, 202, 202	0
4	B	1097/1224 (89%)	0.18	49 (4%)	37	29	12, 121, 202, 202	0
5	C	266/318 (83%)	-0.03	1 (0%)	93	90	20, 115, 194, 202	0
6	E	214/215 (99%)	0.39	15 (7%)	19	14	29, 156, 202, 202	0
7	F	84/155 (54%)	0.15	2 (2%)	62	52	17, 130, 196, 202	0
8	H	133/146 (91%)	0.37	7 (5%)	30	23	56, 150, 202, 202	0
9	I	119/122 (97%)	1.14	25 (21%)	1	2	25, 159, 202, 202	0
10	J	65/70 (92%)	-0.00	1 (1%)	76	67	40, 110, 179, 202	0
11	K	114/120 (95%)	-0.06	0	100	100	12, 118, 178, 199	0
12	L	46/70 (65%)	0.59	7 (15%)	3	4	36, 163, 202, 202	0
All	All	3543/4197 (84%)	0.21	170 (4%)	34	26	12, 131, 202, 202	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	55	THR	6.3
9	I	28	GLU	5.6
9	I	23	ASN	5.6
4	B	133	LYS	5.3
4	B	714	GLU	5.0
3	A	313	GLN	5.0
3	A	1172	LEU	5.0
9	I	105	SER	4.8
6	E	122	LYS	4.6
4	B	715	ALA	4.6
9	I	118	ARG	4.4

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Mol	Chain	Res	Type	RSRZ
9	I	24	ARG	4.4
3	A	1165	GLU	4.4
3	A	1171	GLN	4.3
3	A	1257	ASP	4.2
3	A	1135	ARG	4.1
6	E	118	PRO	4.1
3	A	312	PRO	4.1
3	A	1166	ASP	4.1
3	A	1169	ILE	4.0
4	B	94	LYS	4.0
3	A	701	LEU	4.0
3	A	1173	HIS	4.0
9	I	97	MET	4.0
6	E	93	MET	3.8
3	A	1131	ALA	3.8
4	B	437	GLU	3.8
3	A	1231	ASP	3.8
9	I	22	ASN	3.8
4	B	345	LYS	3.8
3	A	1154	TYR	3.7
6	E	51	GLY	3.7
12	L	44	ASP	3.7
4	B	433	GLN	3.6
7	F	145	ASP	3.6
4	B	869	SER	3.6
6	E	121	MET	3.5
4	B	134	LYS	3.5
8	H	86	ASP	3.5
3	A	186	LYS	3.5
4	B	650	GLU	3.4
9	I	56	ALA	3.4
12	L	50	ASP	3.4
4	B	1161	HIS	3.4
9	I	39	GLY	3.4
6	E	97	VAL	3.3
3	A	1297	GLU	3.3
3	A	1232	ASN	3.3
3	A	1176	LEU	3.3
4	B	353	LYS	3.2
3	A	1168	GLU	3.2
8	H	83	GLN	3.2
4	B	708	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
3	A	1160	SER	3.2
9	I	6	PHE	3.2
3	A	1300	LYS	3.1
9	I	5	ARG	3.1
6	E	115	ASN	3.1
3	A	1298	TYR	3.0
5	C	202	PRO	3.0
4	B	346	GLU	3.0
3	A	1191	TRP	3.0
8	H	133	ASN	2.9
4	B	713	ALA	2.9
4	B	1221	SER	2.9
3	A	888	GLY	2.9
4	B	882	THR	2.9
4	B	741	CYS	2.9
3	A	165	GLY	2.9
3	A	1261	LYS	2.9
4	B	916	THR	2.9
3	A	1260	LEU	2.9
12	L	25	ALA	2.8
6	E	50	MET	2.8
4	B	722	ASP	2.7
3	A	146	MET	2.7
9	I	27	PHE	2.7
3	A	1092	LYS	2.7
3	A	148	CYS	2.7
8	H	7	ASP	2.7
4	B	1075	GLY	2.7
9	I	34	TYR	2.7
4	B	659	ALA	2.7
4	B	432	MET	2.6
4	B	709	ASP	2.6
9	I	37	GLU	2.6
4	B	1074	ASN	2.6
3	A	44	THR	2.6
4	B	425	THR	2.6
6	E	87	SER	2.6
3	A	323	LYS	2.6
6	E	83	CYS	2.6
12	L	43	THR	2.6
3	A	889	SER	2.6
3	A	1192	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
4	B	735	ALA	2.5
8	H	32	THR	2.5
3	A	72	GLU	2.5
4	B	648	HIS	2.5
4	B	1176	ASN	2.5
3	A	145	LYS	2.5
4	B	919	SER	2.5
4	B	428	ILE	2.5
3	A	151	ASP	2.4
12	L	52	GLY	2.4
3	A	1093	LYS	2.4
10	J	28	ASP	2.4
9	I	74	GLU	2.4
3	A	113	LEU	2.4
6	E	58	MET	2.4
3	A	1001	ARG	2.4
3	A	1167	GLU	2.4
3	A	427	GLN	2.4
8	H	31	THR	2.4
3	A	1188	GLN	2.4
3	A	1258	HIS	2.3
4	B	937	ALA	2.4
6	E	114	ASN	2.3
3	A	1299	VAL	2.3
4	B	1186	ASP	2.3
3	A	1036	ARG	2.3
4	B	276	ILE	2.3
3	A	286	HIS	2.3
3	A	705	LYS	2.3
4	B	277	LYS	2.3
3	A	55	ASP	2.3
3	A	680	THR	2.3
4	B	39	ARG	2.3
4	B	246	LYS	2.3
4	B	1164	GLY	2.3
9	I	112	SER	2.3
4	B	106	ASP	2.3
9	I	2	THR	2.3
3	A	1286	LYS	2.3
3	A	1132	LYS	2.2
4	B	165	VAL	2.2
9	I	9	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
4	B	131	ASP	2.2
3	A	49	LYS	2.2
4	B	164	LYS	2.2
4	B	262	GLU	2.2
9	I	11	ASN	2.2
12	L	26	THR	2.2
3	A	153	PRO	2.2
3	A	1125	ALA	2.2
3	A	76	GLU	2.2
4	B	93	GLY	2.2
3	A	718	VAL	2.2
12	L	32	ALA	2.1
3	A	1209	MET	2.1
4	B	917	PRO	2.1
3	A	386	ASP	2.1
4	B	268	THR	2.1
3	A	1212	VAL	2.1
4	B	580	VAL	2.1
6	E	110	PHE	2.1
3	A	466	SER	2.1
9	I	104	LEU	2.1
3	A	788	SER	2.1
6	E	53	PRO	2.1
3	A	717	ASN	2.0
6	E	55	ARG	2.0
9	I	99	LEU	2.0
7	F	85	MET	2.0
4	B	327	ARG	2.0
4	B	738	PHE	2.0
9	I	8	ARG	2.0
9	I	14	LEU	2.0
9	I	33	SER	2.0
8	H	82	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

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
15	UTP	R	3000	29/29	0.80	0.25	-0.88	78,78,78,78	0
13	ZN	I	204	1/1	0.43	0.16	-1.05	90,90,90,90	0
13	ZN	L	105	1/1	0.87	0.17	-1.24	90,90,90,90	0
13	ZN	A	1735	1/1	0.98	0.18	-1.26	90,90,90,90	0
13	ZN	I	203	1/1	0.59	0.25	-1.29	90,90,90,90	0
13	ZN	C	319	1/1	0.96	0.06	-1.66	90,90,90,90	0
13	ZN	A	1734	1/1	0.69	0.14	-1.87	90,90,90,90	0
13	ZN	J	101	1/1	0.75	0.10	-2.55	90,90,90,90	0
13	ZN	B	1307	1/1	0.92	0.06	-	90,90,90,90	0
14	MG	R	2001	1/1	0.96	0.18	-	36,36,36,36	0
14	MG	A	2002	1/1	0.95	0.11	-	44,44,44,44	0

6.5 Other polymers

There are no such residues in this entry.