



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 12:26 PM UTC

PDB ID : 6TED / pdb_00006ted
EMDB ID : EMD-10480
Title : Structure of complete, activated transcription complex Pol II-DSIF-PAF-SPT6
uncovers allosteric elongation activation by RTF1
Authors : Vos, S.M.; Farnung, L.; Cramer, P.
Deposited on : 2019-11-11
Resolution : 3.10 Å (reported)
Based on initial models : 4L1U, 6GMH, 6AFO

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

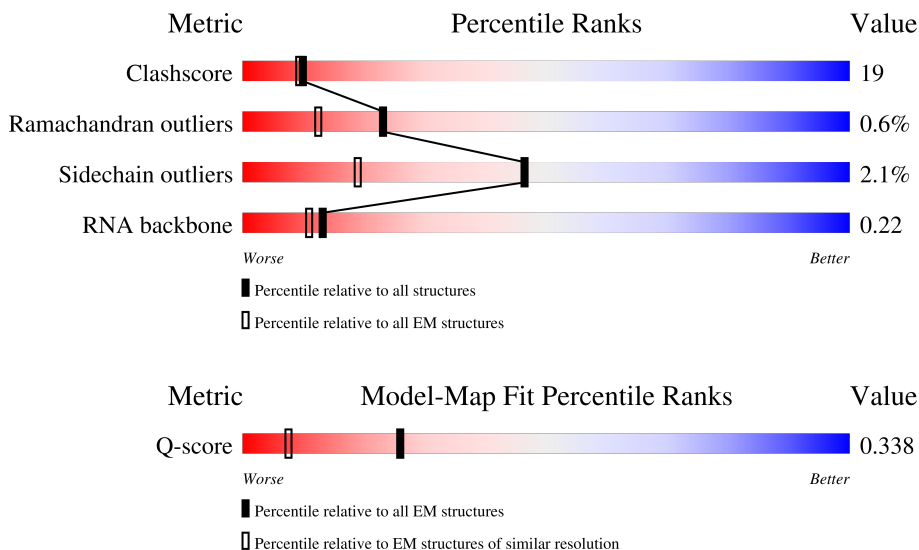
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1984	
2	B	1251	
3	C	275	

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Mol	Chain	Length	Quality of chain
4	D	142	61% 43% 46% 11%
5	E	210	66% 32%
6	F	127	50% 10% 39%
7	G	172	52% 54% 44%
8	H	150	59% 37%
9	I	125	6% 58% 31% 7%
10	J	67	66% 30%
11	K	117	70% 26%
12	L	58	5% 43% 36% 19%
13	M	1729	58% 54% 42%
14	N	48	42% 33% 44% 23%
15	P	46	26% 15% 20% 11% 54%
16	Q	1179	74% 42% 33% 25%
17	R	713	34% 19% 15% 66%
18	T	48	40% 42% 56%
19	U	666	17% 13% 5% 81%
20	V	531	45% 33% 13% 54%
21	W	305	98% 43% 55%
22	X	531	8% 5% 92%
23	Y	121	96% 63% 33%
24	Z	1087	42% 28% 19% 53%

2 Entry composition [i](#)

There are 26 unique types of molecules in this entry. The entry contains 57142 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	N	O	P			S
1	A	1426	11255	7074	2014	2095	2	70	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1122	8980	5684	1576	1656	64	0	0

- Molecule 3 is a protein called RNA polymerase II subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	258	2072	1300	356	410	6	0	0

- Molecule 4 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	126	1004	630	170	200	4	0	0

- Molecule 5 is a protein called RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	209	1720	1089	300	323	8	0	0

- Molecule 6 is a protein called RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	78	626	401	106	114	5	0	0

- Molecule 7 is a protein called RNA polymerase II subunit G.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	171	1333	866	214	245	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	149	1197	759	195	238	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	116	942	582	168	181	11	0	0

- Molecule 10 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	66	524	339	88	91	6	0	0

- Molecule 11 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	115	920	593	152	173	2	0	0

- Molecule 12 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	47	390	240	77	67	6	0	0

- Molecule 13 is a protein called Transcription elongation factor SPT6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	1002	4737	2583	1071	1076	7	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-2	SER	-	expression tag	UNP Q7KZ85
M	-1	ASN	-	expression tag	UNP Q7KZ85
M	0	ALA	-	expression tag	UNP Q7KZ85

- Molecule 14 is a DNA chain called DNA (37-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
14	N	37	773	361	158	217	37	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
15	P	21	452	202	87	142	21	0	0

- Molecule 16 is a protein called RNA polymerase-associated protein CTR9 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Q	890	7226	4579	1264	1352	31	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	1174	GLU	-	expression tag	UNP Q6PD62
Q	1175	ASN	-	expression tag	UNP Q6PD62
Q	1176	LEU	-	expression tag	UNP Q6PD62
Q	1177	TYR	-	expression tag	UNP Q6PD62
Q	1178	PHE	-	expression tag	UNP Q6PD62
Q	1179	GLN	-	expression tag	UNP Q6PD62

- Molecule 17 is a protein called RNA polymerase-associated protein RTF1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	R	244	1832	1148	340	337	7	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-2	SER	-	expression tag	UNP Q92541
R	-1	ASN	-	expression tag	UNP Q92541
R	0	ALA	-	expression tag	UNP Q92541

- Molecule 18 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
18	T	48	974	462	168	296	48	0	0

- Molecule 19 is a protein called RNA polymerase-associated protein LEO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	U	125	852	534	151	166	1	0	0

- Molecule 20 is a protein called RNA polymerase II-associated factor 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	V	244	1703	1061	305	333	4	0	0

- Molecule 21 is a protein called WD repeat-containing protein 61.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	W	300	2333	1483	392	454	4	0	0

- Molecule 22 is a protein called Parafibromin.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
22	X	43	353	220	69	64	0	0

- Molecule 23 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	Y	116	911	570	159	173	9	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-3	GLY	-	expression tag	UNP P63272
Y	-2	PRO	-	expression tag	UNP P63272
Y	-1	GLY	-	expression tag	UNP P63272
Y	0	SER	-	expression tag	UNP P63272

- Molecule 24 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	N	O	P			S
24	Z	510	4023	2550	709	745	1	18	0	0

- Molecule 25 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

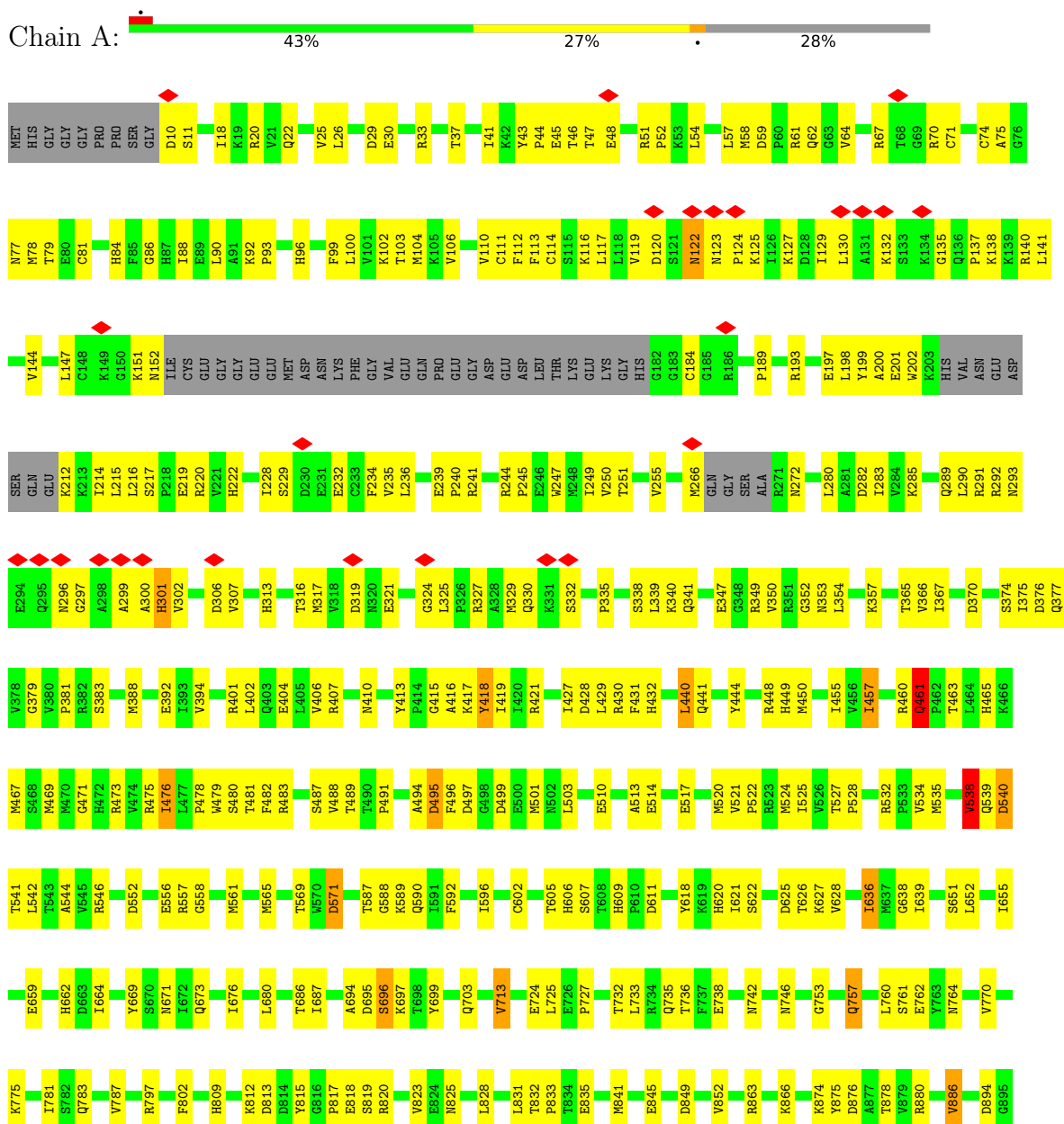
- Molecule 26 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

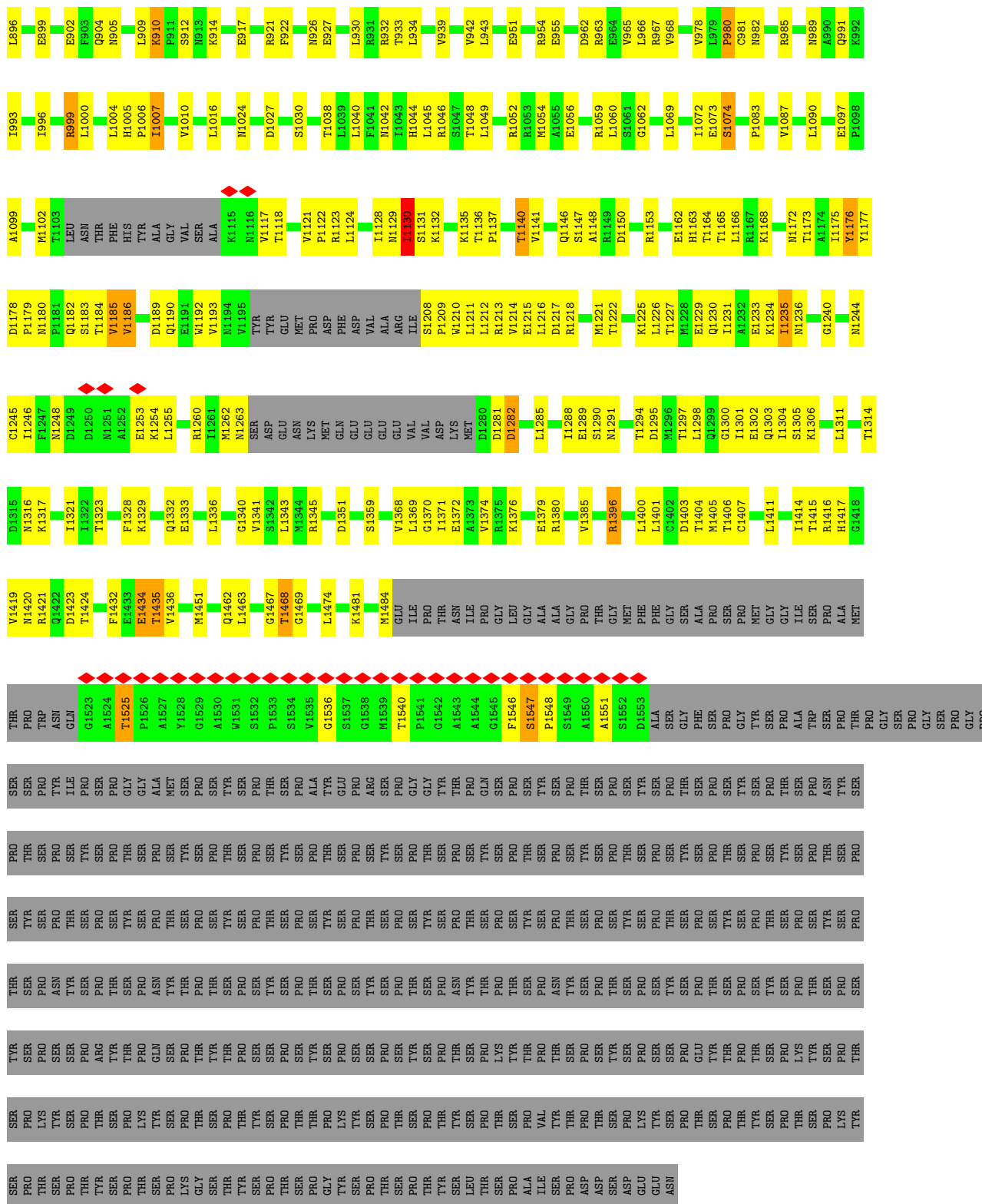
Mol	Chain	Residues	Atoms		AltConf
26	A	1	Total 1	Mg 1	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

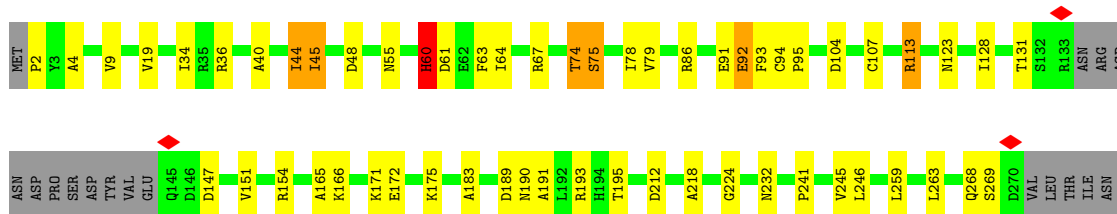
- Molecule 1: DNA-directed RNA polymerase subunit



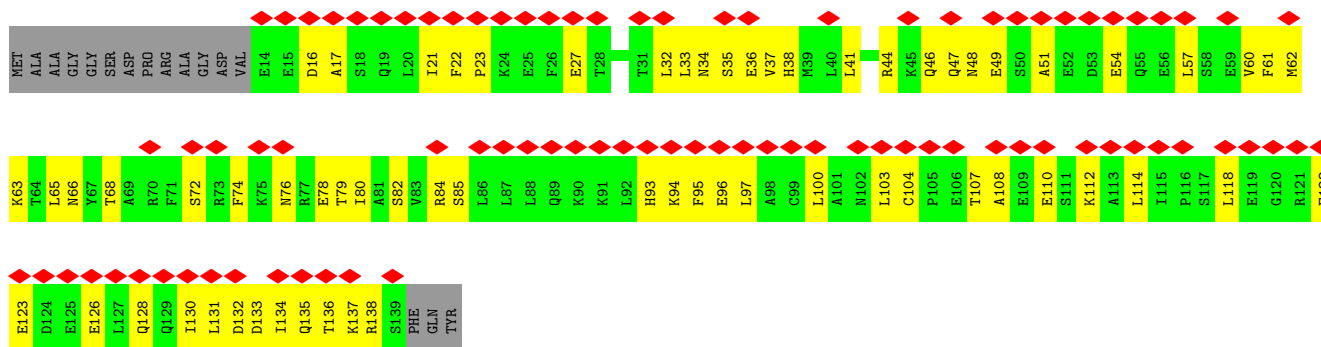
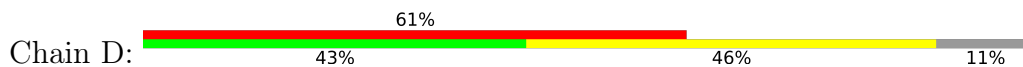


● Molecule 2: DNA-directed RNA polymerase subunit beta

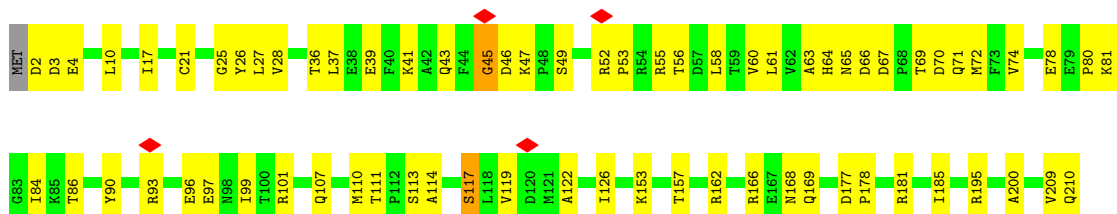




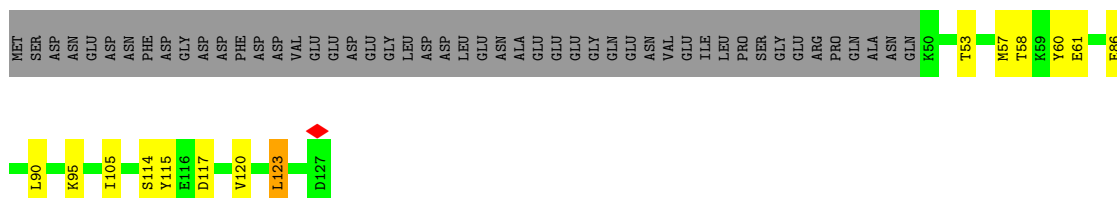
• Molecule 4: RNA polymerase II subunit D



• Molecule 5: RNA polymerase II subunit E

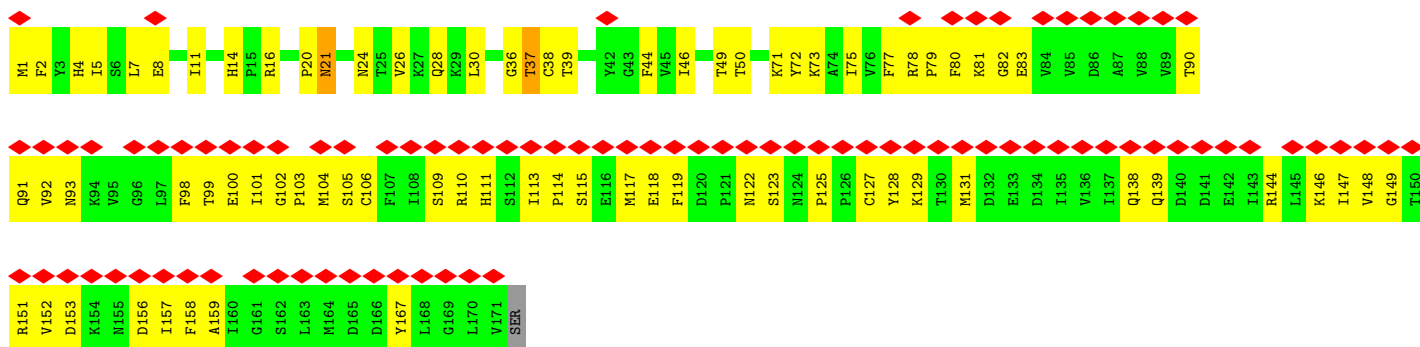


• Molecule 6: RNA polymerase II subunit F

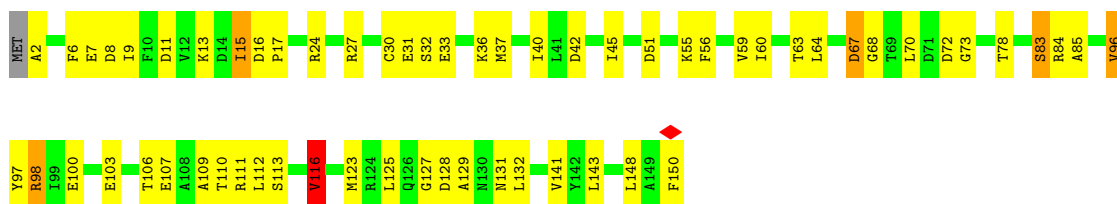


• Molecule 7: RNA polymerase II subunit G

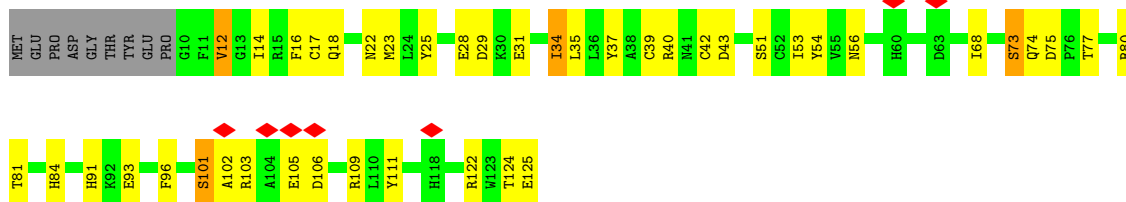




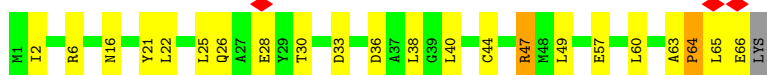
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



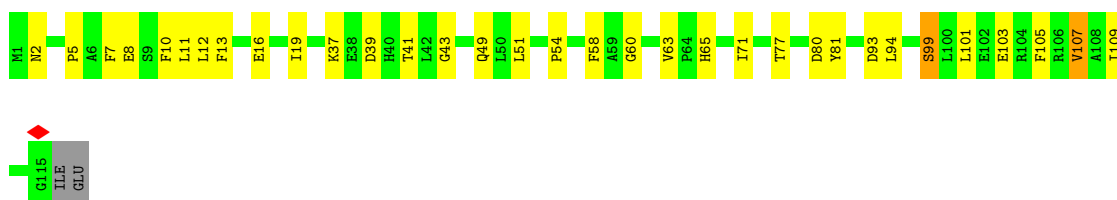
• Molecule 9: DNA-directed RNA polymerase II subunit RPB9



• Molecule 10: Uncharacterized protein



• Molecule 11: Uncharacterized protein



G1438	Y1378	ARG	K1258	CYS	E1076	V1018	L968	K838	G778	Q718
D1439	Q1379	LYS	V1259	PRO	S1079	T1019	Y959	F839	I779	Q719
R1440	H1380	GLN	G1260	PHE	A1080	M1020	C960	F840	R780	F720
K1441	V1381	ARG	M1261	GLN	E1081	C1021	E961	L841	V781	L721
L1442	D1382	THR	T1262	GLN	A1082	H1022	E962	K842	G782	Y722
L1443	V1383	THR	S1143	ASP	D1083	M1023	F963	K843	I783	V723
E1444	R1384	TYR	R1144	ASN	M1084	G1024	N964	K844	I784	Q724
E1445	GLU	LYS	M1145	PRO	P1085	P1025	R965	P845	A785	M725
L1446	GLY	ARG	T1146	GLU	A1086	K1026	V966	H846	F786	A726
I1447	LYS	VAL	E1147	LEU	G1087	V1027	N967	V847	S787	K727
I1448	GLU	I1327	E1148	GLU	A1088	F1028	E968	V848	S788	E728
T1449	ASN	A1328	L1089	VAL	V969	M1029	V969	T849	A789	L729
T1450	ALA	H1329	L1090	TRP	E1090	M1030	L910	R850	R790	K730
K1451	PHE	P1330	E1091	ASN	G1091	C1031	R911	A851	D791	N731
E1452	SER	S1331	I1092	HIS	I1092	A1032	Q912	G852	H792	K732
E1453	THR	F1332	L1093	PHE	L1093	G1033	A913	E853	P793	L733
P1454	THR	H1333	E1094	ASP	L1094	F1034	V914	N854	V794	L734
P1455	TYR	N1334	M1095	GLY	E1094	F1034	N974	N854	V794	L734
T1456	LYS	I1338	P1096	SER	M1095	L1035	R975	N855	F795	A735
F1457	GLY	L1339	E1186	CYS	P1096	K1036	A976	D856	C796	E736
I1458	GLY	A1277	T1157	PRO	E1097	I1037	I977	A857	A797	A737
I1459	GLY	F1340	P1158	GLY	R1098	D1038	A978	Q858	L798	K738
M1401	ALA	K1341	E1159	GLN	L1099	T1039	R979	M859	V799	E739
S1402	ALA	Q1342	E1160	ALA	K1100	A1039	P980	L860	N800	Y740
E1403	ALA	A1343	F1161	SER	D1101	L1039	Y981	I861	G801	V741
E1404	GLY	E1344	L1162	LEU	L1102	G1039	S982	E862	N801	I742
F1405	GLY	K1345	I1163	GLY	D1103	ASP	Q983	D863	G803	K743
E1406	THR	M1346	G1164	THR	L1104	SER	A984	V864	E804	A744
D1407	THR	M1347	K1165	ASP	D1105	THR	L985	K865	V805	C745
L1408	LYS	E1348	L1166	ASP	A1106	ASP	I986	R866	T806	S746
D1409	LEU	T1349	I1167	SER	F1107	TYR	Q987	I867	D807	R747
E1410	ASP	D1233	L1168	ILE	A1108	ILE	Y988	V868	F808	K748
I1411	ARG	N1234	C1169	ALA	E1051	E1051	Y989	H869	L809	L749
V1412	ASN	G1235	M1170	ALA	V1052	V1052	C990	E870	R810	Y750
A1413	ASN	V1236	N1171	ALA	L1053	L1053	Q991	L871	L811	N751
R1414	TRP	T1237	V1171	ALA	D1054	D1054	C931	D872	P812	W752
Y1415	LYS	G1238	T1172	ALA	G1055	G1055	S932	Q873	H813	L753
V1416	LEU	F1239	G1173	ALA	S1056	S1056	ASP	G874	F814	R754
Q1417	PRO	I1240	I1174	ALA	R1057	R1057	E935	Q875	T815	V755
P1418	LYS	P1241	A1175	ALA	V1058	V1058	D936	Q876	LYS	A756
M1419	THR	T1242	H1176	ALA	H1059	H1059	I937	L877	ARG	A756
A1420	TYR	F1244	ARG	ALA	P1060	P1060	L938	S878	THR	P757
S1421	TYR	K1243	PRO	ALA	E1061	E1061	C939	S879	ALA	Y758
F1422	PHE	L1245	GLN	ALA	T1062	T1062	L940	I880	ALA	R759
A1423	ASP	S1246	GLY	ALA	H1120	H1120	L941	I881	TRP	P760
R1424	ASP	D1247	GLU	ALA	I1121	I1121	G881	V882	ARG	D761
D1425	GLU	K1248	TYR	ALA	T1122	T1122	F942	V882	GLU	D762
L1426	ALA	V1249	ASP	ALA	M1065	M1065	H943	E883	GLU	Q763
L1427	ASP	K1251	GLN	ALA	R1066	R1066	P944	L884	VAL	VAL
M1428	HIS	L1252	ILE	ALA	L1004	L1004	L945	V885	GLU	GLU
H1429	LYS	R1253	ARG	ALA	K1005	K1005	V886	E827	GLU	GLU
K1430	GLN	P1253	ASN	ALA	Q1006	Q1006	D886	K828	ASP	ASP
Y1431	GLU	E1254	ASP	ALA	E947	E947	H948	N829	ASP	ASP
Y1432	GLU	E1255	THR	ALA	M1008	M1008	V949	A830	ASP	ASP
Q1433	GLU	E1256	GLY	ALA	T1009	T1009	A890	Q831	ASP	ASP
D1434	LYS	R1256	LEU	ALA	R1010	R1010	I891	D832	ASP	ASP
C1435	LYS	V1257	TRP	ALA	L1130	L1130	K951	I833	GLU	GLU
S1436	LYS		GLN	ALA	E1012	E1012	E952	E834	ASP	ASP
G1437				ALA	R1133	R1133	L954	Y893	GLU	GLU
				ALA	Y1134	Y1134	M894	N894	ASP	ASP
				ALA	D1136	D1136	Q1016	S896	ASP	ASP
				ALA	L1137	L1137	K897		ASP	ASP

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	446195	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.165	Depositor
Minimum map value	-0.086	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.022	Depositor
Map size (\AA)	377.64, 377.64, 377.64	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.049, 1.049, 1.049	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, TPO, MG, SEP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.41	9/11437 (0.1%)	0.97	12/15433 (0.1%)
2	B	1.57	8/9158 (0.1%)	1.08	20/12360 (0.2%)
3	C	1.69	3/2115 (0.1%)	1.07	5/2873 (0.2%)
4	D	0.40	0/1017	0.51	0/1368
5	E	1.23	0/1751	0.88	0/2366
6	F	1.62	1/636 (0.2%)	0.98	0/859
7	G	0.68	0/1364	0.66	0/1853
8	H	1.59	2/1219 (0.2%)	0.98	0/1644
9	I	1.13	0/964	0.88	0/1305
10	J	1.74	1/533 (0.2%)	1.02	0/719
11	K	1.69	1/939 (0.1%)	0.94	0/1271
12	L	1.40	0/395	1.12	1/525 (0.2%)
13	M	0.19	0/4763	0.43	1/6084 (0.0%)
14	N	0.44	0/870	0.46	0/1341
15	P	0.65	0/506	0.73	0/787
16	Q	0.30	0/7365	0.50	0/9927
17	R	0.36	0/1860	0.61	2/2509 (0.1%)
18	T	0.80	0/1087	0.62	1/1674 (0.1%)
19	U	0.36	0/864	0.75	3/1173 (0.3%)
20	V	0.30	0/1728	0.65	2/2357 (0.1%)
21	W	0.32	0/2392	0.50	0/3257
22	X	0.33	0/356	0.55	0/478
23	Y	0.17	0/927	0.40	0/1250
24	Z	0.41	0/4081	0.52	1/5493 (0.0%)
All	All	1.09	25/58327 (0.0%)	0.81	48/78906 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	3
17	R	0	1
All	All	0	6

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	791	GLU	CA-CB	-13.37	1.20	1.53
2	B	94	SER	C-N	-8.45	1.07	1.33
3	C	104	ASP	CA-CB	-8.23	1.40	1.53
1	A	418	TYR	CA-CB	-6.91	1.43	1.53
2	B	504	THR	CB-CG2	-6.75	1.30	1.52
1	A	1396	ARG	CB-CG	-6.42	1.33	1.52
1	A	999	ARG	C-N	-6.32	1.15	1.33
1	A	590	GLN	CG-CD	-6.12	1.36	1.52
8	H	116	VAL	CB-CG1	-5.97	1.32	1.52
6	F	53	THR	C-N	-5.90	1.23	1.33
2	B	922	ARG	CB-CG	-5.64	1.35	1.52
1	A	26	LEU	C-N	-5.62	1.22	1.33
8	H	98	ARG	CB-CG	-5.46	1.36	1.52
2	B	755	GLN	C-N	-5.43	1.18	1.33
2	B	663	GLU	CA-CB	-5.42	1.44	1.53
2	B	924	ARG	CB-CG	-5.42	1.36	1.52
1	A	590	GLN	CB-CG	-5.40	1.36	1.52
10	J	6	ARG	CB-CG	-5.27	1.36	1.52
1	A	377	GLN	CB-CG	-5.22	1.36	1.52
3	C	44	ILE	CA-CB	-5.14	1.51	1.55
3	C	45	ILE	CB-CG2	-5.11	1.35	1.52
11	K	43	GLY	CA-C	-5.08	1.44	1.51
1	A	1140	THR	CA-CB	-5.07	1.36	1.53
1	A	886	VAL	CB-CG1	-5.05	1.35	1.52
2	B	29	VAL	CB-CG2	-5.00	1.36	1.52

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	224	GLY	CA-C-N	8.13	147.25	121.98
3	C	224	GLY	C-N-CA	8.13	147.25	121.98
20	V	258	PRO	N-CA-CB	7.99	110.89	103.46
17	R	507	PRO	N-CA-CB	7.91	111.56	103.25
17	R	506	PRO	N-CA-CB	7.87	110.71	103.08
1	A	636	ILE	N-CA-C	-6.99	105.03	111.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	1330	PRO	N-CA-CB	6.85	110.44	103.25
20	V	238	PRO	N-CA-CB	6.82	110.41	103.25
1	A	538	VAL	N-CA-C	6.70	123.28	109.34
19	U	463	PRO	N-CA-CB	6.65	110.23	103.25
2	B	575	GLY	N-CA-C	6.57	118.71	112.08
1	A	122	ASN	N-CA-C	-6.52	104.73	114.64
1	A	1368	VAL	N-CA-C	-6.44	105.42	111.48
1	A	1396	ARG	CG-CD-NE	-6.35	98.03	112.00
19	U	493	PRO	N-CA-CB	6.33	109.90	103.25
1	A	457	ILE	CG1-CB-CG2	-6.33	91.72	110.70
2	B	629	GLU	CA-C-N	-6.31	113.10	122.56
2	B	629	GLU	C-N-CA	-6.31	113.10	122.56
24	Z	758	PRO	N-CA-CB	6.26	109.82	103.25
2	B	594	MET	CA-C-N	-6.25	114.03	121.90
2	B	594	MET	C-N-CA	-6.25	114.03	121.90
2	B	236	TRP	CA-C-N	-6.23	115.74	122.59
2	B	236	TRP	C-N-CA	-6.23	115.74	122.59
2	B	1122	CYS	N-CA-C	-6.21	99.96	109.65
2	B	790	GLN	CA-C-N	-6.12	113.81	123.23
2	B	790	GLN	C-N-CA	-6.12	113.81	123.23
2	B	371	ARG	CA-CB-CG	-5.83	102.43	114.10
3	C	113	ARG	CA-C-N	-5.74	113.97	122.41
3	C	113	ARG	C-N-CA	-5.74	113.97	122.41
2	B	629	GLU	N-CA-C	5.65	118.53	111.24
1	A	524	MET	CG-SD-CE	-5.47	88.86	100.90
2	B	146	LYS	CB-CA-C	-5.40	104.22	111.89
1	A	461	GLN	N-CA-C	5.38	121.71	109.81
12	L	20	GLY	N-CA-C	-5.33	100.56	113.18
2	B	146	LYS	CA-CB-CG	5.26	124.62	114.10
2	B	839	GLY	N-CA-C	-5.22	105.25	111.36
1	A	1072	ILE	CA-C-N	-5.20	112.90	120.29
1	A	1072	ILE	C-N-CA	-5.20	112.90	120.29
2	B	567	ILE	CG1-CB-CG2	-5.13	95.31	110.70
18	T	33	DC	OP1-P-O3'	5.10	123.31	108.00
2	B	959	GLU	CA-C-N	-5.10	111.42	121.41
2	B	959	GLU	C-N-CA	-5.10	111.42	121.41
19	U	516	ALA	N-CA-C	5.06	121.58	110.80
2	B	648	TYR	CA-C-N	-5.06	111.88	121.54
2	B	648	TYR	C-N-CA	-5.06	111.88	121.54
1	A	1176	TYR	CA-C-N	-5.02	115.08	122.06
1	A	1176	TYR	C-N-CA	-5.02	115.08	122.06
3	C	60	HIS	CB-CA-C	-5.02	100.44	110.42

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1434	GLU	Peptide
1	A	910	LYS	Peptide
2	B	20	ASP	Peptide
2	B	547	GLU	Peptide
2	B	686	GLU	Peptide
17	R	592	ASP	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11255	0	11374	457	0
2	B	8980	0	9019	321	0
3	C	2072	0	2019	47	0
4	D	1004	0	980	55	0
5	E	1720	0	1737	75	0
6	F	626	0	657	11	0
7	G	1333	0	1321	82	0
8	H	1197	0	1156	48	0
9	I	942	0	873	39	0
10	J	524	0	541	19	0
11	K	920	0	942	30	0
12	L	390	0	397	13	0
13	M	4737	0	2262	52	0
14	N	773	0	412	38	0
15	P	452	0	229	24	0
16	Q	7226	0	7169	363	0
17	R	1832	0	1687	119	0
18	T	974	0	541	40	0
19	U	852	0	668	31	0
20	V	1703	0	1426	88	0
21	W	2333	0	2246	156	0
22	X	353	0	371	30	0
23	Y	911	0	908	28	0
24	Z	4023	0	4035	185	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	A	2	0	0	0	0
25	B	1	0	0	0	0
25	C	1	0	0	0	0
25	I	2	0	0	0	0
25	J	1	0	0	0	0
25	L	1	0	0	0	0
25	Y	1	0	0	0	0
26	A	1	0	0	0	0
All	All	57142	0	52970	2126	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (2126) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:953:ASP:OD1	3:C:36:ARG:NH2	1.96	0.98
8:H:37:MET:HE2	8:H:127:GLY:HA3	1.43	0.98
1:A:609:HIS:HD1	1:A:626:THR:HG1	1.04	0.94
16:Q:505:ARG:HH21	20:V:44:PHE:HB2	1.32	0.93
1:A:904:GLN:NE2	1:A:981:CYS:O	2.01	0.91
2:B:105:PRO:HG2	19:U:512:THR:HA	1.51	0.91
16:Q:830:ARG:HA	16:Q:833:LYS:HE2	1.54	0.90
21:W:278:TRP:HB2	21:W:293:GLY:HA2	1.51	0.90
1:A:1227:THR:H	1:A:1230:GLN:HE21	1.19	0.90
14:N:30:DC:H42	18:T:19:DG:H1	1.18	0.89
23:Y:7:PRO:HG3	23:Y:23:LYS:HA	1.53	0.89
2:B:332:LYS:NZ	2:B:333:GLU:OE1	2.07	0.88
21:W:40:LEU:HD12	21:W:66:GLY:HA3	1.53	0.88
16:Q:727:LEU:HB3	16:Q:732:LYS:HB3	1.57	0.87
17:R:388:ARG:NH1	17:R:446:GLU:O	2.08	0.87
16:Q:768:VAL:HG21	16:Q:778:GLU:HG3	1.55	0.86
9:I:103:ARG:NH2	9:I:105:GLU:OE2	2.08	0.86
17:R:387:VAL:HG13	17:R:405:ILE:HD11	1.58	0.86
24:Z:478:VAL:HB	24:Z:518:LEU:HD11	1.58	0.85
2:B:387:HIS:NE2	2:B:671:GLU:OE2	2.10	0.85
1:A:922:PHE:H	1:A:1052:ARG:HD2	1.40	0.85
18:T:41:DC:H4'	24:Z:283:ARG:HE	1.41	0.85
3:C:193:ARG:NH2	3:C:218:ALA:O	2.09	0.85
21:W:35:VAL:HB	21:W:47:TRP:HB2	1.59	0.85
8:H:98:ARG:NH2	8:H:100:GLU:OE1	2.09	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:LEU:HB2	2:B:131:THR:HB	1.59	0.85
23:Y:75:GLN:O	23:Y:111:ARG:NH1	2.09	0.85
16:Q:682:ASP:O	16:Q:686:ASN:ND2	2.09	0.84
1:A:197:GLU:HB2	1:A:215:LEU:HD11	1.60	0.84
17:R:570:TRP:HB3	20:V:133:LYS:HE2	1.61	0.83
1:A:404:GLU:OE2	1:A:407:ARG:NH1	2.12	0.82
9:I:54:TYR:OH	9:I:56:ASN:ND2	2.12	0.82
2:B:613:ARG:NH1	2:B:615:TYR:OH	2.12	0.82
4:D:107:THR:HG23	4:D:110:GLU:H	1.43	0.82
14:N:37:DG:N1	18:T:12:DC:N3	2.27	0.82
1:A:392:GLU:OE2	1:A:401:ARG:NH2	2.11	0.81
5:E:166:ARG:HH22	5:E:168:ASN:HD22	1.26	0.81
16:Q:387:ALA:N	16:Q:390:ASP:OD2	2.13	0.81
21:W:14:ALA:N	21:W:296:GLN:O	2.13	0.81
21:W:172:ILE:HB	21:W:186:LEU:HB2	1.61	0.81
2:B:179:LEU:HD22	2:B:768:ARG:HD3	1.62	0.81
16:Q:643:ASP:OD2	22:X:239:GLN:NE2	2.11	0.81
4:D:76:ASN:HD22	4:D:79:THR:HG23	1.45	0.81
10:J:25:LEU:HB3	17:R:563:ILE:HD11	1.61	0.81
21:W:237:ASN:HD22	21:W:279:GLY:HA2	1.45	0.81
23:Y:3:LEU:O	23:Y:8:LYS:NZ	2.12	0.81
21:W:95:ASN:O	21:W:97:LYS:NZ	2.12	0.81
16:Q:276:ALA:HB1	16:Q:288:VAL:HG23	1.61	0.81
16:Q:737:LYS:HZ2	16:Q:764:LEU:HD13	1.46	0.80
1:A:1182:GLN:O	1:A:1192:TRP:NE1	2.14	0.80
21:W:35:VAL:N	21:W:47:TRP:O	2.12	0.80
2:B:756:LYS:NZ	20:V:134:THR:OG1	2.15	0.80
1:A:1525:TPO:O3P	13:M:1358:ARG:NH2	2.15	0.80
15:P:39:A:H3'	15:P:40:A:H8	1.47	0.80
16:Q:268:ASN:HD22	16:Q:271:VAL:H	1.29	0.79
1:A:1536:GLY:O	13:M:1483:ARG:NH2	2.16	0.79
7:G:111:HIS:HB3	24:Z:494:ARG:HB2	1.64	0.79
21:W:237:ASN:HB3	21:W:280:VAL:HG22	1.65	0.79
16:Q:41:LEU:HD23	16:Q:81:ASP:HB3	1.65	0.79
16:Q:534:TYR:HH	16:Q:553:TRP:HD1	1.31	0.79
1:A:1180:ASN:O	1:A:1183:SER:OG	2.00	0.79
20:V:47:LYS:HB3	22:X:228:GLU:HB2	1.63	0.79
1:A:539:GLN:O	1:A:541:THR:N	2.16	0.78
2:B:297:MET:HG2	2:B:377:LEU:HD11	1.65	0.78
3:C:154:ARG:NH1	10:J:63:ALA:HB2	1.98	0.78
1:A:349:ARG:HE	2:B:1157:LEU:HD22	1.46	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:38:G:H2'	15:P:39:A:H8	1.49	0.78
15:P:40:A:H2'	15:P:41:C:C6	2.19	0.78
1:A:1189:ASP:HA	1:A:1192:TRP:HE3	1.49	0.78
14:N:14:DC:N4	18:T:35:DG:O6	2.16	0.78
16:Q:268:ASN:HD21	16:Q:270:MET:HB3	1.49	0.78
1:A:413:TYR:O	1:A:415:GLY:N	2.17	0.78
16:Q:568:TRP:HE1	16:Q:591:ILE:HD12	1.49	0.78
24:Z:216:VAL:HB	24:Z:226:TYR:HB2	1.65	0.77
9:I:101:SER:OG	9:I:102:ALA:O	2.03	0.77
12:L:16:ILE:HD11	12:L:25:GLU:HB3	1.66	0.77
19:U:394:TYR:O	20:V:172:ARG:NH2	2.17	0.77
24:Z:728:THR:O	24:Z:747:ARG:NH1	2.18	0.77
16:Q:624:LYS:HG3	16:Q:627:ARG:HH21	1.47	0.76
1:A:272:ASN:ND2	18:T:34:DT:O2	2.19	0.76
1:A:1189:ASP:HA	1:A:1192:TRP:CE3	2.20	0.76
2:B:622:CYS:HB3	2:B:666:ASP:HB3	1.68	0.76
1:A:571:ASP:OD1	1:A:571:ASP:N	2.13	0.76
2:B:629:GLU:HG2	2:B:634:LEU:HD21	1.66	0.76
11:K:77:THR:OG1	11:K:81:TYR:O	2.04	0.76
17:R:562:TYR:O	17:R:566:ARG:NE	2.18	0.76
20:V:47:LYS:HE3	22:X:230:VAL:HG22	1.67	0.76
16:Q:353:TYR:OH	20:V:57:ARG:O	2.04	0.76
1:A:659:GLU:OE1	1:A:985:ARG:NH1	2.19	0.75
1:A:1434:GLU:O	1:A:1436:VAL:N	2.19	0.75
24:Z:257:ILE:HA	24:Z:260:MET:HE2	1.68	0.75
16:Q:314:ARG:HH12	16:Q:349:GLN:HE22	1.33	0.75
2:B:834:ARG:NH2	2:B:841:ARG:O	2.20	0.75
1:A:819:SER:O	1:A:819:SER:OG	2.05	0.74
2:B:1142:ASN:HD21	2:B:1145:GLN:HB2	1.52	0.74
1:A:713:VAL:HG21	1:A:817:PRO:HD3	1.67	0.74
8:H:7:GLU:HG2	8:H:59:VAL:HG22	1.68	0.74
14:N:37:DG:O6	18:T:12:DC:N4	2.20	0.74
1:A:296:ASN:OD1	1:A:297:GLY:N	2.20	0.74
1:A:299:ALA:HB3	1:A:302:VAL:HG12	1.69	0.74
1:A:1467:GLY:O	1:A:1469:GLY:N	2.20	0.74
2:B:677:MET:H	2:B:682:LEU:HD22	1.52	0.74
20:V:193:HIS:HB2	20:V:199:VAL:HG12	1.70	0.74
1:A:239:GLU:OE2	1:A:241:ARG:NH1	2.21	0.74
1:A:863:ARG:NH2	1:A:1129:ASN:OD1	2.21	0.74
24:Z:438:GLY:HA3	24:Z:452:PRO:HB2	1.68	0.74
2:B:388:TYR:H	2:B:504:THR:HG21	1.51	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Z:492:ILE:HG22	24:Z:502:LEU:HB3	1.70	0.73
24:Z:554:GLU:OE2	24:Z:559:GLN:NE2	2.21	0.73
15:P:39:A:C3'	15:P:40:A:H8	2.01	0.73
21:W:214:ILE:N	21:W:228:LEU:O	2.21	0.73
24:Z:353:ALA:HB3	24:Z:360:ILE:HB	1.69	0.73
16:Q:424:GLN:HB2	22:X:231:TRP:CE3	2.24	0.73
16:Q:803:MET:HE1	16:Q:807:LEU:HD11	1.70	0.73
24:Z:188:GLU:O	24:Z:192:THR:OG1	2.05	0.73
24:Z:295:TYR:N	24:Z:304:SER:OG	2.17	0.73
1:A:1184:THR:O	1:A:1186:VAL:N	2.22	0.73
21:W:169:ASP:N	21:W:169:ASP:OD1	2.22	0.73
2:B:898:THR:O	2:B:899:SER:OG	2.05	0.72
8:H:32:SER:HB3	8:H:37:MET:H	1.52	0.72
2:B:84:TYR:HB3	2:B:132:VAL:HG23	1.70	0.72
2:B:309:PHE:O	9:I:40:ARG:NH2	2.22	0.72
2:B:650:ASN:N	19:U:460:TYR:OH	2.17	0.72
17:R:564:ASN:HD21	20:V:136:TYR:C	1.96	0.72
4:D:131:LEU:HA	4:D:134:ILE:HD12	1.71	0.72
5:E:81:LYS:NZ	14:N:39:DA:OP1	2.19	0.72
1:A:539:GLN:O	1:A:542:LEU:N	2.21	0.72
21:W:272:ASP:O	21:W:274:GLN:NE2	2.22	0.72
8:H:103:GLU:HG3	8:H:109:ALA:HB2	1.71	0.72
19:U:438:ALA:O	19:U:439:ARG:NH1	2.20	0.72
20:V:110:GLU:HG3	20:V:111:GLU:H	1.53	0.72
1:A:289:GLN:O	1:A:293:ASN:HB2	1.89	0.72
12:L:19:CYS:SG	12:L:20:GLY:N	2.62	0.72
21:W:251:SER:OG	21:W:253:ASP:OD1	2.05	0.72
2:B:348:LEU:O	2:B:361:LYS:NZ	2.22	0.72
7:G:11:ILE:HD11	7:G:26:VAL:HG13	1.70	0.72
23:Y:93:LEU:HD22	23:Y:97:ILE:HD11	1.70	0.72
2:B:595:ASP:OD1	2:B:596:ILE:N	2.20	0.71
16:Q:163:ILE:HB	16:Q:194:PRO:HG3	1.72	0.71
21:W:81:SER:HB3	21:W:91:TRP:HE1	1.55	0.71
16:Q:302:GLU:HG3	16:Q:305:GLN:HE21	1.55	0.71
8:H:128:ASP:OD1	8:H:131:ASN:ND2	2.24	0.71
16:Q:401:LEU:HD22	16:Q:418:LEU:HG	1.72	0.71
17:R:405:ILE:HG23	17:R:426:LEU:HD11	1.72	0.71
5:E:80:PRO:HA	5:E:107:GLN:HB3	1.72	0.71
10:J:64:PRO:O	12:L:23:HIS:NE2	2.23	0.71
18:T:8:DG:H1'	18:T:9:DC:H5'	1.73	0.71
21:W:256:VAL:HB	21:W:270:PHE:HB2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Z:504:SER:OG	24:Z:507:THR:O	2.08	0.71
16:Q:384:LEU:HD13	16:Q:397:ALA:HB2	1.73	0.71
19:U:507:THR:O	19:U:509:ARG:N	2.24	0.71
24:Z:470:LYS:HB2	24:Z:516:ARG:HA	1.72	0.71
5:E:36:THR:N	5:E:39:GLU:OE2	2.16	0.70
9:I:109:ARG:HD3	9:I:124:THR:HG21	1.72	0.70
16:Q:799:VAL:O	16:Q:802:LYS:NZ	2.23	0.70
2:B:1125:MET:HE1	2:B:1156:LYS:HG2	1.73	0.70
17:R:405:ILE:HG12	17:R:426:LEU:HD21	1.72	0.70
7:G:151:ARG:O	7:G:158:PHE:N	2.22	0.70
10:J:44:CYS:O	10:J:47:ARG:NH1	2.25	0.70
1:A:77:ASN:OD1	1:A:78:MET:N	2.25	0.70
16:Q:729:LYS:HE2	16:Q:732:LYS:HD2	1.72	0.70
1:A:244:ARG:HE	1:A:245:PRO:HD2	1.57	0.70
3:C:74:THR:OG1	3:C:74:THR:O	2.09	0.70
1:A:1372:GLU:OE2	5:E:195:ARG:NH1	2.25	0.70
7:G:110:ARG:HH21	7:G:118:GLU:HA	1.56	0.70
9:I:42:CYS:SG	9:I:43:ASP:N	2.65	0.70
24:Z:563:MET:HA	24:Z:637:VAL:HG11	1.73	0.70
24:Z:759:GLY:O	24:Z:761:MET:N	2.24	0.70
2:B:85:LEU:N	2:B:131:THR:O	2.25	0.70
1:A:100:LEU:HD23	1:A:193:ARG:HE	1.57	0.69
1:A:1184:THR:C	1:A:1186:VAL:H	2.00	0.69
19:U:450:LEU:HD21	19:U:452:LEU:HD23	1.73	0.69
4:D:37:VAL:HG21	7:G:2:PHE:CD2	2.27	0.69
24:Z:307:MET:HE3	24:Z:308:ILE:H	1.57	0.69
16:Q:624:LYS:HG3	16:Q:627:ARG:NH2	2.07	0.69
5:E:97:GLU:HB2	5:E:99:ILE:HG12	1.74	0.69
13:M:1379:GLN:HG2	13:M:1469:PRO:HB2	1.73	0.69
17:R:428:LEU:HB2	17:R:437:PHE:CD2	2.27	0.69
24:Z:502:LEU:HG	24:Z:511:LEU:HB3	1.75	0.69
2:B:1040:GLN:NE2	3:C:195:THR:OG1	2.25	0.69
7:G:91:GLN:HG2	7:G:93:ASN:HD21	1.58	0.69
24:Z:525:ALA:HB1	24:Z:552:ARG:HH22	1.58	0.69
1:A:917:GLU:OE2	1:A:921:ARG:NH1	2.25	0.69
13:M:1462:ILE:HD11	13:M:1472:PHE:HB3	1.74	0.69
21:W:113:ALA:HB3	21:W:122:ALA:HB3	1.74	0.69
1:A:999:ARG:NH2	8:H:103:GLU:OE2	2.24	0.69
4:D:34:ASN:O	4:D:68:THR:OG1	2.09	0.69
1:A:1212:LEU:HD21	1:A:1289:GLU:HB3	1.75	0.69
24:Z:450:ILE:HG23	24:Z:452:PRO:HD3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:2:ASP:OD2	5:E:4:GLU:N	2.25	0.69
7:G:152:VAL:HG22	7:G:157:ILE:HG22	1.74	0.69
17:R:410:GLU:OE1	17:R:423:ASN:ND2	2.25	0.69
8:H:36:LYS:HG3	16:Q:709:ARG:HH22	1.57	0.68
17:R:366:ARG:NH1	24:Z:775:TPO:OG1	2.26	0.68
4:D:23:PRO:HG2	7:G:78:ARG:HH12	1.58	0.68
13:M:1488:THR:HB	13:M:1495:ARG:HB3	1.75	0.68
17:R:570:TRP:HD1	20:V:133:LYS:HD2	1.57	0.68
20:V:192:GLN:HB2	20:V:197:PRO:HB3	1.74	0.68
1:A:376:ASP:CG	1:A:473:ARG:HH21	2.01	0.68
13:M:1512:LYS:O	13:M:1516:GLN:NE2	2.24	0.68
16:Q:886:LYS:O	16:Q:890:MET:HG2	1.94	0.68
15:P:39:A:H3'	15:P:40:A:C8	2.29	0.68
1:A:487:SER:OG	1:A:673:GLN:NE2	2.26	0.68
24:Z:433:LEU:HB3	24:Z:436:LEU:HD12	1.75	0.68
24:Z:478:VAL:HG21	24:Z:502:LEU:HD22	1.74	0.68
1:A:357:LYS:NZ	2:B:1112:ASP:OD1	2.26	0.68
5:E:56:THR:OG1	5:E:78:GLU:OE2	2.11	0.68
16:Q:534:TYR:HH	16:Q:553:TRP:CD1	2.11	0.68
21:W:289:ILE:HB	21:W:301:TYR:HB2	1.74	0.68
1:A:686:THR:OG1	1:A:687:ILE:N	2.25	0.68
8:H:2:ALA:C	8:H:84:ARG:HH22	2.02	0.68
16:Q:86:LEU:HD11	16:Q:116:LEU:HB3	1.76	0.68
7:G:123:SER:OG	7:G:125:PRO:O	2.11	0.68
16:Q:590:ARG:HA	16:Q:593:LYS:HG3	1.76	0.67
2:B:633:LEU:HD11	2:B:679:PRO:HB2	1.76	0.67
2:B:649:ASN:HB2	19:U:460:TYR:OH	1.93	0.67
6:F:86:GLU:OE2	6:F:95:LYS:NZ	2.17	0.67
1:A:1212:LEU:HD12	1:A:1285:LEU:HD13	1.77	0.67
14:N:3:DA:H2''	14:N:4:DT:H72	1.75	0.67
16:Q:394:ARG:HB3	16:Q:398:LYS:HE3	1.76	0.67
24:Z:419:ASN:OD1	24:Z:516:ARG:NH1	2.27	0.67
1:A:140:ARG:HH22	1:A:234:PHE:HD1	1.41	0.67
1:A:611:ASP:N	1:A:611:ASP:OD1	2.25	0.67
1:A:1024:ASN:O	5:E:162:ARG:NH2	2.28	0.67
5:E:82:VAL:HG22	5:E:86:THR:OG1	1.93	0.67
21:W:13:GLN:NE2	21:W:15:HIS:O	2.27	0.67
17:R:406:THR:OG1	17:R:427:GLN:O	2.11	0.67
1:A:112:PHE:O	1:A:113:PHE:HB2	1.93	0.67
1:A:116:LYS:NZ	1:A:184:CYS:SG	2.66	0.67
2:B:22:TRP:CE2	2:B:679:PRO:HG3	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:565:THR:HG21	2:B:580:PRO:HB3	1.77	0.67
2:B:1136:GLU:HB2	2:B:1143:LYS:HG2	1.77	0.67
16:Q:484:GLU:HB3	16:Q:487:HIS:HB2	1.76	0.66
24:Z:295:TYR:H	24:Z:304:SER:HG	1.42	0.66
2:B:1157:LEU:O	2:B:1161:GLU:HG3	1.95	0.66
4:D:128:GLN:NE2	4:D:132:ASP:OD1	2.27	0.66
24:Z:184:CYS:SG	24:Z:185:LYS:N	2.68	0.66
7:G:21:ASN:OD1	7:G:21:ASN:N	2.23	0.66
7:G:109:SER:HB3	24:Z:493:VAL:HG21	1.77	0.66
19:U:474:ARG:H	20:V:218:GLN:HA	1.60	0.66
21:W:236:LEU:N	21:W:250:SER:O	2.27	0.66
21:W:292:VAL:HG12	21:W:298:ILE:HG12	1.76	0.66
1:A:200:ALA:HB3	1:A:214:ILE:HG12	1.78	0.66
14:N:37:DG:N2	18:T:12:DC:O2	2.26	0.66
1:A:413:TYR:O	1:A:449:HIS:HD2	1.77	0.66
1:A:1118:THR:O	1:A:1123:ARG:HB2	1.96	0.66
2:B:1003:ASN:O	2:B:1005:ALA:N	2.27	0.66
16:Q:534:TYR:OH	16:Q:556:GLU:OE1	2.12	0.66
3:C:212:ASP:OD1	3:C:212:ASP:N	2.28	0.66
13:M:1373:VAL:HG21	13:M:1379:GLN:HG3	1.76	0.66
21:W:66:GLY:O	21:W:83:SER:OG	2.11	0.66
1:A:539:GLN:NE2	2:B:790:GLN:O	2.28	0.66
14:N:34:DC:H2"	14:N:35:DA:C8	2.30	0.66
16:Q:268:ASN:ND2	16:Q:271:VAL:H	1.93	0.66
16:Q:420:GLN:O	22:X:229:ARG:NH1	2.28	0.66
24:Z:613:GLU:O	24:Z:625:HIS:N	2.28	0.66
14:N:10:DG:H2"	14:N:11:DC:C5	2.30	0.66
21:W:46:VAL:HB	21:W:58:TRP:HB2	1.77	0.66
24:Z:282:LYS:O	24:Z:287:LYS:NZ	2.28	0.65
2:B:354:SER:OG	2:B:355:ASP:N	2.26	0.65
3:C:154:ARG:HH11	10:J:63:ALA:HB2	1.61	0.65
17:R:455:TRP:CD1	17:R:459:MET:HE3	2.31	0.65
21:W:130:VAL:HB	21:W:144:LEU:HD12	1.78	0.65
6:F:105:ILE:HD12	6:F:117:ASP:HB3	1.78	0.65
11:K:13:PHE:HB2	11:K:16:GLU:HG3	1.77	0.65
16:Q:494:ALA:HB1	22:X:224:ILE:HG12	1.78	0.65
17:R:494:GLU:HA	17:R:497:LYS:HD2	1.79	0.65
23:Y:4:GLU:O	23:Y:27:GLN:NE2	2.29	0.65
5:E:27:LEU:O	16:Q:877:GLN:NE2	2.29	0.65
5:E:41:LYS:NZ	5:E:46:ASP:OD1	2.19	0.65
5:E:93:ARG:HA	5:E:96:GLU:OE1	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:30:DC:N3	18:T:19:DG:N2	2.37	0.65
16:Q:342:LEU:HD11	20:V:67:GLU:HG2	1.78	0.65
16:Q:86:LEU:HG	16:Q:120:ALA:HB2	1.76	0.65
2:B:1071:ASN:O	2:B:1073:GLN:N	2.29	0.65
14:N:30:DC:N4	18:T:19:DG:H1	1.93	0.65
16:Q:211:LEU:HD12	16:Q:213:LYS:HZ1	1.62	0.65
8:H:72:ASP:OD1	8:H:73:GLY:N	2.29	0.65
21:W:218:ASP:N	21:W:223:ASN:O	2.29	0.65
23:Y:14:ARG:HH21	23:Y:54:SER:HA	1.61	0.65
24:Z:539:LEU:HD22	24:Z:616:HIS:HB3	1.79	0.65
18:T:39:DC:H2''	18:T:40:DT:H71	1.78	0.65
21:W:195:SER:OG	21:W:236:LEU:O	2.15	0.65
1:A:419:ILE:HG23	1:A:427:ILE:HB	1.79	0.65
16:Q:856:LEU:HD23	16:Q:857:LEU:HD22	1.78	0.65
24:Z:558:PHE:N	24:Z:570:VAL:O	2.30	0.65
2:B:223:SER:OG	2:B:350:HIS:ND1	2.26	0.64
16:Q:605:LEU:O	16:Q:609:ASN:ND2	2.30	0.64
1:A:1099:ALA:HA	1:A:1102:MET:HE3	1.78	0.64
5:E:71:GLN:HB2	5:E:99:ILE:HG22	1.78	0.64
16:Q:568:TRP:CZ3	16:Q:592:LEU:HB2	2.32	0.64
20:V:45:ASP:N	20:V:45:ASP:OD1	2.30	0.64
24:Z:470:LYS:NZ	24:Z:518:LEU:O	2.31	0.64
4:D:76:ASN:HD21	4:D:78:GLU:HB2	1.61	0.64
5:E:113:SER:OG	14:N:40:DG:OP1	2.15	0.64
1:A:609:HIS:ND1	1:A:626:THR:OG1	2.13	0.64
21:W:214:ILE:HB	21:W:228:LEU:HB3	1.78	0.64
17:R:569:GLU:O	17:R:573:VAL:HG23	1.97	0.64
20:V:48:PHE:HB2	22:X:229:ARG:HB2	1.78	0.64
1:A:329:MET:HA	1:A:335:PRO:HA	1.80	0.64
1:A:1140:THR:OG1	1:A:1140:THR:O	2.12	0.64
2:B:100:GLU:OE1	2:B:100:GLU:N	2.24	0.64
7:G:153:ASP:N	7:G:156:ASP:O	2.23	0.64
16:Q:83:MET:HE3	16:Q:124:ILE:HB	1.80	0.64
21:W:26:THR:HG23	21:W:284:GLY:HA2	1.80	0.64
16:Q:710:LYS:HB2	16:Q:712:TYR:CD1	2.32	0.64
2:B:497:LYS:HG3	2:B:498:PRO:HD3	1.80	0.64
14:N:31:DC:H2''	14:N:32:DA:C8	2.32	0.64
2:B:577:HIS:NE2	2:B:583:LEU:HD11	2.13	0.64
24:Z:519:GLN:NE2	24:Z:521:CYS:SG	2.71	0.64
17:R:355:LEU:HG	17:R:357:GLU:H	1.62	0.63
2:B:787:GLY:O	2:B:790:GLN:HG3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:92:ASP:HB3	21:W:95:ASN:OD1	1.98	0.63
2:B:59:VAL:HG23	2:B:408:PHE:CZ	2.33	0.63
2:B:184:TYR:CE2	2:B:191:GLU:HG2	2.33	0.63
3:C:2:PRO:HB3	11:K:54:PRO:HD2	1.79	0.63
14:N:38:DG:H2''	14:N:39:DA:C8	2.34	0.63
1:A:1540:THR:HG23	13:M:1479:ARG:HE	1.62	0.63
2:B:93:LEU:O	19:U:507:THR:HA	1.99	0.63
16:Q:123:ILE:HG13	16:Q:124:ILE:HG12	1.80	0.63
16:Q:398:LYS:O	16:Q:402:LYS:HD3	1.99	0.63
2:B:310:VAL:HG23	2:B:311:ILE:HD12	1.81	0.63
18:T:38:DG:H2''	18:T:39:DC:C5	2.33	0.63
21:W:48:LYS:N	21:W:55:ASP:O	2.27	0.63
5:E:166:ARG:NH2	5:E:168:ASN:HD22	1.95	0.63
7:G:36:GLY:O	24:Z:628:LYS:NZ	2.23	0.63
8:H:8:ASP:OD1	8:H:32:SER:OG	2.05	0.63
17:R:355:LEU:HD12	17:R:356:PRO:HD2	1.81	0.63
17:R:404:GLU:OE1	17:R:455:TRP:NE1	2.32	0.63
24:Z:733:ARG:NH1	24:Z:744:SER:OG	2.31	0.63
16:Q:286:SER:O	16:Q:290:HIS:ND1	2.32	0.63
16:Q:611:TRP:HE1	16:Q:628:HIS:HA	1.63	0.63
1:A:565:MET:HE1	11:K:58:PHE:HE2	1.64	0.63
2:B:67:LEU:H	2:B:83:ARG:HB2	1.64	0.63
16:Q:239:ALA:HB2	16:Q:257:LEU:HB3	1.81	0.63
1:A:694:ALA:HB3	1:A:699:TYR:CE1	2.34	0.62
16:Q:65:GLU:OE1	16:Q:93:TYR:OH	2.15	0.62
16:Q:576:LEU:HD21	16:Q:585:GLN:HE22	1.64	0.62
24:Z:474:MET:HE2	24:Z:494:ARG:HA	1.80	0.62
4:D:46:GLN:HA	4:D:49:GLU:CD	2.24	0.62
16:Q:128:GLN:HE22	20:V:86:LEU:HD13	1.64	0.62
16:Q:835:ASP:OD1	16:Q:839:ARG:NE	2.32	0.62
21:W:206:VAL:HG11	21:W:238:VAL:HG21	1.81	0.62
5:E:64:HIS:N	5:E:70:ASP:O	2.31	0.62
1:A:481:THR:O	1:A:483:ARG:NH1	2.32	0.62
4:D:114:LEU:HD21	7:G:167:TYR:HB2	1.80	0.62
4:D:135:GLN:OE1	4:D:138:ARG:NH1	2.32	0.62
1:A:381:PRO:HB3	1:A:480:SER:HA	1.81	0.62
1:A:922:PHE:H	1:A:1052:ARG:HH11	1.48	0.62
8:H:110:THR:O	8:H:129:ALA:N	2.32	0.62
11:K:5:PRO:HG2	11:K:8:GLU:HG3	1.81	0.62
1:A:556:GLU:OE1	1:A:556:GLU:N	2.33	0.62
2:B:100:GLU:HA	2:B:105:PRO:HG3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:55:ARG:HB2	5:E:78:GLU:HG3	1.82	0.62
9:I:35:LEU:HD21	9:I:53:ILE:HD11	1.81	0.62
2:B:67:LEU:HG	2:B:84:TYR:OH	2.00	0.62
1:A:1016:LEU:HD22	1:A:1069:LEU:HD22	1.82	0.62
16:Q:394:ARG:HD2	16:Q:421:ILE:HG23	1.82	0.62
16:Q:849:LYS:O	16:Q:852:LEU:HG	2.00	0.62
24:Z:506:LEU:HD11	24:Z:552:ARG:HH21	1.63	0.62
2:B:646:ARG:C	2:B:648:TYR:H	2.07	0.62
8:H:83:SER:OG	8:H:84:ARG:N	2.33	0.62
9:I:12:VAL:HG21	9:I:53:ILE:O	2.00	0.62
21:W:206:VAL:HG22	21:W:216:ILE:HG12	1.81	0.62
1:A:962:ASP:CG	1:A:1046:ARG:HH21	2.08	0.61
12:L:56:ASP:O	12:L:58:ARG:N	2.33	0.61
17:R:564:ASN:OD1	20:V:136:TYR:N	2.29	0.61
1:A:797:ARG:NH2	1:A:815:TYR:O	2.32	0.61
1:A:876:ASP:HB3	1:A:878:THR:HG22	1.82	0.61
1:A:1244:ASN:HB2	1:A:1262:MET:HE2	1.80	0.61
5:E:39:GLU:OE1	5:E:39:GLU:N	2.24	0.61
8:H:2:ALA:O	8:H:84:ARG:NH2	2.30	0.61
16:Q:86:LEU:HD12	16:Q:89:LEU:HB2	1.80	0.61
1:A:30:GLU:HA	1:A:33:ARG:HE	1.63	0.61
1:A:200:ALA:HB2	1:A:216:LEU:HD21	1.81	0.61
1:A:1468:THR:H	6:F:60:TYR:HB3	1.66	0.61
2:B:19:PRO:O	2:B:21:LEU:N	2.32	0.61
16:Q:249:ASP:O	16:Q:253:ASN:ND2	2.33	0.61
17:R:364:LEU:HB2	17:R:387:VAL:HG12	1.81	0.61
24:Z:366:TYR:O	24:Z:373:PHE:N	2.28	0.61
2:B:765:GLU:OE1	2:B:770:ARG:NE	2.34	0.61
16:Q:715:GLN:HB2	16:Q:746:VAL:HG11	1.83	0.61
20:V:110:GLU:HG3	20:V:111:GLU:N	2.14	0.61
1:A:88:ILE:O	1:A:90:LEU:N	2.33	0.61
16:Q:38:HIS:HE1	16:Q:73:LEU:HD13	1.66	0.61
16:Q:68:ARG:HE	16:Q:89:LEU:HD12	1.65	0.61
24:Z:390:LEU:HD12	24:Z:393:LEU:HD12	1.82	0.61
1:A:1303:GLN:O	1:A:1340:GLY:HA3	2.01	0.61
3:C:190:ASN:ND2	3:C:195:THR:O	2.20	0.61
16:Q:862:GLU:HA	16:Q:865:LEU:HG	1.82	0.61
2:B:228:SER:O	2:B:405:ARG:NH1	2.34	0.61
3:C:91:GLU:OE1	24:Z:713:SER:HB2	2.01	0.61
5:E:45:GLY:HA3	5:E:53:PRO:HD3	1.82	0.61
16:Q:729:LYS:HB2	16:Q:732:LYS:HD2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:THR:HA	1:A:52:PRO:HA	1.81	0.61
1:A:1481:LYS:O	13:M:1384:ARG:NH1	2.34	0.61
2:B:144:HIS:CD2	2:B:431:LEU:HD21	2.36	0.61
16:Q:158:GLN:HG3	16:Q:159:SER:H	1.66	0.61
1:A:1301:ILE:HG22	1:A:1345:ARG:HH21	1.65	0.60
16:Q:379:LYS:HZ1	20:V:61:TYR:HE2	1.47	0.60
21:W:26:THR:HA	21:W:284:GLY:HA2	1.83	0.60
1:A:222:HIS:HB2	1:A:249:ILE:HD11	1.82	0.60
16:Q:646:ASN:HA	22:X:239:GLN:HA	1.82	0.60
20:V:196:LYS:O	20:V:198:ARG:HG3	2.01	0.60
21:W:53:ARG:NH1	21:W:54:LEU:O	2.34	0.60
23:Y:66:PRO:HB2	23:Y:78:SER:HA	1.82	0.60
24:Z:554:GLU:OE1	24:Z:557:THR:OG1	2.18	0.60
7:G:151:ARG:HB3	7:G:158:PHE:O	2.01	0.60
4:D:48:ASN:HD22	4:D:57:LEU:HG	1.66	0.60
1:A:123:ASN:O	1:A:127:LYS:HG2	2.02	0.60
16:Q:80:LYS:O	16:Q:83:MET:HG3	2.01	0.60
16:Q:222:SER:O	16:Q:226:GLU:HG2	2.01	0.60
21:W:27:ASN:O	21:W:32:SER:OG	2.19	0.60
6:F:114:SER:OG	6:F:115:TYR:N	2.33	0.60
16:Q:163:ILE:HG21	16:Q:189:ALA:HA	1.83	0.60
16:Q:313:ALA:HB2	16:Q:328:TYR:HB2	1.83	0.60
23:Y:19:CYS:SG	23:Y:21:LEU:HB2	2.42	0.60
3:C:55:ASN:ND2	3:C:60:HIS:O	2.34	0.60
16:Q:48:ALA:HB2	16:Q:63:LEU:HD11	1.84	0.60
16:Q:65:GLU:HA	16:Q:89:LEU:HD11	1.82	0.60
21:W:176:ASP:HB2	21:W:183:LEU:HD11	1.83	0.60
1:A:760:LEU:HD22	1:A:764:ASN:ND2	2.16	0.60
20:V:233:VAL:O	20:V:238:PRO:N	2.35	0.60
2:B:784:SER:O	2:B:784:SER:OG	2.14	0.60
10:J:36:ASP:OD1	10:J:36:ASP:N	2.28	0.60
21:W:125:THR:OG1	21:W:131:ASN:ND2	2.34	0.60
1:A:217:SER:OG	1:A:220:ARG:N	2.35	0.60
5:E:45:GLY:CA	5:E:53:PRO:HD3	2.32	0.60
16:Q:581:TRP:O	16:Q:585:GLN:HB2	2.02	0.60
16:Q:620:ARG:HG3	16:Q:625:GLU:HB2	1.84	0.60
24:Z:629:LEU:HB2	24:Z:634:GLY:HA2	1.83	0.60
1:A:894:ASP:OD2	1:A:1396:ARG:NH2	2.35	0.59
1:A:1222:THR:O	1:A:1225:LYS:N	2.34	0.59
3:C:189:ASP:O	3:C:191:ALA:N	2.34	0.59
1:A:1210:TRP:CZ2	1:A:1281:ASP:HB3	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:60:VAL:HA	4:D:63:LYS:HG2	1.82	0.59
7:G:109:SER:HB2	24:Z:503:PHE:CZ	2.37	0.59
2:B:743:ARG:NH1	2:B:745:ASP:OD1	2.35	0.59
16:Q:351:TYR:HB2	16:Q:360:ALA:HB2	1.83	0.59
16:Q:708:LEU:HD21	16:Q:719:VAL:HG21	1.83	0.59
1:A:1128:ILE:HG23	1:A:1414:ILE:HB	1.84	0.59
11:K:49:GLN:NE2	11:K:93:ASP:OD2	2.34	0.59
1:A:64:VAL:HG11	1:A:78:MET:HA	1.84	0.59
8:H:116:VAL:CG1	8:H:123:MET:HE2	2.33	0.59
24:Z:365:ARG:HD3	24:Z:374:LYS:HD2	1.84	0.59
24:Z:499:PHE:HD1	24:Z:512:LYS:HB3	1.67	0.59
16:Q:776:LEU:O	16:Q:779:VAL:HG22	2.03	0.59
1:A:379:GLY:HA2	1:A:475:ARG:O	2.02	0.59
1:A:1231:ILE:O	1:A:1235:ILE:HB	2.03	0.59
2:B:650:ASN:N	2:B:650:ASN:OD1	2.36	0.59
3:C:60:HIS:HB2	3:C:63:PHE:HB2	1.83	0.59
8:H:32:SER:OG	8:H:33:GLU:N	2.33	0.59
16:Q:371:TYR:HE2	16:Q:373:ASN:HD21	1.51	0.59
16:Q:505:ARG:NH2	20:V:44:PHE:HB2	2.12	0.59
1:A:117:LEU:C	1:A:119:VAL:H	2.11	0.59
16:Q:419:ALA:HB2	16:Q:433:ALA:HB3	1.83	0.59
1:A:620:HIS:O	8:H:97:TYR:OH	2.15	0.59
1:A:1004:LEU:HD13	1:A:1062:GLY:HA2	1.85	0.59
16:Q:201:ARG:HH12	16:Q:227:LEU:HD13	1.68	0.59
1:A:1005:HIS:HD2	1:A:1007:ILE:H	1.49	0.59
2:B:177:CYS:SG	2:B:180:ASP:N	2.74	0.59
4:D:103:LEU:O	7:G:144:ARG:NH2	2.36	0.59
16:Q:624:LYS:HA	16:Q:627:ARG:HH21	1.67	0.59
15:P:39:A:C2	15:P:40:A:C5	2.91	0.58
21:W:8:LEU:N	21:W:300:ILE:O	2.30	0.58
1:A:476:ILE:O	1:A:476:ILE:HG13	2.00	0.58
2:B:912:ASN:OD1	2:B:912:ASN:N	2.26	0.58
9:I:17:CYS:N	9:I:22:ASN:O	2.27	0.58
14:N:11:DC:H2''	14:N:12:DG:C8	2.38	0.58
16:Q:884:LYS:O	16:Q:887:ASN:N	2.34	0.58
2:B:298:MET:HE3	9:I:14:ILE:HD12	1.85	0.58
16:Q:774:SER:H	16:Q:830:ARG:NH1	1.99	0.58
17:R:574:GLU:HA	17:R:577:LYS:HG2	1.84	0.58
2:B:565:THR:HA	2:B:610:ARG:HB3	1.86	0.58
5:E:93:ARG:HB2	16:Q:891:PHE:CE1	2.38	0.58
8:H:63:THR:HG21	8:H:68:GLY:HA2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:78:THR:O	8:H:78:THR:OG1	2.21	0.58
17:R:353:VAL:HG12	17:R:469:LEU:HD13	1.86	0.58
19:U:445:ASP:OD2	19:U:447:SER:OG	2.19	0.58
1:A:202:TRP:CE3	1:A:212:LYS:HB2	2.38	0.58
1:A:1052:ARG:NE	1:A:1056:GLU:OE2	2.36	0.58
20:V:88:ASN:OD1	20:V:89:PRO:HD3	2.04	0.58
24:Z:562:ASN:HD21	24:Z:566:LYS:HG3	1.67	0.58
1:A:367:ILE:HA	1:A:482:PHE:O	2.04	0.58
1:A:394:VAL:HG23	1:A:444:TYR:O	2.04	0.58
2:B:743:ARG:HB3	2:B:743:ARG:HH11	1.69	0.58
5:E:66:ASP:OD1	5:E:67:ASP:N	2.36	0.58
17:R:363:ARG:NH2	17:R:365:SER:OG	2.36	0.58
1:A:11:SER:O	2:B:1135:TYR:OH	2.14	0.58
1:A:370:ASP:OD2	11:K:65:HIS:NE2	2.36	0.58
2:B:577:HIS:CD2	2:B:583:LEU:HD11	2.38	0.58
1:A:552:ASP:OD1	8:H:24:ARG:NH1	2.37	0.58
2:B:83:ARG:O	2:B:83:ARG:NH2	2.37	0.58
1:A:1190:GLN:O	1:A:1193:VAL:HG12	2.04	0.58
1:A:1244:ASN:HB2	1:A:1262:MET:CE	2.34	0.58
13:M:1356:ILE:HG22	13:M:1370:THR:HB	1.85	0.58
15:P:37:G:O2'	15:P:38:G:H8	1.86	0.58
15:P:38:G:H2'	15:P:39:A:C8	2.35	0.58
16:Q:95:GLN:NE2	20:V:84:ILE:O	2.37	0.58
17:R:493:GLU:OE1	17:R:493:GLU:N	2.22	0.58
2:B:715:ASP:OD1	2:B:715:ASP:N	2.19	0.58
24:Z:416:ARG:HE	24:Z:466:GLN:HE21	1.52	0.57
2:B:833:THR:C	2:B:835:GLU:H	2.11	0.57
2:B:1115:GLN:HG2	2:B:1150:ARG:HG2	1.86	0.57
16:Q:156:LEU:HD11	16:Q:169:LYS:HE2	1.87	0.57
16:Q:504:ALA:HB2	16:Q:519:LEU:HB3	1.86	0.57
17:R:407:GLY:H	17:R:427:GLN:HB3	1.69	0.57
24:Z:424:ASP:HB2	24:Z:440:ILE:HD12	1.84	0.57
1:A:1177:TYR:OH	1:A:1282:ASP:HA	2.04	0.57
2:B:721:ARG:NH1	2:B:940:GLY:O	2.36	0.57
5:E:90:TYR:HA	16:Q:891:PHE:HZ	1.69	0.57
13:M:1352:GLN:HE22	13:M:1373:VAL:C	2.11	0.57
1:A:392:GLU:HG2	1:A:402:LEU:HD11	1.86	0.57
1:A:699:TYR:O	1:A:703:GLN:HG2	2.05	0.57
2:B:235:ILE:HG13	2:B:348:LEU:HD13	1.85	0.57
7:G:37:THR:HA	24:Z:628:LYS:NZ	2.20	0.57
11:K:63:VAL:HG22	11:K:71:ILE:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:122:ASN:OD1	7:G:123:SER:N	2.38	0.57
16:Q:384:LEU:HG	16:Q:386:ALA:H	1.69	0.57
22:X:233:THR:O	22:X:236:THR:OG1	2.22	0.57
24:Z:280:ARG:HH21	24:Z:288:ASP:HB3	1.69	0.57
1:A:565:MET:HE3	11:K:60:GLY:HA3	1.85	0.57
1:A:589:LYS:NZ	1:A:625:ASP:OD2	2.36	0.57
1:A:823:VAL:HG22	1:A:835:GLU:HB2	1.86	0.57
21:W:27:ASN:HB2	21:W:31:ASN:HD21	1.70	0.57
24:Z:192:THR:HG23	24:Z:245:LEU:HD21	1.85	0.57
1:A:96:HIS:HD2	1:A:99:PHE:CD2	2.23	0.57
1:A:546:ARG:HG2	1:A:546:ARG:O	2.04	0.57
1:A:1146:GLN:NE2	1:A:1150:ASP:OD2	2.36	0.57
1:A:1484:MET:HB2	13:M:1362:LYS:HE3	1.87	0.57
16:Q:474:PHE:HB2	16:Q:503:LEU:HD13	1.85	0.57
1:A:628:VAL:HA	1:A:638:GLY:HA3	1.87	0.57
16:Q:208:PHE:HD1	16:Q:213:LYS:HD2	1.70	0.57
21:W:48:LYS:HB2	21:W:57:GLN:HB2	1.85	0.57
1:A:282:ASP:HB3	1:A:313:HIS:CE1	2.39	0.57
1:A:1146:GLN:OE1	1:A:1153:ARG:HD3	2.05	0.57
20:V:55:GLN:OE1	20:V:57:ARG:NE	2.35	0.57
24:Z:450:ILE:HG21	24:Z:468:LEU:HD11	1.86	0.57
1:A:92:LYS:HD2	1:A:307:VAL:HG11	1.87	0.56
1:A:117:LEU:HG	1:A:232:GLU:OE2	2.05	0.56
17:R:473:ASN:HA	17:R:476:GLU:CD	2.30	0.56
21:W:152:LEU:HD12	21:W:168:ILE:HA	1.85	0.56
1:A:1005:HIS:CD2	1:A:1007:ILE:H	2.23	0.56
3:C:4:ALA:HB2	11:K:93:ASP:HB2	1.86	0.56
16:Q:188:LYS:HB3	16:Q:191:ARG:HH11	1.70	0.56
16:Q:678:ALA:O	16:Q:684:TRP:NE1	2.38	0.56
17:R:560:ILE:HA	17:R:563:ILE:HG22	1.87	0.56
24:Z:501:ILE:HD11	24:Z:510:GLU:HB3	1.87	0.56
1:A:140:ARG:NH2	1:A:234:PHE:HD1	2.03	0.56
1:A:299:ALA:O	1:A:301:HIS:N	2.39	0.56
1:A:538:VAL:O	1:A:538:VAL:HG12	2.06	0.56
1:A:809:HIS:HE1	2:B:506:TRP:CZ2	2.23	0.56
2:B:177:CYS:HB2	2:B:738:THR:OG1	2.06	0.56
2:B:995:GLU:OE1	20:V:131:MET:HB3	2.05	0.56
5:E:55:ARG:O	5:E:56:THR:OG1	2.23	0.56
13:M:1505:ASN:O	13:M:1509:ARG:HG2	2.05	0.56
2:B:285:LEU:HD23	9:I:16:PHE:HZ	1.70	0.56
7:G:110:ARG:HH12	7:G:115:SER:HA	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:12:DG:H2''	14:N:13:DG:H8	1.70	0.56
21:W:68:VAL:HG13	21:W:83:SER:HA	1.87	0.56
2:B:756:LYS:NZ	20:V:134:THR:HG1	2.02	0.56
9:I:25:TYR:O	9:I:37:TYR:HA	2.04	0.56
18:T:33:DC:H2''	18:T:34:DT:OP1	2.04	0.56
20:V:61:TYR:N	20:V:62:LYS:HA	2.21	0.56
19:U:384:VAL:HA	19:U:418:ASN:HB3	1.86	0.56
1:A:353:ASN:OD1	2:B:1071:ASN:ND2	2.39	0.56
2:B:897:ARG:HB2	2:B:900:GLU:HG3	1.88	0.56
16:Q:802:LYS:HE2	16:Q:807:LEU:HB2	1.87	0.56
23:Y:14:ARG:NH1	23:Y:55:SER:OG	2.39	0.56
1:A:886:VAL:HG12	5:E:169:GLN:O	2.06	0.56
1:A:1359:SER:O	1:A:1359:SER:OG	2.16	0.56
1:A:1370:GLY:O	1:A:1374:VAL:HG23	2.06	0.56
8:H:37:MET:HE3	8:H:131:ASN:HD22	1.71	0.56
15:P:39:A:C3'	15:P:40:A:C8	2.87	0.56
16:Q:777:LYS:HE3	16:Q:781:ASN:HD21	1.71	0.56
19:U:395:GLU:HA	20:V:172:ARG:HH21	1.71	0.56
24:Z:478:VAL:HG11	24:Z:492:ILE:HG23	1.87	0.56
1:A:1211:LEU:HD12	1:A:1213:ARG:N	2.21	0.56
1:A:1234:LYS:HE2	1:A:1298:LEU:HA	1.87	0.56
2:B:639:HIS:O	2:B:643:LEU:HB2	2.06	0.56
4:D:104:CYS:HB3	4:D:135:GLN:HE22	1.70	0.56
17:R:415:TYR:CZ	17:R:438:ARG:HB3	2.41	0.56
24:Z:420:PHE:HB3	24:Z:440:ILE:HD13	1.88	0.56
2:B:218:THR:HG23	2:B:238:SER:HB3	1.88	0.56
2:B:1129:ASN:HB3	2:B:1134:THR:HG22	1.87	0.56
18:T:12:DC:H2''	18:T:13:DC:H5'	1.88	0.56
20:V:127:VAL:HG23	20:V:128:VAL:H	1.71	0.56
21:W:163:LEU:O	21:W:175:PHE:N	2.34	0.56
1:A:469:MET:HG3	2:B:1093:CYS:SG	2.46	0.55
3:C:60:HIS:HB2	3:C:63:PHE:H	1.71	0.55
14:N:39:DA:H2''	14:N:40:DG:O4'	2.07	0.55
20:V:95:ASP:OD1	20:V:95:ASP:N	2.39	0.55
1:A:1302:GLU:OE1	1:A:1302:GLU:N	2.38	0.55
2:B:866:ILE:HG22	2:B:867:ILE:HG13	1.87	0.55
21:W:81:SER:HB3	21:W:91:TRP:NE1	2.20	0.55
21:W:112:LEU:HD22	21:W:121:LEU:HD21	1.87	0.55
24:Z:472:PHE:HB3	24:Z:476:ASP:OD2	2.06	0.55
2:B:588:ARG:O	2:B:592:ARG:HD3	2.07	0.55
11:K:39:ASP:OD1	11:K:39:ASP:N	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:492:ILE:O	17:R:496:VAL:HG13	2.07	0.55
21:W:9:PHE:HB3	21:W:300:ILE:CG1	2.35	0.55
24:Z:364:ASN:O	24:Z:374:LYS:NZ	2.39	0.55
24:Z:546:THR:HG23	24:Z:563:MET:HE2	1.88	0.55
1:A:760:LEU:HD13	1:A:764:ASN:HD22	1.71	0.55
2:B:789:ASN:HB3	2:B:795:ILE:HG13	1.88	0.55
16:Q:302:GLU:HG3	16:Q:305:GLN:NE2	2.20	0.55
17:R:592:ASP:O	17:R:594:PHE:N	2.37	0.55
1:A:365:THR:HG22	1:A:366:VAL:H	1.70	0.55
7:G:118:GLU:O	7:G:128:TYR:HA	2.06	0.55
13:M:1476:TYR:OH	13:M:1485:GLU:OE2	2.21	0.55
17:R:564:ASN:ND2	20:V:136:TYR:C	2.64	0.55
21:W:108:ASP:HA	21:W:126:HIS:CE1	2.41	0.55
1:A:1302:GLU:C	1:A:1304:ILE:H	2.15	0.55
2:B:279:VAL:HG23	2:B:312:GLN:O	2.06	0.55
4:D:74:PHE:HE2	4:D:80:ILE:HG12	1.72	0.55
16:Q:451:PRO:HD3	16:Q:480:ARG:HG3	1.88	0.55
16:Q:772:GLU:HA	16:Q:773:LYS:HB2	1.88	0.55
24:Z:542:LEU:HD22	24:Z:570:VAL:HG11	1.87	0.55
1:A:528:PRO:HB3	1:A:899:GLU:HG3	1.87	0.55
1:A:1180:ASN:CG	1:A:1182:GLN:HE21	2.14	0.55
13:M:1344:GLU:HA	13:M:1347:MET:HE2	1.87	0.55
17:R:363:ARG:NE	17:R:446:GLU:HA	2.21	0.55
18:T:31:DT:H2''	18:T:32:DT:H5'	1.89	0.55
22:X:250:PHE:CE1	22:X:253:LEU:HD22	2.42	0.55
1:A:1208:SER:O	1:A:1260:ARG:HD3	2.07	0.55
7:G:46:ILE:HB	7:G:75:ILE:HG13	1.89	0.55
16:Q:772:GLU:HB3	16:Q:774:SER:CB	2.37	0.55
24:Z:416:ARG:NE	24:Z:466:GLN:HE21	2.04	0.55
1:A:460:ARG:HB2	1:A:501:MET:HE3	1.89	0.55
1:A:874:LYS:HG3	1:A:880:ARG:HG3	1.89	0.55
2:B:649:ASN:ND2	19:U:460:TYR:OH	2.40	0.55
13:M:1369:VAL:HG11	13:M:1416:VAL:HG21	1.88	0.55
17:R:569:GLU:O	17:R:572:ILE:HG22	2.07	0.55
1:A:229:SER:OG	1:A:232:GLU:HB2	2.07	0.55
14:N:43:DG:H2''	14:N:44:DG:C8	2.42	0.55
16:Q:94:VAL:HG23	16:Q:140:LEU:HD11	1.89	0.55
16:Q:313:ALA:HB2	16:Q:328:TYR:CB	2.37	0.55
16:Q:761:LEU:HD22	16:Q:785:GLU:HB3	1.89	0.55
17:R:449:GLU:O	17:R:453:MET:HG2	2.07	0.55
7:G:7:LEU:N	7:G:72:TYR:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:17:CYS:HB3	9:I:22:ASN:H	1.72	0.54
13:M:1476:TYR:OH	13:M:1483:ARG:NH1	2.40	0.54
16:Q:568:TRP:CD2	16:Q:592:LEU:HD13	2.42	0.54
17:R:360:ASN:HA	17:R:363:ARG:HB2	1.89	0.54
21:W:31:ASN:HB2	21:W:72:ILE:HG21	1.90	0.54
21:W:41:ASP:OD1	21:W:41:ASP:N	2.40	0.54
1:A:350:VAL:HA	1:A:354:LEU:HB2	1.89	0.54
8:H:27:ARG:HD3	8:H:42:ASP:OD2	2.06	0.54
2:B:714:PRO:HD2	2:B:1001:PRO:HG3	1.88	0.54
2:B:859:ARG:HH12	2:B:901:THR:HG22	1.72	0.54
10:J:57:GLU:OE1	17:R:557:ILE:HG12	2.06	0.54
17:R:471:GLU:HG2	17:R:474:LYS:HE3	1.88	0.54
1:A:62:GLN:HE22	1:A:255:VAL:HG13	1.71	0.54
2:B:342:VAL:HG23	2:B:346:GLU:HB2	1.89	0.54
16:Q:309:CYS:HB3	16:Q:328:TYR:HD1	1.73	0.54
16:Q:546:ASN:HD22	16:Q:577:ALA:HB2	1.73	0.54
24:Z:610:ARG:HD2	24:Z:629:LEU:HD21	1.89	0.54
1:A:290:LEU:HD13	1:A:306:ASP:CG	2.33	0.54
1:A:340:LYS:HG3	1:A:1436:VAL:HG11	1.90	0.54
1:A:522:PRO:O	1:A:662:HIS:HB2	2.07	0.54
2:B:309:PHE:HD2	9:I:40:ARG:NE	2.04	0.54
5:E:166:ARG:HH22	5:E:168:ASN:ND2	1.99	0.54
16:Q:316:PHE:HB2	16:Q:325:ALA:HB2	1.90	0.54
16:Q:525:ARG:HG3	16:Q:526:GLU:HG3	1.88	0.54
16:Q:776:LEU:HD22	16:Q:831:ALA:HA	1.88	0.54
21:W:76:LEU:HD12	21:W:77:PRO:HD2	1.89	0.54
24:Z:235:VAL:O	24:Z:239:ILE:HG12	2.07	0.54
1:A:48:GLU:OE1	1:A:51:ARG:HB2	2.08	0.54
1:A:606:HIS:HB3	1:A:626:THR:HB	1.89	0.54
5:E:111:THR:HG23	5:E:114:ALA:H	1.73	0.54
15:P:39:A:C2	18:T:33:DC:O2	2.61	0.54
17:R:385:CYS:O	17:R:405:ILE:HD12	2.08	0.54
21:W:236:LEU:HD13	21:W:278:TRP:CE3	2.42	0.54
1:A:1130:ILE:HD11	1:A:1405:MET:CE	2.38	0.54
1:A:1141:VAL:HB	1:A:1336:LEU:HB2	1.90	0.54
1:A:1248:ASN:ND2	1:A:1254:LYS:O	2.40	0.54
16:Q:46:ALA:O	16:Q:50:GLU:HG2	2.08	0.54
19:U:450:LEU:CD2	19:U:452:LEU:HD23	2.37	0.54
21:W:19:ILE:HG12	21:W:39:SER:OG	2.06	0.54
1:A:255:VAL:HG23	1:A:280:LEU:HD13	1.89	0.54
16:Q:274:HIS:HA	16:Q:277:ASN:ND2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:505:ARG:HE	20:V:44:PHE:HB3	1.73	0.54
2:B:169:ARG:NH2	20:V:139:THR:OG1	2.40	0.54
2:B:933:ASP:OD2	2:B:1050:ARG:NH2	2.38	0.54
4:D:133:ASP:O	4:D:136:THR:OG1	2.22	0.54
9:I:39:CYS:SG	9:I:40:ARG:N	2.81	0.54
16:Q:364:PHE:HB3	16:Q:380:ILE:HD11	1.90	0.54
21:W:29:LYS:O	21:W:77:PRO:HB3	2.08	0.54
2:B:159:THR:HA	2:B:164:ASN:ND2	2.22	0.54
17:R:452:PHE:CZ	17:R:456:LYS:HE2	2.43	0.54
19:U:379:PRO:HD2	19:U:382:LEU:HD12	1.89	0.54
21:W:233:SER:HG	21:W:251:SER:HB2	1.71	0.54
24:Z:479:LYS:NZ	24:Z:521:CYS:O	2.28	0.54
2:B:108:MET:HE2	2:B:113:ALA:HB2	1.90	0.53
13:M:1463:CYS:O	13:M:1473:LEU:N	2.30	0.53
16:Q:147:GLN:O	16:Q:151:GLN:HG2	2.08	0.53
16:Q:392:GLU:HG2	16:Q:393:LYS:HG2	1.90	0.53
16:Q:553:TRP:HD1	16:Q:556:GLU:OE1	1.91	0.53
1:A:760:LEU:HD11	1:A:781:ILE:HG21	1.90	0.53
2:B:22:TRP:CH2	2:B:679:PRO:HD3	2.43	0.53
2:B:141:GLN:O	2:B:143:GLN:N	2.42	0.53
2:B:792:ASP:CG	2:B:975:ARG:HH22	2.16	0.53
2:B:959:GLU:OE1	2:B:959:GLU:N	2.41	0.53
17:R:356:PRO:HB3	17:R:452:PHE:HB2	1.90	0.53
17:R:560:ILE:O	17:R:563:ILE:HG22	2.08	0.53
1:A:606:HIS:CG	1:A:607:SER:H	2.26	0.53
1:A:727:PRO:HA	1:A:736:THR:HG21	1.89	0.53
3:C:36:ARG:NH1	11:K:41:THR:OG1	2.40	0.53
7:G:100:GLU:OE1	7:G:105:SER:HB3	2.08	0.53
7:G:117:MET:HB3	7:G:128:TYR:HB3	1.89	0.53
9:I:29:ASP:HB3	9:I:34:ILE:HG13	1.89	0.53
16:Q:772:GLU:HB3	16:Q:774:SER:HB3	1.89	0.53
21:W:228:LEU:HD13	21:W:264:ARG:HB3	1.90	0.53
21:W:256:VAL:O	21:W:269:THR:HA	2.07	0.53
1:A:64:VAL:HG12	1:A:81:CYS:SG	2.48	0.53
2:B:388:TYR:CE2	2:B:505:LEU:HD21	2.43	0.53
2:B:420:GLN:C	2:B:422:PHE:H	2.17	0.53
16:Q:190:LEU:O	16:Q:193:ASN:ND2	2.41	0.53
16:Q:454:LEU:HA	16:Q:457:VAL:HG12	1.91	0.53
16:Q:867:GLU:O	16:Q:871:GLN:HG3	2.08	0.53
20:V:45:ASP:HB3	22:X:232:ARG:HE	1.73	0.53
21:W:33:GLU:O	21:W:49:TRP:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Y:40:LEU:HD22	23:Y:42:MET:HB3	1.89	0.53
24:Z:244:ASN:HB3	24:Z:245:LEU:HD22	1.90	0.53
1:A:141:LEU:HA	1:A:144:VAL:HG22	1.89	0.53
5:E:45:GLY:HA3	5:E:52:ARG:HB2	1.91	0.53
8:H:9:ILE:HD12	8:H:148:LEU:HD11	1.90	0.53
12:L:35:ARG:HH21	12:L:40:GLY:CA	2.20	0.53
13:M:1440:ARG:O	13:M:1444:GLU:HG2	2.08	0.53
16:Q:631:ARG:O	16:Q:635:ILE:HG12	2.09	0.53
1:A:802:PHE:HD2	2:B:671:GLU:HG2	1.74	0.53
1:A:1227:THR:N	1:A:1230:GLN:HE21	1.98	0.53
7:G:117:MET:N	7:G:117:MET:SD	2.80	0.53
24:Z:279:VAL:HA	24:Z:386:VAL:HG21	1.90	0.53
1:A:241:ARG:HB2	1:A:241:ARG:CZ	2.39	0.53
1:A:330:GLN:C	1:A:332:SER:H	2.17	0.53
2:B:393:LEU:HD22	2:B:485:LEU:HD22	1.89	0.53
2:B:957:THR:HG22	2:B:1028:LEU:HD22	1.90	0.53
5:E:119:VAL:HA	5:E:122:ALA:HB2	1.90	0.53
2:B:395:LEU:HD11	2:B:532:ILE:HD12	1.91	0.53
16:Q:623:GLU:O	16:Q:627:ARG:NE	2.42	0.53
16:Q:776:LEU:O	16:Q:780:LEU:HD12	2.08	0.53
1:A:86:GLY:C	1:A:255:VAL:HG12	2.34	0.53
1:A:845:GLU:OE2	2:B:500:GLN:NE2	2.42	0.53
2:B:741:HIS:CD2	2:B:742:VAL:HG23	2.43	0.53
2:B:789:ASN:O	2:B:968:ASN:HB2	2.09	0.53
7:G:109:SER:HB3	24:Z:493:VAL:HG11	1.91	0.53
16:Q:511:CYS:O	21:W:229:SER:OG	2.24	0.53
16:Q:769:LEU:HD13	16:Q:824:ALA:HB2	1.91	0.53
16:Q:777:LYS:HA	16:Q:780:LEU:HD13	1.91	0.53
21:W:9:PHE:H	21:W:300:ILE:HB	1.73	0.53
4:D:130:ILE:HA	4:D:133:ASP:OD2	2.09	0.53
9:I:68:ILE:HB	9:I:122:ARG:HD3	1.91	0.53
16:Q:26:GLU:HG3	16:Q:28:ASP:H	1.74	0.53
21:W:108:ASP:HA	21:W:126:HIS:ND1	2.23	0.53
21:W:248:VAL:HG12	21:W:258:VAL:HG22	1.90	0.53
1:A:1180:ASN:ND2	1:A:1182:GLN:HE21	2.07	0.52
7:G:8:GLU:HA	7:G:71:LYS:HA	1.91	0.52
7:G:37:THR:OG1	7:G:38:CYS:N	2.42	0.52
10:J:65:LEU:HD12	10:J:66:GLU:OE1	2.09	0.52
16:Q:244:ASN:ND2	20:V:69:GLN:HA	2.24	0.52
3:C:19:VAL:HG23	3:C:241:PRO:HB2	1.91	0.52
4:D:61:PHE:CE2	4:D:65:LEU:HD21	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:15:ILE:O	8:H:16:ASP:C	2.51	0.52
10:J:40:LEU:HD11	10:J:49:LEU:HD12	1.91	0.52
17:R:355:LEU:HD11	17:R:357:GLU:HG2	1.90	0.52
17:R:403:ALA:HB1	17:R:428:LEU:HB3	1.91	0.52
18:T:17:DT:H2''	18:T:18:DG:C8	2.44	0.52
18:T:35:DG:C2	18:T:36:DC:C2	2.97	0.52
16:Q:384:LEU:HD21	16:Q:386:ALA:HB3	1.91	0.52
16:Q:763:ARG:HG2	20:V:25:GLU:HG3	1.91	0.52
2:B:414:GLU:HG3	2:B:439:ILE:HD11	1.90	0.52
2:B:609:GLU:O	2:B:609:GLU:HG2	2.09	0.52
13:M:1447:LEU:HB3	13:M:1477:GLN:HG3	1.91	0.52
17:R:577:LYS:O	17:R:580:VAL:HG22	2.09	0.52
24:Z:422:PRO:HG3	24:Z:443:VAL:HG21	1.91	0.52
1:A:129:ILE:HD13	1:A:132:LYS:NZ	2.24	0.52
16:Q:420:GLN:HA	22:X:229:ARG:HH22	1.75	0.52
18:T:9:DC:C2'	18:T:10:DT:H71	2.39	0.52
21:W:172:ILE:N	21:W:186:LEU:O	2.42	0.52
21:W:289:ILE:N	21:W:301:TYR:O	2.41	0.52
24:Z:193:ALA:O	24:Z:197:MET:HG3	2.10	0.52
2:B:1136:GLU:HA	2:B:1143:LYS:HA	1.90	0.52
4:D:51:ALA:O	4:D:54:GLU:HB2	2.10	0.52
4:D:82:SER:O	4:D:85:SER:OG	2.25	0.52
5:E:209:VAL:O	5:E:210:GLN:HB2	2.10	0.52
7:G:93:ASN:O	7:G:128:TYR:OH	2.27	0.52
16:Q:239:ALA:HA	16:Q:257:LEU:HD13	1.92	0.52
16:Q:774:SER:O	16:Q:830:ARG:NH2	2.41	0.52
2:B:1010:LYS:HE3	20:V:130:TRP:CZ3	2.43	0.52
4:D:63:LYS:HA	4:D:66:ASN:HD21	1.75	0.52
4:D:63:LYS:HE2	7:G:102:GLY:O	2.10	0.52
16:Q:380:ILE:HD12	16:Q:400:HIS:HE1	1.75	0.52
17:R:458:ALA:HB3	17:R:459:MET:HE2	1.91	0.52
21:W:39:SER:HB2	21:W:41:ASP:OD1	2.10	0.52
21:W:217:TYR:HA	21:W:224:LEU:HA	1.91	0.52
1:A:525:ILE:O	1:A:534:VAL:HG22	2.09	0.52
1:A:1229:GLU:O	1:A:1233:GLU:HG3	2.10	0.52
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.92	0.52
7:G:7:LEU:O	7:G:72:TYR:N	2.27	0.52
16:Q:790:HIS:HA	16:Q:793:PHE:CD2	2.45	0.52
21:W:176:ASP:HB2	21:W:183:LEU:HD21	1.92	0.52
24:Z:588:ASP:HA	24:Z:640:THR:O	2.10	0.52
1:A:1546:PHE:HD2	13:M:1516:GLN:HG3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:388:TYR:OH	2:B:524:LYS:HE3	2.10	0.51
2:B:651:TYR:HB2	19:U:460:TYR:CZ	2.44	0.51
5:E:67:ASP:OD2	5:E:69:THR:OG1	2.22	0.51
16:Q:240:VAL:HG21	16:Q:270:MET:HE3	1.90	0.51
16:Q:768:VAL:HG13	16:Q:769:LEU:HG	1.91	0.51
19:U:394:TYR:C	20:V:172:ARG:HH21	2.18	0.51
1:A:922:PHE:N	1:A:1052:ARG:HH11	2.09	0.51
4:D:63:LYS:HD3	7:G:103:PRO:HA	1.92	0.51
17:R:581:ALA:O	17:R:585:ASN:ND2	2.43	0.51
24:Z:568:VAL:HG13	24:Z:570:VAL:HG13	1.91	0.51
2:B:1062:ARG:CZ	2:B:1074:PRO:HB3	2.39	0.51
7:G:118:GLU:HG2	7:G:129:LYS:O	2.11	0.51
24:Z:206:THR:OG1	24:Z:207:ASP:N	2.43	0.51
24:Z:232:GLN:HE21	24:Z:252:GLN:HB2	1.75	0.51
24:Z:454:HIS:HE2	24:Z:463:PHE:HE2	1.58	0.51
1:A:43:TYR:HB3	1:A:45:GLU:OE1	2.11	0.51
1:A:695:ASP:O	1:A:697:LYS:N	2.39	0.51
10:J:21:TYR:HB2	10:J:38:LEU:HD11	1.92	0.51
13:M:1443:LEU:HD13	13:M:1473:LEU:HD22	1.92	0.51
9:I:81:THR:HG23	9:I:96:PHE:CE1	2.45	0.51
13:M:1473:LEU:HD11	13:M:1484:ILE:HD12	1.92	0.51
14:N:34:DC:H2''	14:N:35:DA:H8	1.76	0.51
24:Z:470:LYS:HD2	24:Z:472:PHE:CZ	2.46	0.51
24:Z:745:VAL:HG11	24:Z:750:LEU:HD21	1.92	0.51
2:B:851:ASP:HB2	12:L:15:MET:HG2	1.91	0.51
2:B:997:GLY:HA2	20:V:131:MET:HG2	1.91	0.51
4:D:123:GLU:OE1	4:D:123:GLU:N	2.44	0.51
16:Q:513:PHE:HB2	21:W:213:TYR:HE1	1.75	0.51
22:X:248:ASN:OD1	22:X:249:ILE:HG13	2.10	0.51
24:Z:478:VAL:HG22	24:Z:490:GLY:O	2.11	0.51
1:A:927:GLU:HG3	1:A:943:LEU:HD11	1.92	0.51
2:B:993:LYS:HG2	2:B:1018:TYR:OH	2.11	0.51
16:Q:744:ARG:HG2	16:Q:748:PRO:HA	1.93	0.51
17:R:417:LEU:N	17:R:420:THR:O	2.40	0.51
20:V:193:HIS:H	20:V:197:PRO:HA	1.73	0.51
21:W:17:ASP:HB2	21:W:41:ASP:HB3	1.93	0.51
21:W:22:VAL:HG23	21:W:37:THR:HG22	1.92	0.51
1:A:428:ASP:OD1	1:A:430:ARG:NH1	2.44	0.51
2:B:177:CYS:SG	2:B:737:ILE:HD11	2.50	0.51
5:E:84:ILE:HG12	5:E:114:ALA:HA	1.92	0.51
16:Q:530:TYR:HD2	16:Q:533:CYS:HB2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:682:ASP:OD1	16:Q:683:VAL:N	2.43	0.51
18:T:36:DC:C2	18:T:37:DC:C5	2.99	0.51
23:Y:45:ASN:HD21	23:Y:48:MET:HB2	1.75	0.51
24:Z:478:VAL:O	24:Z:489:THR:HG23	2.11	0.51
1:A:120:ASP:O	1:A:122:ASN:ND2	2.44	0.51
1:A:419:ILE:HD12	1:A:440:LEU:HD23	1.92	0.51
1:A:1474:LEU:HB2	6:F:105:ILE:HG12	1.93	0.51
2:B:624:PRO:HA	2:B:663:GLU:O	2.09	0.51
7:G:46:ILE:HD11	7:G:77:PHE:CB	2.40	0.51
16:Q:244:ASN:HD22	20:V:69:GLN:HA	1.76	0.51
17:R:493:GLU:O	17:R:496:VAL:HG22	2.11	0.51
21:W:110:TRP:H	21:W:123:THR:HG23	1.76	0.51
24:Z:312:ASP:O	24:Z:315:ARG:HG2	2.11	0.51
1:A:44:PRO:HG2	1:A:285:LYS:HD3	1.93	0.51
1:A:725:LEU:HD23	1:A:733:LEU:HD11	1.93	0.51
1:A:1370:GLY:HA2	5:E:178:PRO:HD2	1.93	0.51
1:A:1423:ASP:OD2	1:A:1423:ASP:N	2.38	0.51
16:Q:815:ARG:O	16:Q:818:SER:OG	2.25	0.51
17:R:454:LYS:NZ	17:R:458:ALA:HB2	2.26	0.51
21:W:44:VAL:HB	21:W:60:LEU:HB2	1.93	0.51
21:W:231:HIS:ND1	21:W:251:SER:HB3	2.26	0.51
22:X:252:ILE:HG13	22:X:253:LEU:N	2.26	0.51
23:Y:40:LEU:HD21	23:Y:52:CYS:SG	2.51	0.51
1:A:410:ASN:HD22	1:A:430:ARG:HD2	1.76	0.50
1:A:1176:TYR:C	1:A:1177:TYR:HD1	2.19	0.50
1:A:1288:ILE:HA	1:A:1291:ASN:ND2	2.27	0.50
1:A:1314:THR:OG1	1:A:1316:ASN:OD1	2.29	0.50
2:B:56:GLN:HG2	2:B:91:ILE:HG22	1.92	0.50
5:E:21:CYS:O	5:E:26:TYR:HB2	2.11	0.50
7:G:91:GLN:HA	7:G:139:GLN:NE2	2.26	0.50
16:Q:93:TYR:HB3	16:Q:113:ALA:HB2	1.93	0.50
17:R:431:GLY:N	17:R:459:MET:HE1	2.26	0.50
19:U:373:LEU:HD23	19:U:375:PHE:H	1.76	0.50
21:W:159:ASP:OD2	21:W:161:LYS:HE3	2.11	0.50
21:W:295:ASP:OD2	21:W:297:GLU:HB2	2.11	0.50
24:Z:436:LEU:HB3	24:Z:454:HIS:CE1	2.45	0.50
2:B:848:LEU:HD23	2:B:865:VAL:HG13	1.93	0.50
16:Q:106:LYS:O	16:Q:110:ILE:HG12	2.12	0.50
21:W:116:PRO:HD3	21:W:156:TYR:HB3	1.92	0.50
24:Z:215:VAL:HG12	24:Z:227:VAL:HG23	1.94	0.50
1:A:202:TRP:HE3	1:A:212:LYS:HB2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:GLY:O	1:A:521:VAL:HG23	2.12	0.50
1:A:1177:TYR:CE1	1:A:1210:TRP:HB3	2.46	0.50
4:D:37:VAL:HG21	7:G:2:PHE:HD2	1.75	0.50
13:M:1398:LEU:HD23	13:M:1400:ILE:HG23	1.93	0.50
13:M:1494:PHE:HE2	13:M:1504:VAL:HG12	1.75	0.50
17:R:452:PHE:HB3	17:R:453:MET:HE2	1.93	0.50
23:Y:63:MET:SD	23:Y:72:SER:HB2	2.51	0.50
1:A:140:ARG:O	1:A:144:VAL:HG13	2.11	0.50
1:A:383:SER:HB3	11:K:2:ASN:HD21	1.76	0.50
2:B:130:LYS:HB3	2:B:142:THR:HG23	1.94	0.50
4:D:61:PHE:O	4:D:65:LEU:HG	2.11	0.50
16:Q:38:HIS:CE1	16:Q:73:LEU:HD22	2.47	0.50
16:Q:164:PRO:HA	16:Q:167:LEU:HB2	1.93	0.50
16:Q:310:TYR:CE2	16:Q:342:LEU:HD13	2.46	0.50
16:Q:635:ILE:O	16:Q:639:VAL:HG22	2.11	0.50
16:Q:880:GLN:HB2	16:Q:884:LYS:HZ3	1.75	0.50
17:R:441:PHE:HA	24:Z:776:PRO:O	2.11	0.50
18:T:9:DC:H2'	18:T:10:DT:H71	1.92	0.50
4:D:33:LEU:HB2	4:D:36:GLU:HB2	1.93	0.50
14:N:39:DA:C6	14:N:40:DG:C6	3.00	0.50
15:P:39:A:H2'	15:P:40:A:C8	2.47	0.50
16:Q:163:ILE:HB	16:Q:164:PRO:HD3	1.94	0.50
16:Q:841:LEU:HD23	16:Q:844:LYS:HD3	1.93	0.50
17:R:404:GLU:O	17:R:428:LEU:HA	2.11	0.50
21:W:231:HIS:ND1	21:W:235:VAL:HG22	2.26	0.50
24:Z:440:ILE:HA	24:Z:450:ILE:HD11	1.94	0.50
1:A:123:ASN:HD22	1:A:125:LYS:HD3	1.75	0.50
1:A:738:GLU:OE2	1:A:797:ARG:NH1	2.45	0.50
2:B:169:ARG:NH2	20:V:139:THR:O	2.43	0.50
2:B:1142:ASN:ND2	2:B:1145:GLN:O	2.45	0.50
2:B:1142:ASN:O	2:B:1144:THR:HG22	2.10	0.50
3:C:9:VAL:HG11	11:K:105:PHE:HD1	1.75	0.50
5:E:47:LYS:O	5:E:53:PRO:HD2	2.11	0.50
5:E:64:HIS:HB2	5:E:70:ASP:OD1	2.12	0.50
15:P:38:G:N3	15:P:39:A:C8	2.80	0.50
18:T:37:DC:H2''	18:T:38:DG:C8	2.46	0.50
1:A:324:GLY:O	1:A:325:LEU:HD22	2.12	0.50
1:A:1147:SER:OG	1:A:1351:ASP:OD1	2.29	0.50
5:E:36:THR:OG1	5:E:39:GLU:OE1	2.29	0.50
16:Q:166:LEU:HA	16:Q:169:LYS:NZ	2.26	0.50
16:Q:837:GLU:O	16:Q:840:GLU:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:414:VAL:HG22	17:R:423:ASN:HB3	1.94	0.50
1:A:651:SER:O	1:A:655:ILE:HG12	2.11	0.50
2:B:44:LEU:HD23	2:B:155:MET:HE3	1.92	0.50
13:M:1347:MET:HB2	13:M:1372:LYS:HE3	1.94	0.50
16:Q:288:VAL:HG13	16:Q:289:GLN:HG3	1.93	0.50
24:Z:444:ASP:HB3	24:Z:448:ILE:HA	1.93	0.50
1:A:894:ASP:HB3	5:E:200:ALA:HB2	1.93	0.49
2:B:1022:LEU:HD23	2:B:1022:LEU:H	1.76	0.49
7:G:46:ILE:HD11	7:G:77:PHE:HB3	1.94	0.49
14:N:39:DA:H2'	14:N:40:DG:C8	2.47	0.49
16:Q:163:ILE:O	16:Q:166:LEU:HG	2.12	0.49
21:W:258:VAL:O	21:W:267:VAL:HG22	2.11	0.49
1:A:833:PRO:HB2	2:B:677:MET:SD	2.52	0.49
2:B:728:MET:SD	2:B:942:LYS:HB3	2.52	0.49
2:B:898:THR:C	2:B:899:SER:HG	2.10	0.49
3:C:86:ARG:NH1	24:Z:716:PRO:O	2.45	0.49
4:D:133:ASP:O	4:D:137:LYS:HG2	2.12	0.49
5:E:177:ASP:O	5:E:181:ARG:HG3	2.11	0.49
16:Q:524:LEU:HD11	16:Q:537:LEU:HD12	1.94	0.49
16:Q:735:GLU:OE1	16:Q:738:GLN:HB2	2.13	0.49
17:R:403:ALA:HB3	17:R:428:LEU:HD13	1.93	0.49
21:W:65:LEU:HG	21:W:85:ASP:HB3	1.94	0.49
22:X:233:THR:HG22	22:X:236:THR:HG23	1.94	0.49
24:Z:529:ASP:HB3	24:Z:553:LEU:HD23	1.94	0.49
1:A:1374:VAL:HG11	1:A:1411:LEU:HD21	1.93	0.49
2:B:218:THR:HG22	2:B:236:TRP:HD1	1.77	0.49
10:J:22:LEU:HD22	17:R:563:ILE:HG21	1.94	0.49
16:Q:743:ALA:O	16:Q:746:VAL:HG22	2.12	0.49
16:Q:829:ALA:HA	16:Q:832:ARG:HD2	1.94	0.49
1:A:742:ASN:O	1:A:746:ASN:ND2	2.45	0.49
2:B:237:VAL:HG11	2:B:369:VAL:HG22	1.94	0.49
19:U:448:MET:HE2	19:U:461:LYS:HB3	1.94	0.49
20:V:126:LYS:HE3	20:V:126:LYS:HA	1.94	0.49
24:Z:470:LYS:HB3	24:Z:472:PHE:HE2	1.78	0.49
24:Z:588:ASP:HB3	24:Z:594:ILE:HG13	1.95	0.49
1:A:316:THR:HA	1:A:319:ASP:O	2.11	0.49
1:A:428:ASP:OD1	1:A:430:ARG:HG3	2.11	0.49
1:A:441:GLN:HG2	1:A:444:TYR:CE2	2.47	0.49
4:D:44:ARG:HA	4:D:47:GLN:OE1	2.12	0.49
16:Q:183:LEU:O	16:Q:187:LYS:HG2	2.13	0.49
17:R:363:ARG:HE	17:R:446:GLU:HG2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:410:GLU:HA	17:R:424:LYS:HA	1.93	0.49
17:R:416:GLN:HE21	17:R:421:ARG:CZ	2.26	0.49
17:R:471:GLU:O	17:R:474:LYS:HG3	2.13	0.49
2:B:537:GLN:HG3	2:B:538:PRO:HD2	1.93	0.49
2:B:626:LEU:HD13	2:B:698:ILE:HG12	1.94	0.49
14:N:35:DA:H2"	14:N:36:DG:H8	1.75	0.49
16:Q:68:ARG:NE	16:Q:89:LEU:HD12	2.27	0.49
21:W:228:LEU:HD11	21:W:259:TRP:CZ3	2.48	0.49
1:A:587:THR:HG22	1:A:588:GLY:N	2.27	0.49
7:G:151:ARG:HG3	24:Z:477:HIS:NE2	2.26	0.49
8:H:60:ILE:HD11	8:H:123:MET:HE1	1.93	0.49
13:M:1374:SER:HB2	13:M:1377:ILE:HD13	1.93	0.49
13:M:1485:GLU:OE1	13:M:1497:ARG:NE	2.34	0.49
16:Q:750:ASP:HB3	16:Q:753:LEU:HG	1.93	0.49
21:W:108:ASP:HB3	21:W:125:THR:HG23	1.95	0.49
1:A:299:ALA:C	1:A:301:HIS:H	2.20	0.49
1:A:1128:ILE:CG2	1:A:1414:ILE:HB	2.43	0.49
2:B:130:LYS:NZ	2:B:429:PHE:O	2.46	0.49
4:D:60:VAL:HG11	7:G:44:PHE:CZ	2.48	0.49
7:G:110:ARG:HD2	7:G:113:ILE:HB	1.95	0.49
12:L:16:ILE:HG13	12:L:26:ASN:O	2.13	0.49
17:R:416:GLN:HG2	17:R:421:ARG:HB3	1.95	0.49
19:U:453:GLY:HA2	20:V:185:ASP:OD2	2.12	0.49
22:X:242:GLY:O	22:X:243:LYS:HE2	2.13	0.49
24:Z:257:ILE:O	24:Z:260:MET:HG2	2.13	0.49
1:A:54:LEU:O	1:A:61:ARG:NH2	2.45	0.49
1:A:496:PHE:HB2	2:B:791:GLU:O	2.12	0.49
1:A:963:ARG:O	1:A:967:ARG:HG3	2.13	0.49
1:A:1000:LEU:O	1:A:1059:ARG:NH1	2.45	0.49
2:B:22:TRP:CZ2	2:B:679:PRO:HG3	2.48	0.49
2:B:824:ASP:O	2:B:872:THR:HG23	2.13	0.49
13:M:783:GLY:N	13:M:797:ALA:O	2.46	0.49
17:R:358:GLU:HA	17:R:361:ARG:NE	2.27	0.49
17:R:389:ILE:O	17:R:400:TYR:HD1	1.95	0.49
24:Z:199:LYS:HG2	24:Z:210:LEU:HD21	1.93	0.49
24:Z:426:VAL:HG21	24:Z:468:LEU:HD13	1.95	0.49
1:A:926:ASN:O	1:A:930:LEU:HG	2.13	0.49
1:A:1007:ILE:HD12	1:A:1007:ILE:HA	1.63	0.49
14:N:37:DG:N2	18:T:12:DC:C2	2.77	0.49
16:Q:128:GLN:HA	16:Q:158:GLN:NE2	2.26	0.49
16:Q:129:ASN:OD1	16:Q:132:LEU:HD13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:416:GLN:HA	17:R:421:ARG:HA	1.94	0.49
21:W:65:LEU:HD12	21:W:84:LEU:C	2.38	0.49
1:A:1311:LEU:HD22	1:A:1332:GLN:HG2	1.95	0.48
2:B:431:LEU:HD23	2:B:431:LEU:H	1.77	0.48
2:B:679:PRO:HG2	2:B:680:ASP:H	1.78	0.48
2:B:816:GLU:OE2	2:B:869:LYS:HE3	2.13	0.48
2:B:1120:ASN:HD22	2:B:1145:GLN:HB3	1.77	0.48
4:D:108:ALA:N	4:D:128:GLN:OE1	2.46	0.48
16:Q:764:LEU:HD22	16:Q:785:GLU:OE1	2.12	0.48
17:R:563:ILE:O	17:R:566:ARG:HG2	2.13	0.48
21:W:35:VAL:O	21:W:47:TRP:N	2.44	0.48
1:A:84:HIS:H	1:A:84:HIS:CD2	2.31	0.48
1:A:1073:GLU:HG3	1:A:1074:SER:N	2.28	0.48
1:A:1087:VAL:HG23	1:A:1400:LEU:HD21	1.95	0.48
2:B:92:TYR:HD1	19:U:506:ALA:HB3	1.79	0.48
2:B:650:ASN:C	19:U:460:TYR:CE2	2.91	0.48
2:B:910:THR:OG1	2:B:911:LEU:N	2.46	0.48
7:G:90:THR:HG23	7:G:99:THR:HA	1.95	0.48
8:H:36:LYS:CE	16:Q:709:ARG:HH12	2.26	0.48
9:I:96:PHE:HA	9:I:111:TYR:O	2.13	0.48
16:Q:663:PHE:HB3	16:Q:690:ILE:HG23	1.95	0.48
21:W:204:LEU:HD22	21:W:216:ILE:HG22	1.95	0.48
23:Y:33:CYS:SG	23:Y:36:CYS:N	2.85	0.48
24:Z:735:GLU:HG3	24:Z:735:GLU:O	2.13	0.48
1:A:1400:LEU:O	1:A:1404:THR:HG23	2.14	0.48
8:H:13:LYS:HG3	8:H:31:GLU:HG2	1.95	0.48
16:Q:188:LYS:HB3	16:Q:191:ARG:NH1	2.29	0.48
16:Q:236:VAL:O	16:Q:240:VAL:HG23	2.13	0.48
16:Q:454:LEU:HB3	16:Q:477:SER:OG	2.13	0.48
16:Q:855:LYS:O	16:Q:858:LYS:HG3	2.13	0.48
23:Y:56:SER:HA	24:Z:271:ALA:HA	1.96	0.48
24:Z:436:LEU:HD13	24:Z:454:HIS:CD2	2.49	0.48
24:Z:746:ASP:OD1	24:Z:747:ARG:N	2.46	0.48
1:A:1467:GLY:C	1:A:1469:GLY:H	2.21	0.48
2:B:299:GLU:HA	2:B:302:LYS:HD3	1.95	0.48
3:C:74:THR:HG23	3:C:128:ILE:O	2.14	0.48
5:E:114:ALA:O	5:E:117:SER:OG	2.23	0.48
16:Q:80:LYS:O	16:Q:84:THR:HG23	2.13	0.48
16:Q:268:ASN:HB3	16:Q:271:VAL:HG12	1.95	0.48
16:Q:854:GLN:HB2	16:Q:855:LYS:NZ	2.28	0.48
19:U:522:THR:O	19:U:524:LYS:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:97:ASN:ND2	20:V:98:VAL:O	2.46	0.48
21:W:89:ARG:HA	21:W:101:SER:HA	1.94	0.48
1:A:111:CYS:SG	1:A:114:CYS:HB2	2.54	0.48
1:A:539:GLN:O	1:A:540:ASP:C	2.56	0.48
1:A:733:LEU:HB2	9:I:106:ASP:HB2	1.96	0.48
1:A:1049:LEU:HG	1:A:1054:MET:HE3	1.96	0.48
17:R:576:GLU:O	17:R:580:VAL:HG13	2.14	0.48
24:Z:548:GLY:CA	24:Z:562:ASN:HA	2.44	0.48
24:Z:615:ARG:HB2	24:Z:616:HIS:CD2	2.49	0.48
4:D:76:ASN:O	4:D:79:THR:OG1	2.31	0.48
11:K:93:ASP:OD1	11:K:93:ASP:N	2.41	0.48
15:P:40:A:C2	18:T:32:DT:N3	2.81	0.48
16:Q:211:LEU:HB2	16:Q:213:LYS:NZ	2.29	0.48
24:Z:342:ALA:HB1	24:Z:346:ARG:NH2	2.28	0.48
1:A:606:HIS:CG	1:A:607:SER:N	2.82	0.48
1:A:922:PHE:N	1:A:1052:ARG:HD2	2.19	0.48
1:A:1173:THR:HG23	1:A:1214:VAL:HG22	1.94	0.48
1:A:1184:THR:C	1:A:1186:VAL:N	2.64	0.48
1:A:1218:ARG:HH22	1:A:1253:GLU:HA	1.77	0.48
2:B:1007:ASN:N	2:B:1007:ASN:OD1	2.42	0.48
7:G:49:THR:OG1	7:G:50:THR:N	2.47	0.48
16:Q:56:LYS:HZ1	16:Q:59:GLU:HG3	1.78	0.48
16:Q:211:LEU:HB2	16:Q:213:LYS:HE3	1.94	0.48
16:Q:346:GLY:HA2	16:Q:349:GLN:HE21	1.79	0.48
16:Q:423:GLU:OE1	22:X:231:TRP:NE1	2.43	0.48
16:Q:568:TRP:CE2	16:Q:592:LEU:HD13	2.49	0.48
17:R:366:ARG:HH22	24:Z:773:SER:H	1.62	0.48
18:T:7:DA:H2"	18:T:8:DG:C8	2.48	0.48
21:W:76:LEU:HG	21:W:78:ILE:HG23	1.95	0.48
21:W:130:VAL:HG22	21:W:151:ILE:HG13	1.95	0.48
24:Z:206:THR:HG23	24:Z:208:THR:H	1.79	0.48
2:B:425:ARG:HH21	2:B:427:LYS:HD3	1.78	0.48
16:Q:542:ARG:NH2	16:Q:574:LEU:HA	2.28	0.48
17:R:359:LEU:HD22	17:R:452:PHE:CE1	2.48	0.48
17:R:370:GLU:HA	17:R:373:CYS:SG	2.54	0.48
21:W:46:VAL:HG11	21:W:58:TRP:HD1	1.78	0.48
21:W:89:ARG:HG2	21:W:101:SER:OG	2.13	0.48
21:W:110:TRP:CD2	21:W:150:PHE:HZ	2.32	0.48
24:Z:310:ARG:CZ	24:Z:337:GLN:HB2	2.44	0.48
24:Z:366:TYR:HB2	24:Z:374:LYS:HA	1.95	0.48
1:A:104:MET:CE	1:A:193:ARG:HD2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:VAL:O	1:A:491:PRO:HD2	2.14	0.48
1:A:1129:ASN:O	1:A:1131:SER:N	2.47	0.48
2:B:355:ASP:OD2	2:B:356:PHE:N	2.46	0.48
2:B:551:GLU:HB3	2:B:556:ILE:HD13	1.96	0.48
14:N:12:DG:C4	14:N:13:DG:C8	3.02	0.48
16:Q:153:HIS:HA	16:Q:169:LYS:HE3	1.96	0.48
16:Q:568:TRP:CZ2	16:Q:591:ILE:HB	2.48	0.48
16:Q:645:LYS:HD2	22:X:242:GLY:O	2.14	0.48
16:Q:835:ASP:O	16:Q:839:ARG:HG3	2.14	0.48
1:A:489:THR:HG23	1:A:494:ALA:HB3	1.96	0.48
1:A:557:ARG:O	1:A:561:MET:HG3	2.14	0.48
2:B:281:ASP:HB3	9:I:22:ASN:HA	1.95	0.48
2:B:1021:HIS:CE1	2:B:1023:ARG:HB2	2.49	0.48
7:G:38:CYS:SG	7:G:39:THR:N	2.87	0.48
7:G:82:GLY:N	7:G:147:ILE:O	2.34	0.48
7:G:101:ILE:N	7:G:104:MET:O	2.43	0.48
8:H:106:THR:OG1	8:H:107:GLU:N	2.47	0.48
16:Q:232:VAL:O	16:Q:236:VAL:HG22	2.13	0.48
16:Q:390:ASP:HB2	16:Q:392:GLU:OE1	2.14	0.48
16:Q:578:LYS:HB2	16:Q:580:GLU:HG3	1.94	0.48
16:Q:682:ASP:OD1	16:Q:683:VAL:HG13	2.14	0.48
16:Q:844:LYS:O	16:Q:848:GLU:HG3	2.14	0.48
17:R:359:LEU:HD11	17:R:386:PHE:CE2	2.49	0.48
19:U:443:TRP:HA	20:V:201:PRO:HA	1.95	0.48
21:W:237:ASN:ND2	21:W:279:GLY:HA2	2.21	0.48
21:W:248:VAL:HG13	21:W:282:TYR:OH	2.14	0.48
21:W:254:LYS:HB3	21:W:273:HIS:O	2.14	0.48
24:Z:426:VAL:HG13	24:Z:440:ILE:HD11	1.95	0.48
1:A:465:HIS:HD2	1:A:467:MET:HE2	1.79	0.47
1:A:495:ASP:HB3	1:A:499:ASP:OD2	2.14	0.47
1:A:896:LEU:HD13	1:A:980:PRO:HG3	1.95	0.47
1:A:1245:CYS:O	1:A:1246:ILE:HD13	2.13	0.47
1:A:1416:ARG:O	1:A:1420:ASN:HB2	2.14	0.47
3:C:92:GLU:HG2	24:Z:711:ARG:CZ	2.43	0.47
16:Q:39:THR:OG1	16:Q:43:ILE:HD13	2.14	0.47
16:Q:576:LEU:CD2	16:Q:585:GLN:HE22	2.27	0.47
16:Q:850:GLU:O	16:Q:854:GLN:NE2	2.44	0.47
17:R:363:ARG:HA	17:R:386:PHE:O	2.14	0.47
17:R:485:TYR:OH	17:R:489:ASP:OD2	2.32	0.47
1:A:141:LEU:HB2	1:A:236:LEU:O	2.14	0.47
2:B:166:LEU:HG	2:B:170:ASP:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:320:PHE:O	2:B:323:SER:OG	2.31	0.47
2:B:719:SER:OG	2:B:720:PRO:HD3	2.13	0.47
2:B:768:ARG:HG3	2:B:771:GLU:OE2	2.15	0.47
7:G:81:LYS:HG3	7:G:148:VAL:C	2.39	0.47
7:G:109:SER:HB2	24:Z:503:PHE:CE2	2.48	0.47
16:Q:128:GLN:NE2	20:V:86:LEU:HD13	2.26	0.47
16:Q:336:ALA:HB1	16:Q:339:SER:OG	2.14	0.47
16:Q:358:GLU:O	16:Q:361:SER:OG	2.32	0.47
16:Q:689:HIS:HA	16:Q:692:VAL:HG12	1.96	0.47
16:Q:753:LEU:O	16:Q:757:VAL:HG13	2.14	0.47
19:U:459:VAL:HG23	19:U:494:HIS:C	2.39	0.47
1:A:46:THR:HB	1:A:58:MET:HB2	1.96	0.47
1:A:376:ASP:HB3	1:A:522:PRO:HD3	1.95	0.47
1:A:1177:TYR:HD2	9:I:28:GLU:OE1	1.97	0.47
2:B:44:LEU:HD23	2:B:155:MET:CE	2.44	0.47
5:E:2:ASP:OD2	5:E:3:ASP:N	2.47	0.47
7:G:80:PHE:HB2	7:G:83:GLU:CD	2.40	0.47
10:J:64:PRO:HG2	10:J:65:LEU:H	1.78	0.47
21:W:191:MET:HB2	21:W:209:SER:HB3	1.96	0.47
1:A:10:ASP:O	2:B:1130:THR:HG21	2.14	0.47
1:A:406:VAL:HG13	1:A:429:LEU:HD11	1.97	0.47
1:A:514:GLU:OE1	2:B:1101:GLN:HB2	2.14	0.47
1:A:527:THR:HG22	1:A:532:ARG:O	2.14	0.47
1:A:760:LEU:HD22	1:A:764:ASN:HD22	1.79	0.47
1:A:1060:LEU:HA	1:A:1060:LEU:HD23	1.60	0.47
1:A:1083:PRO:HD2	6:F:58:THR:HG21	1.96	0.47
1:A:1263:ASN:N	1:A:1263:ASN:OD1	2.47	0.47
3:C:2:PRO:HB3	11:K:54:PRO:CD	2.44	0.47
5:E:78:GLU:OE1	5:E:78:GLU:N	2.48	0.47
8:H:45:ILE:HA	8:H:45:ILE:HD12	1.68	0.47
19:U:443:TRP:NE1	19:U:449:SER:OG	2.47	0.47
21:W:112:LEU:HB3	21:W:121:LEU:HD11	1.96	0.47
24:Z:626:CYS:HB3	24:Z:629:LEU:HD12	1.95	0.47
2:B:313:GLU:HG2	2:B:316:VAL:HG12	1.95	0.47
2:B:680:ASP:O	2:B:684:GLU:HG2	2.14	0.47
4:D:93:HIS:HB3	4:D:96:GLU:OE1	2.14	0.47
7:G:4:HIS:CG	7:G:73:LYS:HE3	2.50	0.47
16:Q:172:ILE:HG22	16:Q:176:LYS:HZ1	1.79	0.47
16:Q:786:LEU:HD21	16:Q:820:LEU:HB3	1.96	0.47
17:R:363:ARG:HG3	17:R:447:PHE:CZ	2.49	0.47
17:R:587:LYS:O	17:R:588:ASN:ND2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:TYR:CE2	1:A:215:LEU:HD13	2.49	0.47
1:A:1162:GLU:HG2	1:A:1163:HIS:N	2.29	0.47
7:G:119:PHE:HA	7:G:128:TYR:CD1	2.49	0.47
15:P:39:A:H2'	15:P:39:A:N3	2.29	0.47
16:Q:68:ARG:HE	16:Q:86:LEU:HD13	1.80	0.47
1:A:70:ARG:HD2	2:B:1131:ARG:HH12	1.79	0.47
1:A:416:ALA:HA	1:A:448:ARG:HA	1.97	0.47
1:A:513:ALA:O	1:A:517:GLU:HG2	2.14	0.47
1:A:1027:ASP:HB3	1:A:1030:SER:HB3	1.96	0.47
1:A:1177:TYR:CD2	9:I:28:GLU:OE1	2.68	0.47
2:B:1007:ASN:O	2:B:1011:ILE:HG13	2.14	0.47
4:D:122:PHE:HD1	4:D:126:GLU:CD	2.23	0.47
14:N:12:DG:C6	14:N:13:DG:C6	3.02	0.47
16:Q:76:ARG:HH11	16:Q:76:ARG:HG3	1.80	0.47
16:Q:143:ASP:N	16:Q:143:ASP:OD1	2.44	0.47
16:Q:721:LEU:HD11	20:V:31:CYS:HA	1.97	0.47
16:Q:737:LYS:HE3	16:Q:760:VAL:HG22	1.96	0.47
21:W:11:GLN:HB3	21:W:298:ILE:HB	1.97	0.47
24:Z:479:LYS:HD3	24:Z:521:CYS:HB2	1.96	0.47
1:A:724:GLU:OE1	1:A:724:GLU:N	2.47	0.47
1:A:951:GLU:HG2	1:A:1007:ILE:HD11	1.97	0.47
1:A:1236:ASN:O	1:A:1240:GLY:N	2.48	0.47
1:A:1415:THR:O	1:A:1419:VAL:HG22	2.14	0.47
2:B:255:ARG:CD	2:B:307:GLU:HG3	2.44	0.47
2:B:347:MET:HG3	2:B:347:MET:O	2.15	0.47
4:D:62:MET:O	4:D:66:ASN:ND2	2.47	0.47
16:Q:167:LEU:HD21	16:Q:189:ALA:HB2	1.96	0.47
16:Q:373:ASN:HB2	16:Q:376:GLU:HG2	1.96	0.47
16:Q:750:ASP:OD1	16:Q:752:VAL:N	2.48	0.47
1:A:621:ILE:HG23	1:A:621:ILE:O	2.14	0.47
1:A:831:LEU:HB3	1:A:835:GLU:HG3	1.97	0.47
2:B:84:TYR:HA	2:B:132:VAL:HA	1.97	0.47
4:D:79:THR:O	4:D:82:SER:OG	2.33	0.47
7:G:147:ILE:HG23	7:G:159:ALA:HB1	1.96	0.47
15:P:38:G:C2'	15:P:39:A:H8	2.24	0.47
16:Q:347:LEU:HB2	16:Q:363:CYS:SG	2.54	0.47
16:Q:411:ASP:HB3	16:Q:415:TRP:CZ3	2.50	0.47
16:Q:624:LYS:HA	16:Q:627:ARG:HE	1.79	0.47
16:Q:712:TYR:O	16:Q:713:LYS:HG3	2.15	0.47
16:Q:833:LYS:O	16:Q:836:GLU:HG3	2.15	0.47
17:R:573:VAL:O	17:R:576:GLU:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:5:TYR:CE1	21:W:303:CYS:HB3	2.50	0.47
24:Z:433:LEU:HD13	24:Z:461:LEU:HD13	1.96	0.47
1:A:1016:LEU:HD23	1:A:1045:LEU:HD21	1.97	0.47
2:B:690:CYS:SG	2:B:693:TYR:CZ	3.08	0.47
2:B:796:MET:HE2	2:B:796:MET:HB3	1.82	0.47
2:B:1136:GLU:CB	2:B:1143:LYS:HG2	2.44	0.47
7:G:113:ILE:HG22	7:G:114:PRO:O	2.15	0.47
8:H:112:LEU:HB2	8:H:132:LEU:HD12	1.97	0.47
9:I:84:HIS:CD2	9:I:125:GLU:OE1	2.68	0.47
16:Q:7:GLU:OE2	16:Q:18:GLU:HB3	2.14	0.47
16:Q:716:ASN:HB3	16:Q:719:VAL:HG22	1.96	0.47
20:V:96:PRO:HA	20:V:97:ASN:HA	1.57	0.47
24:Z:521:CYS:HB3	24:Z:523:GLU:OE1	2.15	0.47
1:A:71:CYS:HB3	1:A:74:CYS:O	2.15	0.46
1:A:239:GLU:HG3	1:A:240:PRO:HD2	1.96	0.46
2:B:451:GLY:HA2	2:B:467:SER:HB3	1.97	0.46
5:E:3:ASP:OD1	5:E:47:LYS:HD2	2.15	0.46
5:E:82:VAL:HG12	5:E:110:MET:CB	2.45	0.46
8:H:112:LEU:HA	8:H:112:LEU:HD23	1.59	0.46
12:L:16:ILE:HD12	12:L:27:GLU:OE2	2.16	0.46
13:M:848:VAL:O	13:M:883:GLU:N	2.48	0.46
14:N:42:DT:H2''	14:N:43:DG:C8	2.51	0.46
21:W:215:LYS:HG2	21:W:227:THR:HG22	1.97	0.46
23:Y:22:VAL:HB	23:Y:84:VAL:HG12	1.97	0.46
24:Z:547:VAL:HG12	24:Z:563:MET:SD	2.54	0.46
1:A:866:LYS:HG3	1:A:1432:PHE:CD1	2.49	0.46
1:A:1162:GLU:O	1:A:1300:GLY:HA3	2.15	0.46
2:B:19:PRO:C	2:B:21:LEU:H	2.23	0.46
2:B:425:ARG:NH2	2:B:427:LYS:HD3	2.30	0.46
4:D:48:ASN:HB3	4:D:57:LEU:HD11	1.97	0.46
7:G:5:ILE:O	7:G:73:LYS:HD2	2.15	0.46
13:M:1362:LYS:HD3	13:M:1363:GLY:N	2.31	0.46
16:Q:211:LEU:HB2	16:Q:213:LYS:HZ2	1.80	0.46
16:Q:366:LYS:HG3	16:Q:369:LYS:HZ3	1.80	0.46
16:Q:380:ILE:HB	16:Q:400:HIS:CE1	2.50	0.46
24:Z:571:ARG:H	24:Z:574:ALA:HB3	1.80	0.46
1:A:1474:LEU:HD12	6:F:105:ILE:HD11	1.97	0.46
2:B:285:LEU:HD12	2:B:285:LEU:HA	1.61	0.46
8:H:30:CYS:SG	8:H:56:PHE:HZ	2.39	0.46
11:K:7:PHE:CD2	11:K:11:LEU:HD12	2.50	0.46
13:M:1447:LEU:HA	13:M:1450:THR:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:43:C:H2'	15:P:44:A:O4'	2.16	0.46
16:Q:30:VAL:HA	16:Q:33:ILE:HG12	1.96	0.46
16:Q:830:ARG:HH21	16:Q:834:GLN:HG3	1.79	0.46
17:R:562:TYR:HB3	17:R:566:ARG:HH21	1.80	0.46
24:Z:340:PHE:HD2	24:Z:370:GLY:HA2	1.81	0.46
1:A:93:PRO:HG2	1:A:219:GLU:OE2	2.15	0.46
1:A:228:ILE:HG23	1:A:232:GLU:HG2	1.96	0.46
1:A:1148:ALA:HB1	1:A:1333:GLU:HB3	1.97	0.46
2:B:285:LEU:HD23	9:I:16:PHE:CZ	2.51	0.46
2:B:329:GLY:HA3	2:B:334:LYS:HB3	1.97	0.46
3:C:78:ILE:H	3:C:78:ILE:HG12	1.48	0.46
5:E:63:ALA:HB3	16:Q:880:GLN:HE22	1.80	0.46
5:E:153:LYS:O	5:E:157:THR:HG23	2.14	0.46
7:G:82:GLY:HA2	7:G:146:LYS:HE3	1.96	0.46
8:H:11:ASP:OD1	8:H:11:ASP:N	2.46	0.46
9:I:29:ASP:CB	9:I:34:ILE:HG13	2.45	0.46
16:Q:637:LYS:O	16:Q:641:ARG:HD3	2.15	0.46
21:W:151:ILE:HG23	21:W:165:SER:OG	2.15	0.46
1:A:1176:TYR:HD1	9:I:51:SER:O	1.99	0.46
1:A:1177:TYR:CE2	1:A:1210:TRP:HE3	2.34	0.46
1:A:1416:ARG:HD2	1:A:1434:GLU:OE2	2.15	0.46
2:B:566:LYS:HA	2:B:576:ILE:HD12	1.97	0.46
2:B:646:ARG:O	2:B:647:GLU:HG2	2.16	0.46
16:Q:386:ALA:HB1	16:Q:394:ARG:HG3	1.97	0.46
16:Q:452:GLU:OE1	16:Q:490:HIS:NE2	2.47	0.46
16:Q:527:HIS:CE1	22:X:220:VAL:HB	2.51	0.46
16:Q:834:GLN:O	16:Q:838:GLU:HG2	2.15	0.46
21:W:25:GLY:HA3	21:W:31:ASN:C	2.40	0.46
1:A:58:MET:HB2	1:A:58:MET:HE2	1.66	0.46
1:A:609:HIS:HA	1:A:626:THR:HG21	1.98	0.46
1:A:1305:SER:OG	1:A:1306:LYS:N	2.48	0.46
2:B:26:CYS:O	2:B:30:ILE:HG12	2.15	0.46
8:H:67:ASP:OD1	8:H:67:ASP:N	2.46	0.46
9:I:17:CYS:SG	9:I:18:GLN:N	2.89	0.46
9:I:75:ASP:OD1	9:I:77:THR:HG22	2.16	0.46
10:J:26:GLN:HA	17:R:566:ARG:HD2	1.98	0.46
16:Q:41:LEU:HD13	16:Q:75:TYR:HE2	1.81	0.46
16:Q:460:LEU:O	16:Q:464:LEU:HG	2.14	0.46
16:Q:855:LYS:HD3	16:Q:855:LYS:HA	1.59	0.46
17:R:574:GLU:HA	17:R:577:LYS:NZ	2.31	0.46
21:W:152:LEU:N	21:W:166:GLY:O	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:252:SER:HA	21:W:276:GLN:HB3	1.98	0.46
24:Z:182:VAL:O	24:Z:224:TYR:HB2	2.14	0.46
1:A:123:ASN:HB3	1:A:125:LYS:HG2	1.98	0.46
1:A:1547:SEP:HA	1:A:1548:PRO:HD3	1.78	0.46
2:B:133:ILE:HD12	2:B:139:GLN:HB3	1.98	0.46
2:B:548:TRP:CZ2	2:B:586:THR:HG21	2.51	0.46
7:G:111:HIS:ND1	24:Z:494:ARG:HB3	2.31	0.46
11:K:99:SER:O	11:K:103:GLU:HG3	2.16	0.46
16:Q:566:ASP:OD1	22:X:234:ARG:HD3	2.16	0.46
18:T:30:DG:H2'	18:T:31:DT:C6	2.50	0.46
19:U:469:ASN:HA	20:V:222:ARG:HA	1.98	0.46
21:W:46:VAL:CB	21:W:58:TRP:HB2	2.45	0.46
21:W:182:LEU:HD21	21:W:185:THR:OG1	2.16	0.46
21:W:233:SER:HB3	21:W:253:ASP:HB3	1.98	0.46
24:Z:571:ARG:HB2	24:Z:574:ALA:HB2	1.98	0.46
1:A:732:THR:HG23	1:A:735:GLN:OE1	2.14	0.46
1:A:1054:MET:SD	1:A:1060:LEU:HD12	2.56	0.46
16:Q:386:ALA:HB2	16:Q:393:LYS:CB	2.46	0.46
16:Q:563:ASP:O	16:Q:565:PRO:HD3	2.15	0.46
24:Z:182:VAL:HG23	24:Z:225:ILE:HG13	1.98	0.46
24:Z:239:ILE:O	24:Z:242:VAL:HG22	2.15	0.46
24:Z:539:LEU:O	24:Z:578:LYS:HB3	2.15	0.46
1:A:112:PHE:CZ	1:A:220:ARG:NH1	2.84	0.46
2:B:170:ASP:OD1	2:B:170:ASP:N	2.43	0.46
5:E:126:ILE:H	5:E:126:ILE:HD12	1.81	0.46
6:F:57:MET:HB2	6:F:123:LEU:HD13	1.98	0.46
8:H:143:LEU:HD12	8:H:143:LEU:HA	1.62	0.46
10:J:25:LEU:HD23	17:R:567:ASN:HD21	1.81	0.46
16:Q:265:ASP:OD1	16:Q:268:ASN:HB2	2.16	0.46
16:Q:289:GLN:O	16:Q:293:LEU:HD23	2.16	0.46
16:Q:872:LYS:O	16:Q:875:LEU:HG	2.16	0.46
18:T:37:DC:H6	18:T:37:DC:H5'	1.81	0.46
18:T:41:DC:H4'	24:Z:283:ARG:NE	2.21	0.46
20:V:88:ASN:O	20:V:90:ASP:N	2.49	0.46
21:W:86:ALA:HB1	21:W:105:GLY:HA2	1.97	0.46
24:Z:705:LEU:HD21	24:Z:747:ARG:HD2	1.96	0.46
1:A:37:THR:O	1:A:37:THR:OG1	2.30	0.46
1:A:117:LEU:HD21	1:A:232:GLU:HG3	1.98	0.46
1:A:347:GLU:HA	1:A:352:GLY:HA3	1.98	0.46
1:A:753:GLY:O	1:A:757:GLN:HG2	2.16	0.46
3:C:60:HIS:HB3	3:C:61:ASP:H	1.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:208:PHE:CD1	16:Q:213:LYS:HD2	2.51	0.46
16:Q:450:PRO:HB2	16:Q:452:GLU:HG2	1.98	0.46
19:U:378:LEU:HD23	19:U:382:LEU:O	2.16	0.46
24:Z:280:ARG:HG3	24:Z:386:VAL:HG13	1.98	0.46
24:Z:294:ASP:HB2	24:Z:306:LYS:HE2	1.98	0.46
24:Z:480:VAL:HG13	24:Z:487:GLY:H	1.81	0.46
1:A:465:HIS:HB3	1:A:1097:GLU:HG3	1.97	0.45
1:A:966:LEU:HA	1:A:966:LEU:HD23	1.74	0.45
1:A:1117:VAL:HA	1:A:1136:THR:HG21	1.97	0.45
2:B:236:TRP:HB2	2:B:259:THR:HB	1.98	0.45
2:B:646:ARG:C	2:B:648:TYR:N	2.73	0.45
2:B:684:GLU:OE2	2:B:684:GLU:HA	2.16	0.45
12:L:52:LEU:HA	12:L:52:LEU:HD12	1.69	0.45
16:Q:620:ARG:NH1	16:Q:659:HIS:O	2.47	0.45
17:R:429:ARG:NE	17:R:431:GLY:O	2.42	0.45
21:W:13:GLN:H	21:W:297:GLU:HG2	1.80	0.45
22:X:253:LEU:O	22:X:256:VAL:HG12	2.16	0.45
1:A:18:ILE:HD12	2:B:1171:MET:HB3	1.99	0.45
1:A:124:PRO:HA	1:A:127:LYS:CG	2.45	0.45
1:A:469:MET:HB3	1:A:469:MET:HE2	1.68	0.45
1:A:1254:LYS:HD3	1:A:1254:LYS:HA	1.77	0.45
1:A:1295:ASP:OD2	1:A:1295:ASP:N	2.46	0.45
1:A:1298:LEU:HA	1:A:1298:LEU:HD23	1.77	0.45
2:B:19:PRO:C	2:B:21:LEU:N	2.74	0.45
2:B:121:SER:HA	2:B:153:PRO:HA	1.98	0.45
2:B:255:ARG:HD3	2:B:307:GLU:HG3	1.98	0.45
2:B:621:ILE:HD13	2:B:621:ILE:HG21	1.66	0.45
2:B:1006:VAL:HG22	20:V:130:TRP:CB	2.45	0.45
4:D:38:HIS:HB2	4:D:68:THR:OG1	2.16	0.45
11:K:71:ILE:HG21	11:K:71:ILE:HD13	1.61	0.45
16:Q:64:LEU:HA	16:Q:64:LEU:HD23	1.82	0.45
17:R:565:GLN:HA	17:R:568:ARG:CZ	2.47	0.45
20:V:38:SER:OG	20:V:39:LEU:N	2.49	0.45
21:W:7:ILE:HA	21:W:301:TYR:HA	1.98	0.45
21:W:233:SER:OG	21:W:252:SER:N	2.44	0.45
23:Y:35:ASN:ND2	23:Y:85:TYR:OH	2.49	0.45
24:Z:470:LYS:HB3	24:Z:472:PHE:CE2	2.51	0.45
1:A:189:PRO:HB2	1:A:201:GLU:H	1.81	0.45
1:A:989:ASN:O	1:A:993:ILE:HG13	2.16	0.45
1:A:1371:ILE:HD11	1:A:1406:THR:HB	1.99	0.45
2:B:317:ALA:O	2:B:321:ILE:HD12	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:650:ASN:C	19:U:460:TYR:HE2	2.25	0.45
2:B:681:ASP:OD2	2:B:681:ASP:N	2.50	0.45
11:K:51:LEU:HA	11:K:51:LEU:HD23	1.62	0.45
14:N:12:DG:C4	14:N:13:DG:N7	2.84	0.45
1:A:317:MET:HE2	1:A:317:MET:HB3	1.80	0.45
1:A:1044:HIS:O	1:A:1048:THR:HG23	2.17	0.45
1:A:1222:THR:C	1:A:1225:LYS:H	2.23	0.45
2:B:757:PRO:HB2	2:B:760:THR:HG22	1.99	0.45
3:C:92:GLU:HG2	24:Z:711:ARG:NH1	2.32	0.45
8:H:70:LEU:HD12	8:H:70:LEU:HA	1.76	0.45
9:I:73:SER:O	9:I:80:ARG:NH2	2.50	0.45
9:I:74:GLN:H	9:I:74:GLN:HG2	1.51	0.45
9:I:91:HIS:CD2	9:I:93:GLU:H	2.35	0.45
16:Q:474:PHE:CB	16:Q:503:LEU:HD13	2.46	0.45
16:Q:591:ILE:HG22	16:Q:592:LEU:HD12	1.97	0.45
23:Y:116:LYS:HD3	23:Y:116:LYS:HA	1.74	0.45
24:Z:469:ARG:NH2	24:Z:497:GLU:O	2.49	0.45
1:A:388:MET:HB3	1:A:388:MET:HE2	1.42	0.45
1:A:539:GLN:C	1:A:541:THR:N	2.74	0.45
1:A:775:LYS:HD2	2:B:974:SER:HB3	1.97	0.45
2:B:332:LYS:HB3	2:B:332:LYS:HE3	1.57	0.45
2:B:388:TYR:HB2	2:B:504:THR:HG23	1.99	0.45
2:B:395:LEU:HA	2:B:395:LEU:HD23	1.67	0.45
3:C:44:ILE:HD13	3:C:44:ILE:HG21	1.48	0.45
7:G:151:ARG:NE	7:G:153:ASP:OD1	2.50	0.45
21:W:235:VAL:HA	21:W:251:SER:HA	1.98	0.45
23:Y:66:PRO:HD3	23:Y:82:PRO:HG3	1.98	0.45
1:A:455:ILE:HD12	1:A:520:MET:HE1	1.98	0.45
2:B:834:ARG:HH22	2:B:842:HIS:HA	1.80	0.45
14:N:12:DG:N1	18:T:38:DG:N2	2.64	0.45
16:Q:246:LYS:HD2	16:Q:246:LYS:HA	1.73	0.45
16:Q:620:ARG:HH22	16:Q:660:LYS:HA	1.81	0.45
17:R:388:ARG:HD3	17:R:445:GLN:HB2	1.99	0.45
17:R:570:TRP:CD1	20:V:133:LYS:HD2	2.43	0.45
20:V:103:ALA:O	20:V:107:LEU:HG	2.17	0.45
20:V:282:ALA:C	20:V:284:GLU:H	2.25	0.45
21:W:29:LYS:HE2	21:W:75:THR:HA	1.99	0.45
21:W:254:LYS:HG2	21:W:275:ASP:C	2.42	0.45
22:X:222:ARG:HA	22:X:225:VAL:HG22	1.97	0.45
23:Y:65:SER:O	23:Y:65:SER:OG	2.33	0.45
1:A:111:CYS:HG	1:A:114:CYS:HB2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:825:ASN:ND2	1:A:835:GLU:OE1	2.47	0.45
1:A:1182:GLN:C	1:A:1192:TRP:HE1	2.18	0.45
1:A:1369:LEU:HD23	1:A:1369:LEU:HA	1.73	0.45
2:B:155:MET:HE3	2:B:183:GLY:HA2	1.99	0.45
2:B:332:LYS:C	2:B:332:LYS:HD2	2.41	0.45
2:B:1134:THR:O	2:B:1134:THR:HG23	2.17	0.45
4:D:74:PHE:CE2	4:D:80:ILE:HG12	2.52	0.45
5:E:26:TYR:CZ	5:E:72:MET:HE3	2.52	0.45
16:Q:763:ARG:HE	20:V:25:GLU:N	2.14	0.45
17:R:566:ARG:HA	17:R:569:GLU:OE1	2.16	0.45
21:W:56:LEU:HD21	21:W:59:SER:OG	2.16	0.45
24:Z:546:THR:HG22	24:Z:547:VAL:N	2.32	0.45
1:A:291:ARG:HG3	1:A:292:ARG:N	2.32	0.45
1:A:1226:LEU:HA	1:A:1230:GLN:NE2	2.31	0.45
2:B:357:CYS:SG	2:B:360:LYS:NZ	2.85	0.45
2:B:651:TYR:N	19:U:460:TYR:OH	2.49	0.45
2:B:714:PRO:CD	2:B:1001:PRO:HG3	2.47	0.45
2:B:1104:ARG:O	2:B:1108:PHE:HB3	2.16	0.45
3:C:45:ILE:HG22	3:C:165:ALA:HB1	1.98	0.45
4:D:32:LEU:HD23	4:D:32:LEU:HA	1.83	0.45
13:M:1463:CYS:SG	13:M:1464:ALA:N	2.90	0.45
16:Q:123:ILE:HG23	16:Q:124:ILE:H	1.82	0.45
16:Q:134:ARG:HA	16:Q:134:ARG:HD2	1.76	0.45
16:Q:170:ALA:HB2	16:Q:185:TYR:HB2	1.99	0.45
17:R:402:VAL:HG23	17:R:451:GLU:HG2	1.98	0.45
20:V:190:ILE:O	20:V:190:ILE:HG13	2.17	0.45
21:W:64:GLN:OE1	21:W:89:ARG:NH2	2.48	0.45
24:Z:243:GLY:O	24:Z:246:ARG:HG2	2.17	0.45
2:B:319:ASN:HD21	2:B:332:LYS:HG2	1.82	0.45
8:H:64:LEU:HD23	8:H:64:LEU:HA	1.79	0.45
16:Q:386:ALA:HB2	16:Q:393:LYS:HB3	1.99	0.45
17:R:356:PRO:HB3	17:R:452:PHE:CB	2.47	0.45
1:A:557:ARG:HG3	1:A:558:GLY:N	2.27	0.45
2:B:479:LEU:O	2:B:483:ARG:HG3	2.17	0.45
5:E:185:ILE:HD12	5:E:209:VAL:HG21	1.98	0.45
16:Q:24:LEU:HD11	16:Q:56:LYS:HZ3	1.82	0.45
16:Q:95:GLN:HG3	20:V:85:ASP:OD1	2.17	0.45
16:Q:131:LEU:HD12	16:Q:155:VAL:HG22	1.98	0.45
16:Q:133:GLY:HA2	16:Q:136:CYS:SG	2.57	0.45
16:Q:200:VAL:HA	20:V:82:VAL:HG22	1.97	0.45
16:Q:380:ILE:HG21	16:Q:396:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:568:TRP:CE3	16:Q:592:LEU:HB2	2.51	0.45
16:Q:736:CYS:O	16:Q:739:THR:HG22	2.17	0.45
23:Y:8:LYS:HE2	23:Y:27:GLN:NE2	2.32	0.45
24:Z:272:ASN:ND2	24:Z:384:GLU:HB2	2.32	0.45
24:Z:729:GLU:O	24:Z:747:ARG:NH2	2.50	0.45
1:A:74:CYS:SG	1:A:81:CYS:HB2	2.56	0.44
1:A:902:GLU:O	1:A:978:VAL:HA	2.17	0.44
1:A:1040:LEU:HA	1:A:1040:LEU:HD12	1.75	0.44
1:A:1118:THR:HG21	1:A:1135:LYS:HB2	1.99	0.44
2:B:407:MET:HE1	2:B:443:GLY:C	2.42	0.44
2:B:655:ASP:O	2:B:659:SER:HB3	2.17	0.44
7:G:4:HIS:CD2	7:G:73:LYS:HE3	2.52	0.44
8:H:111:ARG:HA	8:H:128:ASP:HA	1.99	0.44
8:H:150:PHE:C	22:X:242:GLY:HA3	2.43	0.44
15:P:37:G:H2'	15:P:38:G:C8	2.52	0.44
20:V:75:LEU:HD12	20:V:75:LEU:HA	1.82	0.44
21:W:37:THR:HA	21:W:70:VAL:HG21	1.99	0.44
1:A:57:LEU:HA	1:A:57:LEU:HD23	1.73	0.44
1:A:465:HIS:NE2	1:A:467:MET:HB2	2.31	0.44
2:B:67:LEU:HD13	2:B:420:GLN:OE1	2.17	0.44
2:B:594:MET:HE3	2:B:594:MET:HB3	1.75	0.44
4:D:93:HIS:CE1	4:D:94:LYS:HG3	2.52	0.44
14:N:44:DG:H2''	14:N:45:DG:C8	2.51	0.44
16:Q:716:ASN:OD1	16:Q:717:THR:N	2.50	0.44
17:R:428:LEU:HB2	17:R:437:PHE:CE2	2.52	0.44
21:W:17:ASP:CG	21:W:40:LEU:HB3	2.42	0.44
23:Y:19:CYS:SG	23:Y:35:ASN:ND2	2.84	0.44
24:Z:280:ARG:HB2	24:Z:382:ILE:HG23	2.00	0.44
2:B:139:GLN:OE1	2:B:139:GLN:N	2.49	0.44
2:B:718:GLN:HG2	2:B:720:PRO:HD2	1.99	0.44
3:C:48:ASP:OD1	3:C:175:LYS:NZ	2.51	0.44
16:Q:667:ARG:HD3	16:Q:691:TYR:HE1	1.83	0.44
17:R:353:VAL:HG23	17:R:456:LYS:NZ	2.32	0.44
18:T:11:DC:H2''	18:T:12:DC:C6	2.51	0.44
21:W:203:GLN:OE1	21:W:204:LEU:HG	2.17	0.44
21:W:295:ASP:O	21:W:297:GLU:HG3	2.17	0.44
23:Y:76:ARG:HH11	23:Y:109:LYS:HD3	1.83	0.44
24:Z:639:LYS:HB2	24:Z:642:HIS:HB2	1.99	0.44
1:A:266:MET:HE3	1:A:266:MET:HB3	1.84	0.44
1:A:1129:ASN:O	1:A:1130:ILE:C	2.61	0.44
2:B:92:TYR:N	2:B:92:TYR:CD2	2.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:528:LEU:HD23	2:B:528:LEU:HA	1.78	0.44
3:C:107:CYS:HB3	3:C:154:ARG:O	2.17	0.44
14:N:42:DT:C2	14:N:43:DG:C6	3.06	0.44
16:Q:415:TRP:HA	16:Q:418:LEU:HD12	2.00	0.44
16:Q:868:LYS:HD3	16:Q:868:LYS:HA	1.79	0.44
17:R:353:VAL:HG11	17:R:472:ILE:HD12	1.99	0.44
24:Z:258:LYS:HB3	24:Z:258:LYS:HE2	1.73	0.44
24:Z:614:ILE:HA	24:Z:624:LEU:HA	1.98	0.44
1:A:59:ASP:OD2	1:A:61:ARG:HB2	2.18	0.44
1:A:1124:LEU:HA	1:A:1124:LEU:HD12	1.67	0.44
1:A:1168:LYS:HA	1:A:1168:LYS:HD2	1.89	0.44
2:B:115:LEU:HG	2:B:908:MET:HE3	1.99	0.44
2:B:652:SER:N	2:B:655:ASP:OD1	2.38	0.44
2:B:737:ILE:HD12	2:B:737:ILE:HA	1.79	0.44
5:E:97:GLU:OE1	5:E:97:GLU:N	2.50	0.44
5:E:99:ILE:O	5:E:99:ILE:HG13	2.18	0.44
7:G:30:LEU:HD12	7:G:30:LEU:HA	1.72	0.44
16:Q:841:LEU:HA	16:Q:844:LYS:HG2	1.99	0.44
20:V:193:HIS:HB3	20:V:196:LYS:O	2.18	0.44
24:Z:479:LYS:O	24:Z:519:GLN:HG2	2.17	0.44
24:Z:489:THR:HB	24:Z:505:ASP:OD2	2.17	0.44
1:A:602:CYS:SG	1:A:652:LEU:HD13	2.57	0.44
1:A:982:ASN:HD22	1:A:985:ARG:HB2	1.83	0.44
2:B:897:ARG:CB	2:B:900:GLU:HG3	2.48	0.44
2:B:995:GLU:CD	20:V:131:MET:HB3	2.42	0.44
8:H:40:ILE:O	8:H:123:MET:HA	2.17	0.44
15:P:40:A:H2'	15:P:41:C:H6	1.77	0.44
17:R:366:ARG:HH12	24:Z:775:TPO:HA	1.83	0.44
22:X:222:ARG:O	22:X:226:SER:OG	2.31	0.44
1:A:354:LEU:HD23	1:A:354:LEU:HA	1.70	0.44
5:E:37:LEU:HD21	5:E:41:LYS:HZ3	1.82	0.44
14:N:31:DC:H2''	14:N:32:DA:H8	1.80	0.44
16:Q:847:GLN:O	16:Q:851:LEU:HG	2.17	0.44
20:V:127:VAL:HG23	20:V:128:VAL:N	2.32	0.44
24:Z:242:VAL:HG23	24:Z:245:LEU:HB2	2.00	0.44
1:A:198:LEU:O	1:A:215:LEU:HD12	2.18	0.44
13:M:540:GLY:HA2	13:M:560:GLU:H	1.83	0.44
16:Q:128:GLN:HA	16:Q:158:GLN:HE22	1.82	0.44
16:Q:162:ASN:CG	16:Q:164:PRO:HD2	2.43	0.44
16:Q:750:ASP:OD1	16:Q:753:LEU:N	2.40	0.44
16:Q:750:ASP:O	16:Q:754:MET:HE2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:870:GLU:HA	16:Q:873:LYS:NZ	2.32	0.44
17:R:397:LYS:O	24:Z:777:MET:HE3	2.18	0.44
17:R:455:TRP:O	17:R:459:MET:HG2	2.17	0.44
21:W:171:ILE:HG23	21:W:187:GLU:HG2	1.99	0.44
24:Z:499:PHE:HB3	24:Z:512:LYS:HD2	2.00	0.44
1:A:365:THR:HG22	1:A:366:VAL:N	2.31	0.44
1:A:676:ILE:HD12	1:A:676:ILE:HG23	1.76	0.44
1:A:738:GLU:CD	1:A:797:ARG:HH11	2.26	0.44
2:B:690:CYS:O	2:B:691:SER:OG	2.21	0.44
2:B:1116:VAL:HG11	2:B:1125:MET:HE3	2.00	0.44
6:F:105:ILE:HG21	6:F:105:ILE:HD13	1.63	0.44
11:K:37:LYS:HA	11:K:37:LYS:HD3	1.80	0.44
14:N:37:DG:C2	18:T:12:DC:N3	2.86	0.44
15:P:39:A:N1	15:P:40:A:C6	2.86	0.44
16:Q:527:HIS:CD2	16:Q:530:TYR:HB2	2.53	0.44
16:Q:677:THR:HG22	16:Q:679:ASP:H	1.83	0.44
20:V:182:THR:HA	20:V:185:ASP:OD2	2.17	0.44
21:W:17:ASP:OD2	21:W:40:LEU:HB3	2.17	0.44
1:A:249:ILE:O	1:A:249:ILE:HG13	2.16	0.43
1:A:488:VAL:O	1:A:488:VAL:HG12	2.18	0.43
1:A:812:LYS:HE2	9:I:77:THR:HG23	1.99	0.43
1:A:1484:MET:N	1:A:1484:MET:SD	2.91	0.43
2:B:332:LYS:HZ1	2:B:333:GLU:HB2	1.83	0.43
2:B:556:ILE:HD12	2:B:556:ILE:HA	1.59	0.43
4:D:60:VAL:HG11	7:G:44:PHE:HZ	1.83	0.43
5:E:58:LEU:HD23	5:E:58:LEU:H	1.81	0.43
5:E:61:LEU:HA	5:E:61:LEU:HD12	1.77	0.43
7:G:151:ARG:HH11	24:Z:477:HIS:CD2	2.36	0.43
8:H:11:ASP:HB3	8:H:55:LYS:HG2	2.00	0.43
16:Q:513:PHE:HB2	21:W:213:TYR:CE1	2.53	0.43
16:Q:530:TYR:CE2	16:Q:532:ASP:HB2	2.53	0.43
21:W:191:MET:HG3	21:W:211:ASP:HB3	1.99	0.43
1:A:102:LYS:HE2	1:A:138:LYS:HZ2	1.82	0.43
2:B:145:GLN:O	2:B:146:LYS:C	2.61	0.43
2:B:376:ALA:C	2:B:378:GLY:N	2.76	0.43
2:B:705:GLY:O	2:B:709:SER:HB3	2.18	0.43
4:D:93:HIS:HE1	4:D:94:LYS:HE3	1.83	0.43
7:G:131:MET:SD	7:G:131:MET:N	2.92	0.43
10:J:60:LEU:HD23	10:J:60:LEU:HA	1.79	0.43
13:M:1398:LEU:HD11	13:M:1415:TYR:CD1	2.53	0.43
13:M:1435:CYS:SG	13:M:1442:LYS:HG2	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:120:ALA:HB1	16:Q:130:HIS:HE1	1.83	0.43
16:Q:538:GLY:HA2	16:Q:553:TRP:HE3	1.83	0.43
18:T:47:DG:H2''	18:T:48:DG:H5'	1.99	0.43
20:V:106:LYS:HA	20:V:106:LYS:HD2	1.87	0.43
21:W:281:LYS:HD2	21:W:281:LYS:HA	1.80	0.43
24:Z:389:THR:O	24:Z:393:LEU:HG	2.18	0.43
24:Z:593:ASN:HB3	24:Z:595:HIS:CE1	2.54	0.43
1:A:75:ALA:O	2:B:1131:ARG:NH1	2.52	0.43
1:A:1403:ASP:O	1:A:1407:CYS:HB2	2.18	0.43
2:B:1173:SER:O	2:B:1173:SER:OG	2.36	0.43
4:D:137:LYS:HA	4:D:137:LYS:HD3	1.83	0.43
9:I:53:ILE:HA	9:I:53:ILE:HD13	1.70	0.43
13:M:1476:TYR:CE2	13:M:1483:ARG:HD3	2.54	0.43
16:Q:218:ARG:HD3	16:Q:238:LEU:HD11	2.00	0.43
16:Q:710:LYS:HB2	16:Q:712:TYR:CE1	2.52	0.43
24:Z:188:GLU:OE1	24:Z:188:GLU:N	2.51	0.43
24:Z:420:PHE:HE1	24:Z:470:LYS:HG2	1.83	0.43
24:Z:464:PRO:HD2	24:Z:467:GLU:HB3	1.99	0.43
1:A:106:VAL:O	1:A:110:VAL:HG22	2.19	0.43
1:A:695:ASP:O	1:A:696:SER:OG	2.35	0.43
1:A:818:GLU:OE2	17:R:599:CYS:HA	2.18	0.43
1:A:996:ILE:HD13	1:A:996:ILE:HA	1.62	0.43
2:B:83:ARG:HH22	2:B:133:ILE:CG2	2.31	0.43
2:B:399:LEU:HA	2:B:399:LEU:HD23	1.80	0.43
2:B:576:ILE:HD12	2:B:576:ILE:HA	1.79	0.43
5:E:55:ARG:HA	5:E:58:LEU:CD2	2.48	0.43
16:Q:68:ARG:NH1	16:Q:82:GLN:HE22	2.16	0.43
16:Q:503:LEU:HG	16:Q:507:TYR:CE2	2.53	0.43
1:A:413:TYR:OH	1:A:450:MET:O	2.32	0.43
2:B:472:ARG:HA	2:B:472:ARG:HD2	1.92	0.43
2:B:497:LYS:HG3	2:B:498:PRO:CD	2.46	0.43
2:B:553:LEU:HA	2:B:553:LEU:HD12	1.73	0.43
2:B:1151:MET:HE2	2:B:1155:CYS:SG	2.59	0.43
5:E:3:ASP:OD1	5:E:49:SER:OG	2.20	0.43
5:E:27:LEU:HD12	5:E:27:LEU:HA	1.77	0.43
7:G:104:MET:HG3	7:G:157:ILE:O	2.19	0.43
16:Q:268:ASN:HD22	16:Q:271:VAL:HG12	1.84	0.43
16:Q:456:ASN:OD1	20:V:48:PHE:HA	2.18	0.43
16:Q:772:GLU:HB3	16:Q:774:SER:OG	2.18	0.43
16:Q:877:GLN:OE1	16:Q:881:TYR:CE1	2.72	0.43
17:R:359:LEU:HD22	17:R:452:PHE:HE1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:456:LYS:NZ	17:R:466:LEU:HD13	2.33	0.43
21:W:40:LEU:HA	21:W:66:GLY:HA3	2.01	0.43
21:W:152:LEU:HD12	21:W:167:ALA:O	2.19	0.43
21:W:252:SER:HB3	21:W:276:GLN:OE1	2.18	0.43
23:Y:61:ILE:HD12	23:Y:63:MET:HE2	2.00	0.43
24:Z:291:ALA:HB2	24:Z:307:MET:HG2	2.00	0.43
24:Z:502:LEU:HD21	24:Z:511:LEU:HD22	2.00	0.43
24:Z:557:THR:O	24:Z:558:PHE:CD1	2.71	0.43
2:B:520:VAL:HG13	2:B:520:VAL:O	2.19	0.43
2:B:833:THR:C	2:B:835:GLU:N	2.77	0.43
7:G:91:GLN:HB3	7:G:98:PHE:HD2	1.83	0.43
13:M:1037:ILE:H	13:M:1055:GLY:HA2	1.84	0.43
13:M:1341:LYS:HA	13:M:1341:LYS:HD2	1.85	0.43
14:N:10:DG:H2''	14:N:11:DC:C6	2.54	0.43
16:Q:69:ILE:H	16:Q:69:ILE:HD12	1.84	0.43
16:Q:239:ALA:O	16:Q:243:LEU:HG	2.17	0.43
16:Q:464:LEU:HB2	16:Q:466:ASN:HD22	1.84	0.43
16:Q:527:HIS:HD2	16:Q:530:TYR:HB2	1.83	0.43
16:Q:691:TYR:HB3	16:Q:699:SER:OG	2.19	0.43
23:Y:29:GLU:HG3	23:Y:45:ASN:O	2.19	0.43
24:Z:200:PHE:HA	24:Z:210:LEU:HD13	2.00	0.43
24:Z:540:VAL:HB	24:Z:575:VAL:CG2	2.49	0.43
1:A:417:LYS:HE2	1:A:418:TYR:CE2	2.53	0.43
1:A:479:TRP:CD1	1:A:479:TRP:N	2.87	0.43
1:A:1147:SER:HG	1:A:1351:ASP:CG	2.27	0.43
2:B:472:ARG:HH11	2:B:472:ARG:HD3	1.65	0.43
2:B:545:LEU:HB3	2:B:550:MET:HE3	1.99	0.43
2:B:679:PRO:HG2	2:B:680:ASP:N	2.33	0.43
2:B:907:VAL:HG22	2:B:921:ILE:HG12	2.00	0.43
3:C:94:CYS:SG	3:C:95:PRO:HD2	2.59	0.43
16:Q:762:GLN:O	16:Q:766:THR:HG22	2.18	0.43
1:A:37:THR:HG21	1:A:41:ILE:HD11	2.01	0.43
1:A:841:MET:HE2	1:A:841:MET:HB3	1.77	0.43
1:A:1178:ASP:OD1	1:A:1185:VAL:HG13	2.18	0.43
2:B:254:GLN:O	2:B:303:PRO:HB2	2.19	0.43
2:B:544:PHE:O	2:B:545:LEU:C	2.61	0.43
2:B:577:HIS:CE1	2:B:583:LEU:HD11	2.53	0.43
2:B:625:LEU:HA	2:B:625:LEU:HD23	1.87	0.43
2:B:866:ILE:HG23	2:B:866:ILE:HD12	1.57	0.43
2:B:1142:ASN:ND2	2:B:1145:GLN:HB2	2.27	0.43
7:G:151:ARG:HA	24:Z:477:HIS:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:15:ILE:HG23	8:H:16:ASP:N	2.33	0.43
11:K:12:LEU:HD23	11:K:12:LEU:HA	1.86	0.43
16:Q:380:ILE:HD12	16:Q:400:HIS:CE1	2.53	0.43
17:R:454:LYS:HA	17:R:454:LYS:HD2	1.77	0.43
2:B:100:GLU:HA	2:B:105:PRO:HB3	1.99	0.43
2:B:313:GLU:HG3	2:B:315:ASN:H	1.82	0.43
4:D:33:LEU:HD21	4:D:97:LEU:HD23	2.00	0.43
16:Q:471:LYS:O	16:Q:475:LEU:HD23	2.18	0.43
16:Q:484:GLU:HB2	16:Q:492:TYR:HB3	2.00	0.43
21:W:25:GLY:N	21:W:72:ILE:HD12	2.34	0.43
21:W:84:LEU:HD21	21:W:110:TRP:CZ3	2.53	0.43
21:W:231:HIS:CG	21:W:251:SER:HB3	2.54	0.43
1:A:189:PRO:HA	1:A:201:GLU:O	2.19	0.43
1:A:592:PHE:CD2	1:A:592:PHE:O	2.71	0.43
1:A:770:VAL:HG21	1:A:781:ILE:HD11	2.01	0.43
1:A:783:GLN:HA	1:A:787:VAL:O	2.19	0.43
1:A:1006:PRO:O	1:A:1010:VAL:HG23	2.19	0.43
1:A:1551:ALA:O	13:M:1509:ARG:HD2	2.19	0.43
4:D:17:ALA:HB1	4:D:95:PHE:CZ	2.54	0.43
16:Q:645:LYS:HE3	22:X:243:LYS:NZ	2.33	0.43
16:Q:651:ASN:HB3	20:V:37:ASN:HD21	1.82	0.43
16:Q:651:ASN:ND2	16:Q:682:ASP:OD2	2.52	0.43
16:Q:653:ILE:O	16:Q:656:VAL:HG22	2.19	0.43
17:R:378:PHE:CZ	17:R:382:VAL:HG11	2.54	0.43
18:T:35:DG:N2	18:T:36:DC:O2	2.51	0.43
24:Z:196:LEU:HD12	24:Z:196:LEU:HA	1.79	0.43
24:Z:478:VAL:O	24:Z:489:THR:HA	2.19	0.43
1:A:1132:LYS:H	1:A:1132:LYS:HG2	1.65	0.42
1:A:1221:MET:HE3	1:A:1221:MET:HB3	1.92	0.42
1:A:1463:LEU:HA	1:A:1463:LEU:HD12	1.59	0.42
2:B:501:LEU:HD12	2:B:505:LEU:HD12	2.01	0.42
2:B:649:ASN:OD1	2:B:649:ASN:N	2.46	0.42
2:B:1038:THR:HA	3:C:195:THR:HA	1.99	0.42
15:P:35:A:H5'	15:P:36:G:OP2	2.18	0.42
16:Q:689:HIS:HB2	20:V:35:TYR:HE1	1.84	0.42
16:Q:725:ARG:NE	20:V:31:CYS:SG	2.92	0.42
16:Q:729:LYS:HB2	16:Q:732:LYS:CD	2.46	0.42
16:Q:750:ASP:OD1	16:Q:753:LEU:HG	2.18	0.42
21:W:9:PHE:CE2	21:W:54:LEU:HB3	2.54	0.42
24:Z:261:THR:O	24:Z:264:LEU:HG	2.18	0.42
24:Z:492:ILE:HA	24:Z:502:LEU:HA	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Z:602:VAL:HG21	24:Z:636:PHE:HE2	1.83	0.42
24:Z:705:LEU:HD12	24:Z:724:VAL:HG11	2.01	0.42
1:A:130:LEU:HD11	1:A:235:VAL:HG13	2.01	0.42
1:A:510:GLU:OE1	2:B:1101:GLN:NE2	2.52	0.42
1:A:639:ILE:HG21	1:A:639:ILE:HD13	1.81	0.42
1:A:1179:PRO:HA	1:A:1209:PRO:CB	2.49	0.42
1:A:1323:THR:HG22	1:A:1329:LYS:HD2	2.01	0.42
2:B:568:PHE:CE1	2:B:573:TRP:HB2	2.54	0.42
3:C:67:ARG:NH1	10:J:2:ILE:HG23	2.33	0.42
3:C:75:SER:HB3	3:C:79:VAL:HB	2.01	0.42
4:D:22:PHE:HB2	4:D:27:GLU:OE1	2.18	0.42
16:Q:508:GLU:OE2	16:Q:540:MET:HG3	2.19	0.42
21:W:163:LEU:HB2	21:W:177:ILE:HG23	2.00	0.42
21:W:191:MET:HE2	21:W:210:ASP:O	2.19	0.42
24:Z:439:LYS:O	24:Z:452:PRO:HA	2.19	0.42
1:A:20:ARG:NH1	1:A:22:GLN:OE1	2.52	0.42
1:A:1177:TYR:CE2	1:A:1210:TRP:CE3	3.06	0.42
2:B:43:GLN:O	2:B:155:MET:HE1	2.19	0.42
2:B:186:ILE:HG21	2:B:186:ILE:HD13	1.74	0.42
3:C:268:GLN:HG3	3:C:269:SER:N	2.34	0.42
4:D:16:ASP:H	4:D:21:ILE:CG2	2.32	0.42
16:Q:182:ALA:O	16:Q:186:TYR:CD2	2.72	0.42
16:Q:365:GLU:HG2	16:Q:369:LYS:NZ	2.34	0.42
16:Q:745:HIS:HB2	21:W:20:TRP:CH2	2.53	0.42
20:V:196:LYS:O	20:V:198:ARG:N	2.49	0.42
21:W:113:ALA:C	21:W:121:LEU:HD12	2.44	0.42
21:W:135:VAL:HG23	21:W:136:GLU:HG2	2.01	0.42
21:W:170:GLY:HA2	21:W:193:ILE:HG13	2.01	0.42
24:Z:525:ALA:O	24:Z:552:ARG:NH1	2.49	0.42
1:A:77:ASN:CG	1:A:78:MET:H	2.26	0.42
1:A:338:SER:OG	1:A:341:GLN:HG2	2.20	0.42
1:A:421:ARG:HA	1:A:444:TYR:CD1	2.55	0.42
1:A:421:ARG:HE	1:A:427:ILE:HD11	1.85	0.42
1:A:461:GLN:O	1:A:463:THR:N	2.52	0.42
1:A:1137:PRO:O	1:A:1341:VAL:HG23	2.20	0.42
7:G:127:CYS:SG	7:G:138:GLN:HB3	2.60	0.42
13:M:1344:GLU:HG2	13:M:1347:MET:HE2	2.00	0.42
14:N:35:DA:H2"	14:N:36:DG:C8	2.53	0.42
16:Q:611:TRP:HZ2	16:Q:631:ARG:HH11	1.65	0.42
16:Q:880:GLN:HE21	16:Q:884:LYS:CE	2.32	0.42
17:R:578:ALA:HA	20:V:127:VAL:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:ILE:N	1:A:427:ILE:HD12	2.35	0.42
1:A:569:THR:HG23	1:A:671:ASN:HD21	1.85	0.42
1:A:820:ARG:HH11	1:A:820:ARG:HD3	1.66	0.42
1:A:1343:LEU:HD12	1:A:1343:LEU:HA	1.76	0.42
2:B:319:ASN:ND2	2:B:332:LYS:HG2	2.34	0.42
2:B:544:PHE:CE2	2:B:548:TRP:NE1	2.81	0.42
2:B:544:PHE:CZ	2:B:548:TRP:NE1	2.87	0.42
2:B:574:VAL:O	2:B:574:VAL:HG22	2.20	0.42
2:B:841:ARG:HD3	2:B:841:ARG:HA	1.77	0.42
13:M:1408:LEU:HD23	13:M:1408:LEU:H	1.84	0.42
13:M:1490:THR:OG1	13:M:1493:GLY:N	2.53	0.42
14:N:37:DG:C6	18:T:12:DC:N4	2.79	0.42
15:P:37:G:C2'	15:P:38:G:H8	2.33	0.42
16:Q:62:LYS:HA	16:Q:62:LYS:HD3	1.74	0.42
16:Q:240:VAL:HG11	20:V:72:HIS:O	2.20	0.42
16:Q:598:GLN:HA	16:Q:599:SER:HA	1.76	0.42
16:Q:719:VAL:HG23	16:Q:720:VAL:N	2.35	0.42
17:R:581:ALA:CB	20:V:127:VAL:HG21	2.48	0.42
20:V:182:THR:HA	20:V:185:ASP:CG	2.44	0.42
21:W:11:GLN:HE21	21:W:54:LEU:HD23	1.85	0.42
21:W:288:LYS:HA	21:W:288:LYS:HD3	1.77	0.42
1:A:503:LEU:O	1:A:503:LEU:HD23	2.19	0.42
1:A:909:LEU:O	1:A:910:LYS:HG2	2.20	0.42
1:A:932:ARG:HD3	8:H:106:THR:O	2.19	0.42
1:A:1166:LEU:HA	1:A:1166:LEU:HD23	1.84	0.42
1:A:1401:LEU:O	1:A:1405:MET:HG3	2.19	0.42
2:B:412:LEU:HD23	2:B:412:LEU:HA	1.71	0.42
2:B:428:ASP:OD1	2:B:429:PHE:N	2.52	0.42
2:B:638:ARG:HH21	2:B:639:HIS:CE1	2.38	0.42
3:C:263:LEU:HD13	11:K:19:ILE:HD13	2.00	0.42
5:E:96:GLU:OE1	5:E:96:GLU:N	2.52	0.42
5:E:97:GLU:CD	16:Q:887:ASN:HD21	2.28	0.42
7:G:79:PRO:HG3	7:G:104:MET:HE1	2.02	0.42
7:G:106:CYS:SG	7:G:159:ALA:HB3	2.59	0.42
11:K:101:LEU:HA	11:K:101:LEU:HD12	1.85	0.42
12:L:38:GLU:C	12:L:40:GLY:H	2.28	0.42
14:N:12:DG:C6	18:T:38:DG:N2	2.87	0.42
14:N:14:DC:OP2	24:Z:186:ILE:HD12	2.19	0.42
16:Q:384:LEU:HD11	16:Q:393:LYS:O	2.20	0.42
16:Q:542:ARG:HD2	16:Q:554:PHE:HE2	1.83	0.42
16:Q:553:TRP:HA	16:Q:556:GLU:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:429:ARG:HB2	17:R:434:GLN:HB3	2.02	0.42
17:R:492:ILE:H	17:R:492:ILE:HD12	1.83	0.42
22:X:250:PHE:HA	22:X:253:LEU:HB3	2.02	0.42
23:Y:18:LEU:HD23	23:Y:18:LEU:HA	1.86	0.42
24:Z:178:ASN:OD1	24:Z:179:LEU:N	2.47	0.42
1:A:1038:THR:O	1:A:1042:ASN:ND2	2.52	0.42
2:B:235:ILE:HD12	2:B:235:ILE:HG23	1.64	0.42
2:B:479:LEU:HD23	2:B:479:LEU:HA	1.79	0.42
2:B:557:SER:O	2:B:559:ALA:N	2.53	0.42
2:B:666:ASP:N	2:B:666:ASP:OD1	2.48	0.42
2:B:1062:ARG:CZ	2:B:1065:GLY:H	2.32	0.42
5:E:27:LEU:HD13	5:E:65:ASN:ND2	2.35	0.42
13:M:1421:SER:OG	13:M:1424:ARG:NH2	2.53	0.42
16:Q:365:GLU:HG2	16:Q:369:LYS:HZ1	1.83	0.42
21:W:228:LEU:HD11	21:W:259:TRP:CE3	2.54	0.42
24:Z:450:ILE:O	24:Z:462:GLU:HA	2.20	0.42
1:A:933:THR:OG1	1:A:934:LEU:HG	2.19	0.42
1:A:965:VAL:O	1:A:968:VAL:HG22	2.19	0.42
2:B:241:ALA:O	2:B:242:ARG:C	2.63	0.42
2:B:355:ASP:N	2:B:355:ASP:OD2	2.52	0.42
3:C:131:THR:HG22	3:C:147:ASP:OD1	2.20	0.42
3:C:172:GLU:HG2	11:K:10:PHE:CE1	2.54	0.42
4:D:100:LEU:HD11	4:D:118:LEU:HD21	2.01	0.42
5:E:61:LEU:HD23	16:Q:884:LYS:HG2	2.02	0.42
13:M:1485:GLU:CD	13:M:1497:ARG:HH21	2.28	0.42
16:Q:188:LYS:HA	16:Q:191:ARG:HG2	2.01	0.42
16:Q:310:TYR:OH	20:V:67:GLU:OE2	2.36	0.42
16:Q:773:LYS:HE2	16:Q:827:HIS:HE1	1.84	0.42
17:R:493:GLU:H	17:R:493:GLU:CD	2.16	0.42
20:V:49:ILE:HG22	22:X:227:ARG:HG3	2.01	0.42
21:W:83:SER:HB3	21:W:85:ASP:OD1	2.20	0.42
22:X:221:THR:O	22:X:225:VAL:HG22	2.19	0.42
1:A:374:SER:OG	1:A:375:ILE:N	2.53	0.42
1:A:621:ILE:HG21	1:A:621:ILE:HD13	1.78	0.42
1:A:1417:HIS:HA	1:A:1421:ARG:NH1	2.35	0.42
2:B:839:GLY:O	2:B:891:ASP:HB2	2.20	0.42
7:G:119:PHE:HA	7:G:128:TYR:CE1	2.54	0.42
8:H:132:LEU:HA	8:H:132:LEU:HD23	1.81	0.42
16:Q:132:LEU:HD11	20:V:85:ASP:HA	2.01	0.42
16:Q:211:LEU:HB2	16:Q:213:LYS:CE	2.49	0.42
16:Q:639:VAL:HA	16:Q:642:ASN:OD1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:652:GLY:O	16:Q:656:VAL:HG13	2.20	0.42
17:R:414:VAL:HA	17:R:423:ASN:HB3	2.02	0.42
17:R:429:ARG:NH2	17:R:431:GLY:O	2.51	0.42
17:R:452:PHE:HD2	17:R:453:MET:CE	2.33	0.42
20:V:47:LYS:HA	20:V:47:LYS:HD3	1.75	0.42
21:W:108:ASP:OD1	21:W:126:HIS:ND1	2.53	0.42
21:W:214:ILE:HD12	21:W:228:LEU:HD23	2.02	0.42
24:Z:490:GLY:HA3	24:Z:503:PHE:O	2.20	0.42
1:A:339:LEU:HD23	1:A:339:LEU:HA	1.77	0.42
1:A:680:LEU:HD12	1:A:680:LEU:HA	1.85	0.42
1:A:828:LEU:HD12	1:A:828:LEU:HA	1.85	0.42
1:A:1150:ASP:OD1	1:A:1150:ASP:N	2.48	0.42
1:A:1172:ASN:HB2	1:A:1215:GLU:CD	2.44	0.42
2:B:53:MET:HB3	2:B:57:ARG:HH21	1.84	0.42
2:B:440:ILE:O	2:B:441:SER:C	2.63	0.42
2:B:583:LEU:O	2:B:587:LEU:HD23	2.20	0.42
2:B:847:LYS:HE3	2:B:864:ASP:OD2	2.20	0.42
2:B:848:LEU:C	2:B:848:LEU:HD12	2.44	0.42
3:C:113:ARG:HD2	3:C:113:ARG:HA	1.90	0.42
5:E:64:HIS:ND1	5:E:65:ASN:N	2.68	0.42
10:J:16:ASN:N	10:J:16:ASN:OD1	2.24	0.42
12:L:35:ARG:HH21	12:L:40:GLY:HA3	1.83	0.42
15:P:27:A:O2'	15:P:28:A:O5'	2.36	0.42
16:Q:152:PHE:HD1	16:Q:172:ILE:HD11	1.83	0.42
17:R:452:PHE:O	17:R:456:LYS:HG2	2.20	0.42
20:V:121:SER:O	20:V:121:SER:OG	2.37	0.42
21:W:155:ALA:O	21:W:163:LEU:HG	2.20	0.42
24:Z:176:ASP:OD2	24:Z:176:ASP:N	2.53	0.42
1:A:465:HIS:CD2	1:A:467:MET:HB2	2.54	0.41
1:A:636:ILE:HG23	1:A:636:ILE:HD12	1.66	0.41
1:A:832:THR:HG23	1:A:833:PRO:HD2	2.02	0.41
1:A:1316:ASN:OD1	1:A:1317:LYS:N	2.52	0.41
2:B:309:PHE:CD2	9:I:40:ARG:NE	2.88	0.41
2:B:835:GLU:N	2:B:835:GLU:OE1	2.53	0.41
5:E:10:LEU:HD23	5:E:10:LEU:HA	1.79	0.41
7:G:111:HIS:CD2	24:Z:501:ILE:HD13	2.54	0.41
8:H:83:SER:HG	8:H:85:ALA:H	1.63	0.41
9:I:31:GLU:OE1	9:I:31:GLU:N	2.53	0.41
15:P:36:G:O2'	15:P:37:G:OP2	2.29	0.41
16:Q:707:CYS:SG	16:Q:708:LEU:N	2.93	0.41
16:Q:744:ARG:HG3	16:Q:753:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:563:ILE:HD12	17:R:566:ARG:HD2	2.02	0.41
18:T:6:DC:H1'	18:T:7:DA:C8	2.55	0.41
20:V:51:TYR:CD1	20:V:52:PRO:HD2	2.55	0.41
23:Y:14:ARG:NH1	24:Z:300:GLN:OE1	2.53	0.41
1:A:321:GLU:HG2	1:A:327:ARG:NH2	2.35	0.41
1:A:912:SER:O	1:A:914:LYS:N	2.54	0.41
1:A:1216:LEU:HA	1:A:1216:LEU:HD23	1.86	0.41
2:B:86:LEU:HD12	2:B:86:LEU:HA	1.84	0.41
2:B:544:PHE:O	2:B:547:GLU:N	2.48	0.41
2:B:679:PRO:CG	2:B:680:ASP:N	2.84	0.41
2:B:993:LYS:HD3	20:V:131:MET:SD	2.60	0.41
5:E:3:ASP:CG	5:E:47:LYS:HD2	2.45	0.41
5:E:37:LEU:O	5:E:41:LYS:HG3	2.20	0.41
5:E:166:ARG:NH1	5:E:168:ASN:HB3	2.35	0.41
7:G:24:ASN:O	7:G:28:GLN:HG2	2.20	0.41
9:I:109:ARG:HD3	9:I:124:THR:CG2	2.46	0.41
16:Q:858:LYS:HA	16:Q:861:GLU:HG3	2.03	0.41
24:Z:199:LYS:HG3	24:Z:203:TYR:HD2	1.84	0.41
1:A:993:ILE:HD13	1:A:993:ILE:HG21	1.81	0.41
1:A:1217:ASP:OD2	1:A:1218:ARG:N	2.53	0.41
2:B:199:LYS:HB3	2:B:199:LYS:HE2	1.87	0.41
2:B:376:ALA:C	2:B:378:GLY:H	2.28	0.41
2:B:566:LYS:HG2	2:B:576:ILE:HD11	2.02	0.41
2:B:597:ILE:HG22	2:B:601:VAL:HB	2.01	0.41
2:B:739:ASN:N	2:B:739:ASN:OD1	2.53	0.41
4:D:112:LYS:HE3	4:D:112:LYS:HB2	1.74	0.41
13:M:758:TYR:N	13:M:920:ILE:O	2.49	0.41
16:Q:215:GLU:HG2	16:Q:216:LYS:NZ	2.35	0.41
16:Q:431:LEU:HD23	16:Q:431:LEU:HA	1.83	0.41
16:Q:791:ARG:HH12	21:W:87:HIS:CD2	2.38	0.41
17:R:397:LYS:HA	17:R:397:LYS:HD2	1.85	0.41
17:R:402:VAL:HB	17:R:455:TRP:HB2	2.02	0.41
17:R:485:TYR:HD1	17:R:487:PHE:CE1	2.38	0.41
1:A:140:ARG:NH2	1:A:234:PHE:O	2.50	0.41
1:A:561:MET:SD	11:K:58:PHE:HA	2.59	0.41
1:A:1165:THR:HG22	1:A:1297:THR:H	1.85	0.41
1:A:1255:LEU:HD12	1:A:1255:LEU:N	2.34	0.41
2:B:105:PRO:HG2	19:U:512:THR:CA	2.37	0.41
2:B:573:TRP:CD1	2:B:573:TRP:C	2.96	0.41
3:C:64:ILE:HG23	3:C:64:ILE:HD12	1.70	0.41
3:C:166:LYS:HE2	3:C:166:LYS:HB3	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:41:LEU:HB3	4:D:65:LEU:CD2	2.50	0.41
4:D:84:ARG:HG3	4:D:97:LEU:HD11	2.02	0.41
6:F:90:LEU:HA	6:F:90:LEU:HD23	1.82	0.41
10:J:49:LEU:HD23	10:J:49:LEU:HA	1.82	0.41
16:Q:345:PHE:O	16:Q:349:GLN:HG2	2.20	0.41
16:Q:537:LEU:HB3	16:Q:553:TRP:CZ3	2.55	0.41
16:Q:572:GLY:O	16:Q:576:LEU:HG	2.20	0.41
16:Q:851:LEU:O	16:Q:855:LYS:HG2	2.21	0.41
17:R:429:ARG:HE	17:R:431:GLY:C	2.28	0.41
21:W:8:LEU:HD13	21:W:288:LYS:HE3	2.01	0.41
22:X:246:SER:HA	22:X:249:ILE:HD12	2.02	0.41
24:Z:439:LYS:H	24:Z:453:LYS:H	1.66	0.41
24:Z:526:SER:OG	24:Z:527:GLY:N	2.53	0.41
24:Z:548:GLY:HA3	24:Z:562:ASN:HA	2.01	0.41
24:Z:593:ASN:HB3	24:Z:595:HIS:HE1	1.84	0.41
1:A:544:ALA:HB2	1:A:680:LEU:HD22	2.03	0.41
1:A:618:TYR:HB3	1:A:621:ILE:O	2.21	0.41
1:A:1321:ILE:O	1:A:1328:PHE:O	2.38	0.41
1:A:1467:GLY:O	1:A:1468:THR:C	2.62	0.41
2:B:305:LEU:HD12	2:B:305:LEU:HA	1.74	0.41
2:B:420:GLN:C	2:B:422:PHE:N	2.78	0.41
3:C:259:LEU:HA	3:C:259:LEU:HD12	1.81	0.41
5:E:39:GLU:O	5:E:43:GLN:HB2	2.20	0.41
10:J:30:THR:HG22	10:J:33:ASP:HB2	2.02	0.41
11:K:109:ILE:HD13	11:K:109:ILE:HA	1.88	0.41
16:Q:202:LEU:HD21	16:Q:233:GLY:HA3	2.02	0.41
16:Q:377:THR:OG1	16:Q:400:HIS:O	2.37	0.41
16:Q:424:GLN:HB2	22:X:231:TRP:CZ3	2.54	0.41
18:T:37:DC:C4	18:T:38:DG:C6	3.08	0.41
21:W:84:LEU:HD23	21:W:84:LEU:HA	1.77	0.41
1:A:725:LEU:HD21	1:A:736:THR:HG23	2.02	0.41
1:A:762:GLU:H	1:A:762:GLU:CD	2.28	0.41
2:B:186:ILE:O	2:B:187:ILE:HD13	2.20	0.41
2:B:322:GLY:CA	2:B:339:ALA:HB2	2.50	0.41
2:B:422:PHE:HB3	2:B:429:PHE:CB	2.50	0.41
2:B:506:TRP:CD1	2:B:506:TRP:C	2.97	0.41
2:B:509:VAL:HG11	2:B:524:LYS:HD2	2.01	0.41
2:B:937:SER:OG	2:B:938:ARG:N	2.53	0.41
4:D:110:GLU:O	4:D:114:LEU:HD23	2.21	0.41
13:M:623:LYS:O	13:M:627:ASP:N	2.51	0.41
16:Q:285:TYR:HA	16:Q:288:VAL:HG12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:720:VAL:HG21	16:Q:743:ALA:HB2	2.01	0.41
16:Q:733:LEU:HA	16:Q:733:LEU:HD23	1.72	0.41
17:R:507:PRO:HA	17:R:508:ASN:HA	1.49	0.41
21:W:46:VAL:CG2	21:W:58:TRP:HB2	2.51	0.41
24:Z:601:LYS:HG3	24:Z:611:GLU:OE2	2.20	0.41
24:Z:736:LEU:HA	24:Z:736:LEU:HD23	1.79	0.41
1:A:46:THR:OG1	1:A:47:THR:N	2.53	0.41
1:A:626:THR:O	1:A:627:LYS:HB3	2.21	0.41
1:A:695:ASP:C	1:A:697:LYS:H	2.25	0.41
1:A:849:ASP:HA	1:A:852:VAL:HG22	2.03	0.41
1:A:875:TYR:OH	6:F:61:GLU:OE2	2.28	0.41
2:B:273:PHE:CG	2:B:284:ILE:HG23	2.56	0.41
2:B:312:GLN:OE1	9:I:40:ARG:NH2	2.54	0.41
5:E:111:THR:O	5:E:114:ALA:N	2.52	0.41
7:G:7:LEU:HB2	7:G:72:TYR:CE2	2.55	0.41
13:M:1354:ASP:O	13:M:1372:LYS:HG2	2.20	0.41
13:M:1474:LEU:HD21	13:M:1511:PHE:CE1	2.55	0.41
17:R:440:GLU:HG3	17:R:441:PHE:CE1	2.55	0.41
21:W:27:ASN:ND2	21:W:74:HIS:O	2.53	0.41
24:Z:192:THR:OG1	24:Z:244:ASN:ND2	2.54	0.41
1:A:151:LYS:O	1:A:152:ASN:ND2	2.53	0.41
1:A:465:HIS:CD2	1:A:467:MET:HE2	2.55	0.41
1:A:954:ARG:HH11	1:A:954:ARG:HD2	1.74	0.41
1:A:1290:SER:O	1:A:1294:THR:HG23	2.21	0.41
2:B:817:GLN:HB3	2:B:918:PHE:HD1	1.84	0.41
3:C:34:ILE:HG21	3:C:34:ILE:HD13	1.80	0.41
5:E:17:ILE:HD13	5:E:17:ILE:HA	1.87	0.41
5:E:60:VAL:HG23	5:E:74:VAL:HB	2.03	0.41
5:E:185:ILE:HG21	5:E:185:ILE:HD13	1.67	0.41
7:G:81:LYS:HE2	7:G:149:GLY:HA2	2.03	0.41
8:H:96:VAL:HA	8:H:116:VAL:HA	2.03	0.41
16:Q:235:LEU:HD23	16:Q:261:ALA:HB2	2.02	0.41
16:Q:468:GLY:O	16:Q:472:LYS:HG2	2.20	0.41
16:Q:790:HIS:NE2	16:Q:817:CYS:SG	2.94	0.41
1:A:18:ILE:H	1:A:1462:GLN:HE22	1.69	0.41
1:A:120:ASP:O	1:A:122:ASN:N	2.54	0.41
1:A:290:LEU:HD12	1:A:290:LEU:HA	1.78	0.41
1:A:419:ILE:HD13	1:A:419:ILE:HG21	1.70	0.41
1:A:421:ARG:NE	1:A:427:ILE:HD11	2.36	0.41
1:A:431:PHE:O	1:A:432:HIS:C	2.64	0.41
1:A:461:GLN:O	1:A:461:GLN:NE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:ASP:HB3	2:B:792:ASP:HB3	2.01	0.41
1:A:535:MET:O	1:A:669:TYR:OH	2.29	0.41
1:A:596:ILE:HG21	1:A:596:ILE:HD13	1.76	0.41
1:A:738:GLU:OE1	1:A:797:ARG:HD3	2.21	0.41
1:A:1121:VAL:N	1:A:1122:PRO:CD	2.84	0.41
1:A:1164:THR:O	1:A:1298:LEU:N	2.53	0.41
2:B:222:ARG:HH11	2:B:222:ARG:HD3	1.72	0.41
2:B:889:LYS:HB2	2:B:889:LYS:HE2	1.46	0.41
2:B:1010:LYS:HE3	20:V:130:TRP:CH2	2.56	0.41
3:C:245:VAL:O	3:C:246:LEU:C	2.63	0.41
3:C:246:LEU:HA	3:C:246:LEU:HD23	1.87	0.41
7:G:14:HIS:O	7:G:16:ARG:N	2.54	0.41
7:G:50:THR:HG22	7:G:73:LYS:HB3	2.03	0.41
7:G:92:VAL:H	7:G:139:GLN:HE21	1.68	0.41
11:K:93:ASP:OD1	11:K:94:LEU:N	2.53	0.41
15:P:40:A:C2	15:P:41:C:C4	3.08	0.41
16:Q:258:LEU:HD23	16:Q:258:LEU:HA	1.90	0.41
16:Q:858:LYS:O	16:Q:861:GLU:HG3	2.21	0.41
17:R:388:ARG:HG2	17:R:443:SER:HB2	2.03	0.41
17:R:390:GLY:HA2	17:R:400:TYR:CD1	2.55	0.41
17:R:582:GLU:HA	17:R:585:ASN:HD21	1.85	0.41
21:W:196:LEU:HD13	21:W:205:LEU:HD11	2.01	0.41
21:W:222:ALA:O	21:W:223:ASN:ND2	2.54	0.41
24:Z:389:THR:HG23	24:Z:391:SER:H	1.85	0.41
24:Z:491:LEU:HD23	24:Z:491:LEU:HA	1.83	0.41
24:Z:562:ASN:ND2	24:Z:566:LYS:HG3	2.33	0.41
1:A:33:ARG:H	1:A:33:ARG:HG2	1.69	0.41
1:A:102:LYS:HE2	1:A:138:LYS:NZ	2.36	0.41
1:A:117:LEU:O	1:A:119:VAL:N	2.53	0.41
1:A:939:VAL:O	1:A:943:LEU:HD12	2.21	0.41
1:A:1090:LEU:HD23	1:A:1090:LEU:HA	1.79	0.41
2:B:545:LEU:HD23	2:B:550:MET:HE3	2.03	0.41
7:G:123:SER:HB2	7:G:125:PRO:HD2	2.03	0.41
8:H:6:PHE:CZ	8:H:37:MET:SD	3.14	0.41
11:K:103:GLU:O	11:K:107:VAL:HG13	2.20	0.41
12:L:18:ILE:HD11	12:L:47:LYS:HG3	2.02	0.41
13:M:699:SER:C	13:M:701:GLN:H	2.29	0.41
13:M:1347:MET:HE3	13:M:1378:TYR:CD2	2.56	0.41
16:Q:218:ARG:HH11	16:Q:238:LEU:CD2	2.33	0.41
16:Q:467:LEU:HD12	16:Q:506:LEU:HG	2.02	0.41
16:Q:790:HIS:CD2	16:Q:817:CYS:SG	3.14	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:37:DC:H5'	18:T:37:DC:C6	2.56	0.41
21:W:5:TYR:CD1	21:W:303:CYS:HB3	2.56	0.41
21:W:250:SER:OG	21:W:277:VAL:HG23	2.21	0.41
1:A:217:SER:O	1:A:220:ARG:N	2.53	0.40
1:A:812:LYS:O	1:A:813:ASP:HB2	2.21	0.40
1:A:1212:LEU:CD1	1:A:1285:LEU:HD13	2.48	0.40
1:A:1376:LYS:O	1:A:1380:ARG:HG3	2.21	0.40
1:A:1379:GLU:O	1:A:1379:GLU:HG2	2.16	0.40
1:A:1481:LYS:HA	7:G:20:PRO:HA	2.03	0.40
2:B:123:PRO:HB2	2:B:148:PHE:HE1	1.86	0.40
2:B:557:SER:C	2:B:559:ALA:H	2.29	0.40
3:C:40:ALA:HB1	3:C:171:LYS:HB2	2.02	0.40
3:C:123:ASN:OD1	3:C:123:ASN:C	2.64	0.40
7:G:1:MET:H3	7:G:78:ARG:C	2.30	0.40
16:Q:18:GLU:N	16:Q:18:GLU:OE1	2.53	0.40
16:Q:274:HIS:HA	16:Q:277:ASN:HD21	1.84	0.40
16:Q:296:PHE:CE1	16:Q:305:GLN:HB2	2.56	0.40
16:Q:398:LYS:HE2	16:Q:421:ILE:HG21	2.03	0.40
21:W:251:SER:HG	21:W:255:SER:HG	1.68	0.40
24:Z:525:ALA:CB	24:Z:552:ARG:HH22	2.31	0.40
1:A:99:PHE:O	1:A:103:THR:HG23	2.21	0.40
1:A:247:TRP:N	1:A:247:TRP:CD1	2.87	0.40
1:A:299:ALA:C	1:A:301:HIS:N	2.79	0.40
1:A:991:GLN:HA	1:A:996:ILE:HG12	2.04	0.40
1:A:1288:ILE:HA	1:A:1291:ASN:HD21	1.86	0.40
1:A:1451:MET:HE3	1:A:1451:MET:HB3	1.91	0.40
2:B:583:LEU:N	2:B:583:LEU:HD12	2.36	0.40
4:D:35:SER:OG	4:D:72:SER:HA	2.21	0.40
7:G:110:ARG:HG2	7:G:119:PHE:CZ	2.56	0.40
7:G:152:VAL:HA	7:G:157:ILE:HA	2.03	0.40
16:Q:238:LEU:HD12	16:Q:238:LEU:HA	1.96	0.40
16:Q:393:LYS:HB3	16:Q:393:LYS:HE3	1.70	0.40
18:T:21:DT:H6	18:T:21:DT:H2'	1.67	0.40
21:W:253:ASP:OD1	21:W:253:ASP:N	2.51	0.40
24:Z:551:VAL:HG21	24:Z:632:ASN:OD1	2.20	0.40
24:Z:571:ARG:HB2	24:Z:574:ALA:CB	2.51	0.40
1:A:92:LYS:CD	1:A:307:VAL:HG11	2.52	0.40
1:A:350:VAL:HG21	1:A:1435:THR:HG23	2.03	0.40
1:A:413:TYR:O	1:A:449:HIS:CD2	2.67	0.40
1:A:501:MET:HE2	1:A:501:MET:HB3	1.86	0.40
1:A:713:VAL:CG2	1:A:817:PRO:HD3	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1150:ASP:OD2	1:A:1153:ARG:HG3	2.21	0.40
1:A:1182:GLN:O	1:A:1192:TRP:CE2	2.73	0.40
2:B:157:ARG:NH2	2:B:177:CYS:O	2.54	0.40
2:B:603:MET:HE2	2:B:603:MET:HB2	1.85	0.40
2:B:665:ILE:HA	2:B:665:ILE:HD12	1.78	0.40
2:B:833:THR:HG22	2:B:835:GLU:OE1	2.22	0.40
5:E:101:ARG:HA	5:E:126:ILE:O	2.20	0.40
7:G:110:ARG:NH2	7:G:117:MET:O	2.55	0.40
8:H:125:LEU:HD12	8:H:125:LEU:HA	1.79	0.40
11:K:80:ASP:N	11:K:80:ASP:OD1	2.32	0.40
12:L:13:GLN:HA	12:L:14:PRO:HD3	1.88	0.40
14:N:42:DT:H6	14:N:42:DT:H2'	1.71	0.40
16:Q:3:ARG:HB3	16:Q:4:GLY:H	1.67	0.40
16:Q:24:LEU:HD11	16:Q:56:LYS:NZ	2.36	0.40
16:Q:153:HIS:CE1	16:Q:156:LEU:HD12	2.56	0.40
16:Q:333:THR:HG21	16:Q:347:LEU:HD12	2.02	0.40
16:Q:415:TRP:CZ3	16:Q:440:ILE:HG12	2.57	0.40
17:R:392:GLY:HA2	17:R:397:LYS:O	2.20	0.40
17:R:587:LYS:HE2	17:R:587:LYS:HB2	1.93	0.40
21:W:243:ASP:OD2	21:W:243:ASP:N	2.54	0.40
23:Y:93:LEU:HD23	23:Y:93:LEU:HA	1.87	0.40
24:Z:260:MET:N	24:Z:260:MET:SD	2.94	0.40
1:A:54:LEU:HD12	1:A:54:LEU:HA	1.85	0.40
1:A:135:GLY:O	1:A:137:PRO:HD3	2.21	0.40
1:A:538:VAL:O	1:A:539:GLN:HG2	2.22	0.40
2:B:84:TYR:CB	2:B:132:VAL:HA	2.52	0.40
2:B:95:LYS:HA	2:B:95:LYS:HD2	1.92	0.40
2:B:388:TYR:H	2:B:504:THR:CG2	2.27	0.40
2:B:620:ARG:HH11	2:B:620:ARG:HD2	1.69	0.40
2:B:791:GLU:O	2:B:792:ASP:HB2	2.21	0.40
5:E:25:GLY:O	5:E:65:ASN:HB2	2.22	0.40
13:M:1429:HIS:CE1	13:M:1460:TYR:HH	2.37	0.40
16:Q:95:GLN:OE1	20:V:83:THR:OG1	2.38	0.40
16:Q:689:HIS:HB2	20:V:35:TYR:CE1	2.56	0.40
20:V:58:PHE:HE2	20:V:60:GLN:CD	2.29	0.40
21:W:14:ALA:CB	21:W:298:ILE:HG13	2.52	0.40
21:W:38:GLY:C	21:W:67:VAL:HB	2.46	0.40
24:Z:200:PHE:HB2	24:Z:210:LEU:HD22	2.02	0.40
24:Z:420:PHE:CE1	24:Z:470:LYS:HG2	2.56	0.40
1:A:29:ASP:O	1:A:33:ARG:HG2	2.21	0.40
1:A:955:GLU:OE1	1:A:1010:VAL:HG22	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1163:HIS:CD2	1:A:1297:THR:HG23	2.57	0.40
2:B:50:PHE:HA	2:B:54:SER:HB3	2.02	0.40
2:B:242:ARG:NH2	2:B:252:ILE:HD12	2.37	0.40
5:E:110:MET:HE2	5:E:110:MET:HB3	1.96	0.40
9:I:14:ILE:HG23	9:I:23:MET:HG3	2.03	0.40
16:Q:386:ALA:HB1	16:Q:394:ARG:CG	2.51	0.40
16:Q:636:TYR:CE2	16:Q:652:GLY:HA3	2.56	0.40
18:T:1:DG:H2''	18:T:2:DC:C6	2.56	0.40
21:W:172:ILE:O	21:W:186:LEU:N	2.54	0.40
24:Z:501:ILE:HA	24:Z:511:LEU:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1408/1984 (71%)	1281 (91%)	117 (8%)	10 (1%)	18	49
2	B	1112/1251 (89%)	998 (90%)	105 (9%)	9 (1%)	16	47
3	C	254/275 (92%)	232 (91%)	19 (8%)	3 (1%)	10	37
4	D	124/142 (87%)	118 (95%)	6 (5%)	0	100	100
5	E	207/210 (99%)	199 (96%)	7 (3%)	1 (0%)	24	57
6	F	76/127 (60%)	70 (92%)	6 (8%)	0	100	100
7	G	169/172 (98%)	157 (93%)	12 (7%)	0	100	100
8	H	147/150 (98%)	130 (88%)	16 (11%)	1 (1%)	18	49
9	I	114/125 (91%)	104 (91%)	10 (9%)	0	100	100
10	J	64/67 (96%)	60 (94%)	2 (3%)	2 (3%)	3	18
11	K	113/117 (97%)	107 (95%)	6 (5%)	0	100	100
12	L	45/58 (78%)	39 (87%)	6 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	M	976/1729 (56%)	903 (92%)	72 (7%)	1 (0%)	48	78
16	Q	888/1179 (75%)	836 (94%)	52 (6%)	0	100	100
17	R	240/713 (34%)	225 (94%)	14 (6%)	1 (0%)	30	61
19	U	117/666 (18%)	88 (75%)	21 (18%)	8 (7%)	1	5
20	V	234/531 (44%)	199 (85%)	31 (13%)	4 (2%)	7	30
21	W	298/305 (98%)	268 (90%)	30 (10%)	0	100	100
22	X	41/531 (8%)	41 (100%)	0	0	100	100
23	Y	114/121 (94%)	109 (96%)	5 (4%)	0	100	100
24	Z	497/1087 (46%)	460 (93%)	36 (7%)	1 (0%)	43	73
All	All	7238/11540 (63%)	6624 (92%)	573 (8%)	41 (1%)	23	52

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	540	ASP
1	A	1185	VAL
1	A	1468	THR
2	B	19	PRO
3	C	93	PHE
13	M	1330	PRO
17	R	507	PRO
19	U	506	ALA
19	U	508	HIS
20	V	238	PRO
24	Z	760	GLY
1	A	1435	THR
19	U	481	GLY
19	U	521	LYS
2	B	20	ASP
2	B	142	THR
2	B	1004	ASP
10	J	28	GLU
19	U	463	PRO
19	U	513	LEU
19	U	516	ALA
19	U	523	GLN
20	V	228	GLU
20	V	249	ASP
20	V	291	ASN

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Mol	Chain	Res	Type
1	A	300	ALA
1	A	696	SER
2	B	950	ARG
1	A	495	ASP
1	A	1130	ILE
2	B	679	PRO
2	B	834	ARG
3	C	60	HIS
3	C	92	GLU
2	B	650	ASN
2	B	1001	PRO
1	A	478	PRO
5	E	45	GLY
8	H	17	PRO
10	J	64	PRO
1	A	980	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1245/1761 (71%)	1214 (98%)	31 (2%)	42	69
2	B	986/1084 (91%)	939 (95%)	47 (5%)	23	54
3	C	235/252 (93%)	232 (99%)	3 (1%)	61	77
4	D	109/126 (86%)	109 (100%)	0	100	100
5	E	191/192 (100%)	188 (98%)	3 (2%)	55	75
6	F	68/111 (61%)	66 (97%)	2 (3%)	37	66
7	G	146/153 (95%)	144 (99%)	2 (1%)	59	76
8	H	130/131 (99%)	122 (94%)	8 (6%)	16	46
9	I	104/112 (93%)	100 (96%)	4 (4%)	29	60
10	J	55/56 (98%)	54 (98%)	1 (2%)	51	73
11	K	104/106 (98%)	102 (98%)	2 (2%)	50	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	43/55 (78%)	39 (91%)	4 (9%)	8	31
13	M	154/1524 (10%)	154 (100%)	0	100	100
16	Q	761/1011 (75%)	759 (100%)	2 (0%)	86	87
17	R	168/625 (27%)	167 (99%)	1 (1%)	78	83
19	U	63/590 (11%)	63 (100%)	0	100	100
20	V	144/462 (31%)	143 (99%)	1 (1%)	76	82
21	W	255/260 (98%)	253 (99%)	2 (1%)	73	81
22	X	40/467 (9%)	40 (100%)	0	100	100
23	Y	102/105 (97%)	101 (99%)	1 (1%)	68	79
24	Z	434/939 (46%)	432 (100%)	2 (0%)	81	85
All	All	5537/10122 (55%)	5421 (98%)	116 (2%)	46	71

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	VAL
1	A	67	ARG
1	A	79	THR
1	A	147	LEU
1	A	250	VAL
1	A	251	THR
1	A	283	ILE
1	A	301	HIS
1	A	440	LEU
1	A	457	ILE
1	A	461	GLN
1	A	476	ILE
1	A	538	VAL
1	A	571	ASP
1	A	605	THR
1	A	622	SER
1	A	664	ILE
1	A	713	VAL
1	A	757	GLN
1	A	761	SER
1	A	905	ASN
1	A	942	VAL
1	A	1007	ILE

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Mol	Chain	Res	Type
1	A	1074	SER
1	A	1130	ILE
1	A	1175	ILE
1	A	1186	VAL
1	A	1235	ILE
1	A	1282	ASP
1	A	1385	VAL
1	A	1424	THR
2	B	20	ASP
2	B	90	GLN
2	B	92	TYR
2	B	115	LEU
2	B	147	THR
2	B	154	ILE
2	B	163	LEU
2	B	170	ASP
2	B	176	GLU
2	B	180	ASP
2	B	198	GLU
2	B	218	THR
2	B	267	VAL
2	B	291	ASP
2	B	311	ILE
2	B	331	THR
2	B	348	LEU
2	B	351	VAL
2	B	354	SER
2	B	359	THR
2	B	386	ASP
2	B	411	LEU
2	B	440	ILE
2	B	504	THR
2	B	556	ILE
2	B	567	ILE
2	B	574	VAL
2	B	597	ILE
2	B	626	LEU
2	B	649	ASN
2	B	650	ASN
2	B	659	SER
2	B	665	ILE
2	B	715	ASP

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Mol	Chain	Res	Type
2	B	731	GLN
2	B	738	THR
2	B	743	ARG
2	B	750	VAL
2	B	759	VAL
2	B	784	SER
2	B	909	VAL
2	B	931	ILE
2	B	958	CYS
2	B	1118	VAL
2	B	1130	THR
2	B	1148	LEU
2	B	1174	VAL
3	C	74	THR
3	C	75	SER
3	C	151	VAL
5	E	28	VAL
5	E	82	VAL
5	E	117	SER
6	F	120	VAL
6	F	123	LEU
7	G	21	ASN
7	G	37	THR
8	H	15	ILE
8	H	51	ASP
8	H	67	ASP
8	H	83	SER
8	H	96	VAL
8	H	113	SER
8	H	116	VAL
8	H	141	VAL
9	I	12	VAL
9	I	34	ILE
9	I	73	SER
9	I	101	SER
10	J	47	ARG
11	K	99	SER
11	K	107	VAL
12	L	34	ILE
12	L	39	CYS
12	L	43	ILE
12	L	44	MET

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Mol	Chain	Res	Type
16	Q	552	ASP
16	Q	820	LEU
17	R	422	THR
20	V	45	ASP
21	W	43	LEU
21	W	169	ASP
23	Y	115	ILE
24	Z	614	ILE
24	Z	720	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (129) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	A	122	ASN
1	A	123	ASN
1	A	143	HIS
1	A	152	ASN
1	A	288	ASN
1	A	320	ASN
1	A	423	ASN
1	A	449	HIS
1	A	704	ASN
1	A	780	ASN
1	A	791	GLN
1	A	792	ASN
1	A	804	HIS
1	A	809	HIS
1	A	935	GLN
1	A	991	GLN
1	A	1005	HIS
1	A	1032	GLN
1	A	1182	GLN
1	A	1190	GLN
1	A	1230	GLN
1	A	1236	ASN
1	A	1420	ASN
2	B	43	GLN
2	B	52	GLN
2	B	111	ASN
2	B	117	ASN
2	B	175	ASN

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Mol	Chain	Res	Type
2	B	197	GLN
2	B	319	ASN
2	B	481	HIS
2	B	500	GLN
2	B	585	ASN
2	B	631	GLN
2	B	649	ASN
2	B	842	HIS
2	B	1003	ASN
2	B	1040	GLN
2	B	1094	GLN
2	B	1120	ASN
2	B	1142	ASN
3	C	60	HIS
3	C	83	GLN
3	C	111	GLN
3	C	114	HIS
3	C	262	GLN
4	D	19	GLN
4	D	34	ASN
4	D	48	ASN
4	D	66	ASN
4	D	76	ASN
4	D	129	GLN
5	E	30	GLN
5	E	65	ASN
5	E	107	GLN
5	E	129	GLN
5	E	168	ASN
7	G	93	ASN
7	G	139	GLN
8	H	131	ASN
8	H	133	HIS
9	I	18	GLN
9	I	56	ASN
9	I	84	HIS
9	I	91	HIS
11	K	49	GLN
13	M	1352	GLN
16	Q	23	GLN
16	Q	38	HIS
16	Q	40	GLN

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Mol	Chain	Res	Type
16	Q	105	ASN
16	Q	128	GLN
16	Q	151	GLN
16	Q	153	HIS
16	Q	161	ASN
16	Q	244	ASN
16	Q	268	ASN
16	Q	278	HIS
16	Q	294	HIS
16	Q	298	ASN
16	Q	305	GLN
16	Q	319	GLN
16	Q	349	GLN
16	Q	373	ASN
16	Q	407	GLN
16	Q	466	ASN
16	Q	527	HIS
16	Q	573	ASN
16	Q	585	GLN
16	Q	609	ASN
16	Q	616	HIS
16	Q	617	GLN
16	Q	706	ASN
16	Q	714	HIS
16	Q	781	ASN
16	Q	860	GLN
16	Q	877	GLN
16	Q	880	GLN
16	Q	887	ASN
17	R	416	GLN
17	R	432	ASN
17	R	484	ASN
17	R	585	ASN
17	R	588	ASN
19	U	451	HIS
20	V	37	ASN
20	V	72	HIS
20	V	97	ASN
20	V	122	GLN
20	V	193	HIS
21	W	11	GLN
21	W	15	HIS

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Mol	Chain	Res	Type
21	W	27	ASN
21	W	131	ASN
21	W	173	ASN
21	W	246	HIS
21	W	268	HIS
21	W	273	HIS
23	Y	27	GLN
23	Y	35	ASN
23	Y	45	ASN
24	Z	232	GLN
24	Z	244	ASN
24	Z	466	GLN
24	Z	519	GLN
24	Z	534	HIS
24	Z	595	HIS
24	Z	616	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	20/46 (43%)	7 (35%)	3 (15%)

All (7) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	28	A
15	P	29	C
15	P	30	C
15	P	31	G
15	P	36	G
15	P	37	G
15	P	39	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	P	28	A
15	P	36	G
15	P	38	G

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	TPO	Z	775	24	8,10,11	1.60	1 (12%)	10,14,16	2.21	1 (10%)
1	TPO	A	1525	1	8,10,11	1.65	1 (12%)	10,14,16	2.02	1 (10%)
1	SEP	A	1547	1	8,9,10	1.55	1 (12%)	7,12,14	1.11	1 (14%)

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
24	TPO	Z	775	24	-	1/9/11/13	-
1	TPO	A	1525	1	-	4/9/11/13	-
1	SEP	A	1547	1	-	0/6/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1525	TPO	P-O1P	3.56	1.61	1.50
24	Z	775	TPO	P-O1P	3.49	1.61	1.50
1	A	1547	SEP	P-O1P	3.40	1.61	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Z	775	TPO	P-OG1-CB	-6.55	105.53	123.33
1	A	1525	TPO	P-OG1-CB	-5.56	108.22	123.33
1	A	1547	SEP	OG-CB-CA	2.01	110.10	108.14

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1525	TPO	N-CA-CB-CG2
1	A	1525	TPO	N-CA-CB-OG1
1	A	1525	TPO	C-CA-CB-CG2
24	Z	775	TPO	C-CA-CB-CG2
1	A	1525	TPO	O-C-CA-CB

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	Z	775	TPO	2	0
1	A	1525	TPO	1	0
1	A	1547	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	3
19	U	1
20	V	1
13	M	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	U	497:ASP	C	505:SER	N	25.86
1	V	299:GLU	C	310:ASN	N	12.74
1	M	1334:ASN	C	1338:ILE	N	5.29
1	B	755:GLN	C	756:LYS	N	1.18
1	B	108:MET	C	109:MET	N	1.17
1	A	999:ARG	C	1000:LEU	N	1.15
1	B	94:SER	C	95:LYS	N	1.07

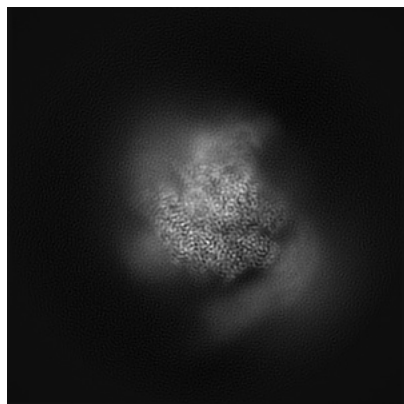
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10480. These allow visual inspection of the internal detail of the map and identification of artifacts.

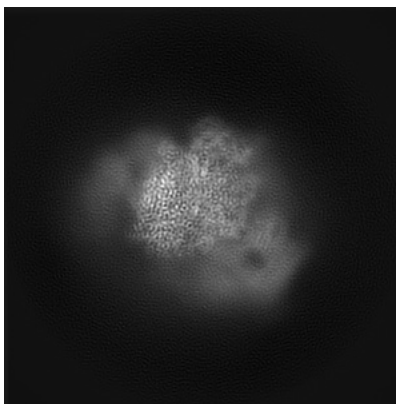
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

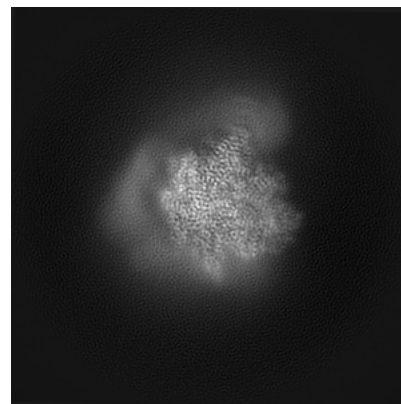
6.1.1 Primary map



X

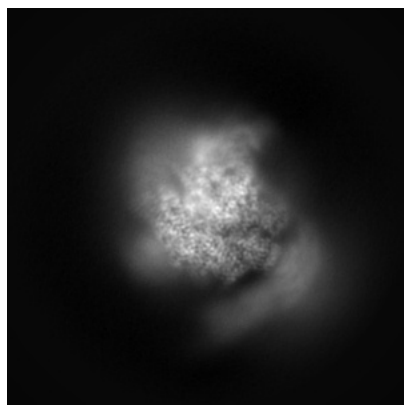


Y

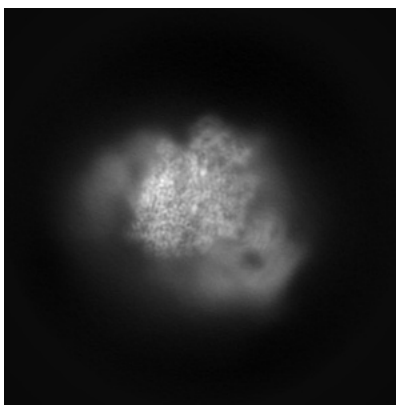


Z

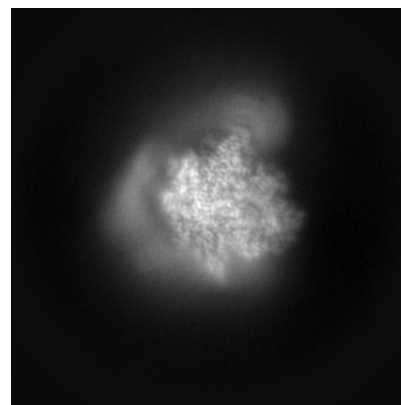
6.1.2 Raw map



X



Y

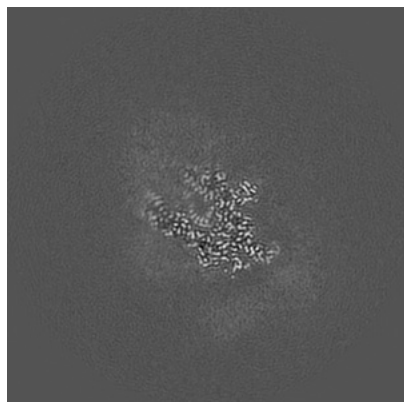


Z

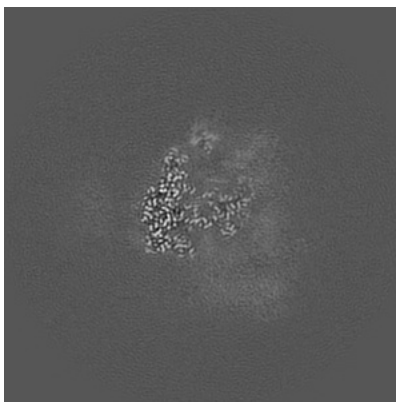
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

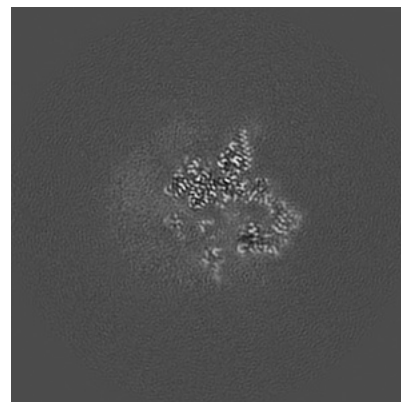
6.2.1 Primary map



X Index: 180

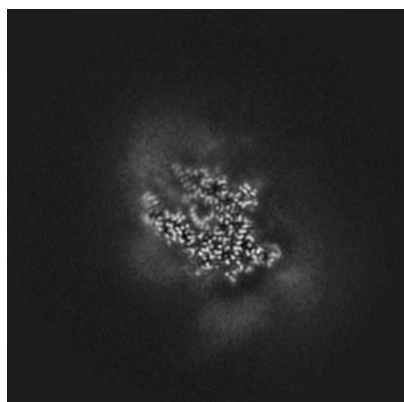


Y Index: 180

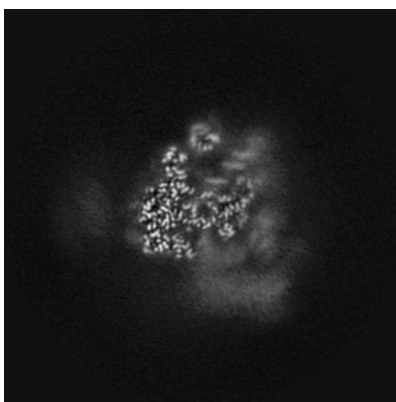


Z Index: 180

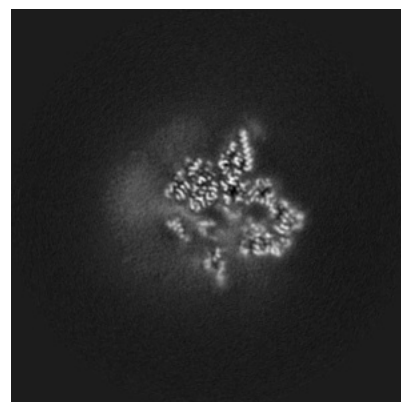
6.2.2 Raw map



X Index: 180



Y Index: 180

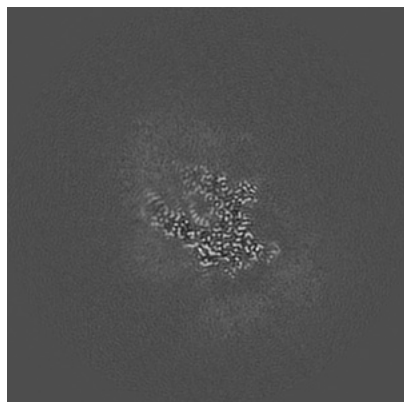


Z Index: 180

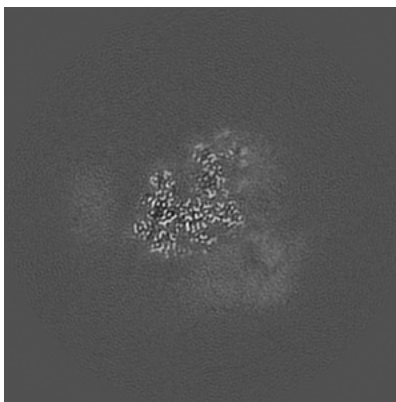
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

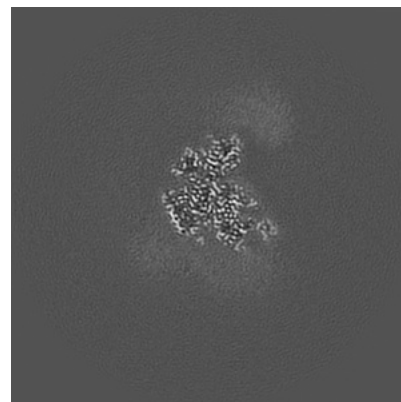
6.3.1 Primary map



X Index: 179

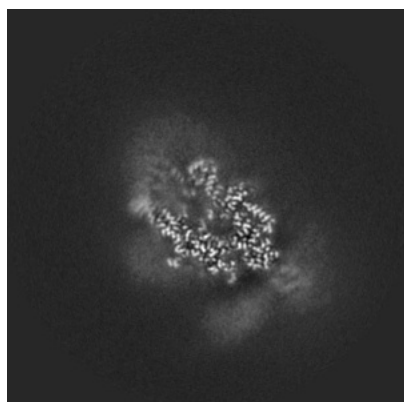


Y Index: 193

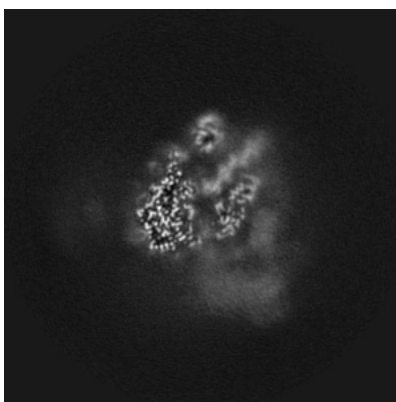


Z Index: 143

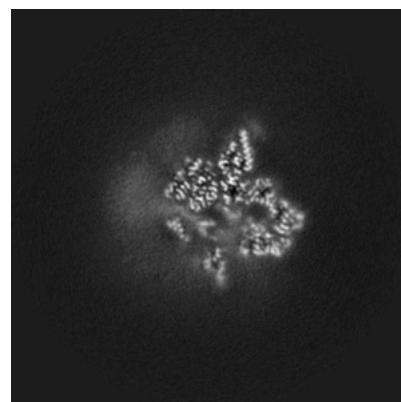
6.3.2 Raw map



X Index: 189



Y Index: 174

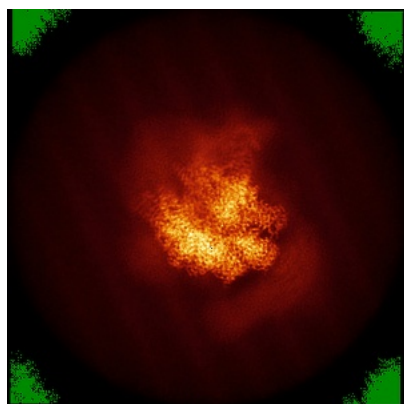


Z Index: 180

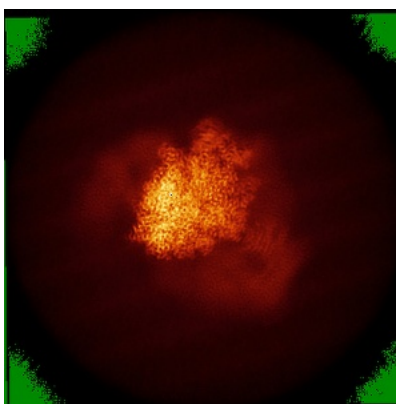
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

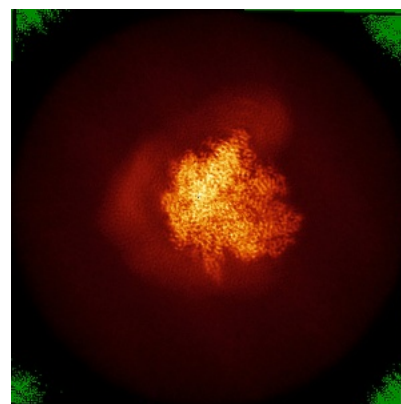
6.4.1 Primary map



X

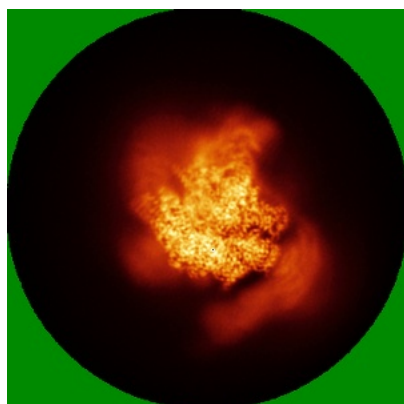


Y

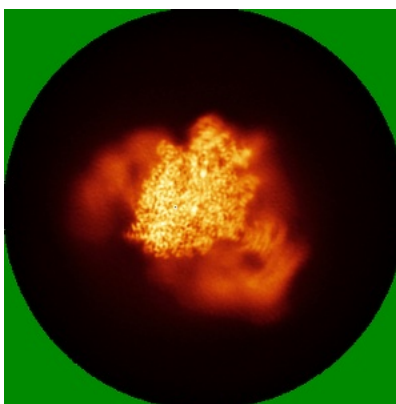


Z

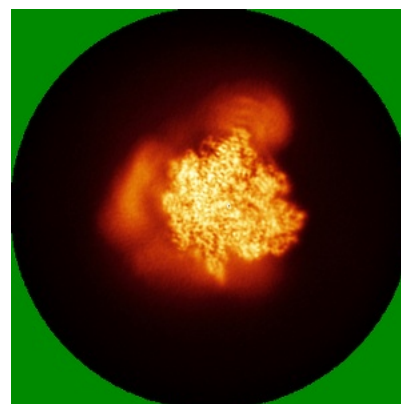
6.4.2 Raw map



X



Y

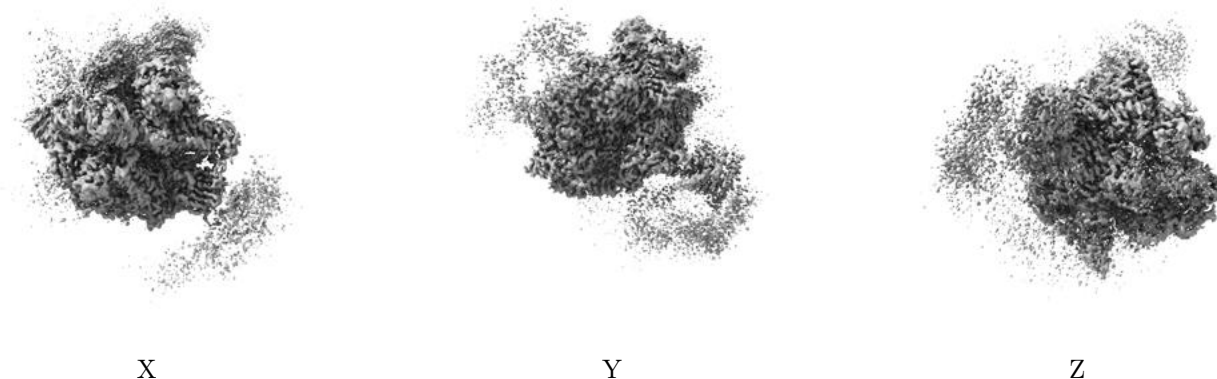


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

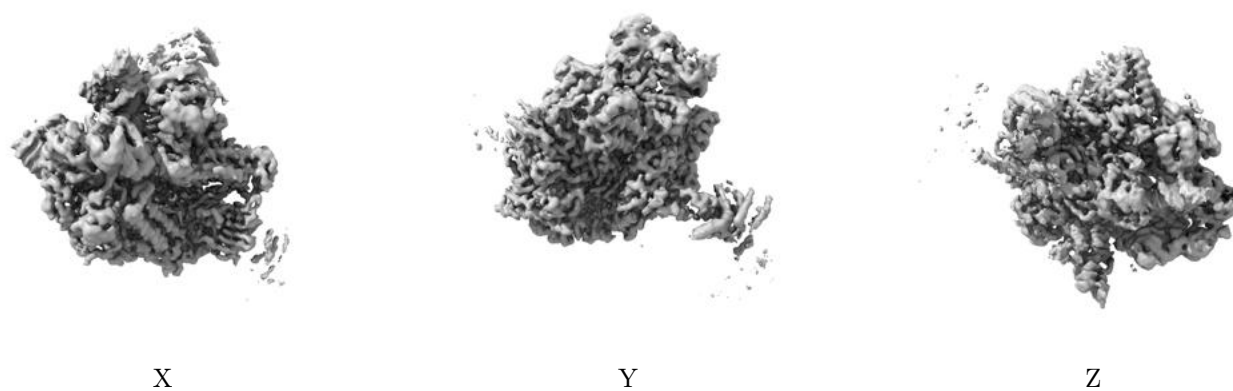
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

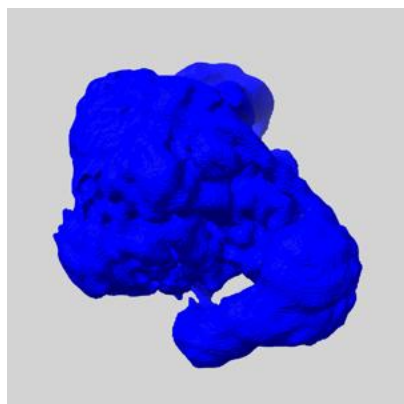
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

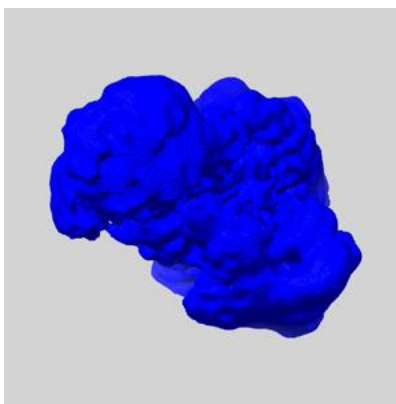
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

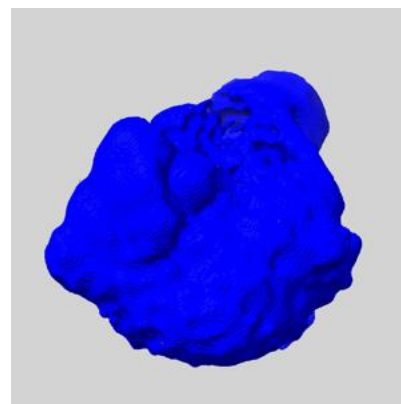
6.6.1 emd_10480_msk_1.map [i](#)



X

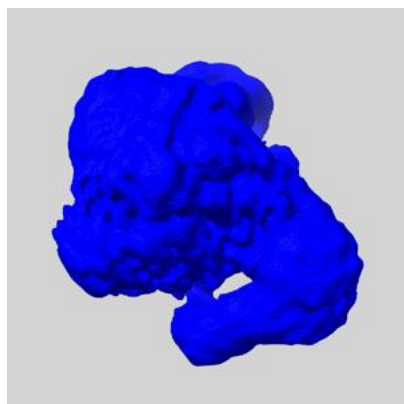


Y

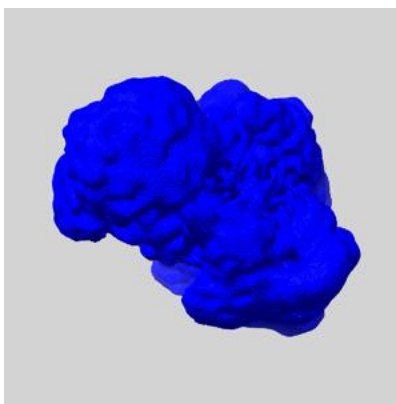


Z

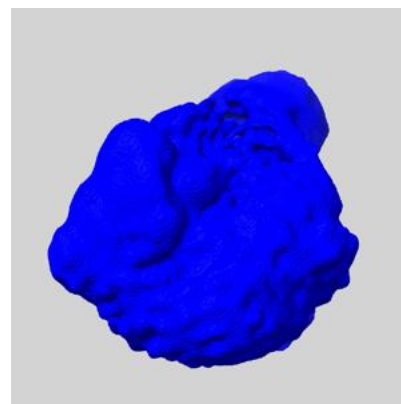
6.6.2 emd_10480_msk_2.map [i](#)



X



Y

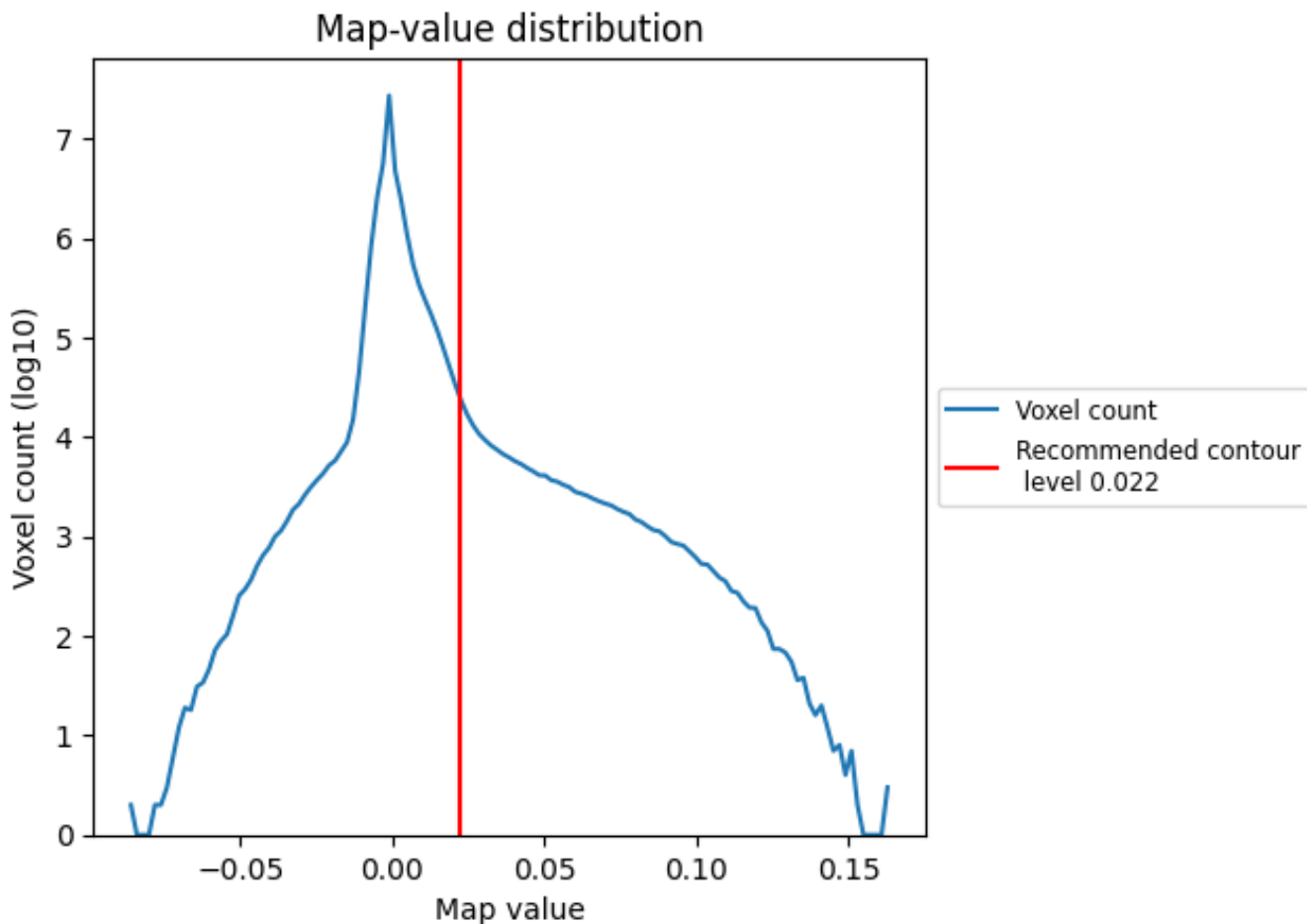


Z

7 Map analysis [i](#)

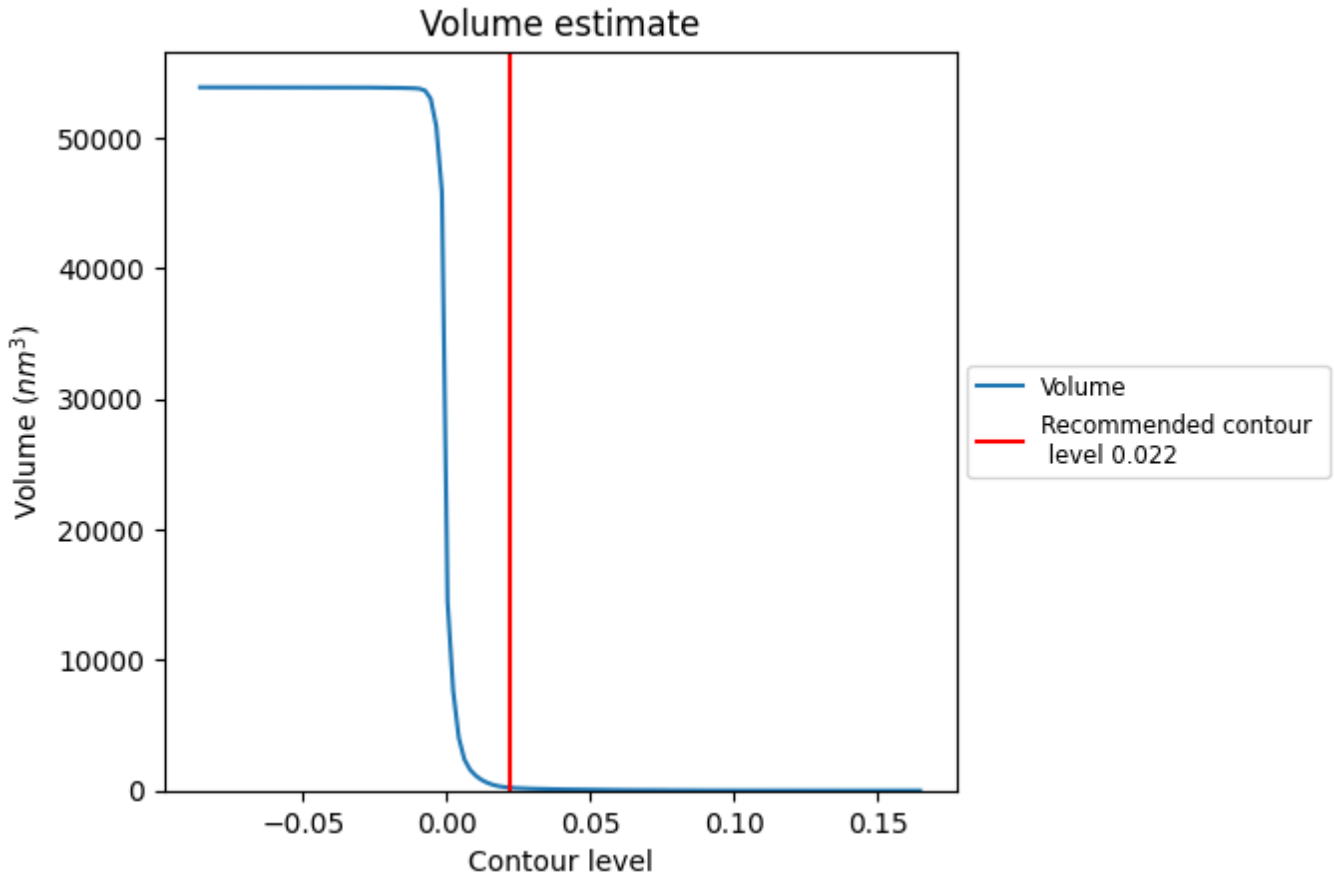
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

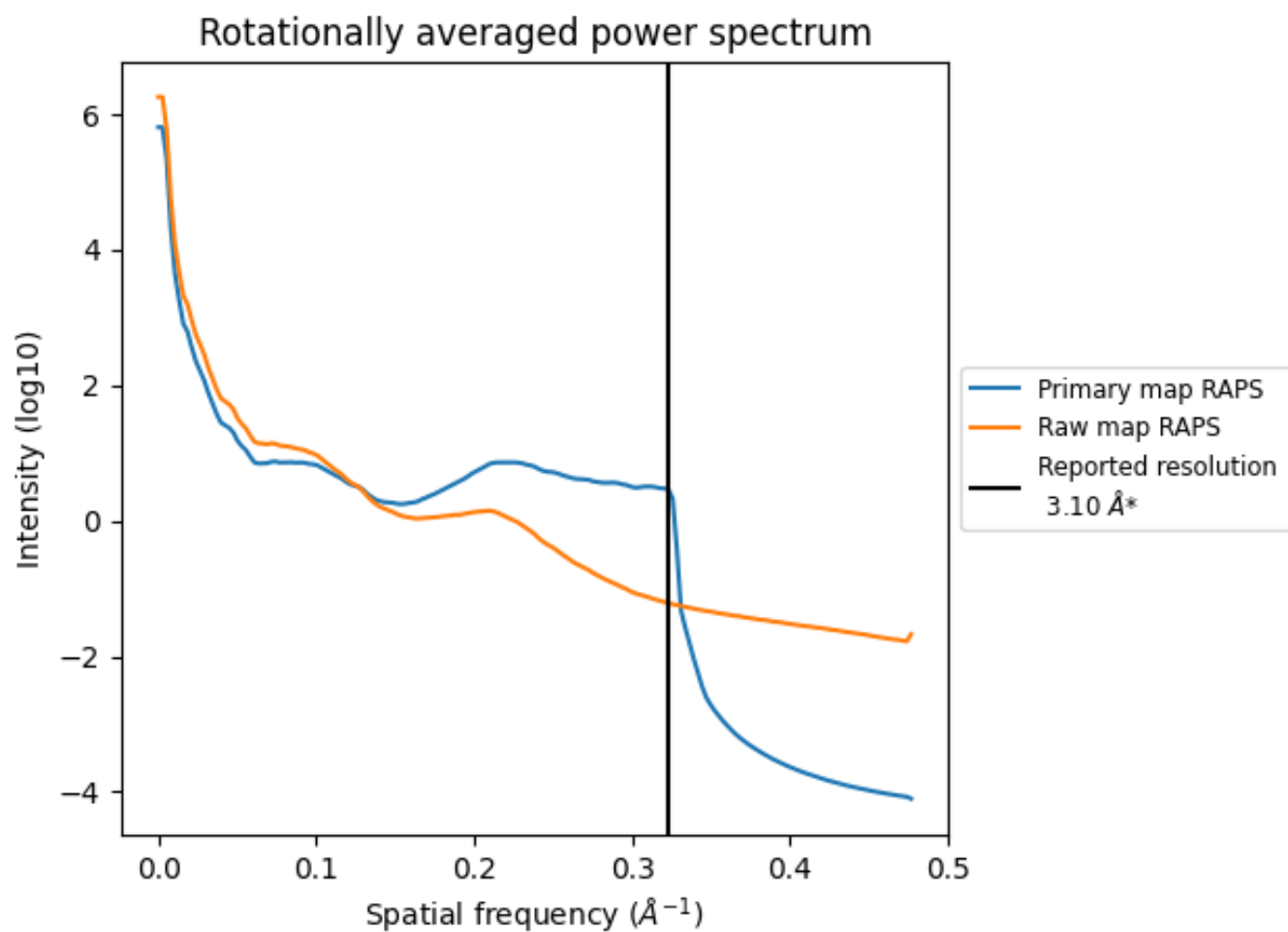
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 223 nm³; this corresponds to an approximate mass of 202 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum i

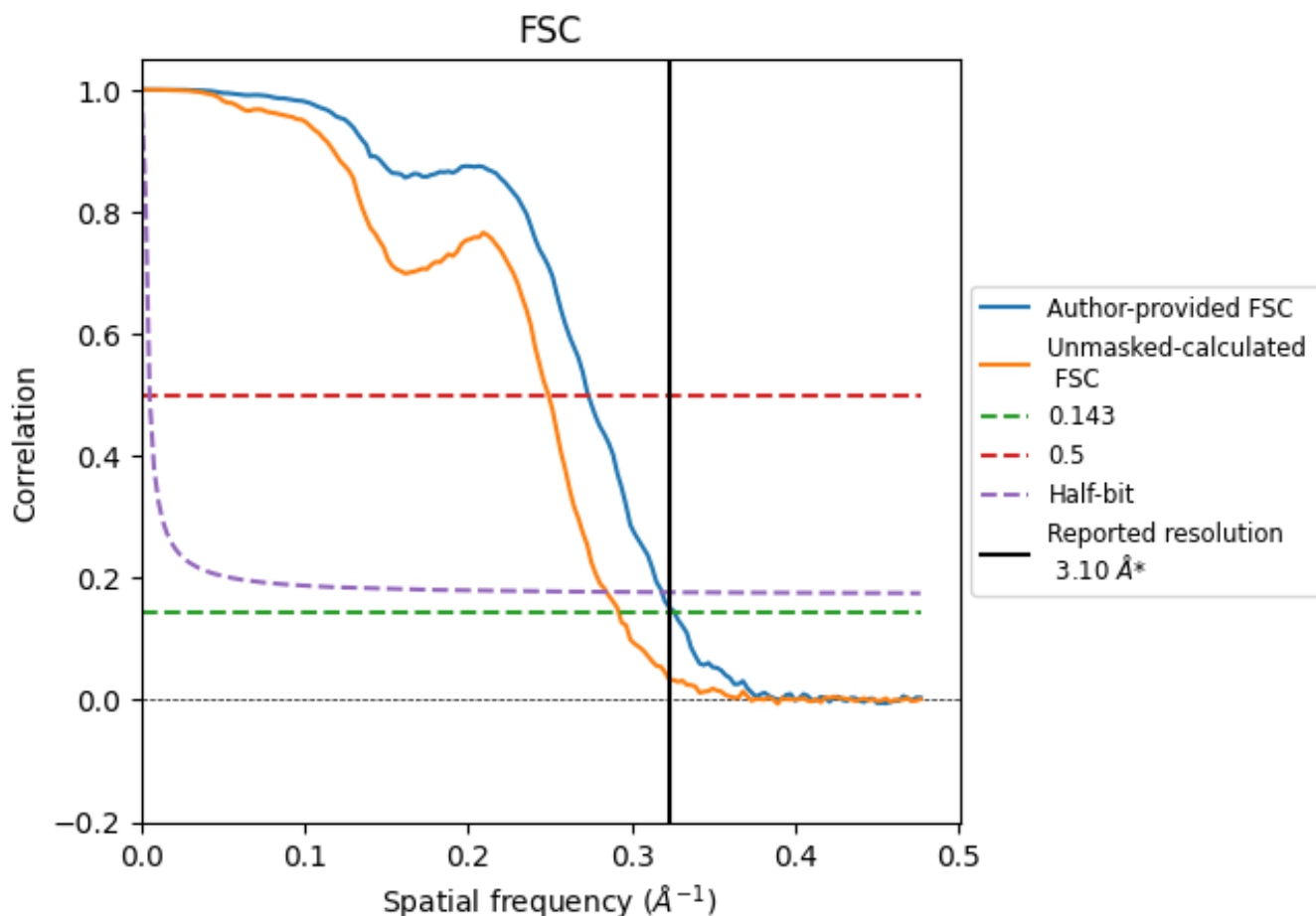


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

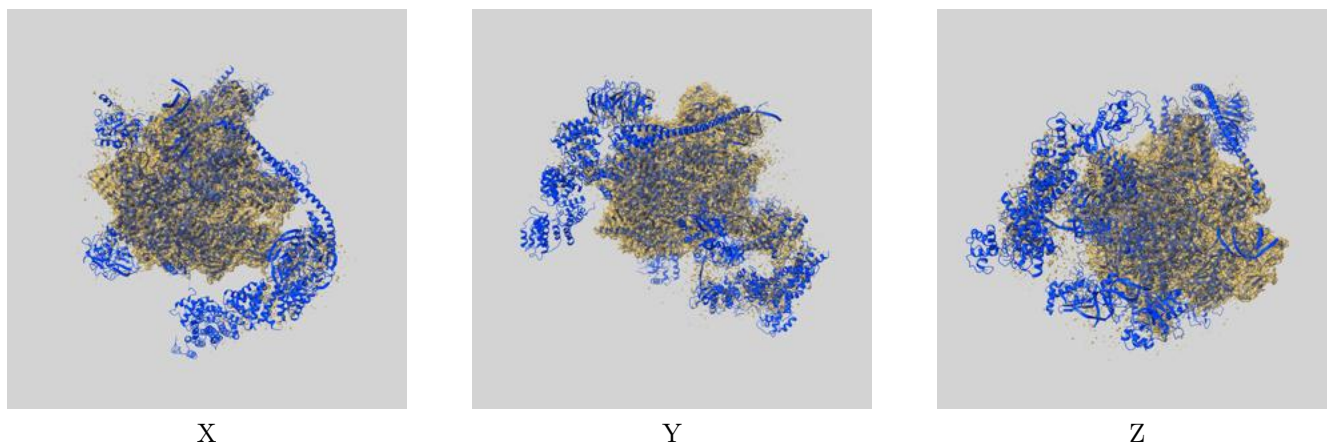
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.07	3.66	3.14
Unmasked-calculated*	3.42	4.01	3.51

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.42 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

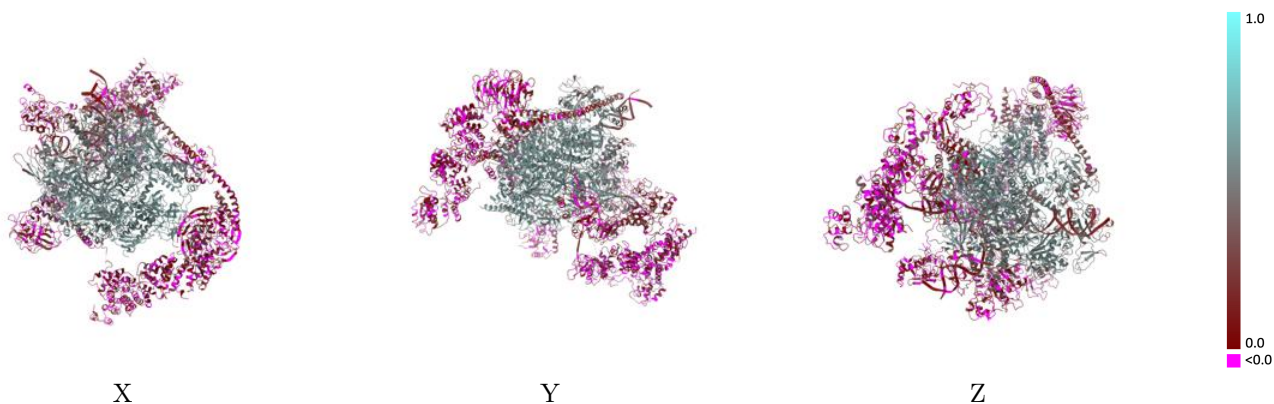
This section contains information regarding the fit between EMDB map EMD-10480 and PDB model 6TED. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



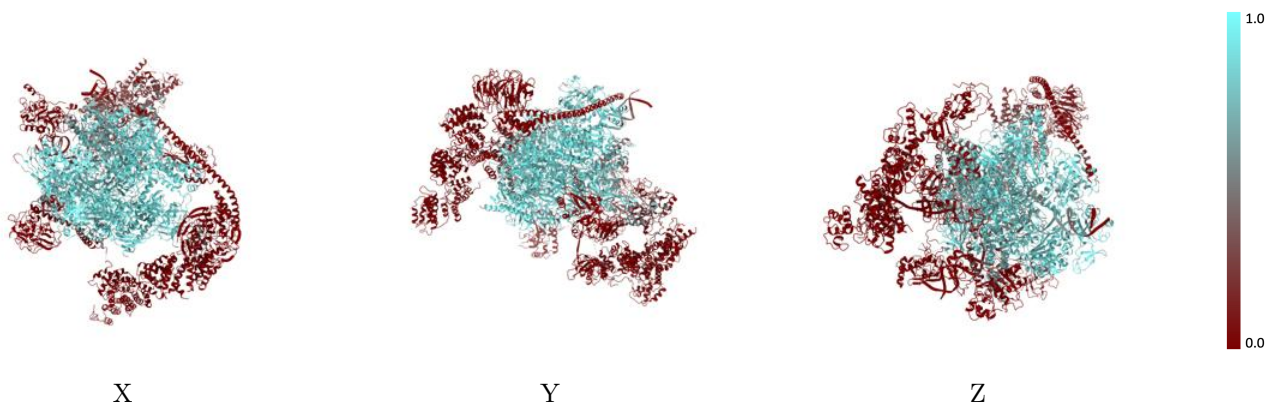
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



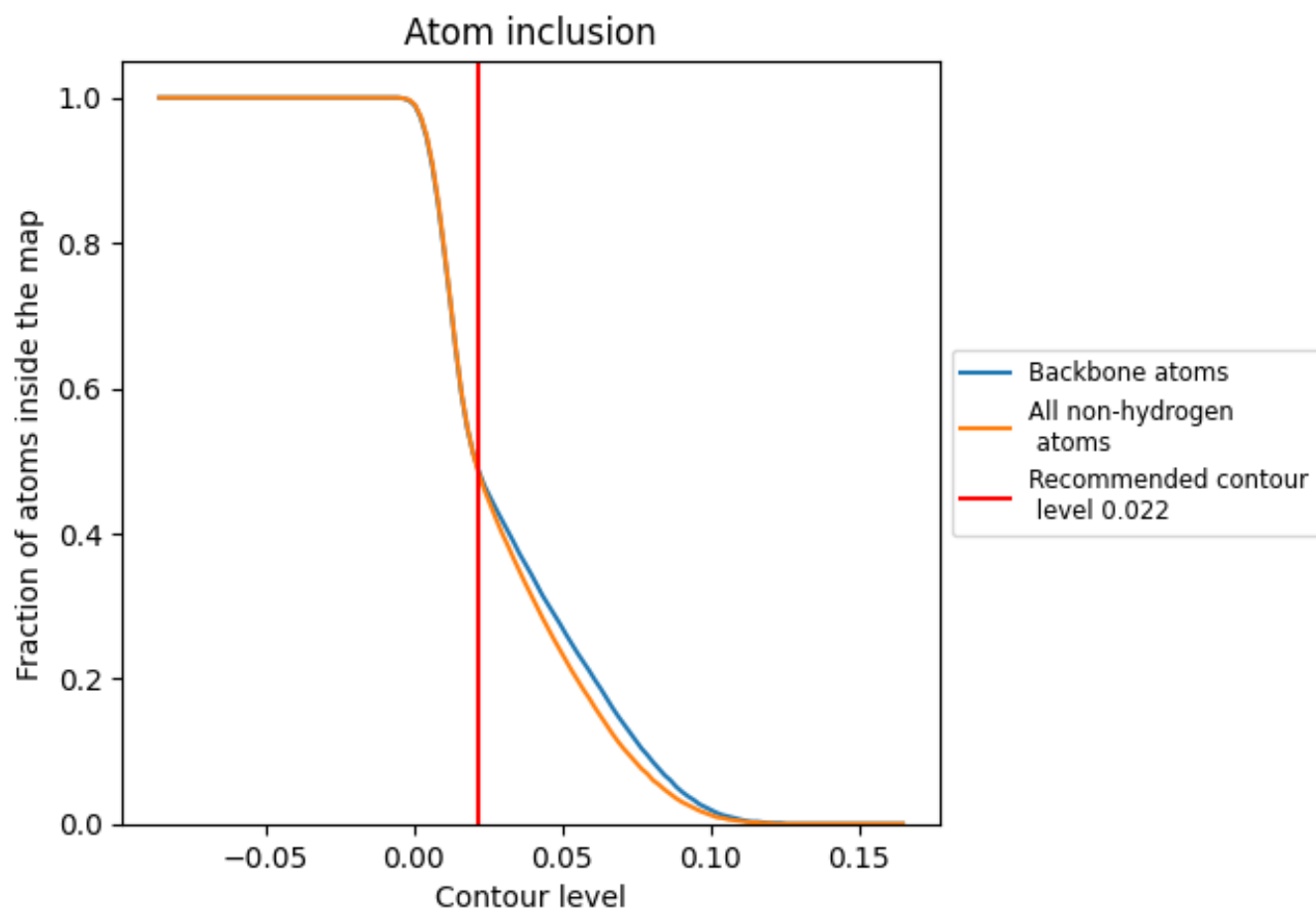
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.022).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 48% of all backbone atoms, 48% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4810	 0.3380
A	 0.8490	 0.5370
B	 0.8820	 0.5560
C	 0.9110	 0.5800
D	 0.2730	 0.1850
E	 0.8540	 0.5210
F	 0.8960	 0.5740
G	 0.4390	 0.3110
H	 0.8510	 0.5590
I	 0.8470	 0.5110
J	 0.9180	 0.5730
K	 0.9210	 0.5890
L	 0.8480	 0.5090
M	 0.0150	 0.0750
N	 0.3470	 0.2200
P	 0.4250	 0.2780
Q	 0.0280	 0.1020
R	 0.0120	 0.0880
T	 0.5190	 0.3100
U	 0.0550	 0.1140
V	 0.0260	 0.1270
W	 0.0110	 0.0430
X	 0.0240	 0.1060
Y	 0.0060	 0.0770
Z	 0.0990	 0.1660

