



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 07:57 PM UTC

PDB ID : 7Z30 / pdb_00007z30
EMDB ID : EMD-14469
Title : Structure of yeast RNA Polymerase III-Ty1 integrase complex at 2.9 Å (focus subunit C11 terminal Zn-ribbon in the funnel pore).
Authors : Nguyen, P.Q.; Fernandez-Tornero, C.
Deposited on : 2022-03-01
Resolution : 2.90 Å(reported)

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
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

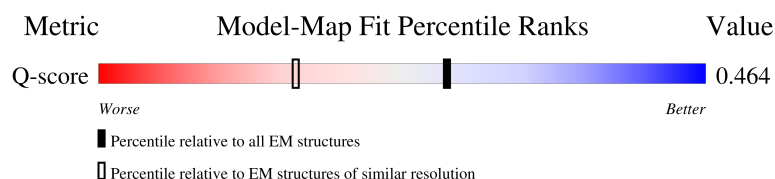
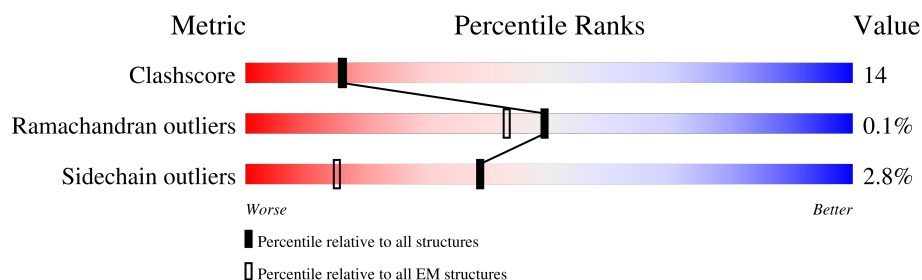
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	1460	24% 68% 27% ..
2	B	1149	13% 65% 30% ..
3	C	335	73% 25% .
4	D	161	86% 55% 35% 10%

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Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	212	
8	H	146	
9	I	110	
10	J	70	
11	K	142	
12	L	70	
13	M	282	
14	N	422	
15	O	654	
16	P	317	
17	Q	251	
18	W	635	
19	X	17	

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 40685 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 III subunit RPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1419	Total	C	N	O	S	0	0
			11123	7013	1962	2089	59		

- Molecule 2 is a protein called DNA-directed RNA polymerase III subunit RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1102	Total	C	N	O	S	0	0
			8701	5507	1499	1635	60		

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	335	Total	C	N	O	S	0	0
			2655	1681	454	511	9		

- Molecule 4 is a protein called DNA-directed RNA polymerase III subunit RPC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	145	Total	C	N	O	S	0	0
			1140	723	191	220	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	215	Total	C	N	O	S	0	0
			1759	1116	310	321	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	83	Total	C	N	O	S	0	0
			671	429	114	125	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase III subunit RPC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	191	Total	C	N	O	S	0	0
			1544	1007	250	281	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	138	Total	C	N	O	S	0	0
			1103	694	186	218	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	110	Total	C	N	O	S	0	0
			872	546	145	170	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			549	350	95	98	6		

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	101	Total	C	N	O	S	0	0
			792	496	130	161	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	50	Total	C	N	O	S	0	0
			381	235	76	66	4		

- Molecule 13 is a protein called DNA-directed RNA polymerase III subunit RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	183	Total	C	N	O	S	0	0
			1492	953	250	288	1		

- Molecule 14 is a protein called DNA-directed RNA polymerase III subunit RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	151	Total	C	N	O	S	0	0
			1169	738	215	213	3		

- Molecule 15 is a protein called DNA-directed RNA polymerase III subunit RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	568	Total	C	N	O	S	0	0
			4558	2897	784	858	19		

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	136	Total	C	N	O	S	0	0
			1126	736	175	211	4		

- Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	104	Total	C	N	O	S	0	0
			829	535	137	154	3		

- Molecule 18 is a protein called Integrase.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	17	Total	C	N	O	S	0	0
			141	86	27	27	1		

- Molecule 19 is a protein called Unknown RNA Polymerase III chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	X	14	Total	C	N	O	0	0
			70	42	14	14		

- Molecule 20 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
20	A	2	Total	Zn	0
			2	2	
20	B	1	Total	Zn	0
			1	1	
20	I	2	Total	Zn	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
20	J	1	Total 1	Zn 1	0
20	L	1	Total 1	Zn 1	0

- Molecule 21 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
21	A	1	Total 1	Mg 1	0
21	I	1	Total 1	Mg 1	0

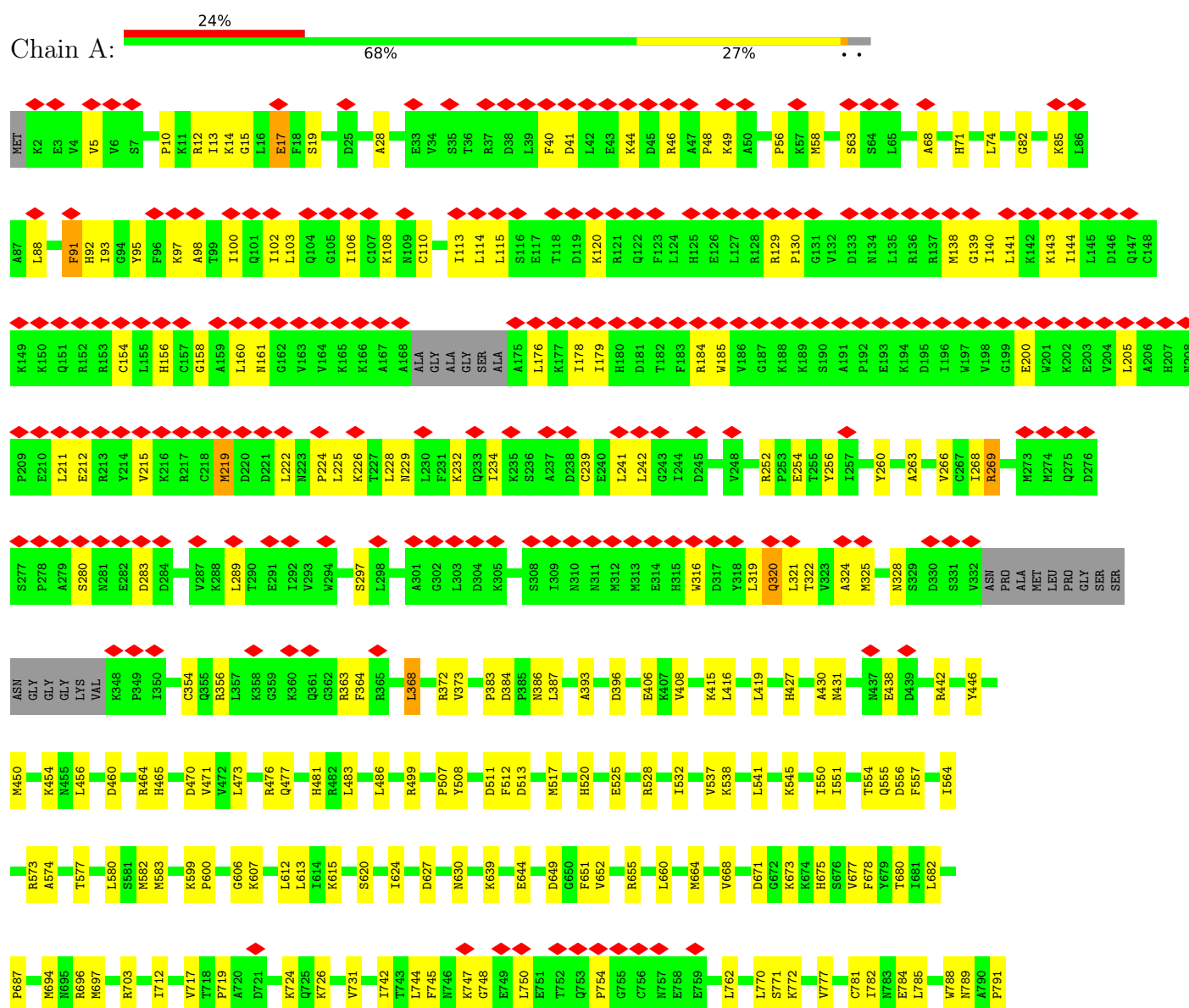
- Molecule 22 is water.

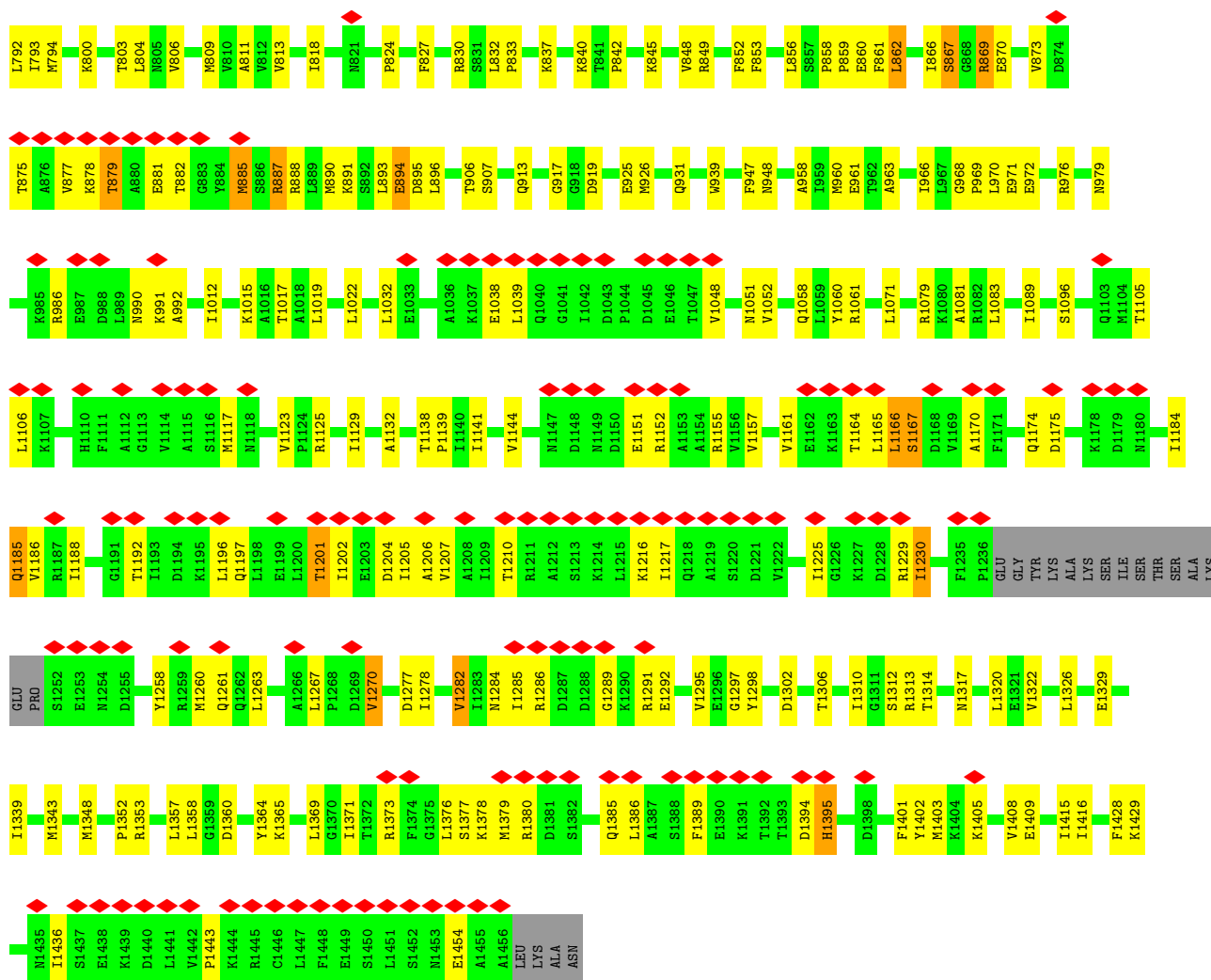
Mol	Chain	Residues	Atoms		AltConf
22	A	1	Total 1	O 1	0

3 Residue-property plots

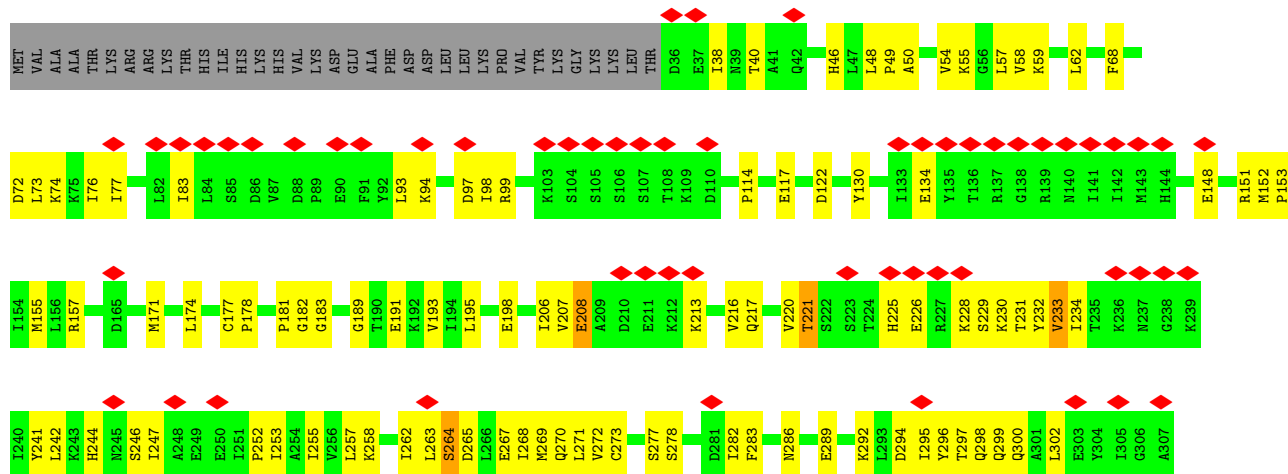
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

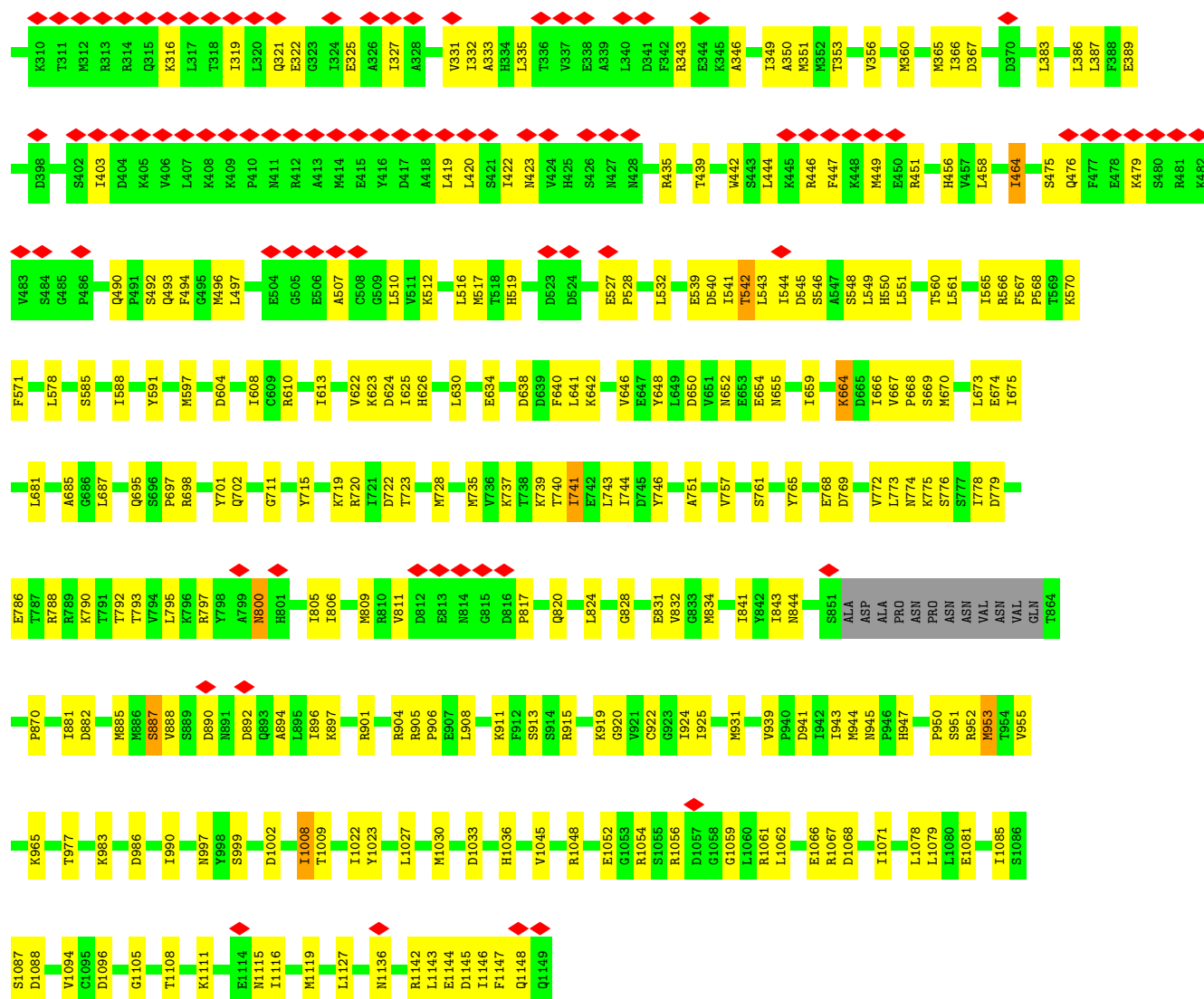
- Molecule 1: DNA-directed RNA polymerase III subunit RPC1



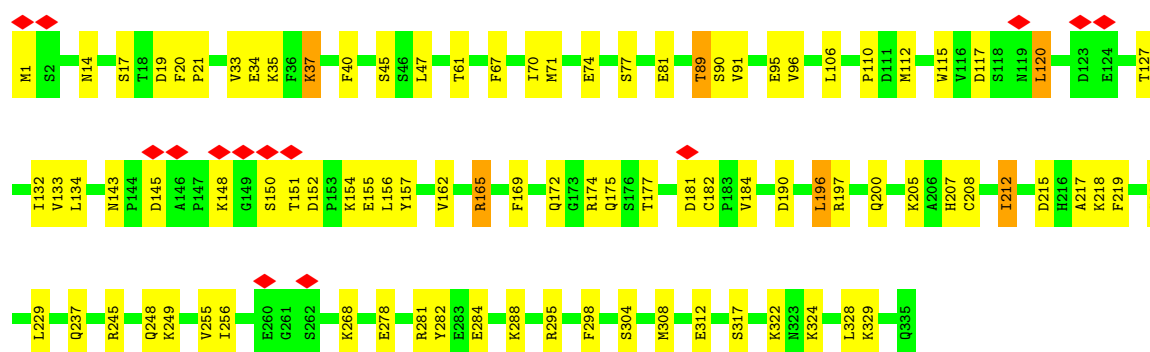


• Molecule 2: DNA-directed RNA polymerase III subunit RPC2

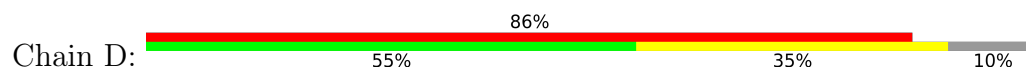


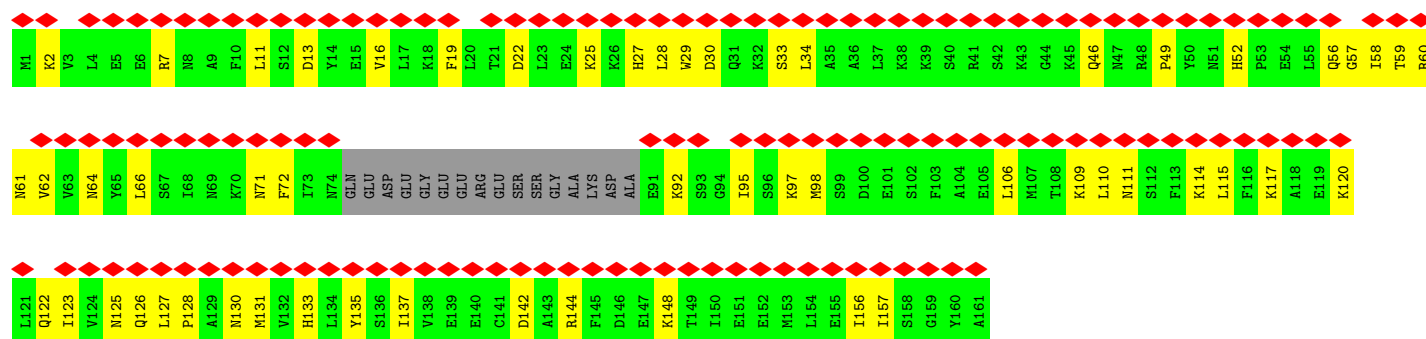


• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

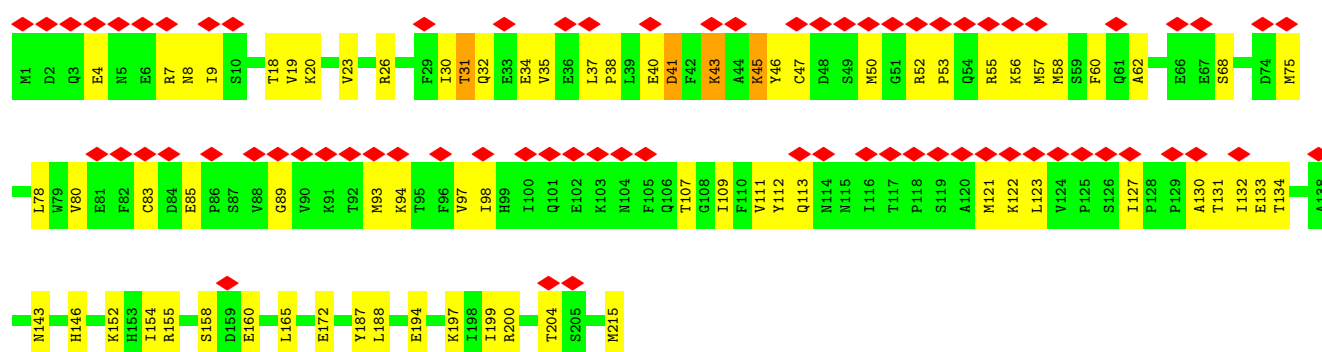


• Molecule 4: DNA-directed RNA polymerase III subunit RPC9

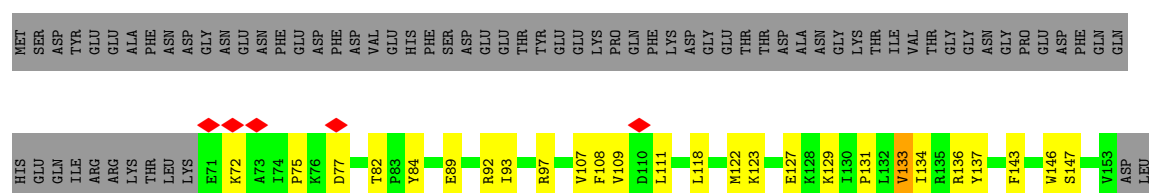
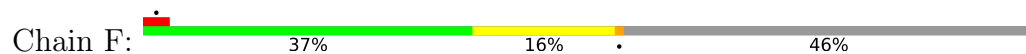




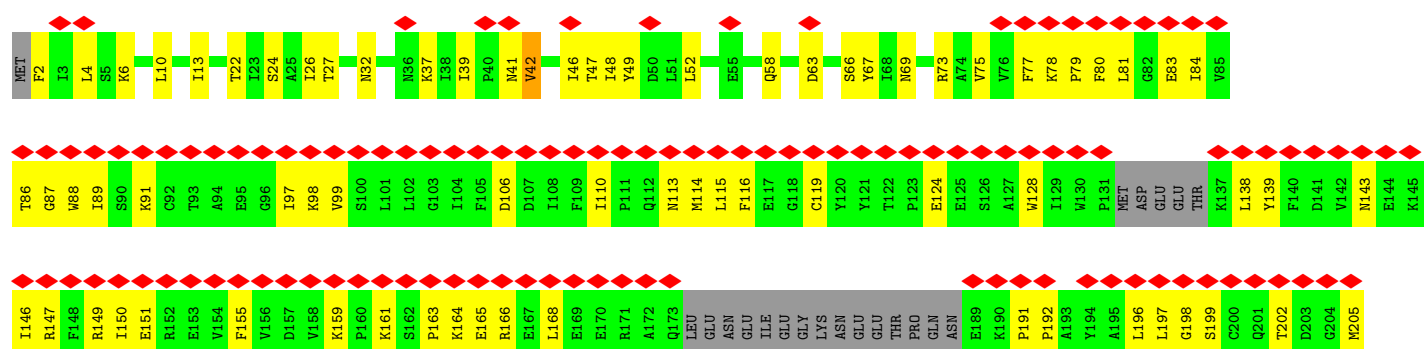
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



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

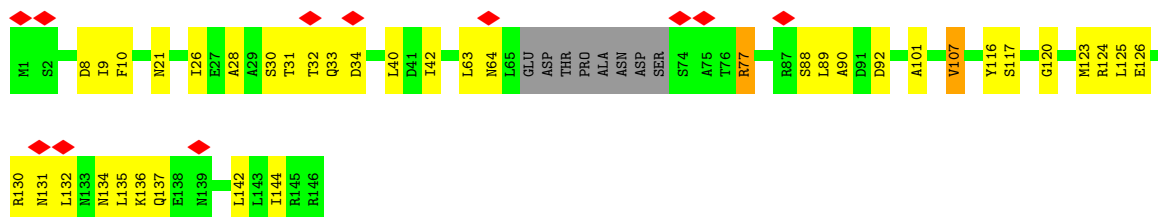


• Molecule 7: DNA-directed RNA polymerase III subunit RPC8

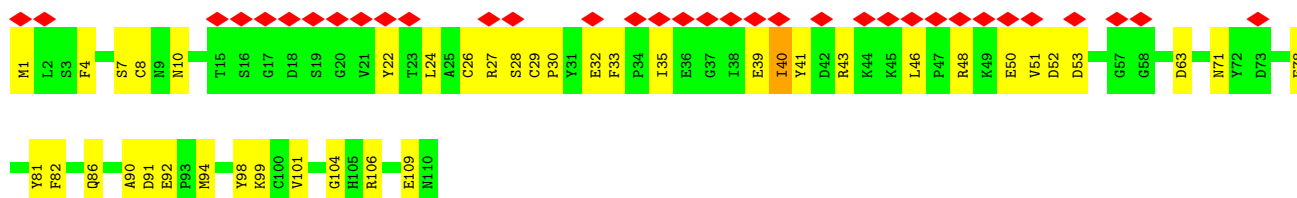




- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



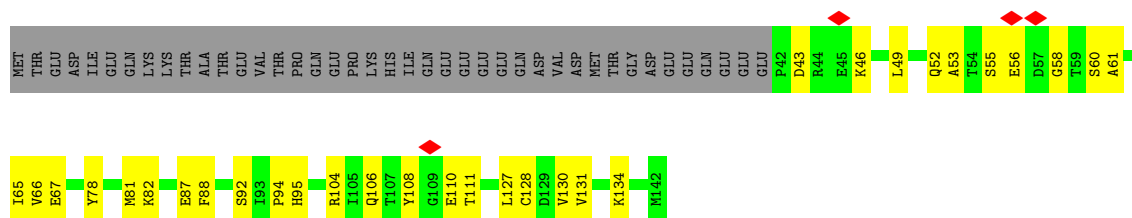
- Molecule 9: DNA-directed RNA polymerase III subunit RPC10



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

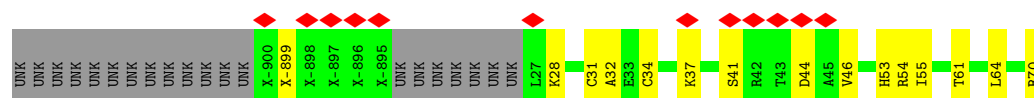


- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

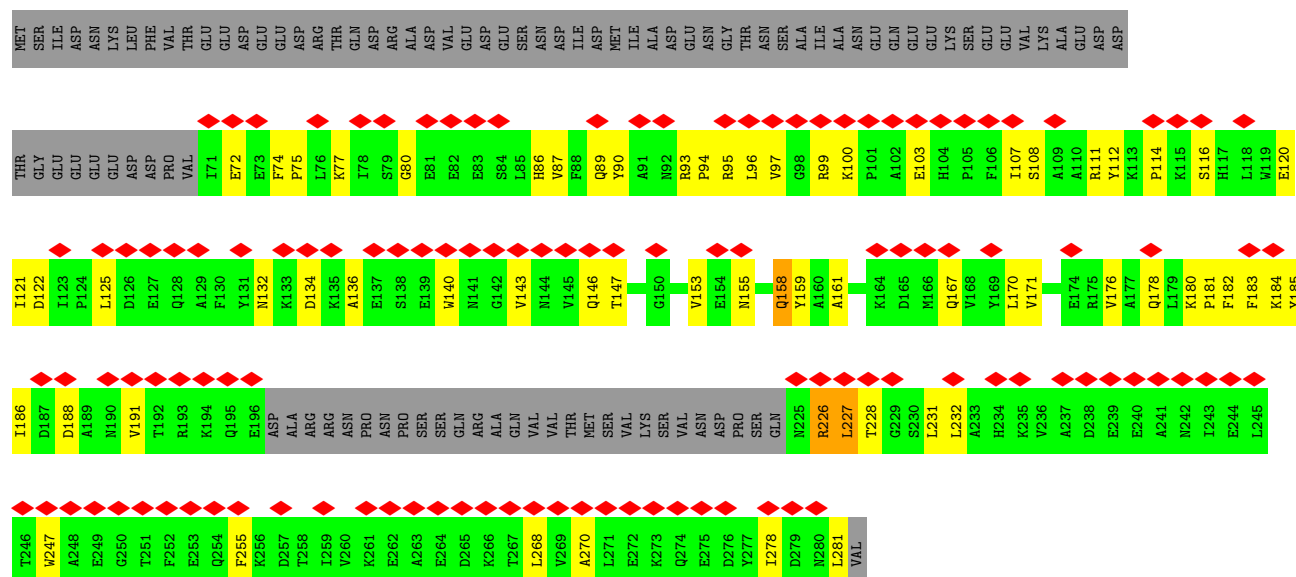
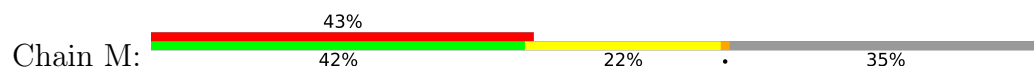


- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

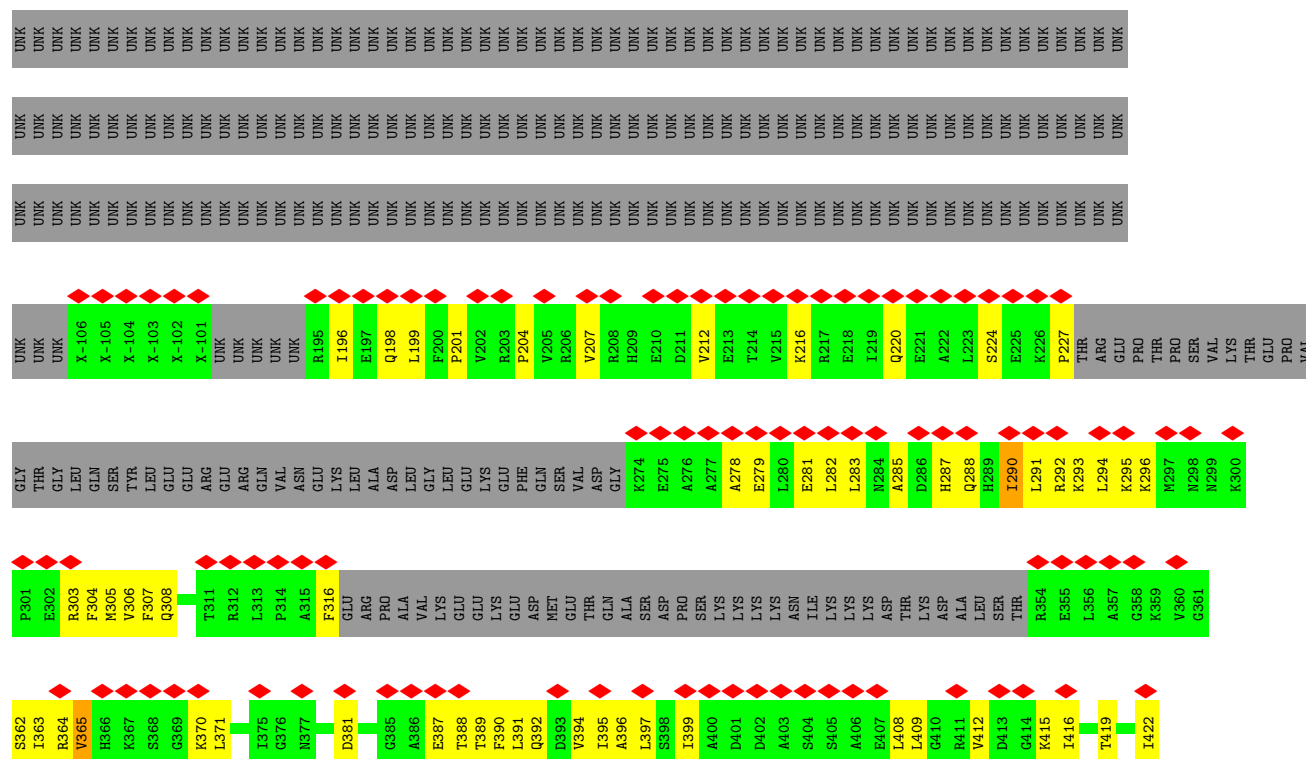




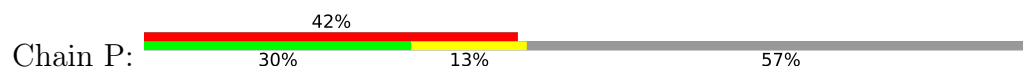
• Molecule 13: DNA-directed RNA polymerase III subunit RPC5



• Molecule 14: DNA-directed RNA polymerase III subunit RPC4



Chain O:



GLU	ASP	ASN	GLU	THR	GLU	ILE	LYS	V609	S610	R611	D612	T613	W614	N615	T616	K617	M618	M619	R620	S621	L622	E623	P624	P625	ARG	SER	LYS	LYS	ARG	ILE	HIS	LEU	ILE	ALA
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Chain X:

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	643858	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42.45	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.154	Depositor
Minimum map value	-0.086	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0227	Depositor
Map size ($\text{\AA}$)	317.99997, 317.99997, 317.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.24	0/11322	0.44	1/15295 (0.0%)
2	B	0.20	0/8853	0.40	0/11940
3	C	0.43	0/2711	0.57	0/3676
4	D	0.15	0/1158	0.45	0/1550
5	E	0.26	0/1795	0.48	0/2416
6	F	0.16	0/683	0.36	0/923
7	G	0.18	0/1583	0.48	1/2146 (0.0%)
8	H	0.18	0/1121	0.41	0/1517
9	I	0.21	0/893	0.46	0/1208
10	J	0.14	0/558	0.34	0/750
11	K	0.17	0/803	0.36	0/1083
12	L	0.14	0/353	0.46	0/468
13	M	0.21	0/1524	0.43	0/2061
14	N	0.17	0/1152	0.46	0/1546
15	O	0.17	0/4627	0.44	0/6243
16	P	0.13	0/1157	0.36	0/1571
17	Q	0.16	0/850	0.45	0/1148
18	W	0.09	0/144	0.31	0/195
All	All	0.22	0/41287	0.44	2/55736 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
3	C	0	1
13	M	0	1
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1371	ILE	N-CA-C	-6.51	105.99	112.17
7	G	42	VAL	N-CA-C	-5.86	108.15	113.71

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	869	ARG	Sidechain
1	A	888	ARG	Sidechain
3	C	174	ARG	Sidechain
13	M	226	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11123	0	11245	326	0
2	B	8701	0	8822	290	0
3	C	2655	0	2628	56	0
4	D	1140	0	1112	49	0
5	E	1759	0	1788	54	0
6	F	671	0	692	19	0
7	G	1544	0	1540	77	0
8	H	1103	0	1079	27	0
9	I	872	0	817	42	0
10	J	549	0	559	12	0
11	K	792	0	790	23	0
12	L	381	0	385	11	0
13	M	1492	0	1456	55	0
14	N	1169	0	1208	67	0
15	O	4558	0	4735	180	0
16	P	1126	0	1079	35	0
17	Q	829	0	819	28	0
18	W	141	0	137	3	0
19	X	70	0	20	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	A	2	0	0	0	0
20	B	1	0	0	0	0
20	I	2	0	0	0	0
20	J	1	0	0	0	0
20	L	1	0	0	0	0
21	A	1	0	0	0	0
21	I	1	0	0	0	0
22	A	1	0	0	0	0
All	All	40685	0	40911	1171	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 14.

All (1171) 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:232:TYR:OH	2:B:353:THR:HG22	1.44	1.18
19:X:1008:UNK:O	19:X:1010:UNK:N	2.04	0.91
2:B:269:MET:O	2:B:273:CYS:HB2	1.72	0.89
17:Q:51:GLU:HA	17:Q:54:LEU:HD12	1.55	0.87
2:B:299:GLN:HA	2:B:302:LEU:HD12	1.58	0.85
2:B:1045:VAL:HG23	19:X:1009:UNK:O	1.78	0.83
7:G:113:ASN:ND2	7:G:114:MET:SD	2.51	0.83
13:M:228:THR:HA	13:M:232:LEU:HB2	1.59	0.83
16:P:171:ASP:HB3	16:P:174:PHE:HB3	1.61	0.83
1:A:754:PRO:HB3	9:I:53:ASP:HB3	1.61	0.82
5:E:55:ARG:HA	5:E:58:MET:HE3	1.61	0.81
15:O:256:PRO:HA	15:O:259:LEU:HD23	1.62	0.81
1:A:393:ALA:HB3	1:A:499:ARG:HB2	1.62	0.81
15:O:506:ARG:HD3	16:P:250:ASP:HB2	1.64	0.79
2:B:171:MET:HE3	2:B:178:PRO:HA	1.64	0.79
4:D:11:LEU:HD21	7:G:4:LEU:HG	1.65	0.79
2:B:198:GLU:HB3	2:B:475:SER:HA	1.64	0.78
1:A:17:GLU:HG3	1:A:1405:LYS:HG2	1.66	0.78
5:E:9:ILE:HD12	5:E:43:LYS:HD3	1.64	0.78
15:O:578:ARG:HH22	15:O:648:TRP:HB2	1.49	0.77
1:A:878:LYS:HD2	1:A:1105:THR:HA	1.66	0.76
2:B:527:GLU:HG2	2:B:528:PRO:HD3	1.68	0.76
4:D:122:GLN:HE22	7:G:84:ILE:H	1.32	0.76
1:A:875:THR:HA	1:A:878:LYS:HD3	1.69	0.75
4:D:117:LYS:HZ1	17:Q:105:ILE:HD12	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:LEU:HD13	1:A:226:LYS:HD3	1.69	0.75
3:C:132:ILE:HD12	3:C:184:VAL:HG21	1.69	0.74
7:G:10:LEU:HD11	7:G:67:TYR:HB3	1.69	0.74
1:A:907:SER:HB2	1:A:1409:GLU:HG3	1.66	0.74
17:Q:133:PRO:HD2	17:Q:136:LEU:HD12	1.68	0.74
1:A:613:LEU:O	1:A:696:ARG:NH1	2.20	0.73
7:G:115:LEU:HD23	7:G:116:PHE:H	1.54	0.73
9:I:99:LYS:HB2	9:I:106:ARG:HD2	1.71	0.73
1:A:1175:ASP:OD2	1:A:1261:GLN:NE2	2.20	0.73
17:Q:53:SER:OG	17:Q:57:LYS:NZ	2.23	0.72
1:A:325:MET:HE3	1:A:325:MET:H	1.52	0.72
2:B:271:LEU:O	2:B:550:HIS:NE2	2.20	0.72
7:G:110:ILE:HG22	7:G:198:GLY:H	1.55	0.72
15:O:288:MET:HE1	15:O:326:ILE:HD13	1.70	0.72
1:A:85:LYS:HD3	1:A:260:TYR:HE1	1.54	0.71
13:M:136:ALA:HB1	13:M:143:VAL:HG21	1.71	0.71
1:A:256:TYR:HE2	1:A:1401:PHE:HA	1.55	0.71
9:I:4:PHE:HE1	14:N:204:PRO:HD3	1.55	0.71
2:B:221:THR:HG21	2:B:333:ALA:HA	1.72	0.71
4:D:13:ASP:OD2	4:D:125:ASN:ND2	2.24	0.71
15:O:164:ILE:HG22	15:O:282:ILE:HG21	1.73	0.71
2:B:234:ILE:HD11	2:B:356:VAL:HG13	1.72	0.70
4:D:106:LEU:HB3	4:D:110:LEU:HD23	1.73	0.70
1:A:1167:SER:HA	9:I:46:LEU:HD23	1.71	0.70
4:D:95:ILE:HA	4:D:98:MET:HE1	1.74	0.70
11:K:53:ALA:O	11:K:104:ARG:NH1	2.24	0.70
1:A:968:GLY:HA2	1:A:971:GLU:HB2	1.73	0.69
16:P:163:PRO:HG3	16:P:233:VAL:HG11	1.75	0.69
2:B:548:SER:HA	2:B:551:LEU:HD12	1.72	0.69
1:A:108:LYS:O	15:O:572:HIS:NE2	2.25	0.69
2:B:244:HIS:HD2	2:B:246:SER:H	1.41	0.69
2:B:232:TYR:HH	2:B:353:THR:HG22	1.56	0.69
5:E:46:TYR:HA	5:E:57:MET:HE1	1.75	0.69
15:O:303:ARG:HH12	15:O:465:PHE:HB2	1.56	0.68
1:A:958:ALA:HA	1:A:961:GLU:HG3	1.74	0.68
1:A:1185:GLN:HE22	1:A:1229:ARG:HG2	1.59	0.68
1:A:848:VAL:HA	1:A:860:GLU:HG2	1.74	0.68
7:G:97:ILE:HG22	7:G:110:ILE:HD11	1.75	0.68
1:A:1454:GLU:OE1	4:D:111:ASN:ND2	2.26	0.68
1:A:176:LEU:O	1:A:320:GLN:NE2	2.27	0.68
5:E:112:TYR:HE1	5:E:134:THR:HG23	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:578:ARG:O	15:O:582:GLU:HG2	1.94	0.68
2:B:1036:HIS:HB2	2:B:1054:ARG:HD2	1.76	0.68
4:D:117:LYS:NZ	17:Q:105:ILE:HD12	2.09	0.68
4:D:30:ASP:HB2	4:D:60:ARG:HH22	1.58	0.67
2:B:72:ASP:O	2:B:76:ILE:HG12	1.94	0.67
2:B:774:ASN:ND2	2:B:775:LYS:O	2.28	0.67
5:E:23:VAL:HG13	5:E:30:ILE:HD13	1.77	0.67
15:O:289:LYS:HE2	15:O:326:ILE:HB	1.77	0.67
1:A:1170:ALA:HB3	9:I:46:LEU:HD22	1.77	0.67
15:O:492:TYR:CZ	15:O:573:SER:HB2	2.29	0.67
1:A:1394:ASP:OD1	1:A:1395:HIS:N	2.28	0.66
13:M:180:LYS:HG3	13:M:181:PRO:HD2	1.77	0.66
13:M:87:VAL:HG22	14:N:394:VAL:HG12	1.75	0.66
15:O:137:ILE:HD11	17:Q:57:LYS:HD3	1.78	0.66
14:N:290:ILE:HD11	14:N:416:ILE:HD12	1.78	0.66
1:A:200:GLU:HG2	15:O:515:LYS:HB3	1.78	0.66
2:B:1045:VAL:CG2	19:X:1009:UNK:O	2.44	0.66
6:F:107:VAL:HG21	6:F:111:LEU:HD21	1.77	0.66
13:M:247:TRP:HZ2	14:N:408:LEU:HD12	1.61	0.66
1:A:476:ARG:HG3	1:A:517:MET:HG2	1.78	0.66
15:O:140:ILE:HG21	15:O:160:VAL:HG21	1.78	0.66
5:E:20:LYS:HE3	5:E:34:GLU:HB2	1.76	0.65
16:P:215:TYR:HB2	16:P:260:CYS:HB3	1.78	0.65
1:A:556:ASP:OD2	2:B:945:ASN:ND2	2.26	0.65
11:K:88:PHE:HB3	11:K:106:GLN:HB2	1.79	0.65
1:A:979:ASN:HB3	5:E:160:GLU:HG2	1.79	0.65
1:A:373:VAL:HG11	2:B:1062:LEU:HD12	1.78	0.65
2:B:915:ARG:HD2	2:B:1023:TYR:HD2	1.62	0.65
9:I:35:ILE:HD11	9:I:40:ILE:HD11	1.79	0.65
1:A:372:ARG:NH1	2:B:1059:GLY:O	2.28	0.65
1:A:624:ILE:HD12	1:A:680:THR:HG22	1.79	0.65
15:O:210:PRO:HG2	15:O:213:ASP:HB2	1.79	0.64
1:A:583:MET:HE2	1:A:613:LEU:HD12	1.78	0.64
15:O:61:ALA:HB1	15:O:98:LEU:HD21	1.80	0.64
1:A:742:ILE:HD13	1:A:762:LEU:HD21	1.77	0.64
2:B:695:GLN:HG2	2:B:697:PRO:HD2	1.80	0.64
1:A:12:ARG:HG2	2:B:1146:ILE:HG23	1.79	0.64
1:A:1079:ARG:HD2	6:F:84:TYR:CZ	2.32	0.64
1:A:1022:LEU:HD22	1:A:1060:TYR:HD1	1.62	0.64
2:B:264:SER:HB3	2:B:267:GLU:HG2	1.79	0.64
1:A:1022:LEU:HD22	1:A:1060:TYR:CD1	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1056:ARG:NH1	19:X:1008:UNK:CB	2.60	0.63
4:D:131:MET:HE3	4:D:135:TYR:HB2	1.80	0.63
15:O:365:ASP:OD1	15:O:368:ARG:NH2	2.31	0.63
14:N:305:MET:HE2	14:N:416:ILE:HD11	1.79	0.63
1:A:1429:LYS:HG3	6:F:137:TYR:HE2	1.64	0.63
13:M:112:TYR:CE2	14:N:397:LEU:HD21	2.33	0.63
1:A:917:GLY:HA3	1:A:1353:ARG:HG2	1.81	0.63
1:A:1155:ARG:NH2	9:I:52:ASP:O	2.32	0.63
11:K:56:GLU:N	11:K:56:GLU:OE2	2.30	0.63
12:L:31:CYS:CB	12:L:34:CYS:SG	2.87	0.63
13:M:103:GLU:OE1	14:N:198:GLN:NE2	2.32	0.62
7:G:207:LEU:HG	7:G:209:SER:H	1.64	0.62
15:O:168:SER:HB3	15:O:279:SER:HB2	1.80	0.62
1:A:40:PHE:HB3	1:A:46:ARG:HA	1.80	0.62
1:A:1017:THR:HG23	1:A:1032:LEU:HD11	1.81	0.62
5:E:18:THR:HG23	5:E:143:ASN:HB3	1.81	0.62
12:L:28:LYS:HD2	12:L:37:LYS:HG3	1.80	0.62
14:N:399:ILE:HD12	14:N:399:ILE:O	2.00	0.62
2:B:1067:ARG:NH2	2:B:1068:ASP:OD1	2.32	0.62
15:O:169:LEU:HD21	15:O:174:TYR:HD2	1.64	0.62
6:F:109:VAL:HG21	6:F:123:LYS:HG2	1.81	0.62
15:O:294:LYS:NZ	15:O:298:ASN:HD22	1.96	0.62
2:B:343:ARG:NH2	2:B:544:ILE:O	2.33	0.62
16:P:175:ILE:HA	16:P:178:LEU:HD12	1.82	0.62
9:I:7:SER:O	13:M:146:GLN:NE2	2.33	0.61
16:P:193:ASN:HB2	16:P:197:ASN:HB2	1.81	0.61
1:A:28:ALA:HA	15:O:32:MET:HE1	1.81	0.61
2:B:800:ASN:OD1	2:B:800:ASN:N	2.32	0.61
14:N:290:ILE:O	14:N:294:LEU:HG	2.00	0.61
1:A:664:MET:HA	1:A:664:MET:HE2	1.82	0.61
1:A:1184:ILE:HG13	1:A:1260:MET:HE3	1.81	0.61
2:B:551:LEU:HD23	14:N:216:LYS:HG2	1.81	0.61
2:B:776:SER:HB2	3:C:217:ALA:HB2	1.83	0.61
15:O:360:THR:HG22	15:O:477:TYR:HB3	1.83	0.61
15:O:83:ILE:HG22	15:O:85:GLY:H	1.65	0.61
15:O:338:ASP:HB2	15:O:345:PHE:HE1	1.64	0.61
4:D:127:LEU:HB3	4:D:133:HIS:HB3	1.82	0.61
15:O:494:TYR:CE2	16:P:294:PHE:HA	2.35	0.61
4:D:126:GLN:NE2	7:G:84:ILE:O	2.30	0.60
5:E:50:MET:HE3	5:E:50:MET:H	1.66	0.60
1:A:386:ASN:ND2	2:B:765:TYR:OH	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:698:ARG:HD2	2:B:952:ARG:HB3	1.84	0.60
1:A:557:PHE:HB3	1:A:697:MET:HE3	1.83	0.60
15:O:262:ILE:HG13	15:O:263:LEU:HD12	1.81	0.60
2:B:302:LEU:HB3	2:B:325:GLU:HG2	1.82	0.60
12:L:31:CYS:HB3	12:L:34:CYS:SG	2.41	0.60
15:O:617:GLU:HG2	15:O:618:LEU:HG	1.82	0.60
1:A:473:LEU:HB2	1:A:520:HIS:HB2	1.82	0.60
3:C:89:THR:HG22	3:C:200:GLN:HA	1.82	0.60
7:G:202:THR:H	7:G:205:MET:HE2	1.67	0.60
1:A:541:LEU:HD12	1:A:682:LEU:HD13	1.82	0.59
2:B:1148:GLN:HA	7:G:69:ASN:HD21	1.67	0.59
15:O:585:MET:O	15:O:589:LEU:HD22	2.02	0.59
2:B:1105:GLY:HA2	2:B:1116:ILE:HG21	1.84	0.59
2:B:257:LEU:HD23	2:B:268:ILE:HG23	1.83	0.59
13:M:107:ILE:HD12	13:M:121:ILE:HD11	1.85	0.59
15:O:643:ARG:NH2	17:Q:51:GLU:OE1	2.35	0.59
1:A:160:LEU:HD11	1:A:185:TRP:HD1	1.66	0.59
15:O:537:LEU:O	15:O:541:ILE:HG12	2.02	0.59
15:O:96:VAL:HG23	17:Q:136:LEU:HD13	1.84	0.59
1:A:200:GLU:HG3	15:O:515:LYS:HZ2	1.67	0.59
2:B:622:VAL:O	2:B:626:HIS:ND1	2.33	0.59
1:A:1141:ILE:HB	1:A:1295:VAL:HG22	1.84	0.59
4:D:58:ILE:HD13	7:G:46:ILE:HA	1.84	0.59
13:M:97:VAL:HG21	14:N:198:GLN:HG3	1.84	0.59
2:B:77:ILE:HD13	2:B:98:ILE:HB	1.85	0.59
2:B:997:ASN:OD1	2:B:999:SER:OG	2.21	0.59
5:E:93:MET:HE3	5:E:123:LEU:HD12	1.84	0.58
2:B:566:ARG:HH21	14:N:282:LEU:HD21	1.68	0.58
1:A:678:PHE:HB3	1:A:694:MET:HE2	1.85	0.58
1:A:1286:ARG:HD2	1:A:1292:GLU:HG2	1.85	0.58
2:B:207:VAL:HA	2:B:217:GLN:HB2	1.84	0.58
2:B:464:ILE:HG13	2:B:687:LEU:HD21	1.85	0.58
2:B:570:LYS:HZ3	14:N:283:LEU:HG	1.68	0.58
2:B:570:LYS:NZ	14:N:283:LEU:HG	2.18	0.58
5:E:52:ARG:HD2	5:E:53:PRO:HD2	1.85	0.58
2:B:667:VAL:HG22	2:B:668:PRO:HD2	1.86	0.58
2:B:811:VAL:HA	2:B:817:PRO:HA	1.84	0.58
6:F:118:LEU:O	6:F:122:MET:HG3	2.03	0.58
2:B:157:ARG:NH2	2:B:177:CYS:O	2.35	0.58
13:M:147:THR:O	13:M:182:PHE:N	2.36	0.58
5:E:127:ILE:HG12	5:E:130:ALA:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:131:LEU:HD21	15:O:648:TRP:HZ2	1.68	0.58
15:O:64:VAL:HG13	15:O:79:LEU:HD11	1.84	0.58
15:O:539:SER:O	15:O:542:ARG:NH1	2.37	0.57
15:O:589:LEU:HA	15:O:592:LYS:HG2	1.87	0.57
13:M:86:HIS:CE1	14:N:397:LEU:HD22	2.38	0.57
1:A:832:LEU:HD11	1:A:862:LEU:HD22	1.86	0.57
1:A:968:GLY:O	1:A:972:GLU:HG3	2.04	0.57
1:A:1204:ASP:HA	1:A:1207:VAL:HG22	1.86	0.57
1:A:1216:LYS:HB3	1:A:1217:ILE:HD12	1.85	0.57
5:E:62:ALA:HB3	5:E:78:LEU:HB3	1.87	0.57
15:O:549:GLN:NE2	15:O:567:ARG:HH21	2.01	0.57
1:A:919:ASP:OD2	1:A:1353:ARG:NH2	2.35	0.57
2:B:931:MET:HE3	2:B:943:ILE:HG13	1.85	0.57
7:G:80:PHE:CZ	17:Q:105:ILE:HD11	2.38	0.57
9:I:28:SER:HA	13:M:186:ILE:HD11	1.86	0.57
14:N:394:VAL:HG23	14:N:409:LEU:HB2	1.86	0.57
1:A:782:ILE:HG13	1:A:803:THR:HG23	1.87	0.57
2:B:1052:GLU:O	19:X:1004:UNK:O	2.22	0.57
7:G:115:LEU:HD23	7:G:116:PHE:N	2.19	0.57
2:B:887:SER:OG	2:B:888:VAL:N	2.37	0.57
15:O:567:ARG:HD2	15:O:569:LYS:HG2	1.87	0.57
7:G:147:ARG:HB3	7:G:205:MET:HA	1.87	0.57
15:O:39:GLN:HA	15:O:42:LEU:HD13	1.87	0.57
2:B:793:THR:HG21	2:B:843:ILE:HG21	1.86	0.57
2:B:356:VAL:O	2:B:360:MET:HG3	2.05	0.56
17:Q:128:ASN:HB2	17:Q:131:LEU:HD12	1.87	0.56
1:A:599:LYS:HG3	1:A:600:PRO:HA	1.86	0.56
2:B:94:LYS:HB3	2:B:134:GLU:HB2	1.86	0.56
2:B:207:VAL:HG13	2:B:366:ILE:HA	1.88	0.56
2:B:965:LYS:NZ	2:B:1002:ASP:OD2	2.33	0.56
3:C:172:GLN:H	3:C:175:GLN:HB2	1.71	0.56
4:D:71:ASN:HB3	7:G:208:VAL:HG21	1.86	0.56
5:E:165:LEU:HD11	5:E:172:GLU:HG3	1.86	0.56
9:I:32:GLU:HB2	13:M:132:ASN:HB2	1.88	0.56
15:O:44:PRO:HB2	15:O:582:GLU:HG3	1.86	0.56
15:O:643:ARG:HH11	16:P:291:PHE:HD1	1.54	0.56
2:B:809:MET:HG3	2:B:809:MET:O	2.05	0.56
8:H:40:LEU:HD13	8:H:123:MET:HB2	1.86	0.56
13:M:74:PHE:HB2	14:N:363:ILE:HG23	1.88	0.56
2:B:365:MET:HE2	2:B:365:MET:HA	1.87	0.56
2:B:542:THR:HB	13:M:153:VAL:HG21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:77:ARG:HE	8:H:77:ARG:HA	1.71	0.56
3:C:115:TRP:HH2	3:C:212:ILE:HG12	1.71	0.56
1:A:384:ASP:HB2	1:A:499:ARG:HB3	1.88	0.56
1:A:1289:GLY:O	1:A:1291:ARG:NH1	2.38	0.56
15:O:35:SER:O	15:O:40:ARG:NH2	2.38	0.56
15:O:588:LEU:HD11	15:O:644:LEU:HD13	1.86	0.56
1:A:887:ARG:HH12	1:A:1389:PHE:HA	1.71	0.56
1:A:963:ALA:HB2	1:A:1012:ILE:HG21	1.88	0.56
2:B:687:LEU:HD12	2:B:741:ILE:HG22	1.86	0.56
2:B:885:MET:HE3	2:B:887:SER:HB3	1.87	0.56
13:M:72:GLU:H	14:N:365:VAL:HG13	1.71	0.56
14:N:396:ALA:HB2	14:N:409:LEU:HD11	1.87	0.56
15:O:211:ILE:HD12	15:O:330:LEU:HD23	1.88	0.56
15:O:624:LEU:O	15:O:628:LYS:HD3	2.06	0.56
1:A:818:ILE:HD11	1:A:824:PRO:HD2	1.88	0.56
2:B:68:PHE:HA	2:B:72:ASP:HB2	1.87	0.56
3:C:70:ILE:HG23	3:C:74:GLU:HB2	1.88	0.56
2:B:667:VAL:HG12	2:B:670:MET:HG3	1.88	0.55
15:O:529:LYS:HD2	15:O:532:ASP:HB2	1.87	0.55
1:A:580:LEU:HD11	1:A:612:LEU:HD13	1.89	0.55
2:B:776:SER:HA	2:B:779:ASP:HB2	1.88	0.55
14:N:392:GLN:HB2	14:N:412:VAL:HB	1.88	0.55
15:O:168:SER:HA	15:O:281:THR:HG22	1.89	0.55
1:A:613:LEU:HD11	1:A:697:MET:HA	1.88	0.55
2:B:841:ILE:HG12	2:B:870:PRO:HB2	1.87	0.55
14:N:387:GLU:OE2	14:N:387:GLU:N	2.27	0.55
1:A:882:THR:HG22	1:A:1123:VAL:HG11	1.87	0.55
15:O:502:PRO:HA	15:O:505:MET:HE2	1.88	0.55
2:B:97:ASP:OD1	2:B:99:ARG:NH1	2.40	0.55
3:C:197:ARG:O	3:C:200:GLN:HG3	2.07	0.55
1:A:1061:ARG:NH1	1:A:1061:ARG:HG2	2.21	0.55
13:M:270:ALA:HA	14:N:316:PHE:HA	1.89	0.55
1:A:15:GLY:HA2	1:A:1408:VAL:HG23	1.87	0.55
1:A:833:PRO:HB2	2:B:659:ILE:HD12	1.89	0.55
1:A:1051:ASN:O	8:H:131:ASN:ND2	2.40	0.55
2:B:220:VAL:HG22	2:B:229:SER:HB2	1.87	0.55
2:B:349:ILE:O	2:B:353:THR:HG23	2.07	0.55
9:I:86:GLN:HE21	9:I:90:ALA:HA	1.71	0.55
14:N:198:GLN:OE1	14:N:198:GLN:N	2.40	0.55
1:A:17:GLU:OE1	2:B:1142:ARG:HG2	2.06	0.55
1:A:1058:GLN:NE2	8:H:134:ASN:O	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:87:ASP:OD1	15:O:89:ASP:N	2.40	0.55
1:A:97:LYS:HA	1:A:97:LYS:HE2	1.89	0.54
2:B:297:THR:HG22	13:M:183:PHE:HB2	1.88	0.54
15:O:137:ILE:CD1	17:Q:57:LYS:HD3	2.37	0.54
1:A:427:HIS:O	1:A:465:HIS:ND1	2.39	0.54
15:O:96:VAL:HB	17:Q:136:LEU:HD22	1.88	0.54
1:A:1151:GLU:HG3	1:A:1152:ARG:HG3	1.89	0.54
2:B:565:ILE:HG12	2:B:566:ARG:O	2.08	0.54
3:C:117:ASP:HB3	3:C:120:LEU:HD11	1.89	0.54
13:M:99:ARG:HH21	14:N:227:PRO:HA	1.72	0.54
15:O:492:TYR:O	15:O:496:ILE:HG12	2.08	0.54
15:O:492:TYR:CE1	15:O:496:ILE:HD11	2.41	0.54
1:A:93:ILE:HG12	1:A:324:ALA:HA	1.89	0.54
1:A:809:MET:HG3	2:B:953:MET:HG2	1.89	0.54
7:G:89:ILE:HG22	7:G:99:VAL:HA	1.90	0.54
2:B:267:GLU:HA	2:B:270:GLN:HB2	1.89	0.54
2:B:217:GLN:O	2:B:232:TYR:HB3	2.07	0.54
15:O:509:ARG:HG2	15:O:509:ARG:HH11	1.73	0.54
1:A:948:ASN:O	1:A:1061:ARG:NH2	2.41	0.54
2:B:57:LEU:HD11	2:B:516:LEU:HD12	1.90	0.54
2:B:1056:ARG:HH12	19:X:1008:UNK:CB	2.21	0.54
1:A:92:HIS:HB3	1:A:95:TYR:HB2	1.89	0.54
7:G:110:ILE:HD12	7:G:110:ILE:O	2.08	0.54
1:A:48:PRO:HB2	1:A:56:PRO:HD3	1.88	0.54
1:A:1061:ARG:HG2	1:A:1061:ARG:HH11	1.72	0.54
4:D:122:GLN:HE22	7:G:84:ILE:N	2.04	0.54
7:G:42:VAL:O	7:G:78:LYS:HE2	2.08	0.54
16:P:244:CYS:HA	16:P:247:LEU:HG	1.90	0.54
1:A:785:LEU:HD23	1:A:792:LEU:HB2	1.89	0.53
3:C:256:ILE:HA	3:C:268:LYS:H	1.72	0.53
8:H:64:ASN:HA	8:H:88:SER:HB2	1.91	0.53
3:C:229:LEU:HD13	3:C:295:ARG:HA	1.90	0.53
7:G:91:LYS:HB3	7:G:98:LYS:HB3	1.88	0.53
15:O:53:VAL:HG21	15:O:65:ILE:HG21	1.90	0.53
2:B:890:ASP:OD1	2:B:890:ASP:N	2.40	0.53
15:O:139:GLU:O	15:O:143:GLN:HB2	2.09	0.53
1:A:12:ARG:HH21	1:A:14:LYS:HA	1.72	0.53
11:K:110:GLU:HG3	11:K:111:THR:HG23	1.89	0.53
12:L:41:SER:N	12:L:44:ASP:OD2	2.40	0.53
15:O:133:SER:O	15:O:137:ILE:HG13	2.08	0.53
15:O:506:ARG:HD3	16:P:250:ASP:CB	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:232:TYR:CE1	2:B:356:VAL:HG21	2.44	0.53
7:G:147:ARG:HB3	7:G:206:GLY:H	1.73	0.53
15:O:215:TRP:CD1	15:O:335:LEU:HB3	2.43	0.53
1:A:464:ARG:NH1	1:A:470:ASP:OD2	2.39	0.53
13:M:158:GLN:HE22	14:N:308:GLN:HE21	1.57	0.53
13:M:227:LEU:HD13	13:M:231:LEU:HB3	1.90	0.53
2:B:496:MET:HB3	2:B:608:ILE:HG12	1.91	0.53
7:G:80:PHE:CG	7:G:81:LEU:N	2.77	0.53
2:B:447:PHE:HB3	2:B:449:MET:HE1	1.90	0.53
13:M:95:ARG:NH2	14:N:224:SER:OG	2.38	0.53
15:O:549:GLN:HE22	15:O:567:ARG:HH21	1.56	0.53
1:A:1138:THR:O	1:A:1138:THR:OG1	2.25	0.53
2:B:54:VAL:HG23	2:B:55:LYS:HG3	1.91	0.53
2:B:739:LYS:HG2	2:B:977:THR:HG21	1.91	0.53
5:E:45:LYS:HE3	5:E:46:TYR:HE1	1.74	0.53
7:G:165:GLU:N	7:G:165:GLU:OE1	2.41	0.53
6:F:136:ARG:HD2	6:F:146:TRP:CD1	2.44	0.52
1:A:893:LEU:HD23	1:A:896:LEU:HD22	1.91	0.52
1:A:960:MET:HE3	1:A:960:MET:HA	1.90	0.52
1:A:1436:ILE:HD11	7:G:22:THR:HB	1.91	0.52
2:B:737:LYS:HB2	2:B:741:ILE:HG12	1.90	0.52
9:I:8:CYS:SG	9:I:10:ASN:HB2	2.48	0.52
1:A:1019:LEU:HD13	1:A:1060:TYR:HB2	1.91	0.52
9:I:86:GLN:HB2	9:I:94:MET:HG2	1.90	0.52
1:A:862:LEU:HD13	2:B:494:PHE:HD2	1.74	0.52
2:B:476:GLN:O	2:B:479:LYS:HE3	2.10	0.52
2:B:772:VAL:HB	2:B:943:ILE:HB	1.91	0.52
15:O:124:GLU:O	15:O:127:ILE:HG12	2.09	0.52
2:B:262:ILE:HG22	2:B:268:ILE:HG13	1.91	0.52
17:Q:47:ILE:HG13	17:Q:51:GLU:HB2	1.90	0.52
1:A:891:LYS:HE2	1:A:1389:PHE:HB2	1.91	0.52
2:B:831:GLU:HB3	12:L:61:THR:HB	1.91	0.52
15:O:289:LYS:NZ	15:O:324:PRO:O	2.42	0.52
2:B:76:ILE:HG23	2:B:389:GLU:OE1	2.10	0.52
2:B:741:ILE:HB	2:B:746:TYR:HB3	1.91	0.52
3:C:215:ASP:OD2	12:L:70:ARG:NH2	2.33	0.52
10:J:21:TYR:HB2	10:J:39:LEU:HD11	1.92	0.52
15:O:541:ILE:HD12	15:O:548:ILE:HD11	1.92	0.52
2:B:638:ASP:O	2:B:642:LYS:HG2	2.10	0.52
13:M:159:TYR:HB3	13:M:170:LEU:HD12	1.91	0.52
15:O:326:ILE:HG23	15:O:327:ARG:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:16:VAL:HG21	7:G:2:PHE:HD2	1.74	0.52
15:O:44:PRO:HB3	15:O:583:TRP:HB2	1.92	0.52
2:B:244:HIS:HD1	2:B:332:ILE:HG13	1.74	0.52
2:B:449:MET:N	2:B:449:MET:HE3	2.25	0.52
2:B:931:MET:HB3	2:B:939:VAL:CG2	2.39	0.52
5:E:8:ASN:ND2	5:E:52:ARG:HH12	2.08	0.52
1:A:1365:LYS:HZ1	1:A:1379:MET:HB3	1.75	0.51
9:I:78:GLU:OE2	9:I:78:GLU:N	2.43	0.51
1:A:1369:LEU:HD13	1:A:1378:LYS:HB3	1.91	0.51
2:B:258:LYS:HG2	2:B:263:LEU:HA	1.92	0.51
7:G:32:ASN:N	7:G:32:ASN:HD22	2.07	0.51
2:B:335:LEU:HD21	2:B:560:THR:HG21	1.91	0.51
14:N:364:ARG:HG2	14:N:364:ARG:HH11	1.76	0.51
14:N:365:VAL:HA	14:N:371:LEU:HD22	1.92	0.51
15:O:310:GLN:NE2	15:O:313:LYS:HE2	2.25	0.51
15:O:625:ASN:O	15:O:629:MET:HG3	2.10	0.51
1:A:794:MET:SD	2:B:950:PRO:HG3	2.51	0.51
5:E:9:ILE:HG22	5:E:53:PRO:HG3	1.91	0.51
15:O:338:ASP:HB2	15:O:345:PHE:CE1	2.44	0.51
1:A:717:VAL:HG11	1:A:809:MET:HE2	1.91	0.51
2:B:117:GLU:HG3	12:L:55:ILE:HD11	1.92	0.51
5:E:89:GLY:O	5:E:93:MET:HE2	2.09	0.51
15:O:163:VAL:HG23	15:O:169:LEU:HB3	1.91	0.51
1:A:256:TYR:CE2	1:A:1401:PHE:HA	2.39	0.51
1:A:268:ILE:HD12	2:B:1127:LEU:HD12	1.93	0.51
2:B:666:ILE:HD11	2:B:673:LEU:HD22	1.93	0.51
2:B:1111:LYS:HE2	15:O:29:GLU:HG3	1.92	0.51
3:C:90:SER:OG	3:C:91:VAL:N	2.44	0.51
4:D:115:LEU:HA	4:D:144:ARG:HH12	1.75	0.51
7:G:163:PRO:HA	7:G:166:ARG:HE	1.76	0.51
8:H:40:LEU:HG	8:H:42:ILE:HG13	1.93	0.51
1:A:252:ARG:HB3	1:A:254:GLU:OE2	2.10	0.51
3:C:47:LEU:HD23	18:W:609:VAL:HB	1.93	0.51
9:I:1:MET:HA	9:I:1:MET:HE2	1.92	0.51
15:O:585:MET:HE1	15:O:648:TRP:CE2	2.45	0.51
1:A:1174:GLN:HE22	9:I:41:TYR:HD2	1.58	0.51
1:A:1329:GLU:OE2	5:E:200:ARG:NH2	2.44	0.51
2:B:820:GLN:HG2	2:B:841:ILE:HD12	1.92	0.51
7:G:114:MET:SD	7:G:114:MET:N	2.84	0.51
14:N:292:ARG:HH21	14:N:293:LYS:HE3	1.75	0.51
14:N:388:THR:OG1	14:N:392:GLN:NE2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:494:TYR:HE2	16:P:293:ILE:O	1.92	0.51
1:A:10:PRO:HB2	2:B:1146:ILE:HD11	1.92	0.51
1:A:556:ASP:OD1	2:B:761:SER:OG	2.23	0.51
1:A:573:ARG:NH2	11:K:87:GLU:HB2	2.26	0.51
1:A:102:ILE:HD12	1:A:242:LEU:HB3	1.93	0.51
1:A:473:LEU:HD11	2:B:1078:LEU:HD21	1.92	0.51
13:M:86:HIS:HB2	14:N:395:ILE:HG13	1.93	0.51
13:M:90:TYR:HD2	14:N:391:LEU:HB3	1.76	0.51
15:O:584:ASN:O	15:O:588:LEU:HG	2.11	0.51
16:P:193:ASN:O	16:P:196:LYS:HG2	2.11	0.51
1:A:41:ASP:N	1:A:44:LYS:HE2	2.27	0.50
1:A:396:ASP:OD1	1:A:396:ASP:N	2.43	0.50
1:A:573:ARG:HH21	11:K:87:GLU:HB2	1.76	0.50
1:A:852:PHE:CE2	2:B:953:MET:HE3	2.46	0.50
2:B:604:ASP:OD1	2:B:604:ASP:N	2.44	0.50
8:H:132:LEU:HD23	8:H:132:LEU:H	1.76	0.50
1:A:408:VAL:HG21	1:A:456:LEU:HD22	1.92	0.50
1:A:1360:ASP:O	1:A:1364:TYR:HB3	2.12	0.50
1:A:1373:ARG:HA	1:A:1389:PHE:HE2	1.77	0.50
2:B:286:ASN:O	2:B:289:GLU:HG3	2.12	0.50
1:A:93:ILE:H	1:A:93:ILE:HD12	1.75	0.50
1:A:538:LYS:HB3	1:A:687:PRO:HB2	1.94	0.50
1:A:1196:LEU:HG	9:I:51:VAL:HG12	1.93	0.50
15:O:577:MET:HE1	16:P:312:PHE:HE1	1.76	0.50
1:A:319:LEU:HA	1:A:322:THR:HG22	1.93	0.50
2:B:152:MET:HE3	2:B:153:PRO:HD2	1.93	0.50
4:D:115:LEU:HD12	4:D:144:ARG:HH12	1.77	0.50
5:E:187:TYR:HD1	5:E:188:LEU:HD12	1.76	0.50
15:O:136:ILE:O	15:O:140:ILE:HG12	2.11	0.50
18:W:610:SER:O	18:W:611:ARG:NE	2.43	0.50
1:A:1139:PRO:HG3	1:A:1298:TYR:CZ	2.47	0.50
2:B:83:ILE:HG22	2:B:93:LEU:HB3	1.93	0.50
8:H:8:ASP:OD1	8:H:9:ILE:N	2.44	0.50
15:O:164:ILE:HD12	15:O:165:SER:N	2.27	0.50
1:A:431:ASN:OD1	1:A:465:HIS:NE2	2.43	0.50
1:A:477:GLN:NE2	2:B:1066:GLU:OE2	2.42	0.50
1:A:1339:ILE:HD13	1:A:1358:LEU:HD23	1.94	0.50
5:E:34:GLU:N	5:E:34:GLU:OE1	2.45	0.50
13:M:86:HIS:HE1	14:N:397:LEU:HD22	1.74	0.50
2:B:540:ASP:OD1	2:B:541:ILE:N	2.45	0.50
2:B:549:LEU:HD23	2:B:550:HIS:CE1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1:MET:SD	3:C:14:ASN:HB2	2.52	0.50
5:E:85:GLU:OE2	5:E:85:GLU:N	2.21	0.50
1:A:41:ASP:H	1:A:44:LYS:HE2	1.77	0.50
7:G:79:PRO:HA	7:G:83:GLU:OE1	2.11	0.50
15:O:160:VAL:O	15:O:163:VAL:HG12	2.12	0.50
1:A:95:TYR:HE2	2:B:1136:ASN:HB3	1.77	0.49
2:B:265:ASP:HA	2:B:268:ILE:HD12	1.94	0.49
2:B:272:VAL:HG21	2:B:283:PHE:CZ	2.47	0.49
3:C:308:MET:HB3	3:C:312:GLU:OE2	2.12	0.49
4:D:142:ASP:OD1	4:D:142:ASP:N	2.44	0.49
7:G:89:ILE:HG13	7:G:143:ASN:H	1.76	0.49
8:H:10:PHE:HB3	8:H:28:ALA:HB1	1.94	0.49
1:A:368:LEU:HB3	1:A:1416:ILE:HG12	1.94	0.49
1:A:969:PRO:HA	1:A:972:GLU:OE2	2.12	0.49
1:A:1174:GLN:HG3	1:A:1185:GLN:HG3	1.94	0.49
14:N:287:HIS:O	14:N:290:ILE:HG22	2.12	0.49
15:O:305:GLY:HA3	16:P:205:ASN:HD21	1.77	0.49
1:A:652:VAL:HG21	1:A:668:VAL:HG21	1.94	0.49
1:A:719:PRO:HG2	1:A:724:LYS:HD3	1.93	0.49
2:B:62:LEU:HA	2:B:155:MET:HE1	1.94	0.49
2:B:623:LYS:HG3	2:B:625:ILE:HG22	1.94	0.49
3:C:237:GLN:HB2	3:C:288:LYS:HD3	1.93	0.49
15:O:454:ASN:O	15:O:458:LYS:HG3	2.12	0.49
1:A:877:VAL:HB	1:A:1106:LEU:HD21	1.94	0.49
1:A:1174:GLN:OE1	9:I:43:ARG:HB2	2.13	0.49
2:B:244:HIS:HB3	2:B:247:ILE:HG12	1.95	0.49
9:I:27:ARG:O	9:I:28:SER:OG	2.24	0.49
14:N:220:GLN:O	14:N:387:GLU:HG3	2.13	0.49
16:P:256:VAL:HG13	16:P:260:CYS:HB2	1.94	0.49
1:A:115:LEU:HD11	1:A:144:ILE:HG23	1.93	0.49
1:A:283:ASP:OD1	1:A:283:ASP:N	2.45	0.49
1:A:906:THR:HB	1:A:1380:ARG:HH22	1.78	0.49
5:E:143:ASN:HD21	5:E:146:HIS:CE1	2.30	0.49
10:J:1:MET:HG3	10:J:57:ILE:HB	1.95	0.49
1:A:1343:MET:HB2	1:A:1348:MET:HB2	1.93	0.49
3:C:127:THR:HA	12:L:-899:UNK:HA	1.93	0.49
4:D:127:LEU:HD21	7:G:147:ARG:HD2	1.95	0.49
9:I:4:PHE:CE1	14:N:204:PRO:HD3	2.41	0.49
15:O:293:SER:O	15:O:297:ILE:HG12	2.13	0.49
15:O:527:LEU:HD22	16:P:246:VAL:HG21	1.95	0.49
4:D:57:GLY:O	4:D:61:ASN:ND2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:56:LYS:HA	5:E:56:LYS:HE2	1.95	0.49
10:J:31:ASP:HB2	10:J:34:THR:HG22	1.93	0.49
15:O:594:LYS:O	15:O:598:GLU:HG3	2.12	0.49
1:A:947:PHE:CZ	8:H:136:LYS:HD2	2.48	0.49
1:A:1186:VAL:HG13	1:A:1230:ILE:HG23	1.95	0.49
1:A:1225:ILE:HG12	1:A:1229:ARG:O	2.13	0.49
1:A:1284:ASN:OD1	1:A:1285:ILE:N	2.45	0.49
2:B:207:VAL:HG12	2:B:367:ASP:OD1	2.11	0.49
8:H:124:ARG:NH1	8:H:126:GLU:OE2	2.39	0.49
17:Q:129:LEU:O	17:Q:137:TYR:OH	2.20	0.49
1:A:750:LEU:HD11	1:A:762:LEU:HD13	1.94	0.49
1:A:1352:PRO:HG3	5:E:204:THR:HG21	1.95	0.49
2:B:507:ALA:HA	2:B:510:LEU:HD12	1.95	0.49
3:C:17:SER:HB3	3:C:19:ASP:OD1	2.13	0.49
13:M:255:PHE:CD2	14:N:409:LEU:HD23	2.47	0.49
15:O:169:LEU:HD22	15:O:170:THR:H	1.77	0.49
15:O:509:ARG:HG2	15:O:509:ARG:NH1	2.28	0.49
15:O:292:ARG:O	15:O:295:GLN:HG2	2.13	0.48
15:O:619:LEU:HB3	15:O:624:LEU:HB3	1.96	0.48
1:A:91:PHE:CD2	1:A:224:PRO:HG3	2.48	0.48
2:B:701:TYR:HD1	9:I:90:ALA:HB3	1.78	0.48
4:D:16:VAL:HG11	7:G:2:PHE:CE2	2.48	0.48
7:G:128:TRP:HD1	7:G:139:TYR:HB2	1.78	0.48
15:O:455:SER:O	15:O:459:ILE:HG23	2.13	0.48
1:A:41:ASP:HB2	1:A:44:LYS:HG2	1.94	0.48
1:A:430:ALA:HA	1:A:464:ARG:HA	1.95	0.48
1:A:726:LYS:HE3	1:A:726:LYS:HB3	1.53	0.48
2:B:48:LEU:HD13	2:B:517:MET:HG3	1.95	0.48
3:C:21:PRO:HD2	11:K:82:LYS:HA	1.96	0.48
9:I:39:GLU:OE1	9:I:39:GLU:N	2.45	0.48
15:O:643:ARG:NH1	16:P:291:PHE:HA	2.28	0.48
16:P:224:PHE:CD1	16:P:224:PHE:C	2.89	0.48
1:A:13:ILE:HG13	2:B:1119:MET:HE1	1.96	0.48
1:A:160:LEU:HD11	1:A:185:TRP:CD1	2.47	0.48
1:A:966:ILE:HD12	1:A:1071:LEU:HD12	1.96	0.48
2:B:252:PRO:HB2	2:B:289:GLU:OE2	2.14	0.48
2:B:294:ASP:N	2:B:294:ASP:OD1	2.46	0.48
7:G:80:PHE:HE2	17:Q:107:ARG:HD2	1.77	0.48
14:N:212:VAL:O	14:N:216:LYS:HB2	2.14	0.48
14:N:381:ASP:OD1	14:N:419:THR:OG1	2.20	0.48
15:O:553:ARG:HB2	15:O:562:ALA:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:LYS:HB2	1:A:639:LYS:HE2	1.58	0.48
1:A:1278:ILE:HD12	1:A:1297:GLY:HA3	1.94	0.48
1:A:1428:PHE:CZ	6:F:89:GLU:HA	2.49	0.48
2:B:711:GLY:HA3	2:B:751:ALA:HA	1.94	0.48
15:O:183:MET:SD	15:O:183:MET:N	2.86	0.48
15:O:238:ARG:NH1	15:O:242:LYS:HG2	2.28	0.48
15:O:314:ILE:HD12	15:O:314:ILE:H	1.77	0.48
1:A:1310:ILE:HG22	1:A:1313:ARG:H	1.78	0.48
1:A:1379:MET:HE1	1:A:1380:ARG:NH1	2.28	0.48
2:B:681:LEU:HB3	2:B:685:ALA:HB3	1.96	0.48
9:I:71:ASN:N	9:I:71:ASN:HD22	2.11	0.48
2:B:545:ASP:HB3	14:N:390:PHE:CE1	2.49	0.48
7:G:80:PHE:CE2	17:Q:107:ARG:HD2	2.49	0.48
13:M:87:VAL:HB	13:M:176:VAL:HG23	1.96	0.48
15:O:160:VAL:O	15:O:164:ILE:HG13	2.13	0.48
15:O:608:ARG:HG2	15:O:610:ASP:OD1	2.14	0.48
5:E:4:GLU:OE2	5:E:4:GLU:HA	2.13	0.48
15:O:332:GLN:HG2	15:O:337:GLN:HE22	1.79	0.48
5:E:215:MET:HE3	5:E:215:MET:HB2	1.78	0.48
8:H:101:ALA:HB2	8:H:116:TYR:CE2	2.48	0.48
15:O:634:GLU:O	15:O:637:VAL:HG12	2.14	0.48
1:A:179:ILE:HD12	1:A:219:MET:HE3	1.94	0.48
1:A:926:MET:HE2	1:A:1353:ARG:NH1	2.29	0.48
1:A:1184:ILE:HD13	1:A:1263:LEU:HD22	1.95	0.48
3:C:132:ILE:HG21	3:C:184:VAL:HG11	1.95	0.48
3:C:255:VAL:HG12	3:C:256:ILE:HG23	1.95	0.48
4:D:127:LEU:HD11	7:G:84:ILE:HG21	1.94	0.48
5:E:31:THR:OG1	5:E:32:GLN:N	2.46	0.48
11:K:66:VAL:HG23	11:K:67:GLU:HG3	1.96	0.48
5:E:83:CYS:O	5:E:113:GLN:NE2	2.47	0.47
13:M:147:THR:HG21	13:M:184:LYS:HE3	1.96	0.47
15:O:203:ILE:HG13	15:O:207:HIS:ND1	2.29	0.47
1:A:1125:ARG:NH2	1:A:1317:ASN:O	2.41	0.47
8:H:31:THR:O	8:H:32:THR:OG1	2.29	0.47
10:J:45:CYS:O	10:J:48:ARG:HG3	2.14	0.47
1:A:226:LYS:HE3	15:O:547:GLU:OE2	2.14	0.47
1:A:1201:THR:OG1	1:A:1202:ILE:N	2.47	0.47
15:O:491:VAL:O	15:O:495:VAL:HG23	2.14	0.47
1:A:511:ASP:OD2	9:I:92:GLU:OE2	2.33	0.47
1:A:777:VAL:HG12	1:A:811:ALA:HB1	1.97	0.47
1:A:1192:THR:HG23	1:A:1196:LEU:HD13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:650:ASP:O	2:B:654:GLU:HG3	2.15	0.47
15:O:29:GLU:OE1	15:O:29:GLU:N	2.47	0.47
1:A:744:LEU:HB3	1:A:750:LEU:HD21	1.95	0.47
2:B:244:HIS:ND1	2:B:332:ILE:HG13	2.30	0.47
4:D:60:ARG:HG3	4:D:64:ASN:HD22	1.79	0.47
16:P:174:PHE:CE2	16:P:178:LEU:HD11	2.49	0.47
7:G:81:LEU:HD23	7:G:81:LEU:O	2.13	0.47
7:G:89:ILE:HG12	7:G:146:ILE:HD11	1.95	0.47
15:O:54:LYS:HD2	15:O:59:GLU:HA	1.97	0.47
15:O:200:LEU:HB3	15:O:280:LEU:HD22	1.95	0.47
15:O:294:LYS:HZ3	15:O:298:ASN:HD22	1.63	0.47
15:O:629:MET:O	15:O:632:GLU:HG3	2.14	0.47
1:A:438:GLU:OE2	1:A:442:ARG:NH2	2.41	0.47
2:B:207:VAL:HA	2:B:217:GLN:CB	2.45	0.47
2:B:253:ILE:HG12	2:B:353:THR:HG22	1.97	0.47
2:B:277:SER:N	14:N:207:VAL:O	2.47	0.47
2:B:1147:PHE:CD1	7:G:58:GLN:HG3	2.49	0.47
3:C:134:LEU:HD12	3:C:208:CYS:SG	2.55	0.47
7:G:202:THR:HB	7:G:205:MET:HE2	1.95	0.47
1:A:1415:ILE:HD13	2:B:1067:ARG:HD2	1.96	0.47
2:B:226:GLU:HB3	2:B:228:LYS:NZ	2.29	0.47
2:B:567:PHE:CZ	14:N:283:LEU:HD23	2.50	0.47
2:B:778:ILE:HG12	2:B:906:PRO:HG2	1.97	0.47
4:D:29:TRP:O	4:D:33:SER:OG	2.26	0.47
7:G:52:LEU:HD21	7:G:73:ARG:HD3	1.96	0.47
9:I:48:ARG:NH1	9:I:50:GLU:OE2	2.47	0.47
1:A:1310:ILE:O	1:A:1314:THR:OG1	2.29	0.47
2:B:497:LEU:HD13	2:B:512:LYS:HD2	1.97	0.47
2:B:715:TYR:CZ	10:J:59:LYS:HG2	2.50	0.47
2:B:904:ARG:HH12	2:B:1033:ASP:CG	2.22	0.47
11:K:55:SER:OG	11:K:58:GLY:O	2.31	0.47
14:N:285:ALA:O	14:N:288:GLN:HG2	2.15	0.47
15:O:460:LEU:HD22	15:O:467:PHE:HD2	1.79	0.47
1:A:297:SER:HB3	17:Q:31:ASN:HB2	1.97	0.47
1:A:416:LEU:HD23	1:A:419:LEU:HD12	1.95	0.47
1:A:668:VAL:HG13	1:A:677:VAL:HG23	1.96	0.47
1:A:747:LYS:HD2	1:A:748:GLY:N	2.30	0.47
1:A:856:LEU:HD23	1:A:861:PHE:HA	1.96	0.47
3:C:71:MET:HG2	3:C:317:SER:HB3	1.96	0.47
3:C:162:VAL:HG23	3:C:196:LEU:HD11	1.97	0.47
3:C:248:GLN:HB2	3:C:256:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LEU:HD12	1:A:241:LEU:HD13	1.96	0.46
1:A:252:ARG:HD2	15:O:43:ASN:HB2	1.96	0.46
1:A:1117:MET:SD	1:A:1282:VAL:HG11	2.55	0.46
2:B:225:HIS:HA	2:B:447:PHE:HE1	1.80	0.46
2:B:911:LYS:HD3	2:B:919:LYS:HD2	1.97	0.46
3:C:212:ILE:HD13	3:C:212:ILE:HA	1.79	0.46
4:D:92:LYS:HB3	4:D:97:LYS:HZ3	1.80	0.46
4:D:127:LEU:HD22	4:D:133:HIS:CE1	2.51	0.46
7:G:149:ARG:O	7:G:198:GLY:HA2	2.14	0.46
11:K:87:GLU:HB3	11:K:108:TYR:CZ	2.50	0.46
13:M:278:ILE:HD13	14:N:422:ILE:HG23	1.97	0.46
1:A:106:ILE:O	1:A:161:ASN:ND2	2.48	0.46
1:A:234:ILE:O	15:O:43:ASN:ND2	2.39	0.46
1:A:745:PHE:HB2	1:A:750:LEU:HD11	1.98	0.46
1:A:800:LYS:HG2	2:B:947:HIS:O	2.16	0.46
2:B:253:ILE:HG12	2:B:353:THR:CG2	2.45	0.46
2:B:567:PHE:HA	14:N:279:GLU:OE1	2.14	0.46
3:C:40:PHE:HD2	11:K:134:LYS:HG3	1.80	0.46
12:L:32:ALA:HB3	12:L:53:HIS:CD2	2.50	0.46
16:P:164:TRP:HD1	16:P:175:ILE:HD12	1.79	0.46
16:P:255:LYS:HA	16:P:255:LYS:HE3	1.97	0.46
1:A:74:LEU:O	2:B:1048:ARG:NH2	2.48	0.46
1:A:269:ARG:NH1	1:A:289:LEU:HD21	2.31	0.46
1:A:813:VAL:O	1:A:848:VAL:HB	2.14	0.46
1:A:1258:TYR:CD2	2:B:292:LYS:HD3	2.50	0.46
7:G:89:ILE:H	7:G:146:ILE:HD11	1.81	0.46
1:A:607:LYS:HD2	8:H:120:GLY:HA3	1.95	0.46
1:A:788:TRP:HA	1:A:793:ILE:HD11	1.96	0.46
1:A:1129:ILE:HG21	1:A:1339:ILE:HG13	1.97	0.46
2:B:58:VAL:HG21	2:B:181:PRO:HB3	1.97	0.46
2:B:1094:VAL:HG12	2:B:1143:LEU:HD11	1.98	0.46
4:D:122:GLN:NE2	7:G:83:GLU:HA	2.30	0.46
6:F:82:THR:O	6:F:136:ARG:NH1	2.36	0.46
16:P:253:LEU:HD13	16:P:261:TYR:CG	2.50	0.46
17:Q:140:MET:HE2	17:Q:140:MET:HB2	1.74	0.46
1:A:845:LYS:HB3	1:A:845:LYS:HE2	1.70	0.46
2:B:122:ASP:HA	2:B:189:GLY:HA3	1.98	0.46
2:B:350:ALA:O	2:B:353:THR:OG1	2.30	0.46
2:B:610:ARG:HH12	2:B:674:GLU:CD	2.23	0.46
11:K:78:TYR:CZ	11:K:82:LYS:HD2	2.51	0.46
13:M:278:ILE:HA	13:M:281:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:LEU:HD22	1:A:212:GLU:HG3	1.97	0.46
1:A:731:VAL:HG11	1:A:849:ARG:HG3	1.96	0.46
1:A:853:PHE:HA	2:B:955:VAL:HG11	1.96	0.46
1:A:1132:ALA:HB1	1:A:1320:LEU:HD21	1.97	0.46
4:D:62:VAL:O	4:D:66:LEU:HG	2.15	0.46
6:F:127:GLU:HB3	6:F:129:LYS:HG3	1.97	0.46
7:G:164:LYS:O	7:G:168:LEU:HG	2.15	0.46
9:I:81:TYR:HD2	9:I:99:LYS:HG2	1.81	0.46
1:A:513:ASP:HA	2:B:920:GLY:HA2	1.98	0.46
1:A:615:LYS:NZ	1:A:620:SER:O	2.47	0.46
2:B:55:LYS:HD3	2:B:519:HIS:CE1	2.51	0.46
2:B:739:LYS:H	2:B:977:THR:HG22	1.79	0.46
2:B:913:SER:HB2	2:B:1027:LEU:HD11	1.97	0.46
2:B:1052:GLU:O	19:X:1004:UNK:N	2.49	0.46
4:D:2:LYS:HE2	4:D:2:LYS:HB2	1.86	0.46
5:E:60:PHE:C	5:E:60:PHE:CD1	2.93	0.46
7:G:159:LYS:HG2	7:G:161:LYS:HD2	1.97	0.46
15:O:57:LEU:HD22	15:O:98:LEU:HD23	1.97	0.46
1:A:268:ILE:O	1:A:356:ARG:NH2	2.47	0.46
1:A:1174:GLN:HG3	1:A:1185:GLN:CG	2.46	0.46
2:B:40:THR:OG1	2:B:624:ASP:HB3	2.15	0.46
2:B:49:PRO:HG3	2:B:743:LEU:HD21	1.97	0.46
2:B:824:LEU:HD21	2:B:844:ASN:HD22	1.80	0.46
2:B:915:ARG:HD2	2:B:1023:TYR:CD2	2.47	0.46
3:C:33:VAL:O	3:C:34:GLU:HB2	2.15	0.46
3:C:324:LYS:HB3	3:C:324:LYS:HE2	1.70	0.46
5:E:46:TYR:CD2	5:E:58:MET:HB3	2.51	0.46
1:A:450:MET:HE1	1:A:454:LYS:HE2	1.97	0.46
1:A:882:THR:HG22	1:A:1123:VAL:CG1	2.45	0.46
2:B:292:LYS:HE2	2:B:292:LYS:HB2	1.76	0.46
2:B:322:GLU:O	2:B:325:GLU:HG3	2.16	0.46
15:O:110:THR:HG23	15:O:116:LYS:HB2	1.98	0.46
1:A:564:ILE:O	1:A:606:GLY:HA3	2.16	0.46
1:A:1184:ILE:HG21	1:A:1267:LEU:HD13	1.98	0.46
1:A:1188:ILE:HD13	1:A:1205:ILE:HD12	1.98	0.46
3:C:110:PRO:C	3:C:112:MET:H	2.24	0.46
5:E:80:VAL:HG12	5:E:109:ILE:HB	1.98	0.46
13:M:108:SER:O	13:M:122:ASP:HB2	2.16	0.46
1:A:19:SER:HB2	1:A:1403:MET:HE3	1.98	0.45
1:A:68:ALA:HA	1:A:71:HIS:CE1	2.52	0.45
1:A:211:LEU:O	1:A:215:VAL:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1071:ILE:HG13	2:B:1079:LEU:HD11	1.98	0.45
3:C:81:GLU:HA	3:C:218:LYS:HZ2	1.81	0.45
5:E:131:THR:C	5:E:132:ILE:HD13	2.42	0.45
9:I:39:GLU:H	9:I:39:GLU:CD	2.23	0.45
13:M:103:GLU:H	13:M:103:GLU:CD	2.24	0.45
14:N:278:ALA:HA	14:N:281:GLU:HG2	1.97	0.45
1:A:63:SER:HA	1:A:74:LEU:H	1.80	0.45
1:A:537:VAL:HG13	1:A:551:ILE:HD13	1.98	0.45
1:A:630:ASN:ND2	1:A:649:ASP:O	2.49	0.45
1:A:1185:GLN:HE22	1:A:1229:ARG:CG	2.29	0.45
2:B:234:ILE:HD11	2:B:356:VAL:CG1	2.44	0.45
15:O:116:LYS:HD2	15:O:117:THR:N	2.31	0.45
15:O:552:PRO:HB3	15:O:557:ARG:HA	1.97	0.45
2:B:779:ASP:OD1	2:B:905:ARG:NH2	2.36	0.45
5:E:43:LYS:O	5:E:47:CYS:HB2	2.16	0.45
6:F:97:ARG:HD2	6:F:97:ARG:HA	1.78	0.45
9:I:86:GLN:NE2	9:I:90:ALA:HA	2.30	0.45
13:M:247:TRP:CZ2	14:N:408:LEU:HD12	2.46	0.45
15:O:376:LEU:HD22	15:O:453:ILE:HD12	1.99	0.45
16:P:185:PHE:HB2	16:P:224:PHE:CE2	2.52	0.45
17:Q:20:PRO:HG2	17:Q:23:LEU:HB2	1.98	0.45
1:A:14:LYS:HB2	2:B:1144:GLU:HG2	1.98	0.45
1:A:1207:VAL:O	1:A:1210:THR:OG1	2.27	0.45
2:B:50:ALA:HB2	2:B:630:LEU:HD11	1.99	0.45
2:B:1142:ARG:HA	2:B:1142:ARG:HD3	1.62	0.45
8:H:34:ASP:N	8:H:34:ASP:OD1	2.47	0.45
15:O:195:CYS:HB2	15:O:263:LEU:HD21	1.99	0.45
15:O:585:MET:HE1	15:O:648:TRP:CD2	2.51	0.45
1:A:1164:THR:C	1:A:1165:LEU:HD22	2.42	0.45
7:G:2:PHE:CE1	7:G:77:PHE:HD1	2.35	0.45
7:G:46:ILE:HB	7:G:75:VAL:HG23	1.97	0.45
7:G:63:ASP:OD2	7:G:67:TYR:OH	2.25	0.45
7:G:191:PRO:HG2	7:G:192:PRO:HD3	1.98	0.45
13:M:80:GLY:HA3	13:M:171:VAL:HG13	1.99	0.45
15:O:294:LYS:HZ1	15:O:298:ASN:HD22	1.61	0.45
1:A:890:MET:HG3	1:A:894:GLU:HG3	1.98	0.45
2:B:597:MET:HE1	14:N:216:LYS:HE2	1.99	0.45
5:E:80:VAL:HA	5:E:109:ILE:HB	1.99	0.45
6:F:123:LYS:HB2	6:F:123:LYS:HE2	1.71	0.45
15:O:570:GLU:OE2	15:O:570:GLU:N	2.50	0.45
1:A:102:ILE:HD11	1:A:1401:PHE:HZ	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:THR:HG21	11:K:88:PHE:HA	1.99	0.45
2:B:901:ARG:NH1	3:C:95:GLU:OE2	2.50	0.45
4:D:148:LYS:HA	4:D:148:LYS:HD3	1.78	0.45
1:A:939:TRP:CD1	1:A:1015:LYS:HE3	2.52	0.45
1:A:1443:PRO:HG3	7:G:52:LEU:HD11	1.98	0.45
2:B:740:THR:O	2:B:744:ILE:HG12	2.17	0.45
2:B:769:ASP:O	2:B:920:GLY:HA3	2.17	0.45
2:B:278:SER:O	2:B:282:ILE:HG12	2.17	0.45
2:B:719:LYS:HB3	2:B:719:LYS:HE2	1.62	0.45
2:B:723:THR:HA	2:B:790:LYS:HG2	1.98	0.45
2:B:832:VAL:HA	2:B:881:ILE:HG22	1.99	0.45
2:B:911:LYS:HD2	2:B:1027:LEU:HD12	1.99	0.45
7:G:24:SER:HA	7:G:27:THR:HG22	1.99	0.45
7:G:81:LEU:HA	7:G:150:ILE:HG23	1.99	0.45
9:I:98:TYR:HE2	9:I:109:GLU:HB3	1.80	0.45
14:N:287:HIS:CD2	14:N:370:LYS:HA	2.52	0.45
15:O:238:ARG:HH12	15:O:242:LYS:HG2	1.82	0.45
15:O:512:ARG:NH1	15:O:568:CYS:SG	2.90	0.45
1:A:555:GLN:NE2	2:B:768:GLU:H	2.15	0.45
1:A:976:ARG:O	1:A:976:ARG:HG2	2.17	0.45
2:B:1088:ASP:OD1	2:B:1088:ASP:N	2.49	0.45
5:E:94:LYS:O	5:E:98:ILE:HG12	2.17	0.45
9:I:30:PRO:HB3	13:M:136:ALA:HB2	1.99	0.45
11:K:49:LEU:HD11	11:K:61:ALA:HB1	2.00	0.45
15:O:107:LEU:HG	15:O:210:PRO:HD2	1.99	0.45
15:O:181:ASP:HA	15:O:184:LYS:HD3	1.98	0.45
1:A:93:ILE:HD12	1:A:93:ILE:N	2.32	0.44
1:A:913:GLN:NE2	1:A:1360:ASP:OD2	2.43	0.44
2:B:383:LEU:HB3	2:B:442:TRP:CH2	2.51	0.44
2:B:1008:ILE:HG13	2:B:1009:THR:HG23	1.99	0.44
3:C:143:ASN:H	3:C:157:TYR:HA	1.82	0.44
3:C:205:LYS:HE2	3:C:205:LYS:HB3	1.82	0.44
13:M:161:ALA:HB2	13:M:170:LEU:HD13	1.99	0.44
2:B:701:TYR:CE2	9:I:91:ASP:HB3	2.53	0.44
4:D:7:ARG:CZ	17:Q:103:ASP:HA	2.47	0.44
5:E:38:PRO:HB2	5:E:41:ASP:HB3	1.99	0.44
7:G:98:LYS:NZ	7:G:106:ASP:O	2.49	0.44
1:A:120:LYS:HD2	1:A:120:LYS:HA	1.84	0.44
1:A:770:LEU:HD11	1:A:842:PRO:HB3	1.99	0.44
2:B:73:LEU:HA	2:B:73:LEU:HD23	1.77	0.44
2:B:157:ARG:HD2	2:B:182:GLY:HA3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:257:LEU:HD23	2:B:268:ILE:HG12	1.99	0.44
15:O:60:ARG:NH1	15:O:90:SER:HB2	2.33	0.44
15:O:76:VAL:HG11	15:O:92:LYS:NZ	2.32	0.44
15:O:318:LEU:HD12	15:O:366:LEU:HD22	2.00	0.44
15:O:345:PHE:HA	15:O:348:GLU:CD	2.42	0.44
1:A:511:ASP:O	1:A:512:PHE:C	2.61	0.44
1:A:712:ILE:HD11	1:A:791:PRO:HG3	1.98	0.44
2:B:543:LEU:HD21	13:M:155:ASN:ND2	2.32	0.44
5:E:32:GLN:HA	5:E:35:VAL:HB	1.99	0.44
6:F:137:TYR:CD1	6:F:143:PHE:HB3	2.52	0.44
7:G:150:ILE:HD13	7:G:196:LEU:HG	2.00	0.44
13:M:77:LYS:HE3	13:M:167:GLN:HB3	1.99	0.44
15:O:131:LEU:HD21	15:O:648:TRP:CZ2	2.51	0.44
1:A:789:ASN:HB3	1:A:792:LEU:HB3	1.99	0.44
4:D:117:LYS:HD2	4:D:117:LYS:HA	1.61	0.44
15:O:105:LYS:O	15:O:121:TYR:N	2.41	0.44
15:O:610:ASP:OD1	15:O:611:VAL:N	2.51	0.44
1:A:58:MET:HE3	1:A:82:GLY:HA3	1.99	0.44
1:A:140:ILE:O	1:A:144:ILE:HG13	2.17	0.44
1:A:747:LYS:HD2	1:A:747:LYS:C	2.43	0.44
1:A:862:LEU:O	1:A:866:ILE:HG13	2.17	0.44
2:B:548:SER:OG	14:N:387:GLU:OE1	2.27	0.44
5:E:154:ILE:O	5:E:197:LYS:N	2.42	0.44
6:F:127:GLU:N	6:F:127:GLU:OE2	2.50	0.44
15:O:310:GLN:HA	15:O:313:LYS:HZ3	1.82	0.44
1:A:95:TYR:OH	2:B:1136:ASN:O	2.25	0.44
1:A:98:ALA:O	1:A:102:ILE:HG12	2.17	0.44
1:A:129:ARG:HD3	1:A:130:PRO:HD2	2.00	0.44
1:A:991:LYS:HA	1:A:991:LYS:HD3	1.71	0.44
2:B:1096:ASP:N	2:B:1115:ASN:O	2.43	0.44
8:H:135:LEU:HB2	8:H:137:GLN:NE2	2.33	0.44
10:J:48:ARG:HH11	10:J:49:MET:HG2	1.81	0.44
15:O:310:GLN:HE22	15:O:313:LYS:HE2	1.83	0.44
15:O:500:LEU:HD22	15:O:540:LEU:HD12	2.00	0.44
1:A:143:LYS:HA	1:A:143:LYS:HD2	1.85	0.44
1:A:483:LEU:HD22	1:A:550:ILE:HG21	1.99	0.44
2:B:327:ILE:O	2:B:331:VAL:HG23	2.18	0.44
2:B:591:TYR:CE1	2:B:652:ASN:HB3	2.53	0.44
5:E:93:MET:O	5:E:97:VAL:HG23	2.18	0.44
7:G:151:GLU:OE2	7:G:199:SER:HB3	2.18	0.44
13:M:94:PRO:HA	14:N:390:PHE:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:GLY:O	1:A:263:ALA:N	2.51	0.44
1:A:266:VAL:HA	1:A:269:ARG:HD2	1.99	0.44
1:A:471:VAL:HB	1:A:528:ARG:HG3	1.99	0.44
1:A:784:GLU:OE2	1:A:784:GLU:HA	2.17	0.44
1:A:878:LYS:O	1:A:879:THR:C	2.61	0.44
2:B:351:MET:HE1	2:B:549:LEU:HD21	1.99	0.44
2:B:882:ASP:HB3	2:B:901:ARG:HE	1.83	0.44
16:P:225:ILE:HD12	16:P:225:ILE:HA	1.90	0.44
17:Q:48:THR:H	17:Q:51:GLU:HG3	1.83	0.44
1:A:1377:SER:O	1:A:1377:SER:OG	2.31	0.43
2:B:295:ILE:HD11	9:I:10:ASN:ND2	2.33	0.43
2:B:806:ILE:O	2:B:828:GLY:HA3	2.18	0.43
3:C:89:THR:CG2	3:C:200:GLN:HA	2.48	0.43
3:C:245:ARG:O	3:C:249:LYS:HG2	2.17	0.43
15:O:93:THR:O	15:O:96:VAL:HG12	2.18	0.43
16:P:240:ILE:HD12	16:P:243:LEU:HD12	2.00	0.43
1:A:12:ARG:HG2	2:B:1146:ILE:CG2	2.48	0.43
1:A:184:ARG:HG2	1:A:185:TRP:CE2	2.53	0.43
2:B:208:GLU:HG2	2:B:216:VAL:O	2.18	0.43
2:B:788:ARG:NH2	2:B:882:ASP:OD2	2.50	0.43
3:C:19:ASP:O	11:K:82:LYS:NZ	2.50	0.43
3:C:33:VAL:C	3:C:35:LYS:H	2.25	0.43
5:E:37:LEU:HA	5:E:37:LEU:HD12	1.84	0.43
7:G:39:ILE:HB	7:G:42:VAL:HB	1.99	0.43
9:I:33:PHE:CE2	14:N:201:PRO:HD3	2.53	0.43
10:J:49:MET:HE3	10:J:49:MET:HB3	1.86	0.43
15:O:161:GLN:O	15:O:164:ILE:HD12	2.17	0.43
1:A:364:PHE:HA	1:A:368:LEU:HB2	2.01	0.43
1:A:599:LYS:NZ	8:H:90:ALA:O	2.34	0.43
1:A:827:PHE:CE1	2:B:492:SER:HA	2.54	0.43
2:B:298:GLN:O	2:B:302:LEU:HG	2.18	0.43
2:B:797:ARG:HH12	2:B:892:ASP:CG	2.25	0.43
2:B:944:MET:HB2	2:B:944:MET:HE3	1.80	0.43
13:M:140:TRP:HB3	13:M:185:TYR:HB2	1.99	0.43
15:O:180:SER:HB3	15:O:183:MET:HE2	2.00	0.43
15:O:328:ASP:C	15:O:330:LEU:H	2.25	0.43
15:O:599:ASN:HD21	15:O:630:VAL:HG11	1.83	0.43
1:A:1302:ASP:O	1:A:1306:THR:OG1	2.35	0.43
2:B:74:LYS:HA	2:B:77:ILE:HG22	2.00	0.43
5:E:52:ARG:HD2	5:E:52:ARG:HA	1.83	0.43
5:E:78:LEU:CD1	5:E:107:THR:HB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:112:TYR:CE1	5:E:134:THR:HG23	2.47	0.43
15:O:38:GLU:OE2	15:O:39:GLN:NE2	2.52	0.43
15:O:164:ILE:CG2	15:O:282:ILE:HG21	2.46	0.43
15:O:361:PHE:CD1	15:O:366:LEU:HD21	2.53	0.43
15:O:376:LEU:HD13	15:O:453:ILE:HD11	2.01	0.43
1:A:450:MET:HE3	1:A:450:MET:O	2.18	0.43
2:B:532:LEU:HD11	2:B:578:LEU:HD12	2.00	0.43
3:C:95:GLU:HG2	3:C:96:VAL:N	2.33	0.43
3:C:197:ARG:HA	3:C:197:ARG:HD3	1.65	0.43
5:E:19:VAL:O	5:E:23:VAL:HG12	2.19	0.43
5:E:78:LEU:HD12	5:E:78:LEU:HA	1.81	0.43
15:O:259:LEU:HD13	15:O:261:GLN:HG3	1.99	0.43
1:A:372:ARG:HA	2:B:1061:ARG:HA	2.01	0.43
1:A:771:SER:HB2	9:I:63:ASP:CG	2.44	0.43
1:A:830:ARG:HD3	1:A:837:LYS:HA	1.98	0.43
1:A:986:ARG:O	1:A:986:ARG:HG3	2.19	0.43
5:E:26:ARG:HH12	5:E:133:GLU:CD	2.24	0.43
7:G:6:LYS:HG2	7:G:73:ARG:HG2	2.01	0.43
7:G:81:LEU:HD13	17:Q:107:ARG:NE	2.34	0.43
8:H:107:VAL:HG21	8:H:126:GLU:OE1	2.18	0.43
11:K:43:ASP:OD2	11:K:46:LYS:HB2	2.18	0.43
13:M:134:ASP:OD1	13:M:134:ASP:N	2.52	0.43
1:A:532:ILE:HD12	1:A:532:ILE:HA	1.90	0.43
1:A:573:ARG:HB3	3:C:20:PHE:HE2	1.82	0.43
1:A:582:MET:SD	1:A:703:ARG:HB3	2.59	0.43
1:A:1038:GLU:HG3	1:A:1039:LEU:HD12	1.99	0.43
1:A:1339:ILE:O	1:A:1343:MET:HG2	2.18	0.43
2:B:775:LYS:HB2	2:B:925:ILE:HG22	2.00	0.43
2:B:1108:THR:O	2:B:1108:THR:OG1	2.34	0.43
5:E:4:GLU:CD	5:E:7:ARG:HH21	2.26	0.43
7:G:119:CYS:HB3	7:G:128:TRP:CE3	2.54	0.43
15:O:60:ARG:HH12	15:O:90:SER:HB2	1.83	0.43
15:O:585:MET:HG3	15:O:644:LEU:HD22	1.99	0.43
1:A:114:LEU:HD11	1:A:161:ASN:ND2	2.33	0.43
1:A:992:ALA:O	5:E:199:ILE:HG13	2.19	0.43
2:B:319:ILE:HD12	2:B:319:ILE:HA	1.90	0.43
2:B:565:ILE:HD13	2:B:571:PHE:HB2	2.01	0.43
3:C:278:GLU:O	3:C:281:ARG:HG2	2.19	0.43
5:E:152:LYS:HE3	5:E:154:ILE:HD11	2.01	0.43
7:G:147:ARG:O	7:G:205:MET:HB2	2.18	0.43
14:N:196:ILE:HB	14:N:199:LEU:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:504:ALA:HB2	15:O:536:THR:HB	2.00	0.43
15:O:605:LYS:HB2	15:O:605:LYS:HE2	1.59	0.43
13:M:89:GLN:HE21	13:M:178:GLN:HG2	1.84	0.43
2:B:55:LYS:HE2	2:B:648:TYR:OH	2.19	0.43
2:B:241:TYR:HE1	2:B:252:PRO:HG3	1.84	0.43
8:H:125:LEU:HG	8:H:130:ARG:HH12	1.84	0.43
8:H:131:ASN:OD1	8:H:131:ASN:N	2.51	0.43
15:O:193:GLN:HG2	15:O:197:MET:HE1	2.01	0.43
1:A:88:LEU:HB3	1:A:316:TRP:CE2	2.54	0.42
2:B:1081:GLU:HA	2:B:1085:ILE:HB	2.01	0.42
6:F:108:PHE:HE2	6:F:131:PRO:HG3	1.84	0.42
18:W:619:MET:HG2	18:W:622:LEU:HG	2.00	0.42
19:X:1008:UNK:C	19:X:1010:UNK:N	2.78	0.42
1:A:225:LEU:HB2	1:A:316:TRP:HH2	1.84	0.42
1:A:785:LEU:HD21	1:A:806:VAL:HG11	2.01	0.42
2:B:217:GLN:HG2	2:B:356:VAL:HG23	2.00	0.42
2:B:319:ILE:HD12	2:B:321:GLN:NE2	2.34	0.42
2:B:778:ILE:HG23	2:B:906:PRO:HG2	2.00	0.42
2:B:1045:VAL:CB	19:X:1009:UNK:O	2.66	0.42
4:D:71:ASN:HD22	7:G:86:THR:HG21	1.84	0.42
4:D:120:LYS:HA	4:D:120:LYS:HD3	1.73	0.42
6:F:72:LYS:HA	6:F:72:LYS:HD3	1.79	0.42
7:G:49:TYR:N	7:G:73:ARG:O	2.44	0.42
15:O:153:LYS:C	15:O:153:LYS:HD2	2.44	0.42
15:O:301:LYS:HE2	15:O:313:LYS:HE3	2.00	0.42
17:Q:123:ASP:HB3	17:Q:140:MET:HA	2.02	0.42
1:A:386:ASN:HB2	11:K:95:HIS:HD2	1.84	0.42
1:A:1083:LEU:HD11	1:A:1089:ILE:HD13	2.01	0.42
2:B:213:LYS:HB3	2:B:213:LYS:HE3	1.88	0.42
2:B:568:PRO:HD2	14:N:279:GLU:OE1	2.19	0.42
2:B:735:MET:HE3	2:B:735:MET:O	2.20	0.42
2:B:773:LEU:HB2	2:B:922:CYS:SG	2.60	0.42
2:B:986:ASP:O	2:B:990:ILE:HG13	2.19	0.42
3:C:165:ARG:HH21	3:C:190:ASP:HA	1.84	0.42
4:D:27:HIS:HA	4:D:29:TRP:CH2	2.54	0.42
7:G:13:ILE:HD11	7:G:26:ILE:HG13	2.00	0.42
1:A:226:LYS:HE3	15:O:547:GLU:CD	2.44	0.42
1:A:406:GLU:OE1	1:A:415:LYS:NZ	2.52	0.42
1:A:885:MET:HE3	1:A:885:MET:HB3	1.73	0.42
2:B:545:ASP:OD1	2:B:548:SER:HB2	2.19	0.42
17:Q:57:LYS:HE3	17:Q:57:LYS:HB3	1.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:LEU:HB2	1:A:508:TYR:OH	2.19	0.42
1:A:896:LEU:HD23	1:A:1357:LEU:HD11	2.01	0.42
2:B:151:ARG:HA	2:B:151:ARG:HD2	1.86	0.42
2:B:242:LEU:HD21	2:B:332:ILE:HD11	2.01	0.42
2:B:622:VAL:HG13	2:B:640:PHE:HE2	1.84	0.42
3:C:70:ILE:HA	3:C:74:GLU:HG3	2.00	0.42
4:D:123:ILE:HD12	4:D:157:ILE:HG21	2.01	0.42
6:F:133:VAL:HA	6:F:147:SER:HA	2.01	0.42
13:M:114:PRO:C	13:M:116:SER:H	2.28	0.42
15:O:353:GLU:HG3	15:O:477:TYR:CE2	2.54	0.42
2:B:55:LYS:HB3	2:B:59:LYS:HD3	2.02	0.42
2:B:383:LEU:HD11	2:B:451:ARG:HH12	1.84	0.42
15:O:593:GLU:OE2	15:O:593:GLU:HA	2.18	0.42
17:Q:27:ASP:OD1	17:Q:28:VAL:N	2.53	0.42
1:A:848:VAL:HG13	1:A:860:GLU:HB3	2.01	0.42
1:A:1166:LEU:CD2	1:A:1270:VAL:HG22	2.49	0.42
2:B:351:MET:HE2	2:B:561:LEU:HD22	2.01	0.42
3:C:282:TYR:O	3:C:284:GLU:N	2.53	0.42
5:E:45:LYS:O	5:E:57:MET:HE1	2.19	0.42
6:F:93:ILE:HD13	6:F:93:ILE:HA	1.86	0.42
7:G:128:TRP:CD1	7:G:139:TYR:HB2	2.55	0.42
9:I:99:LYS:NZ	9:I:104:GLY:HA2	2.35	0.42
14:N:304:PHE:CE2	14:N:394:VAL:HG21	2.55	0.42
14:N:307:PHE:CE1	14:N:416:ILE:HG13	2.55	0.42
1:A:890:MET:HG2	2:B:1068:ASP:CG	2.44	0.42
2:B:74:LYS:NZ	2:B:97:ASP:HA	2.35	0.42
2:B:216:VAL:HG23	2:B:233:VAL:HG12	2.01	0.42
2:B:262:ILE:HG13	2:B:346:ALA:HB1	2.02	0.42
2:B:386:LEU:HD12	2:B:387:LEU:N	2.35	0.42
14:N:306:VAL:HG23	14:N:415:LYS:HA	2.02	0.42
15:O:65:ILE:HD12	15:O:65:ILE:HA	1.84	0.42
15:O:464:ASN:ND2	16:P:254:GLU:HG2	2.34	0.42
1:A:383:PRO:HB3	1:A:512:PHE:CE2	2.55	0.42
1:A:483:LEU:HB3	1:A:507:PRO:HB3	2.02	0.42
1:A:890:MET:HG2	2:B:1068:ASP:OD1	2.19	0.42
1:A:925:GLU:HB2	1:A:1081:ALA:HA	2.00	0.42
1:A:1139:PRO:HG3	1:A:1298:TYR:CE2	2.55	0.42
2:B:114:PRO:HB3	2:B:174:LEU:HD22	2.01	0.42
2:B:327:ILE:HD12	2:B:327:ILE:HA	1.97	0.42
3:C:115:TRP:CH2	3:C:212:ILE:HG12	2.51	0.42
3:C:133:VAL:HG22	3:C:207:HIS:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:28:LEU:HD13	4:D:52:HIS:HD2	1.85	0.42
4:D:127:LEU:HD13	4:D:133:HIS:CD2	2.54	0.42
5:E:121:MET:SD	5:E:122:LYS:HG2	2.59	0.42
5:E:155:ARG:HD3	5:E:194:GLU:OE1	2.20	0.42
13:M:268:LEU:HG	14:N:316:PHE:HB3	2.02	0.42
15:O:253:ILE:O	15:O:257:ASN:HB3	2.20	0.42
16:P:256:VAL:CG1	16:P:260:CYS:HB2	2.50	0.42
1:A:141:LEU:HD13	1:A:1402:TYR:CE2	2.55	0.42
1:A:239:CYS:SG	1:A:252:ARG:NH2	2.93	0.42
1:A:473:LEU:HD11	2:B:1078:LEU:HD11	2.01	0.42
1:A:644:GLU:HA	1:A:651:PHE:HB3	2.02	0.42
1:A:830:ARG:NH2	2:B:655:ASN:O	2.53	0.42
2:B:403:ILE:HD13	2:B:403:ILE:HA	1.93	0.42
3:C:77:SER:HB3	3:C:219:PHE:O	2.20	0.42
4:D:72:PHE:HB3	4:D:128:PRO:HD2	2.01	0.42
14:N:389:THR:O	14:N:389:THR:HG23	2.19	0.42
15:O:174:TYR:O	15:O:178:VAL:HG23	2.20	0.42
15:O:464:ASN:OD1	15:O:465:PHE:N	2.53	0.42
15:O:552:PRO:HG3	15:O:557:ARG:HG2	2.01	0.42
1:A:772:LYS:HE2	1:A:772:LYS:HB2	1.68	0.41
1:A:976:ARG:HH11	1:A:976:ARG:HG3	1.85	0.41
2:B:720:ARG:HB3	2:B:722:ASP:OD1	2.19	0.41
8:H:63:LEU:HD12	8:H:89:LEU:HB3	2.01	0.41
8:H:125:LEU:HG	8:H:130:ARG:NH1	2.34	0.41
11:K:127:LEU:O	11:K:131:VAL:HG23	2.19	0.41
13:M:96:LEU:HB2	13:M:100:LYS:O	2.19	0.41
15:O:136:ILE:HA	15:O:287:PHE:CE1	2.54	0.41
1:A:154:CYS:H	1:A:158:GLY:HA2	1.85	0.41
1:A:321:LEU:O	1:A:324:ALA:N	2.43	0.41
1:A:545:LYS:HB2	1:A:1096:SER:HB3	2.01	0.41
1:A:1322:VAL:HG13	1:A:1326:LEU:HD12	2.01	0.41
2:B:834:MET:HG2	12:L:61:THR:HG21	2.02	0.41
9:I:26:CYS:HB3	9:I:29:CYS:SG	2.60	0.41
15:O:87:ASP:OD1	15:O:87:ASP:C	2.63	0.41
1:A:627:ASP:OD1	1:A:655:ARG:NH2	2.52	0.41
1:A:1166:LEU:HD23	1:A:1267:LEU:O	2.20	0.41
2:B:786:GLU:OE1	2:B:788:ARG:NH1	2.46	0.41
3:C:134:LEU:HD23	3:C:169:PHE:HA	2.01	0.41
4:D:114:LYS:HA	4:D:114:LYS:HD3	1.84	0.41
8:H:26:ILE:HD13	8:H:42:ILE:HD12	2.02	0.41
15:O:465:PHE:HD1	15:O:465:PHE:HA	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:518:SER:O	15:O:522:ILE:HG12	2.21	0.41
1:A:788:TRP:HE1	8:H:21:ASN:HD22	1.68	0.41
1:A:858:PRO:N	1:A:859:PRO:HD2	2.35	0.41
2:B:195:LEU:HG	2:B:456:HIS:HD2	1.85	0.41
2:B:567:PHE:HB3	2:B:570:LYS:HB2	2.02	0.41
2:B:630:LEU:HA	2:B:634:GLU:O	2.20	0.41
2:B:711:GLY:HA2	2:B:728:MET:HB2	2.01	0.41
2:B:983:LYS:HE2	2:B:983:LYS:HB2	1.86	0.41
7:G:47:THR:OG1	7:G:48:ILE:N	2.53	0.41
9:I:81:TYR:CZ	9:I:101:VAL:HG12	2.55	0.41
14:N:281:GLU:HG3	14:N:282:LEU:N	2.34	0.41
15:O:285:ASP:O	15:O:289:LYS:HG2	2.21	0.41
15:O:459:ILE:HG22	16:P:210:PRO:HB3	2.02	0.41
15:O:619:LEU:HD23	15:O:619:LEU:HA	1.72	0.41
17:Q:69:PRO:HB3	17:Q:120:ILE:HG23	2.01	0.41
1:A:103:LEU:HB3	1:A:108:LYS:HE3	2.03	0.41
1:A:387:LEU:HD21	1:A:393:ALA:N	2.35	0.41
1:A:1048:VAL:HG13	1:A:1052:VAL:HG22	2.01	0.41
2:B:931:MET:HB3	2:B:939:VAL:HG22	2.01	0.41
4:D:19:PHE:HA	4:D:22:ASP:OD2	2.20	0.41
4:D:25:LYS:O	4:D:29:TRP:NE1	2.53	0.41
10:J:57:ILE:O	10:J:61:LEU:HG	2.21	0.41
12:L:46:VAL:HG12	12:L:54:ARG:HH21	1.85	0.41
13:M:155:ASN:HD21	13:M:158:GLN:HG2	1.85	0.41
14:N:227:PRO:C	14:N:296:LYS:HZ3	2.28	0.41
14:N:308:GLN:N	14:N:416:ILE:O	2.48	0.41
15:O:77:ARG:HH21	15:O:80:VAL:HG11	1.85	0.41
15:O:345:PHE:O	15:O:348:GLU:HG2	2.20	0.41
15:O:509:ARG:HB3	16:P:249:TYR:CD1	2.55	0.41
16:P:163:PRO:HD2	16:P:164:TRP:CZ3	2.55	0.41
1:A:138:MET:HG3	1:A:139:GLY:N	2.35	0.41
1:A:368:LEU:HD13	1:A:368:LEU:HA	1.77	0.41
1:A:673:LYS:HA	1:A:673:LYS:HD3	1.88	0.41
1:A:745:PHE:CE2	1:A:840:LYS:HE3	2.56	0.41
2:B:641:LEU:HD23	2:B:646:VAL:O	2.21	0.41
2:B:941:ASP:OD2	10:J:48:ARG:NH2	2.53	0.41
6:F:75:PRO:HB2	6:F:77:ASP:OD1	2.20	0.41
7:G:41:ASN:HA	7:G:155:PHE:CD1	2.56	0.41
7:G:89:ILE:HG13	7:G:143:ASN:N	2.36	0.41
11:K:92:SER:O	11:K:94:PRO:HD3	2.20	0.41
14:N:199:LEU:HD23	14:N:199:LEU:HA	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:505:MET:HE2	15:O:505:MET:HB2	1.81	0.41
1:A:5:VAL:HG21	7:G:39:ILE:HG13	2.03	0.41
1:A:232:LYS:HE3	16:P:315:TRP:CH2	2.56	0.41
1:A:574:ALA:HB2	11:K:81:MET:HG2	2.03	0.41
1:A:789:ASN:ND2	1:A:791:PRO:HD2	2.35	0.41
1:A:1277:ASP:C	1:A:1278:ILE:HD13	2.45	0.41
2:B:130:TYR:CE1	2:B:148:GLU:HB2	2.55	0.41
2:B:319:ILE:CD1	13:M:227:LEU:HD21	2.50	0.41
4:D:109:LYS:HD3	4:D:156:ILE:HG13	2.02	0.41
7:G:138:LEU:HD13	7:G:139:TYR:N	2.35	0.41
13:M:125:LEU:HD21	13:M:146:GLN:HB2	2.03	0.41
13:M:188:ASP:HA	13:M:191:VAL:HG12	2.03	0.41
15:O:60:ARG:HG2	17:Q:75:MET:HE2	2.03	0.41
15:O:376:LEU:HD23	15:O:456:HIS:CE1	2.56	0.41
15:O:621:PRO:O	15:O:624:LEU:HG	2.20	0.41
1:A:372:ARG:O	2:B:1087:SER:OG	2.33	0.41
2:B:191:GLU:OE1	2:B:458:LEU:HD23	2.21	0.41
2:B:389:GLU:HG2	2:B:446:ARG:CZ	2.51	0.41
2:B:419:LEU:O	2:B:422:ILE:HG22	2.21	0.41
2:B:444:LEU:HD12	2:B:449:MET:SD	2.60	0.41
2:B:585:SER:O	2:B:588:ILE:HD12	2.20	0.41
2:B:757:VAL:HG21	2:B:1022:ILE:HB	2.02	0.41
2:B:885:MET:HE2	2:B:897:LYS:HB2	2.03	0.41
7:G:150:ILE:HA	7:G:197:LEU:O	2.21	0.41
15:O:194:LEU:HA	15:O:197:MET:HE2	2.02	0.41
15:O:308:THR:O	15:O:311:VAL:HG12	2.21	0.41
15:O:613:GLY:N	15:O:615:GLU:OE2	2.51	0.41
1:A:408:VAL:HG23	1:A:460:ASP:O	2.21	0.41
1:A:481:HIS:CD2	1:A:481:HIS:H	2.39	0.41
1:A:660:LEU:O	8:H:117:SER:OG	2.35	0.41
1:A:673:LYS:HD2	1:A:675:HIS:NE2	2.36	0.41
1:A:890:MET:HE3	2:B:1068:ASP:HB3	2.03	0.41
2:B:46:HIS:C	2:B:49:PRO:HD2	2.46	0.41
2:B:255:ILE:HD12	2:B:296:TYR:CE2	2.55	0.41
2:B:420:LEU:HA	2:B:423:ASN:HD22	1.86	0.41
2:B:702:GLN:CD	2:B:915:ARG:HA	2.45	0.41
2:B:793:THR:HG23	2:B:896:ILE:HB	2.01	0.41
2:B:834:MET:HE2	2:B:834:MET:HB3	1.73	0.41
2:B:908:LEU:HD12	2:B:908:LEU:HA	1.93	0.41
3:C:37:LYS:HG2	11:K:130:VAL:HG13	2.01	0.41
3:C:61:THR:HA	3:C:298:PHE:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:67:PHE:O	3:C:71:MET:HG3	2.21	0.41
3:C:328:LEU:HD21	11:K:65:ILE:HD13	2.02	0.41
4:D:28:LEU:HD12	4:D:28:LEU:HA	1.94	0.41
5:E:46:TYR:HE2	5:E:58:MET:HA	1.85	0.41
13:M:75:PRO:HA	14:N:362:SER:HA	2.03	0.41
13:M:95:ARG:HA	14:N:391:LEU:HD13	2.02	0.41
15:O:532:ASP:HA	15:O:535:SER:OG	2.21	0.41
15:O:544:ASN:HB2	15:O:576:PHE:HB2	2.03	0.41
1:A:110:CYS:SG	1:A:156:HIS:HB3	2.61	0.41
1:A:229:ASN:HB3	15:O:544:ASN:OD1	2.21	0.41
1:A:827:PHE:CE1	1:A:833:PRO:HD3	2.56	0.41
1:A:1206:ALA:O	1:A:1210:THR:HG23	2.21	0.41
4:D:56:GLN:HA	4:D:59:THR:HG22	2.02	0.41
7:G:79:PRO:HA	7:G:83:GLU:CD	2.46	0.41
8:H:30:SER:HB3	8:H:33:GLN:O	2.21	0.41
8:H:142:LEU:HD21	8:H:144:ILE:HD11	2.03	0.41
9:I:22:TYR:O	9:I:35:ILE:HD13	2.21	0.41
14:N:303:ARG:O	14:N:304:PHE:HD1	2.04	0.41
1:A:44:LYS:NZ	1:A:49:LYS:HB2	2.35	0.40
1:A:100:ILE:HD11	1:A:178:ILE:HG12	2.04	0.40
1:A:363:ARG:HA	1:A:363:ARG:HD3	1.90	0.40
2:B:38:ILE:HG22	2:B:624:ASP:HB2	2.03	0.40
2:B:262:ILE:HG23	2:B:267:GLU:CD	2.46	0.40
2:B:908:LEU:HD11	2:B:924:ILE:HA	2.03	0.40
3:C:329:LYS:HE2	3:C:329:LYS:HB3	1.91	0.40
9:I:24:LEU:HD21	9:I:40:ILE:HD13	2.02	0.40
14:N:291:LEU:CD1	14:N:295:LYS:HD2	2.51	0.40
15:O:62:ALA:O	15:O:65:ILE:HG22	2.21	0.40
19:X:1011:UNK:O	19:X:1013:UNK:N	2.54	0.40
1:A:386:ASN:OD1	1:A:703:ARG:NH2	2.52	0.40
1:A:818:ILE:HG22	1:A:867:SER:HA	2.03	0.40
2:B:206:ILE:HD12	2:B:206:ILE:HA	1.86	0.40
2:B:232:TYR:CD1	2:B:356:VAL:HG21	2.56	0.40
2:B:613:ILE:HG13	2:B:675:ILE:HG12	2.02	0.40
2:B:664:LYS:HE2	2:B:664:LYS:HB3	1.70	0.40
2:B:795:LEU:HB2	2:B:894:ALA:HB3	2.03	0.40
7:G:80:PHE:HD1	7:G:83:GLU:OE1	2.03	0.40
9:I:43:ARG:HB2	9:I:43:ARG:HE	1.67	0.40
1:A:14:LYS:HB3	1:A:14:LYS:HE2	1.82	0.40
1:A:525:GLU:OE1	1:A:528:ARG:NH2	2.54	0.40
1:A:804:LEU:HD11	9:I:82:PHE:CZ	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:155:MET:HE2	2:B:155:MET:HB3	1.87	0.40
2:B:155:MET:HE3	2:B:183:GLY:HA2	2.03	0.40
3:C:322:LYS:HB2	11:K:128:CYS:HB3	2.04	0.40
6:F:134:ILE:HG22	6:F:136:ARG:HG3	2.03	0.40
7:G:124:GLU:HG3	7:G:124:GLU:O	2.22	0.40
10:J:44:TYR:HA	10:J:47:ARG:HB2	2.04	0.40
13:M:143:VAL:HG12	13:M:185:TYR:CD2	2.57	0.40
15:O:628:LYS:HE2	15:O:628:LYS:HB2	1.97	0.40
15:O:643:ARG:HH12	16:P:291:PHE:HA	1.86	0.40
16:P:164:TRP:CD1	16:P:175:ILE:HD12	2.55	0.40
1:A:184:ARG:HG2	1:A:185:TRP:CD2	2.57	0.40
1:A:328:ASN:HB2	1:A:354:CYS:SG	2.61	0.40
1:A:1155:ARG:HB2	1:A:1197:GLN:OE1	2.22	0.40
1:A:1380:ARG:HD3	1:A:1385:GLN:OE1	2.22	0.40
2:B:701:TYR:CZ	9:I:91:ASP:HB3	2.56	0.40
2:B:1030:MET:HE3	2:B:1030:MET:HB2	1.99	0.40
4:D:34:LEU:HD23	4:D:34:LEU:HA	1.98	0.40
4:D:123:ILE:HG22	4:D:137:ILE:HD13	2.03	0.40
4:D:130:ASN:HB3	4:D:133:HIS:CG	2.57	0.40
7:G:87:GLY:C	7:G:88:TRP:HD1	2.29	0.40
7:G:147:ARG:NH1	7:G:208:VAL:HA	2.36	0.40
10:J:12:LYS:HE3	10:J:41:LEU:HD23	2.03	0.40
13:M:111:ARG:HB2	13:M:120:GLU:HB2	2.03	0.40
15:O:156:VAL:HA	15:O:159:ILE:HG22	2.04	0.40
1:A:106:ILE:HG22	1:A:113:ILE:HA	2.02	0.40
1:A:115:LEU:HD23	1:A:115:LEU:HA	1.83	0.40
1:A:1157:VAL:O	1:A:1161:VAL:HG22	2.22	0.40
2:B:228:LYS:HE3	2:B:228:LYS:HB3	1.89	0.40
2:B:258:LYS:HA	2:B:262:ILE:O	2.21	0.40
2:B:296:TYR:CD1	2:B:300:GLN:HB3	2.57	0.40
2:B:316:LYS:HA	2:B:316:LYS:HD2	1.89	0.40
2:B:435:ARG:O	2:B:439:THR:HG23	2.21	0.40
2:B:490:GLN:O	2:B:493:GLN:HG2	2.20	0.40
3:C:162:VAL:CG2	3:C:196:LEU:HD11	2.52	0.40
10:J:30:LEU:HB3	10:J:34:THR:HG23	2.04	0.40
15:O:492:TYR:HD1	15:O:577:MET:HG3	1.87	0.40
16:P:245:GLU:O	16:P:248:VAL:HG12	2.21	0.40
16:P:269:LEU:HG	16:P:297:PHE:CE2	2.57	0.40
17:Q:103:ASP:OD1	17:Q:103:ASP:N	2.48	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	1411/1460 (97%)	1326 (94%)	84 (6%)	1 (0%)	48	77
2	B	1098/1149 (96%)	1046 (95%)	52 (5%)	0	100	100
3	C	333/335 (99%)	318 (96%)	15 (4%)	0	100	100
4	D	141/161 (88%)	126 (89%)	13 (9%)	2 (1%)	9	30
5	E	213/215 (99%)	204 (96%)	9 (4%)	0	100	100
6	F	81/155 (52%)	81 (100%)	0	0	100	100
7	G	185/212 (87%)	168 (91%)	17 (9%)	0	100	100
8	H	134/146 (92%)	124 (92%)	10 (8%)	0	100	100
9	I	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
10	J	65/70 (93%)	62 (95%)	3 (5%)	0	100	100
11	K	99/142 (70%)	93 (94%)	6 (6%)	0	100	100
12	L	42/70 (60%)	39 (93%)	3 (7%)	0	100	100
13	M	179/282 (64%)	169 (94%)	10 (6%)	0	100	100
14	N	139/422 (33%)	135 (97%)	4 (3%)	0	100	100
15	O	564/654 (86%)	538 (95%)	26 (5%)	0	100	100
16	P	132/317 (42%)	125 (95%)	7 (5%)	0	100	100
17	Q	100/251 (40%)	86 (86%)	13 (13%)	1 (1%)	12	39
18	W	15/635 (2%)	15 (100%)	0	0	100	100
All	All	5039/6786 (74%)	4759 (94%)	276 (6%)	4 (0%)	49	77

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	46	GLN
4	D	49	PRO
17	Q	33	ILE
1	A	879	THR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	1230/1257 (98%)	1193 (97%)	37 (3%)	36	70
2	B	965/1006 (96%)	943 (98%)	22 (2%)	44	76
3	C	296/296 (100%)	275 (93%)	21 (7%)	13	40
4	D	123/145 (85%)	123 (100%)	0	100	100
5	E	197/197 (100%)	188 (95%)	9 (5%)	24	57
6	F	73/137 (53%)	71 (97%)	2 (3%)	39	73
7	G	170/190 (90%)	168 (99%)	2 (1%)	63	86
8	H	121/128 (94%)	118 (98%)	3 (2%)	42	74
9	I	98/98 (100%)	97 (99%)	1 (1%)	68	89
10	J	62/65 (95%)	61 (98%)	1 (2%)	55	83
11	K	91/130 (70%)	89 (98%)	2 (2%)	45	77
12	L	39/39 (100%)	38 (97%)	1 (3%)	40	73
13	M	159/249 (64%)	155 (98%)	4 (2%)	42	74
14	N	125/200 (62%)	123 (98%)	2 (2%)	55	83
15	O	521/593 (88%)	507 (97%)	14 (3%)	39	73
16	P	126/285 (44%)	122 (97%)	4 (3%)	34	68
17	Q	92/212 (43%)	91 (99%)	1 (1%)	65	88
18	W	17/586 (3%)	17 (100%)	0	100	100
All	All	4505/5813 (78%)	4379 (97%)	126 (3%)	38	72

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	GLU
1	A	91	PHE
1	A	219	MET
1	A	228	LEU
1	A	269	ARG
1	A	280	SER

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Mol	Chain	Res	Type
1	A	320	GLN
1	A	368	LEU
1	A	446	TYR
1	A	554	THR
1	A	671	ASP
1	A	781	CYS
1	A	862	LEU
1	A	867	SER
1	A	869	ARG
1	A	870	GLU
1	A	873	VAL
1	A	881	GLU
1	A	885	MET
1	A	887	ARG
1	A	894	GLU
1	A	895	ASP
1	A	931	GLN
1	A	970	LEU
1	A	990	ASN
1	A	1144	VAL
1	A	1166	LEU
1	A	1167	SER
1	A	1185	GLN
1	A	1201	THR
1	A	1230	ILE
1	A	1270	VAL
1	A	1282	VAL
1	A	1312	SER
1	A	1376	LEU
1	A	1386	LEU
1	A	1395	HIS
2	B	193	VAL
2	B	208	GLU
2	B	221	THR
2	B	230	LYS
2	B	231	THR
2	B	233	VAL
2	B	264	SER
2	B	464	ILE
2	B	539	GLU
2	B	542	THR
2	B	546	SER

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Mol	Chain	Res	Type
2	B	664	LYS
2	B	669	SER
2	B	741	ILE
2	B	792	THR
2	B	800	ASN
2	B	805	ILE
2	B	887	SER
2	B	951	SER
2	B	953	MET
2	B	1008	ILE
2	B	1145	ASP
3	C	37	LYS
3	C	45	SER
3	C	89	THR
3	C	106	LEU
3	C	120	LEU
3	C	145	ASP
3	C	148	LYS
3	C	150	SER
3	C	151	THR
3	C	152	ASP
3	C	154	LYS
3	C	155	GLU
3	C	156	LEU
3	C	165	ARG
3	C	177	THR
3	C	181	ASP
3	C	182	CYS
3	C	196	LEU
3	C	212	ILE
3	C	223	SER
3	C	304	SER
5	E	31	THR
5	E	40	GLU
5	E	41	ASP
5	E	43	LYS
5	E	45	LYS
5	E	68	SER
5	E	75	MET
5	E	111	VAL
5	E	158	SER
6	F	92	ARG

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Mol	Chain	Res	Type
6	F	133	VAL
7	G	37	LYS
7	G	66	SER
8	H	77	ARG
8	H	92	ASP
8	H	107	VAL
9	I	40	ILE
10	J	10	CYS
11	K	52	GLN
11	K	60	SER
12	L	64	LEU
13	M	93	ARG
13	M	158	GLN
13	M	226	ARG
13	M	227	LEU
14	N	290	ILE
14	N	365	VAL
15	O	57	LEU
15	O	67	MET
15	O	94	THR
15	O	129	ILE
15	O	130	LEU
15	O	131	LEU
15	O	146	VAL
15	O	257	ASN
15	O	279	SER
15	O	319	THR
15	O	486	VAL
15	O	565	LEU
15	O	599	ASN
15	O	642	SER
16	P	179	LEU
16	P	212	VAL
16	P	218	THR
16	P	254	GLU
17	Q	121	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	HIS
1	A	151	GLN

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Mol	Chain	Res	Type
1	A	229	ASN
1	A	437	ASN
1	A	455	ASN
1	A	555	GLN
1	A	618	HIS
1	A	619	ASN
1	A	725	GLN
1	A	753	GLN
1	A	816	GLN
1	A	948	ASN
1	A	1254	ASN
1	A	1453	ASN
2	B	116	HIS
2	B	244	HIS
2	B	275	ASN
2	B	321	GLN
2	B	382	GLN
2	B	423	ASN
2	B	441	ASN
2	B	456	HIS
2	B	493	GLN
2	B	519	HIS
2	B	695	GLN
2	B	708	GLN
2	B	774	ASN
2	B	814	ASN
2	B	844	ASN
2	B	883	GLN
2	B	1025	GLN
2	B	1148	GLN
3	C	88	ASN
3	C	158	ASN
3	C	161	HIS
3	C	172	GLN
3	C	175	GLN
3	C	301	ASN
4	D	61	ASN
4	D	64	ASN
4	D	71	ASN
4	D	122	GLN
4	D	130	ASN
5	E	8	ASN

Continued on next page...

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Mol	Chain	Res	Type
5	E	136	ASN
5	E	143	ASN
5	E	179	GLN
7	G	32	ASN
7	G	69	ASN
8	H	21	ASN
8	H	52	GLN
8	H	64	ASN
8	H	83	GLN
8	H	137	GLN
9	I	61	ASN
9	I	71	ASN
9	I	105	HIS
11	K	118	GLN
12	L	66	GLN
13	M	86	HIS
13	M	89	GLN
13	M	117	HIS
13	M	132	ASN
13	M	155	ASN
13	M	156	ASN
13	M	158	GLN
13	M	178	GLN
13	M	190	ASN
13	M	225	ASN
14	N	298	ASN
14	N	299	ASN
14	N	377	ASN
14	N	392	GLN
15	O	222	HIS
15	O	225	ASN
15	O	298	ASN
15	O	310	GLN
15	O	549	GLN
15	O	584	ASN
16	P	176	ASN
16	P	205	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

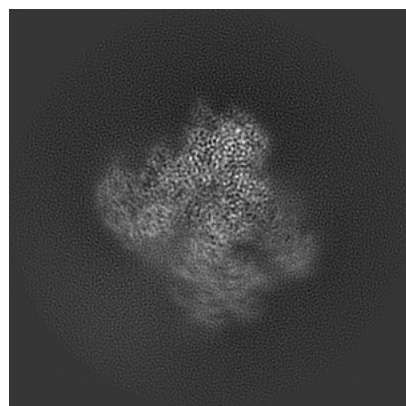
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14469. These allow visual inspection of the internal detail of the map and identification of artifacts.

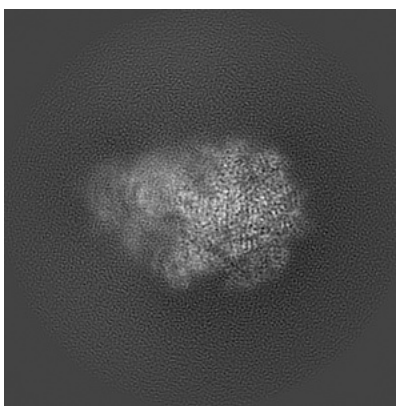
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

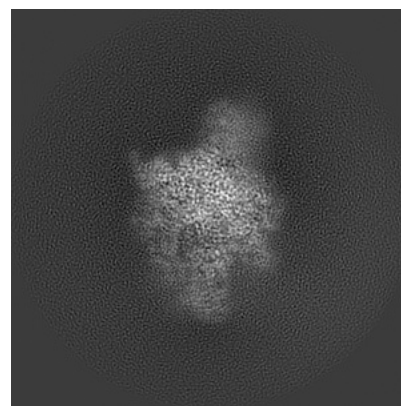
6.1.1 Primary map



X

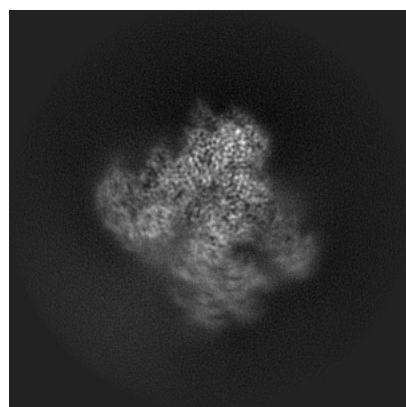


Y

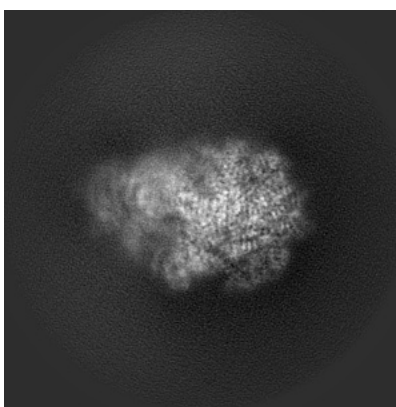


Z

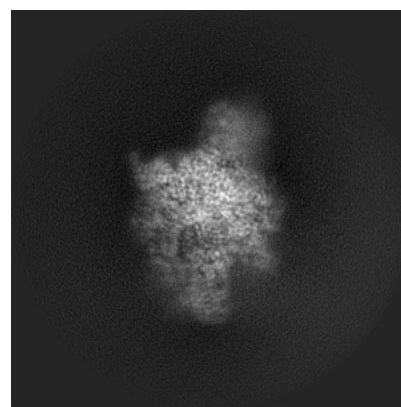
6.1.2 Raw map



X



Y

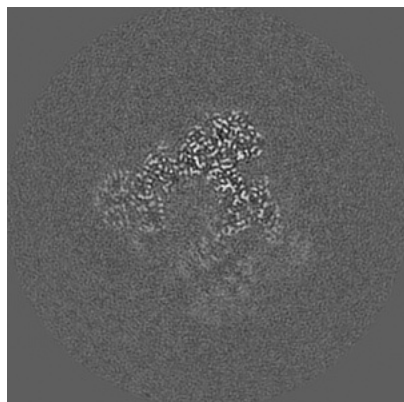


Z

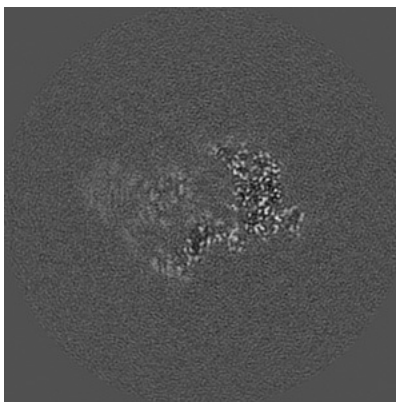
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

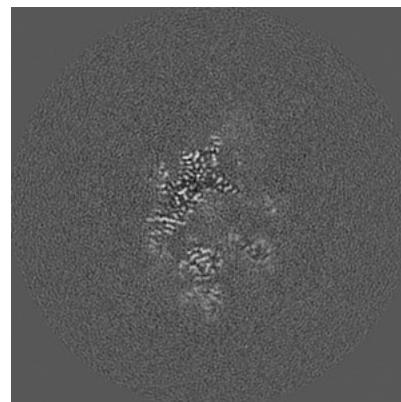
6.2.1 Primary map



X Index: 150

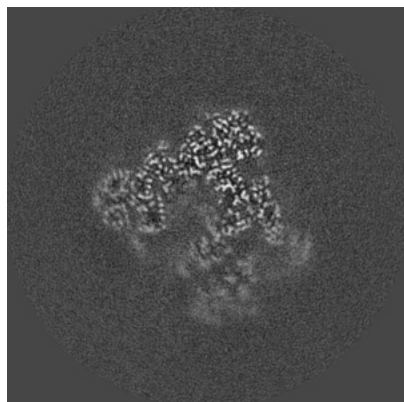


Y Index: 150

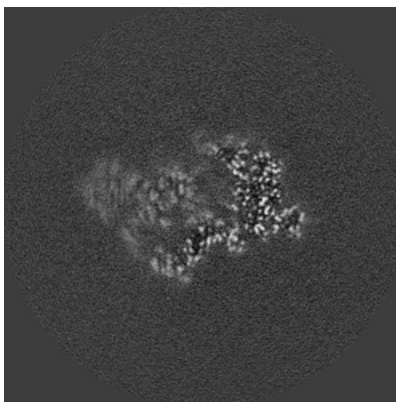


Z Index: 150

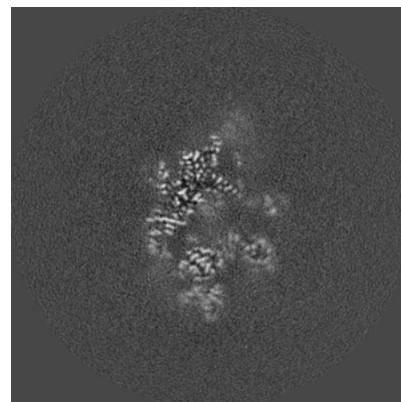
6.2.2 Raw map



X Index: 150



Y Index: 150

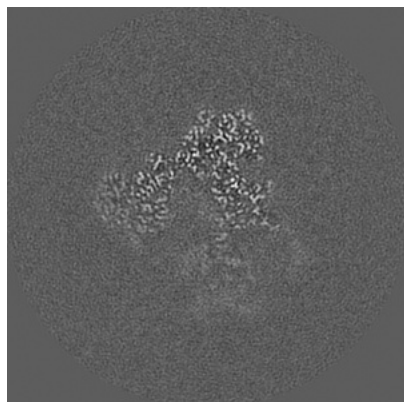


Z Index: 150

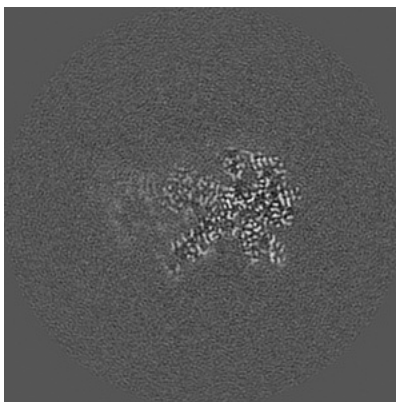
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

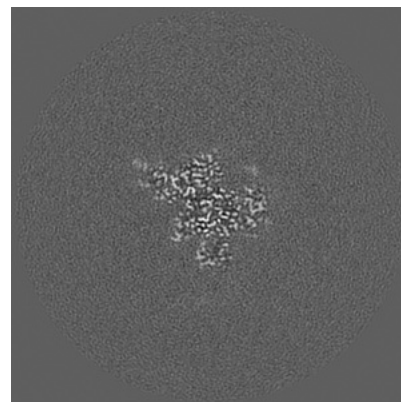
6.3.1 Primary map



X Index: 147

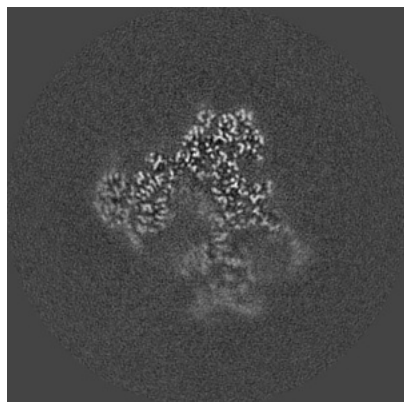


Y Index: 161

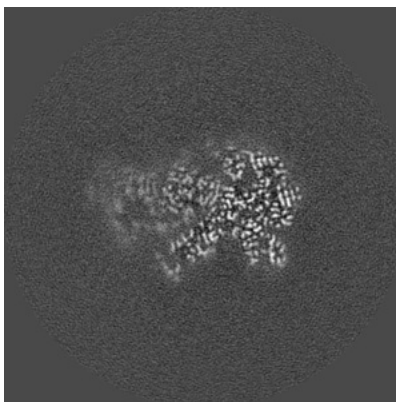


Z Index: 188

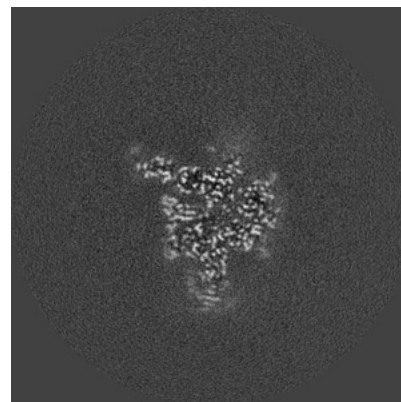
6.3.2 Raw map



X Index: 147



Y Index: 161

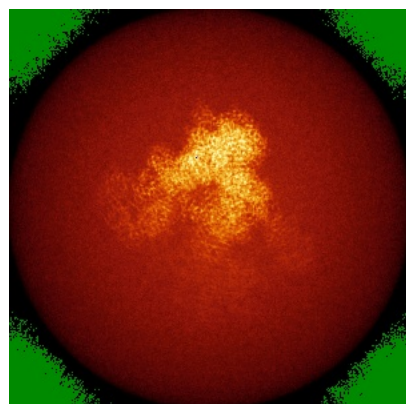


Z Index: 173

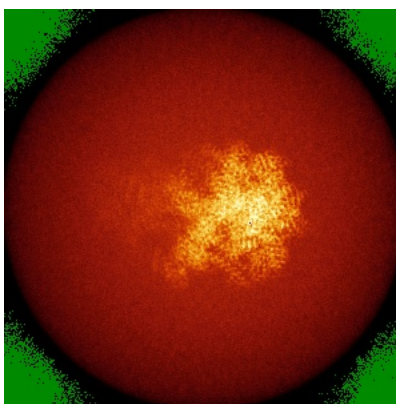
The images above show the largest variance slices of the map in three orthogonal directions.

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

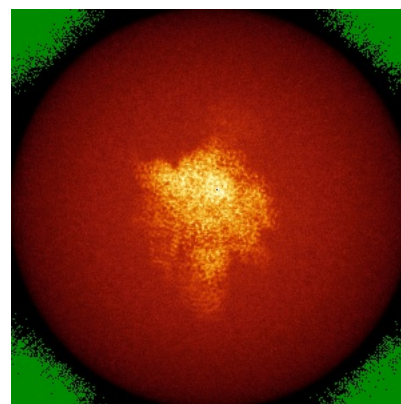
6.4.1 Primary map



X

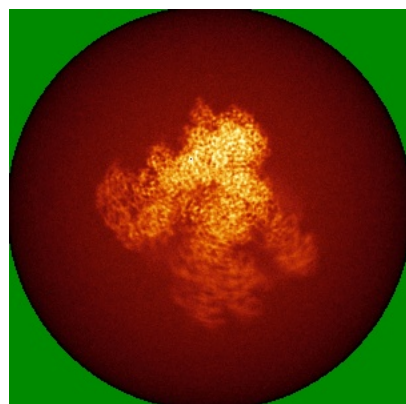


Y

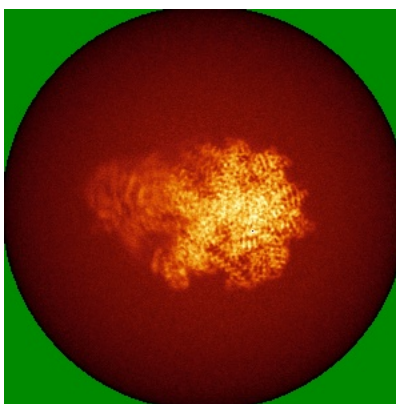


Z

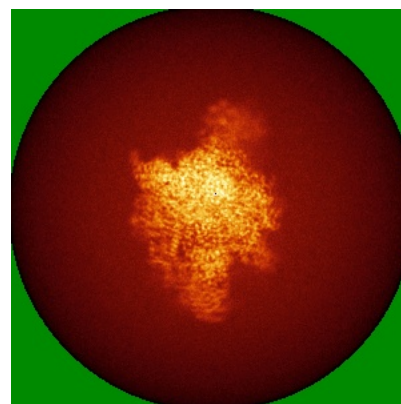
6.4.2 Raw map



X



Y

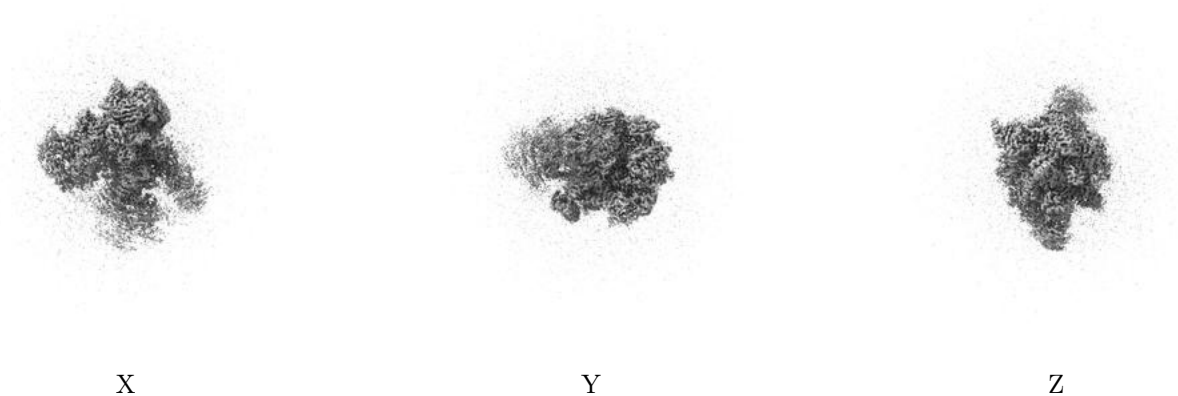


Z

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.

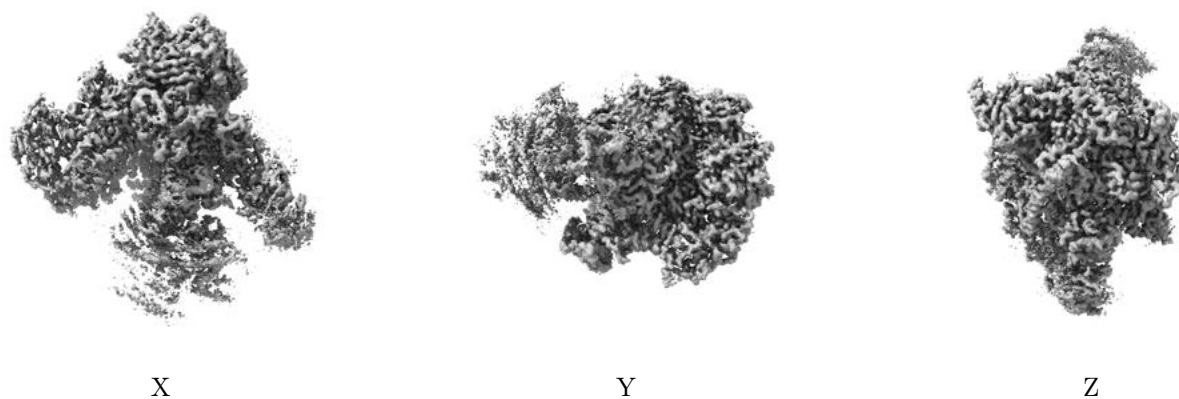
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0227. 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.

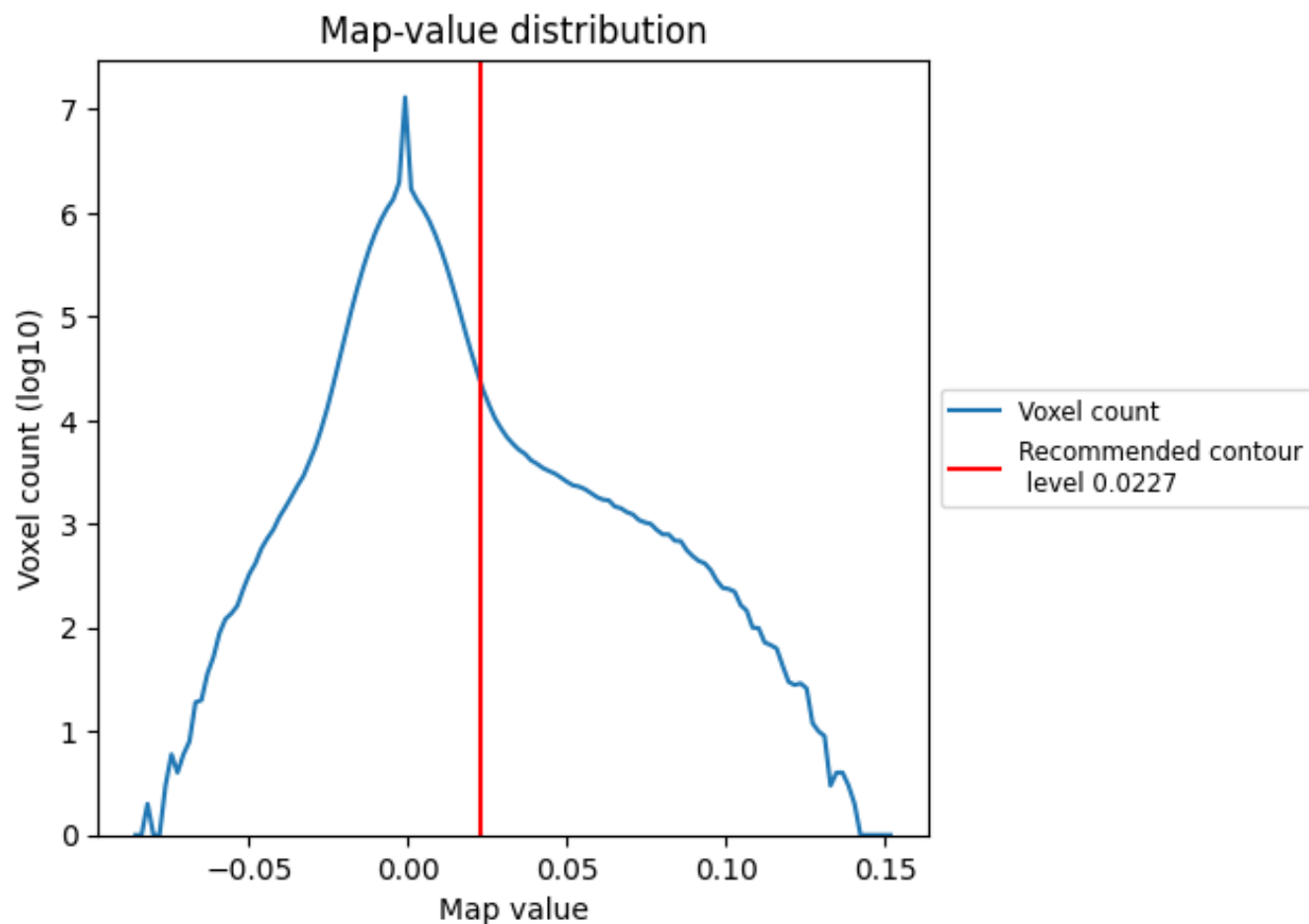
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

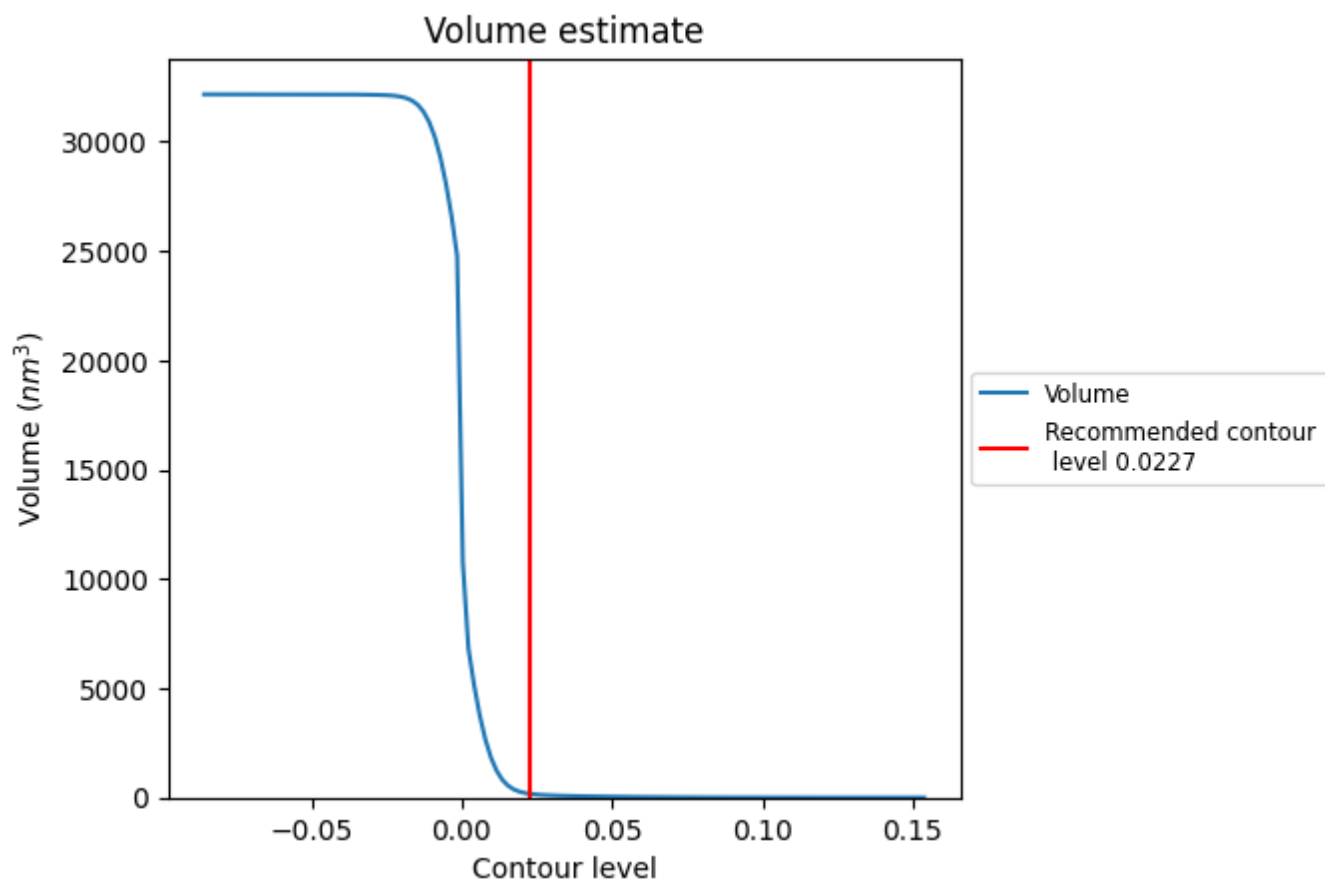
This section contains the results of statistical analysis of the map.

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.

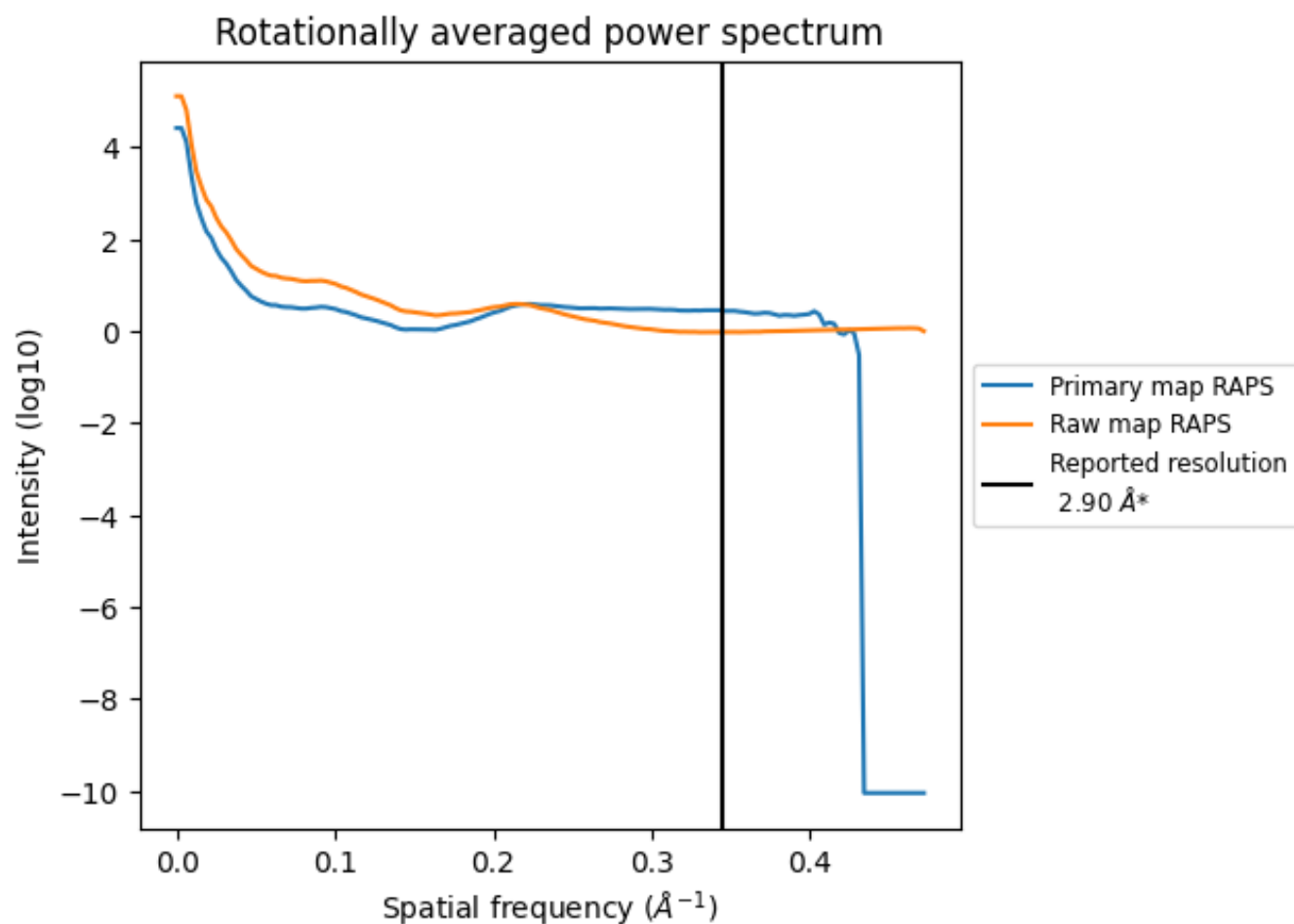
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 170 nm³; this corresponds to an approximate mass of 153 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 ⓘ

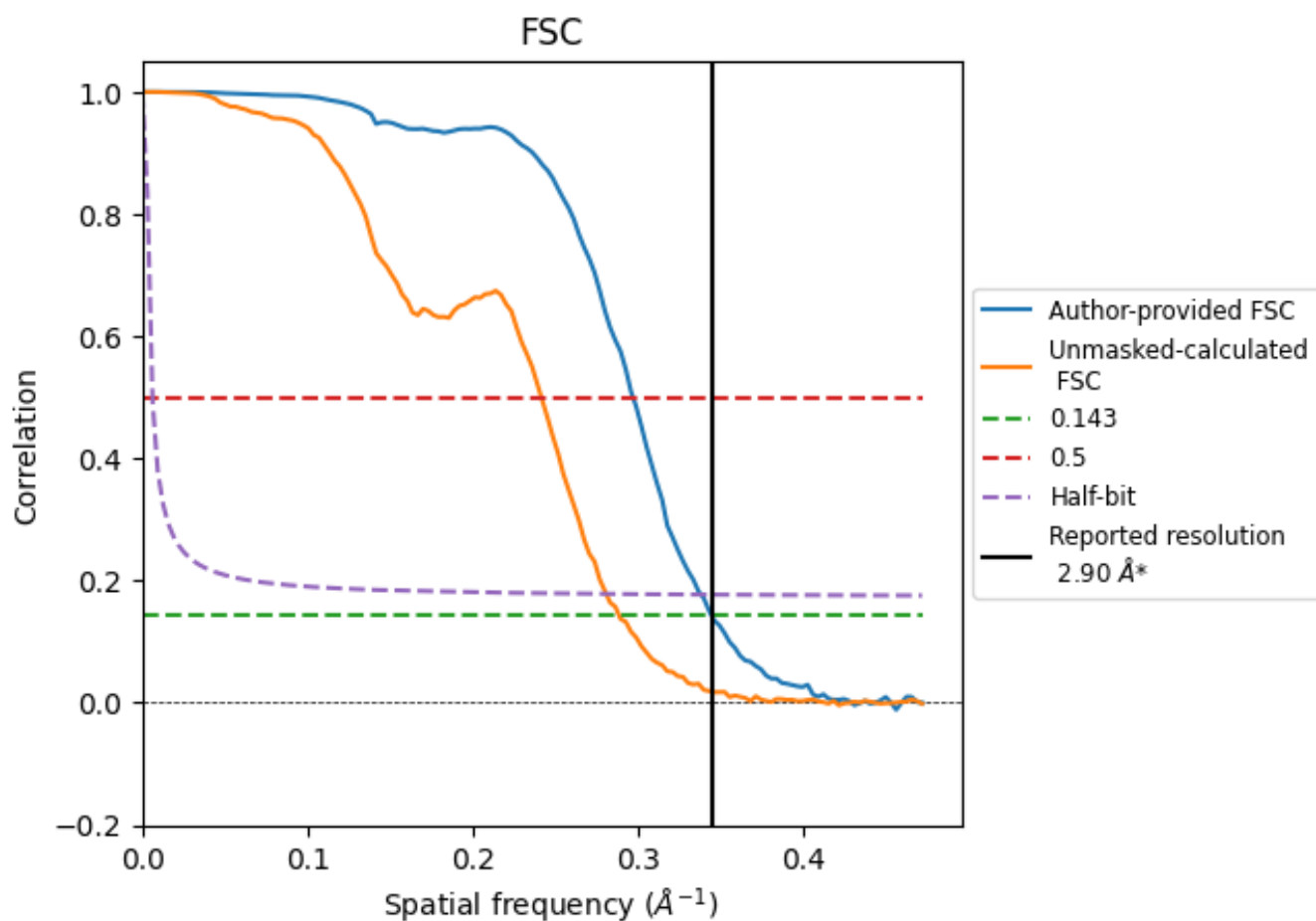


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	2.90	-
Author-provided FSC curve	2.90	3.37	2.96
Unmasked-calculated*	3.47	4.14	3.56

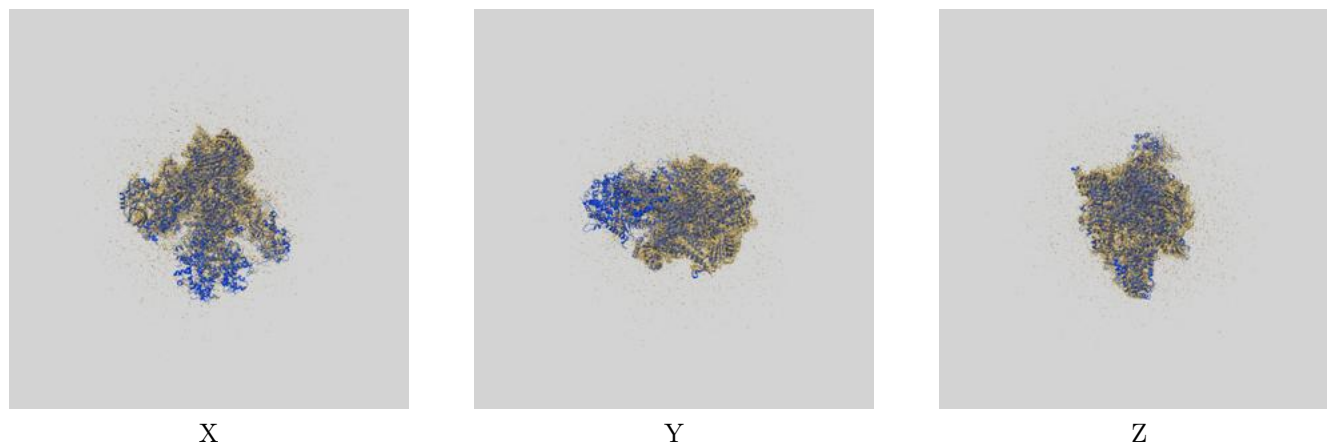
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.5 CUT-OFF 3.37 differs from the reported value 2.9 by more than 10 %

The value from deposited half-maps intersecting FSC 0.5 CUT-OFF 4.14 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

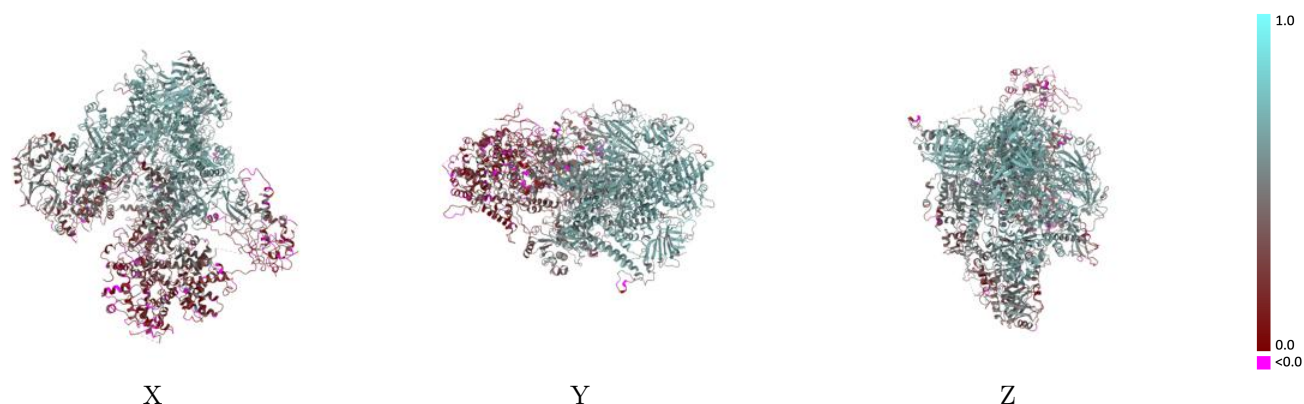
This section contains information regarding the fit between EMDB map EMD-14469 and PDB model 7Z30. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



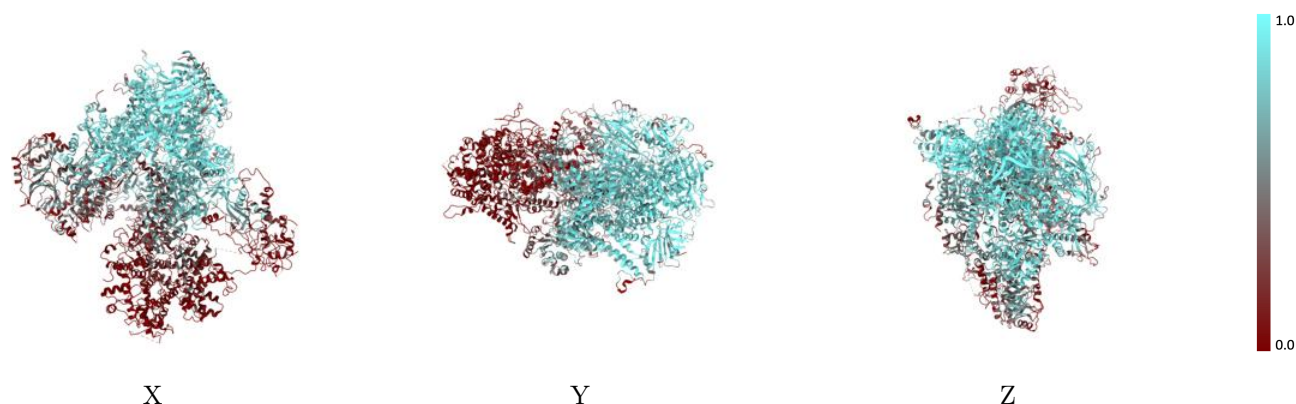
The images above show the 3D surface view of the map at the recommended contour level 0.0227 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



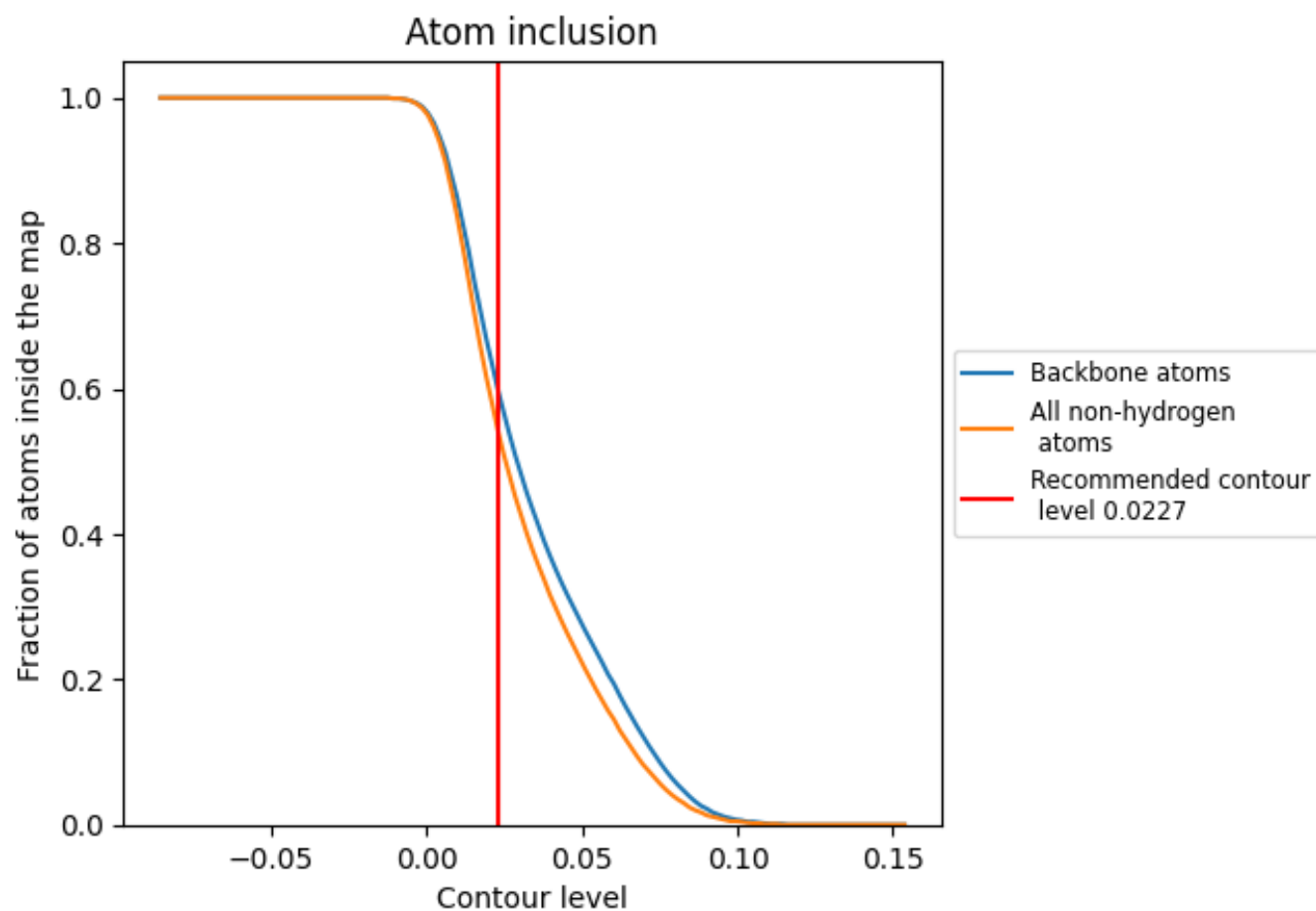
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0227).

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 55% 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 (0.0227) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5460	 0.4640
A	 0.6540	 0.5110
B	 0.7460	 0.5610
C	 0.8360	 0.6070
D	 0.1140	 0.2090
E	 0.5620	 0.4740
F	 0.8360	 0.6120
G	 0.3110	 0.3430
H	 0.7930	 0.5860
I	 0.6080	 0.5060
J	 0.8880	 0.6280
K	 0.8560	 0.6280
L	 0.6880	 0.5550
M	 0.3090	 0.3720
N	 0.2980	 0.3870
O	 0.0910	 0.2370
P	 0.0370	 0.1680
Q	 0.0540	 0.2240
W	 0.0880	 0.2960
X	 0.3290	 0.4520

