



Full wwPDB EM Validation Report ⓘ

Mar 14, 2026 – 01:42 AM UTC

PDB ID : 8UIS / pdb_00008uis
EMDB ID : EMD-42303
Title : Structure of transcription complex Pol II-DSIF-NELF-TFIIS
Authors : Su, B.G.; Vos, S.M.
Deposited on : 2023-10-10
Resolution : 3.23 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

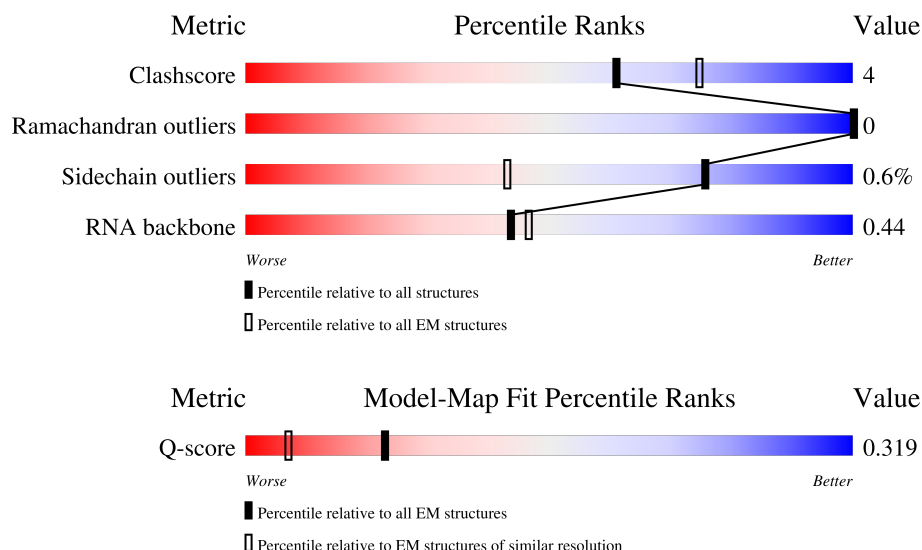
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.23 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	14612 (2.73 - 3.73)

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	N	50	
2	P	22	
3	T	50	

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Mol	Chain	Length	Quality of chain
4	W	590	
5	Z	1087	
6	A	1970	
7	B	1174	
8	C	271	
9	D	142	
10	E	210	
11	F	127	
12	G	172	
13	H	150	
14	I	125	
15	J	67	
16	K	117	
17	L	58	
18	S	301	
19	U	528	

2 Entry composition [i](#)

There are 21 unique types of molecules in this entry. The entry contains 79960 atoms, of which 39727 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 DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	N	27	Total	C	H	N	O	P	0	0
			855	263	304	100	161	27		

- Molecule 2 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	P	14	Total	C	H	N	O	P	0	0
			447	132	151	51	99	14		

- Molecule 3 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	T	38	Total	C	H	N	O	P	0	0
			1209	371	426	148	226	38		

- Molecule 4 is a protein called Negative elongation factor C/D.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	W	381	Total	C	H	N	O	S	0	0
			6058	1928	3047	507	557	19		

- Molecule 5 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	Z	273	Total	C	H	N	O	S	0	0
			4375	1369	2201	392	402	11		

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	A	1415	Total	C	H	N	O	S	0	0
			22549	7052	11339	2005	2082	71		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
7	B	1136	Total	C	H	N	O	S	0	0
			18194	5739	9118	1597	1676	64		

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	C	255	Total	C	H	N	O	S	0	0
			4039	1285	1995	349	404	6		

- Molecule 9 is a protein called RNA polymerase Rpb4/RPC9 core domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	D	124	Total	C	H	N	O	S	0	0
			2016	632	1004	173	203	4		

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	E	207	Total	C	H	N	O	S	0	0
			3438	1083	1729	298	320	8		

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	F	77	Total	C	H	N	O	S	0	0
			1271	397	653	105	111	5		

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	G	171	Total	C	H	N	O	S	0	0
			2709	875	1358	219	249	8		

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	H	148	Total	C	H	N	O	S	0	0
			2333	750	1147	194	237	5		

- Molecule 14 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	I	114	Total	C	H	N	O	S	0	0
			1790	571	862	166	180	11		

- Molecule 15 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	J	65	Total	C	H	N	O	S	0	0
			1049	334	534	87	88	6		

- Molecule 16 is a protein called RNA polymerase II subunit J.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	K	115	Total	C	H	N	O	S	0	0
			1862	593	942	152	173	2		

- Molecule 17 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	L	44	Total	C	H	N	O	S	0	0
			753	231	380	72	64	6		

- Molecule 18 is a protein called Transcription elongation factor A protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	S	122	Total	C	H	N	O	S	0	0
			1950	589	981	181	191	8		

- Molecule 19 is a protein called Negative elongation factor A.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	U	196	Total	C	H	N	O	S	0	0
			3054	953	1556	253	284	8		

- 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	C	1	Total	Zn	0
			1	1	

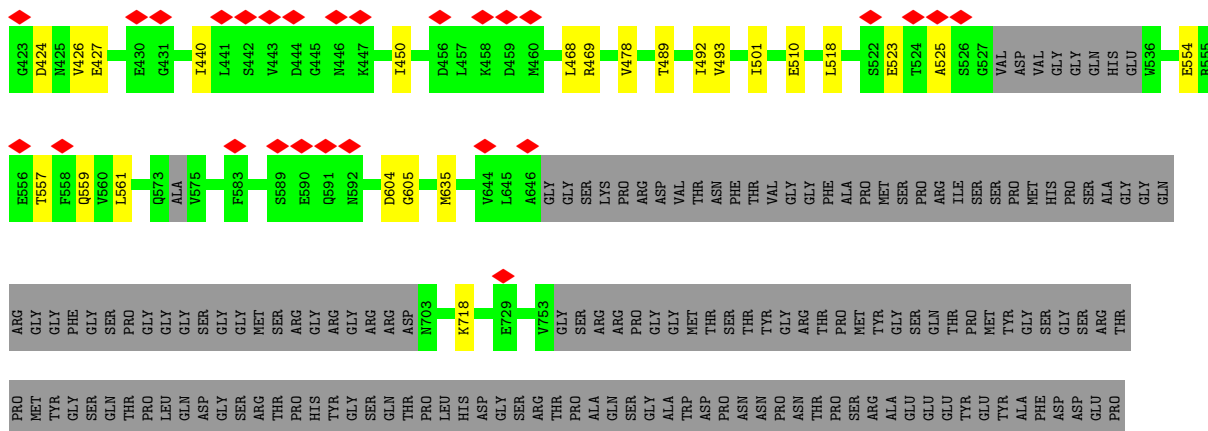
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Mol	Chain	Residues	Atoms		AltConf
20	I	2	Total 2	Zn 2	0
20	J	1	Total 1	Zn 1	0
20	L	1	Total 1	Zn 1	0

- Molecule 21 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

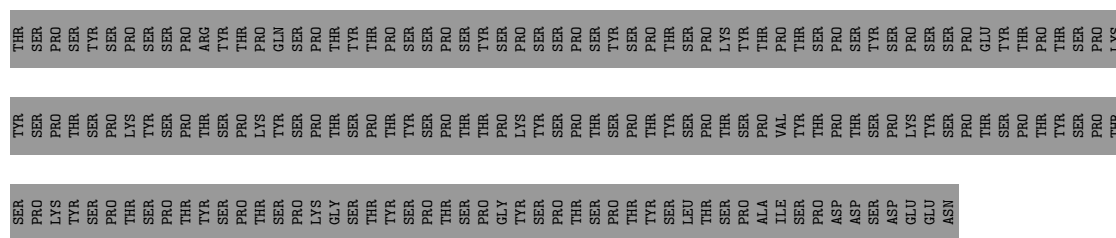
Mol	Chain	Residues	Atoms		AltConf
21	A	1	Total 1	Mg 1	0



LEU
GLU
ALA

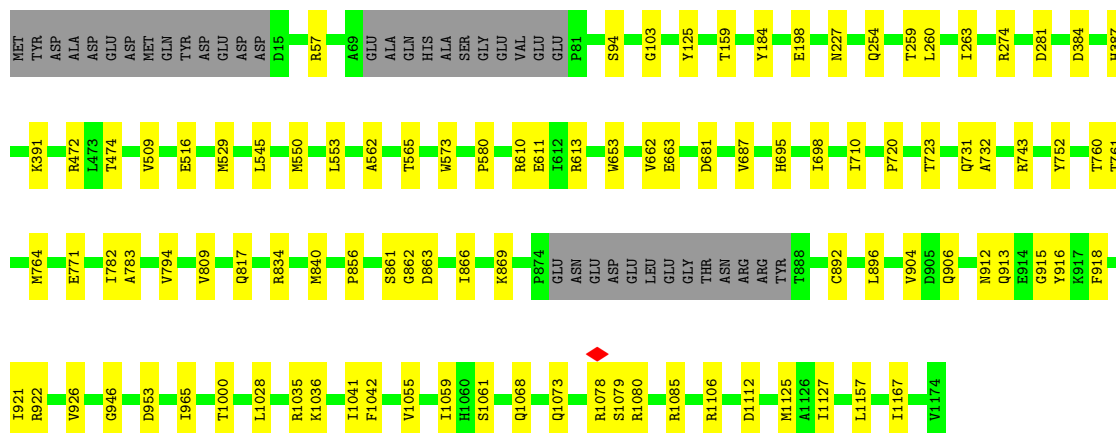
Chain A: 63% 9% 28%





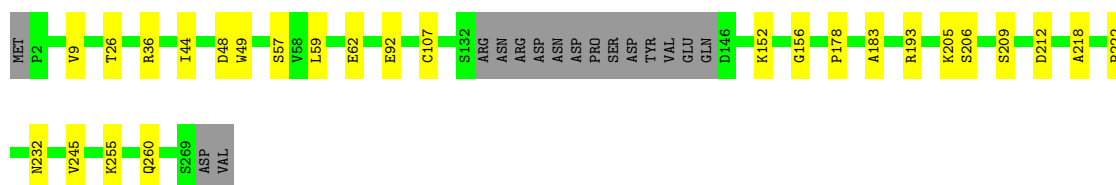
• Molecule 7: DNA-directed RNA polymerase subunit beta

Chain B: 88% 8% .



• Molecule 8: DNA-directed RNA polymerase II subunit RPB3

Chain C: 85% 10% 6%



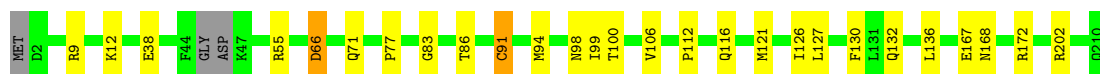
• Molecule 9: RNA polymerase Rpb4/ RPC9 core domain-containing protein

Chain D: 77% 10% 13%



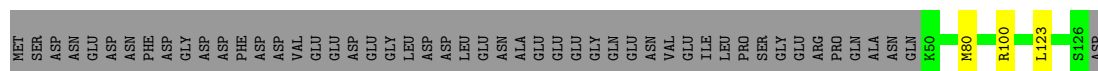
• Molecule 10: DNA-directed RNA polymerase II subunit E

Chain E: 86% 12% ..



• Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:  58% 39%



- Molecule 12: DNA-directed RNA polymerase II subunit RPB7

Chain G:  86% 13%



- Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:  82% 17%



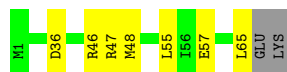
- Molecule 14: DNA-directed RNA polymerase II subunit RPB9

Chain I:  77% 14% 9%

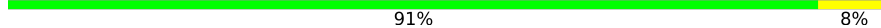


- Molecule 15: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:  87% 10%



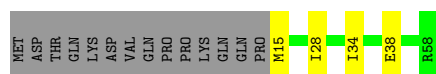
- Molecule 16: RNA polymerase II subunit J

Chain K:  91% 8%



- Molecule 17: RNA polymerase II subunit K

Chain L:  69% 7% 24%



- Molecule 18: Transcription elongation factor A protein 1

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	160410	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 ($e^-/\text{\AA}^2$)	51	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.597	Depositor
Minimum map value	-0.410	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	420.864, 420.864, 420.864	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	N	0.52	0/616	0.78	0/945
2	P	0.40	0/329	0.77	0/510
3	T	0.61	0/879	0.93	0/1355
4	W	0.26	0/3068	0.50	0/4157
5	Z	0.19	0/2206	0.39	0/2968
6	A	0.22	0/11414	0.44	0/15410
7	B	0.22	0/9257	0.43	0/12493
8	C	0.21	0/2087	0.41	0/2836
9	D	0.23	0/1025	0.42	0/1376
10	E	0.22	0/1739	0.43	0/2347
11	F	0.22	0/628	0.40	0/848
12	G	0.24	0/1382	0.44	0/1874
13	H	0.19	0/1207	0.43	0/1628
14	I	0.22	0/949	0.49	0/1284
15	J	0.20	0/524	0.48	0/707
16	K	0.20	0/939	0.40	0/1271
17	L	0.22	0/378	0.43	0/500
18	S	0.24	0/977	0.46	0/1307
19	U	0.27	0/1521	0.48	0/2063
All	All	0.25	0/41125	0.47	0/55879

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	551	304	306	3	0
2	P	296	151	152	4	0
3	T	783	426	427	5	0
4	W	3011	3047	3053	49	0
5	Z	2174	2201	2201	17	0
6	A	11210	11339	11336	123	0
7	B	9076	9118	9117	66	0
8	C	2044	1995	1994	16	0
9	D	1012	1004	1004	8	0
10	E	1709	1729	1729	18	0
11	F	618	653	653	2	0
12	G	1351	1358	1358	15	0
13	H	1186	1147	1147	15	0
14	I	928	862	860	12	0
15	J	515	534	534	4	0
16	K	920	942	942	8	0
17	L	373	380	379	3	0
18	S	969	981	981	9	0
19	U	1498	1556	1556	28	0
20	A	2	0	0	0	0
20	B	1	0	0	0	0
20	C	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
All	All	40233	39727	39729	347	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 4.

All (347) 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)
4:W:439:ARG:HD3	4:W:483:GLN:OE1	1.70	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:439:ARG:CD	4:W:483:GLN:OE1	2.28	0.81
4:W:198:LEU:HD13	19:U:92:MET:HE1	1.67	0.75
3:T:20:DT:O4	6:A:854:THR:OG1	2.06	0.72
6:A:481:THR:O	6:A:483:ARG:NH1	2.23	0.71
4:W:248:LEU:HD11	19:U:124:LEU:HD13	1.73	0.70
12:G:89:VAL:HG13	12:G:97:LEU:HD11	1.74	0.69
4:W:321:ASP:OD1	4:W:375:ARG:NH2	2.25	0.69
9:D:36:GLU:OE1	9:D:84:ARG:NH2	2.26	0.69
2:P:14:U:O2	6:A:334:ARG:NH1	2.27	0.68
4:W:481:HIS:O	4:W:489:GLN:NE2	2.27	0.68
7:B:611:GLU:OE1	7:B:613:ARG:NH1	2.27	0.68
17:L:15:MET:SD	17:L:15:MET:N	2.67	0.67
7:B:862:GLY:O	7:B:1078:ARG:NH2	2.28	0.67
13:H:49:PRO:O	13:H:147:LYS:NZ	2.27	0.66
7:B:529:MET:HE1	7:B:698:ILE:HD12	1.78	0.66
4:W:313:LEU:HG	4:W:328:ILE:HD11	1.77	0.66
8:C:205:LYS:NZ	8:C:212:ASP:O	2.29	0.66
7:B:896:LEU:O	7:B:1078:ARG:NH2	2.29	0.66
7:B:1035:ARG:NH1	7:B:1036:LYS:O	2.30	0.65
12:G:41:LYS:O	12:G:78:ARG:NH1	2.30	0.65
7:B:274:ARG:NH2	7:B:281:ASP:OD1	2.28	0.65
14:I:60:HIS:ND1	14:I:103:ARG:O	2.29	0.65
4:W:322:PRO:O	4:W:375:ARG:NH1	2.29	0.65
4:W:504:LEU:HD12	4:W:512:VAL:HG11	1.79	0.65
6:A:70:ARG:NH1	6:A:76:GLY:O	2.30	0.64
19:U:68:VAL:HG13	19:U:75:LEU:HD12	1.79	0.64
6:A:486:LEU:HB3	6:A:538:VAL:HG21	1.79	0.64
7:B:198:GLU:OE2	7:B:391:LYS:NZ	2.25	0.63
6:A:1430:CYS:O	6:A:1435:THR:HG22	1.97	0.63
6:A:1206:ARG:NH2	6:A:1207:ILE:O	2.31	0.63
6:A:94:VAL:N	6:A:250:VAL:O	2.31	0.63
14:I:68:ILE:O	14:I:122:ARG:NH1	2.33	0.61
4:W:540:VAL:O	19:U:167:ARG:NH1	2.33	0.61
6:A:1234:LYS:NZ	6:A:1297:THR:O	2.34	0.61
7:B:94:SER:HB3	19:U:262:LEU:HD21	1.83	0.61
10:E:94:MET:O	10:E:98:ASN:N	2.33	0.60
3:T:23:DG:OP1	7:B:1085:ARG:N	2.34	0.60
6:A:421:ARG:NH2	6:A:436:SER:O	2.34	0.60
6:A:322:LEU:HD23	6:A:325:LEU:HD12	1.83	0.60
6:A:687:ILE:HD11	6:A:766:PHE:CD2	2.37	0.59
19:U:89:TRP:HA	19:U:92:MET:HE3	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:20:DT:H72	6:A:854:THR:HG23	1.83	0.59
6:A:686:THR:HG23	7:B:782:ILE:O	2.03	0.59
6:A:687:ILE:HD13	6:A:769:MET:CE	2.32	0.59
7:B:1059:ILE:O	7:B:1080:ARG:NH2	2.36	0.59
10:E:55:ARG:NH2	10:E:132:GLN:OE1	2.35	0.59
6:A:1314:THR:OG1	6:A:1316:ASN:OD1	2.14	0.58
10:E:106:VAL:N	10:E:130:PHE:O	2.36	0.58
6:A:576:GLN:O	6:A:590:GLN:NE2	2.37	0.58
7:B:771:GLU:O	15:J:55:LEU:HD21	2.04	0.58
19:U:24:TRP:O	19:U:55:LYS:NZ	2.37	0.58
2:P:21:C:H42	3:T:22:DC:H42	1.51	0.58
6:A:1422:GLN:O	6:A:1429:LYS:NZ	2.27	0.58
7:B:869:LYS:NZ	7:B:892:CYS:SG	2.77	0.57
6:A:1453:GLY:O	6:A:1457:ASN:ND2	2.38	0.57
10:E:106:VAL:O	10:E:132:GLN:N	2.37	0.57
4:W:407:LEU:HD23	4:W:450:VAL:HG13	1.87	0.57
6:A:495:ASP:OD1	6:A:495:ASP:N	2.37	0.57
5:Z:427:GLU:OE2	5:Z:469:ARG:NH2	2.38	0.57
7:B:926:VAL:HG21	8:C:62:GLU:HG3	1.86	0.57
6:A:340:LYS:HG3	6:A:1436:VAL:HG11	1.87	0.57
4:W:281:LEU:HD11	4:W:297:GLY:HA3	1.86	0.56
7:B:953:ASP:OD1	8:C:36:ARG:NH2	2.38	0.56
19:U:29:ILE:O	19:U:33:LEU:N	2.38	0.56
4:W:305:LEU:HD13	4:W:356:TYR:HE2	1.69	0.56
7:B:752:TYR:HE1	7:B:809:VAL:HG23	1.70	0.56
10:E:94:MET:HE1	10:E:127:LEU:HD11	1.87	0.56
6:A:366:VAL:HG11	7:B:1055:VAL:HG12	1.87	0.56
5:Z:450:ILE:HG21	5:Z:468:LEU:HD11	1.87	0.56
7:B:254:GLN:OE1	7:B:254:GLN:N	2.39	0.56
6:A:349:ARG:HD2	7:B:1157:LEU:HD22	1.87	0.56
6:A:1364:GLU:O	6:A:1368:VAL:HG12	2.06	0.55
4:W:497:LEU:HD22	4:W:533:PHE:CD2	2.40	0.55
7:B:794:VAL:O	7:B:946:GLY:N	2.37	0.55
9:D:16:ASP:N	9:D:21:ILE:O	2.38	0.55
6:A:1480:CYS:HA	11:F:80:MET:HE3	1.87	0.55
8:C:9:VAL:HG11	16:K:105:PHE:CD1	2.41	0.55
6:A:428:ASP:O	6:A:432:HIS:ND1	2.40	0.55
6:A:631:GLU:OE2	13:H:95:LYS:NZ	2.29	0.55
4:W:534:VAL:HG21	4:W:557:LEU:HD13	1.87	0.55
6:A:340:LYS:HD2	6:A:1436:VAL:HG21	1.89	0.55
16:K:89:ASN:N	16:K:89:ASN:HD22	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1301:ILE:HD13	6:A:1345:ARG:HB3	1.89	0.55
10:E:83:GLY:O	10:E:86:THR:OG1	2.25	0.54
9:D:90:LYS:NZ	9:D:126:GLU:OE2	2.40	0.54
10:E:91:CYS:SG	10:E:121:MET:HE1	2.48	0.54
12:G:79:PRO:HB3	12:G:104:MET:HE1	1.88	0.54
6:A:906:LEU:N	6:A:975:SER:OG	2.41	0.54
7:B:861:SER:OG	7:B:863:ASP:OD1	2.24	0.54
8:C:183:ALA:HB3	8:C:232:ASN:HB3	1.88	0.54
13:H:106:THR:OG1	13:H:107:GLU:OE1	2.24	0.54
14:I:65:LEU:O	14:I:122:ARG:NH1	2.40	0.54
19:U:14:HIS:O	19:U:18:GLY:N	2.41	0.54
14:I:17:CYS:HA	14:I:24:LEU:HD21	1.89	0.54
6:A:467:MET:SD	6:A:467:MET:N	2.81	0.54
11:F:100:ARG:NH1	11:F:123:LEU:O	2.41	0.54
5:Z:554:GLU:OE2	5:Z:559:GLN:NE2	2.42	0.53
13:H:89:GLU:N	13:H:89:GLU:OE1	2.41	0.53
4:W:260:ARG:HG2	19:U:136:MET:HE2	1.91	0.53
7:B:834:ARG:HA	7:B:840:MET:HE2	1.91	0.53
6:A:350:VAL:CG1	6:A:1435:THR:HG21	2.39	0.53
4:W:470:LEU:HD11	4:W:500:MET:HE3	1.89	0.53
12:G:92:VAL:HG12	12:G:119:PHE:CE1	2.43	0.53
2:P:21:C:OP1	7:B:731:GLN:NE2	2.42	0.53
1:N:45:DC:N4	3:T:5:DT:O4	2.42	0.53
4:W:423:VAL:O	4:W:427:VAL:HG23	2.09	0.53
5:Z:554:GLU:OE1	5:Z:557:THR:OG1	2.27	0.53
6:A:460:ARG:HB2	6:A:501:MET:HE3	1.92	0.52
18:S:227:GLU:OE1	18:S:227:GLU:N	2.43	0.52
7:B:57:ARG:NH1	7:B:227:ASN:OD1	2.43	0.52
6:A:680:LEU:O	6:A:684:GLY:N	2.42	0.52
4:W:460:THR:HG23	4:W:506:ARG:NE	2.25	0.52
6:A:851:ALA:O	6:A:854:THR:HG22	2.10	0.52
6:A:1210:TRP:NE1	14:I:28:GLU:OE1	2.43	0.52
12:G:10:GLU:HB3	12:G:67:LEU:HD11	1.91	0.52
6:A:74:CYS:SG	6:A:84:HIS:NE2	2.81	0.52
14:I:12:VAL:O	14:I:50:ASN:ND2	2.42	0.52
6:A:66:GLU:N	6:A:66:GLU:OE1	2.41	0.52
10:E:167:GLU:OE1	10:E:167:GLU:N	2.41	0.52
6:A:90:LEU:HD22	6:A:94:VAL:HG22	1.91	0.52
4:W:504:LEU:HD12	4:W:512:VAL:CG1	2.40	0.51
6:A:1217:ASP:OD1	6:A:1219:LYS:NZ	2.42	0.51
7:B:794:VAL:HG13	7:B:965:ILE:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:412:SER:OG	4:W:413:THR:N	2.41	0.51
12:G:30:LEU:O	12:G:34:VAL:HG22	2.10	0.51
6:A:1169:VAL:HG12	6:A:1220:HIS:HB3	1.93	0.51
6:A:1168:LYS:O	6:A:1220:HIS:ND1	2.44	0.51
6:A:1429:LYS:HB2	6:A:1438:VAL:HG11	1.92	0.51
4:W:308:ALA:HB2	13:H:13:LYS:O	2.10	0.51
7:B:760:THR:OG1	7:B:764:MET:SD	2.59	0.51
10:E:12:LYS:NZ	10:E:136:LEU:O	2.43	0.51
12:G:122:ASN:OD1	12:G:123:SER:N	2.44	0.51
13:H:50:VAL:HG12	13:H:147:LYS:CE	2.41	0.51
6:A:1229:GLU:OE1	18:S:189:ASN:ND2	2.43	0.50
16:K:37:LYS:N	16:K:69:HIS:O	2.45	0.50
19:U:60:THR:CG2	19:U:97:LEU:HD21	2.41	0.50
4:W:497:LEU:HD22	4:W:533:PHE:HD2	1.77	0.50
7:B:474:THR:OG1	7:B:732:ALA:O	2.30	0.50
6:A:1284:PHE:CZ	6:A:1288:ILE:HD11	2.47	0.50
6:A:84:HIS:CE1	7:B:1127:ILE:HG22	2.47	0.50
6:A:1443:ALA:HB2	7:B:1167:ILE:HG23	1.94	0.50
6:A:1199:MET:HB2	18:S:147:MET:HE1	1.94	0.49
7:B:565:THR:HG21	7:B:580:PRO:HB3	1.93	0.49
13:H:112:LEU:HB2	13:H:132:LEU:HD12	1.94	0.49
6:A:1130:ILE:HD13	6:A:1411:LEU:HD12	1.94	0.49
6:A:1054:MET:HE1	6:A:1060:LEU:HD12	1.94	0.49
6:A:614:ASP:OD1	6:A:615:SER:N	2.46	0.49
6:A:82:PRO:HB2	7:B:1125:MET:HE1	1.94	0.49
6:A:583:ARG:NH1	8:C:222:PRO:O	2.45	0.49
7:B:125:TYR:OH	19:U:262:LEU:HD22	2.13	0.49
7:B:1068:GLN:N	7:B:1073:GLN:O	2.40	0.49
6:A:383:SER:N	16:K:2:ASN:OD1	2.44	0.48
4:W:256:SER:HB3	19:U:137:LEU:HD23	1.95	0.48
4:W:460:THR:HG23	4:W:506:ARG:CZ	2.43	0.48
19:U:48:LEU:O	19:U:53:LYS:NZ	2.46	0.48
4:W:207:THR:O	4:W:211:THR:HG23	2.14	0.48
6:A:1368:VAL:HG13	6:A:1369:LEU:HG	1.95	0.48
7:B:817:GLN:HA	7:B:918:PHE:HB2	1.95	0.48
9:D:87:LEU:HD22	9:D:97:LEU:HB3	1.96	0.48
5:Z:561:LEU:HD23	5:Z:635:MET:HG3	1.94	0.48
9:D:64:THR:HG22	12:G:103:PRO:HD3	1.95	0.48
19:U:117:VAL:HA	19:U:120:ILE:HD12	1.95	0.48
6:A:70:ARG:NH1	6:A:75:ALA:O	2.47	0.48
7:B:720:PRO:O	7:B:723:THR:OG1	2.24	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:1028:LEU:HD13	7:B:1041:ILE:HB	1.94	0.48
10:E:9:ARG:HG3	10:E:136:LEU:HD21	1.95	0.48
19:U:13:LEU:HD22	19:U:56:LEU:HD13	1.96	0.48
4:W:260:ARG:CG	19:U:136:MET:HE2	2.44	0.47
4:W:418:ILE:O	4:W:462:HIS:NE2	2.46	0.47
6:A:148:CYS:SG	6:A:149:LYS:N	2.88	0.47
6:A:760:LEU:HD11	6:A:781:ILE:HG21	1.94	0.47
5:Z:478:VAL:HB	5:Z:518:LEU:HD22	1.96	0.47
6:A:84:HIS:ND1	7:B:1127:ILE:HG22	2.30	0.47
10:E:168:ASN:O	10:E:172:ARG:NH2	2.48	0.47
6:A:686:THR:HG21	7:B:1042:PHE:H	1.78	0.47
16:K:80:ASP:OD1	16:K:80:ASP:N	2.46	0.47
4:W:414:LEU:HD21	4:W:454:LEU:HD13	1.96	0.47
4:W:470:LEU:O	4:W:474:VAL:HG13	2.14	0.47
7:B:866:ILE:HG21	7:B:896:LEU:HD21	1.96	0.47
8:C:57:SER:OG	8:C:59:LEU:O	2.33	0.47
7:B:681:ASP:OD1	7:B:681:ASP:N	2.45	0.47
8:C:152:LYS:NZ	15:J:57:GLU:OE2	2.31	0.47
12:G:138:GLN:N	12:G:138:GLN:OE1	2.46	0.47
7:B:103:GLY:HA3	19:U:267:ALA:HB2	1.97	0.47
4:W:317:PHE:CZ	4:W:328:ILE:HD12	2.50	0.47
6:A:492:TYR:CD2	6:A:501:MET:HE1	2.50	0.46
6:A:689:ILE:O	6:A:692:SER:OG	2.29	0.46
6:A:1192:TRP:HZ3	6:A:1246:ILE:HG22	1.80	0.46
6:A:1472:ASP:N	6:A:1472:ASP:OD1	2.47	0.46
7:B:259:THR:O	7:B:259:THR:OG1	2.32	0.46
10:E:112:PRO:O	10:E:116:GLN:NE2	2.47	0.46
13:H:28:LEU:HD11	13:H:50:VAL:HG21	1.96	0.46
6:A:505:LEU:O	7:B:1106:ARG:NH2	2.48	0.46
5:Z:478:VAL:HG21	5:Z:492:ILE:HG23	1.96	0.46
6:A:350:VAL:HG13	6:A:1435:THR:HG21	1.97	0.46
7:B:761:THR:HG23	7:B:1000:THR:HA	1.98	0.46
15:J:36:ASP:OD1	15:J:46:ARG:NH1	2.49	0.46
7:B:184:TYR:OH	7:B:472:ARG:NH2	2.49	0.46
7:B:743:ARG:O	7:B:922:ARG:NH1	2.48	0.46
6:A:1151:ALA:HB2	6:A:1334:TRP:CZ2	2.51	0.46
17:L:28:ILE:HG21	17:L:34:ILE:HG22	1.98	0.46
4:W:442:GLN:N	4:W:484:LEU:HD11	2.30	0.46
6:A:1452:LYS:N	6:A:1456:GLU:OE2	2.49	0.46
4:W:349:ASN:O	4:W:353:LYS:N	2.46	0.45
6:A:388:MET:HE2	7:B:1061:SER:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:599:HIS:ND1	6:A:632:ASN:OD1	2.47	0.45
7:B:1079:SER:OG	7:B:1080:ARG:N	2.46	0.45
6:A:693:ILE:HD13	6:A:828:LEU:HD21	1.97	0.45
6:A:746:ASN:OD1	6:A:749:ARG:NH2	2.49	0.45
4:W:246:SER:HB3	4:W:283:LEU:HD21	1.97	0.45
4:W:455:LEU:CD1	4:W:473:LEU:HD21	2.47	0.45
6:A:611:ASP:OD1	6:A:612:ASP:N	2.49	0.45
7:B:783:ALA:HB2	7:B:1041:ILE:HG23	1.99	0.45
5:Z:440:ILE:HG23	5:Z:450:ILE:HD11	1.98	0.45
7:B:906:GLN:OE1	7:B:922:ARG:NH2	2.49	0.45
18:S:194:ARG:NH2	18:S:223:MET:O	2.50	0.45
6:A:102:LYS:NZ	6:A:141:LEU:HD22	2.31	0.45
18:S:147:MET:O	18:S:195:ILE:HD11	2.16	0.45
6:A:1201:ASP:OD1	6:A:1201:ASP:N	2.48	0.45
6:A:1243:LEU:HD21	6:A:1288:ILE:HD13	1.98	0.45
8:C:107:CYS:O	8:C:156:GLY:N	2.49	0.45
7:B:384:ASP:OD2	7:B:387:HIS:N	2.50	0.45
9:D:18:SER:O	9:D:117:SER:OG	2.33	0.45
10:E:100:THR:O	10:E:126:ILE:N	2.50	0.45
6:A:592:PHE:CE2	6:A:596:ILE:HD11	2.52	0.45
6:A:1169:VAL:HG11	6:A:1226:LEU:HD12	1.98	0.45
6:A:1235:ILE:HA	6:A:1296:MET:HE1	1.99	0.45
14:I:29:ASP:O	14:I:33:ARG:N	2.50	0.44
6:A:1086:MET:SD	6:A:1466:ALA:HB1	2.57	0.44
6:A:1428:MET:HE1	6:A:1456:GLU:H	1.82	0.44
4:W:393:VAL:HG11	4:W:423:VAL:HG13	1.99	0.44
4:W:468:GLN:OE1	4:W:468:GLN:N	2.50	0.44
6:A:589:LYS:NZ	6:A:638:GLY:O	2.50	0.44
12:G:108:ILE:HD11	12:G:145:LEU:HD22	2.00	0.44
13:H:56:PHE:CE1	13:H:145:MET:HE2	2.53	0.44
2:P:13:G:H1'	6:A:264:VAL:HG11	1.99	0.44
4:W:248:LEU:CD1	19:U:124:LEU:HD13	2.44	0.44
5:Z:501:ILE:HD13	12:G:111:HIS:NE2	2.32	0.44
6:A:1182:GLN:O	6:A:1190:GLN:NE2	2.50	0.44
9:D:79:THR:OG1	9:D:139:SER:OG	2.32	0.44
4:W:305:LEU:HD11	4:W:337:PHE:HA	2.00	0.44
6:A:733:LEU:HD23	14:I:106:ASP:HB2	1.99	0.44
6:A:58:MET:HE1	6:A:263:ALA:HB2	1.99	0.44
6:A:97:VAL:HG23	6:A:100:LEU:HD12	1.99	0.44
6:A:728:THR:HG23	6:A:736:THR:HG23	2.00	0.44
6:A:909:LEU:O	6:A:967:ARG:NH2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1203:ASP:OD1	6:A:1203:ASP:N	2.51	0.44
6:A:1453:GLY:N	6:A:1456:GLU:OE2	2.45	0.44
14:I:36:LEU:HD23	14:I:47:GLU:HA	1.99	0.44
1:N:42:DT:H2"	1:N:43:DT:H71	1.98	0.44
6:A:1026:ASP:O	6:A:1031:ARG:NH2	2.49	0.44
6:A:1374:VAL:HG11	6:A:1411:LEU:HD11	1.99	0.44
6:A:888:GLN:OE1	6:A:892:GLY:N	2.52	0.43
6:A:1192:TRP:CZ3	6:A:1246:ILE:HG22	2.53	0.43
7:B:912:ASN:OD1	7:B:916:TYR:N	2.45	0.43
4:W:408:VAL:HG12	19:U:181:LYS:HG2	1.99	0.43
4:W:367:VAL:HA	19:U:148:ALA:HB2	2.00	0.43
6:A:347:GLU:OE1	6:A:347:GLU:N	2.52	0.43
6:A:1448:SER:OG	6:A:1449:ASP:N	2.52	0.43
7:B:553:LEU:HD11	7:B:573:TRP:CG	2.54	0.43
12:G:104:MET:HE2	12:G:157:ILE:HG22	1.99	0.43
19:U:41:ILE:HG23	19:U:56:LEU:HD21	1.99	0.43
4:W:240:PHE:HZ	19:U:120:ILE:HD11	1.83	0.43
6:A:31:LEU:HD11	6:A:254:PRO:HG3	1.99	0.43
6:A:602:CYS:SG	6:A:603:ILE:N	2.91	0.43
6:A:622:SER:O	13:H:27:ARG:NH2	2.52	0.43
6:A:1036:ASN:HD21	10:E:202:ARG:CZ	2.31	0.43
14:I:86:CYS:SG	14:I:87:GLN:N	2.92	0.43
6:A:121:SER:HA	6:A:126:ILE:HG21	1.99	0.43
6:A:1169:VAL:O	6:A:1217:ASP:N	2.48	0.43
6:A:24:GLY:O	6:A:1443:ALA:HB1	2.18	0.43
7:B:710:ILE:HA	7:B:764:MET:HE2	2.01	0.43
14:I:106:ASP:OD1	14:I:106:ASP:N	2.51	0.43
15:J:47:ARG:NH2	15:J:48:MET:HE1	2.34	0.43
6:A:22:GLN:NE2	6:A:23:PHE:O	2.52	0.43
8:C:260:GLN:HB2	16:K:91:ILE:HG21	2.01	0.43
13:H:41:LEU:HD23	13:H:145:MET:HE1	2.00	0.42
5:Z:501:ILE:HD11	5:Z:510:GLU:HB3	2.01	0.42
6:A:1201:ASP:N	6:A:1203:ASP:OD1	2.52	0.42
7:B:913:GLN:O	7:B:913:GLN:NE2	2.52	0.42
10:E:55:ARG:NH1	10:E:77:PRO:O	2.53	0.42
12:G:92:VAL:HG13	12:G:128:TYR:CD2	2.54	0.42
7:B:260:LEU:HB2	7:B:263:ILE:HD12	2.00	0.42
4:W:261:ILE:O	4:W:265:VAL:HG23	2.19	0.42
4:W:509:VAL:HG13	4:W:510:LEU:HD12	2.00	0.42
6:A:457:ILE:HD11	6:A:515:ILE:HD12	2.01	0.42
6:A:1428:MET:HE2	6:A:1428:MET:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:167:GLU:OE2	18:S:171:GLN:NE2	2.50	0.42
5:Z:420:PHE:HB3	5:Z:440:ILE:HD13	2.01	0.42
5:Z:523:GLU:N	5:Z:523:GLU:OE1	2.52	0.42
6:A:1428:MET:HE1	6:A:1456:GLU:N	2.35	0.42
7:B:653:TRP:CH2	7:B:662:VAL:HG21	2.55	0.42
7:B:912:ASN:OD1	7:B:915:GLY:N	2.52	0.42
8:C:193:ARG:NH2	8:C:218:ALA:O	2.52	0.42
13:H:51:ASP:OD1	13:H:52:LEU:N	2.52	0.42
6:A:1146:GLN:O	6:A:1150:ASP:N	2.49	0.42
7:B:516:GLU:OE1	7:B:516:GLU:N	2.47	0.42
8:C:44:ILE:HG21	8:C:178:PRO:HB3	2.01	0.42
4:W:246:SER:OG	4:W:283:LEU:HD11	2.20	0.42
6:A:1184:THR:N	6:A:1190:GLN:OE1	2.52	0.42
8:C:48:ASP:OD1	8:C:49:TRP:N	2.49	0.42
4:W:323:PRO:O	4:W:362:TYR:OH	2.38	0.41
7:B:562:ALA:O	7:B:610:ARG:NH1	2.53	0.41
7:B:663:GLU:OE2	7:B:695:HIS:NE2	2.50	0.41
7:B:856:PRO:HA	7:B:904:VAL:HG13	2.02	0.41
8:C:206:SER:O	8:C:209:SER:OG	2.32	0.41
14:I:31:GLU:OE1	14:I:31:GLU:N	2.49	0.41
19:U:60:THR:OG1	19:U:75:LEU:HD13	2.19	0.41
6:A:352:GLY:O	7:B:1085:ARG:NH1	2.53	0.41
10:E:71:GLN:HB2	10:E:99:ILE:HD12	2.01	0.41
12:G:92:VAL:HG11	12:G:127:CYS:CA	2.50	0.41
6:A:530:SER:OG	6:A:532:ARG:NE	2.53	0.41
8:C:255:LYS:HE3	16:K:42:LEU:HD21	2.02	0.41
4:W:240:PHE:CZ	19:U:120:ILE:HD11	2.55	0.41
7:B:1112:ASP:OD1	7:B:1112:ASP:N	2.53	0.41
10:E:66:ASP:OD1	10:E:66:ASP:N	2.54	0.41
6:A:1428:MET:HE3	6:A:1456:GLU:OE1	2.19	0.41
19:U:21:ASP:OD1	19:U:22:GLU:N	2.53	0.41
7:B:545:LEU:HD13	7:B:550:MET:SD	2.60	0.41
9:D:87:LEU:HD21	9:D:101:ALA:HB2	2.01	0.41
17:L:38:GLU:OE1	17:L:38:GLU:N	2.54	0.41
6:A:1169:VAL:HG11	6:A:1226:LEU:CD1	2.50	0.41
6:A:1210:TRP:O	6:A:1260:ARG:NH1	2.54	0.41
5:Z:493:VAL:HG11	12:G:109:SER:OG	2.21	0.41
6:A:601:ASN:ND2	6:A:989:ASN:OD1	2.54	0.41
6:A:868:MET:HG2	6:A:1404:THR:HG21	2.03	0.41
6:A:1173:THR:HG23	6:A:1214:VAL:HG12	2.03	0.41
7:B:904:VAL:HG23	7:B:921:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:536:GLU:O	4:W:540:VAL:HG22	2.21	0.41
5:Z:489:THR:CG2	5:Z:525:ALA:HB2	2.50	0.41
6:A:729:PRO:HB3	18:S:249:GLN:HA	2.03	0.41
5:Z:604:ASP:OD1	5:Z:605:GLY:N	2.53	0.40
10:E:38:GLU:OE1	10:E:38:GLU:N	2.50	0.40
13:H:102:ASP:OD2	13:H:110:THR:OG1	2.37	0.40
13:H:118:TYR:OH	13:H:123:MET:SD	2.76	0.40
8:C:245:VAL:HG11	16:K:105:PHE:CZ	2.56	0.40
18:S:132:ARG:N	18:S:167:GLU:OE2	2.54	0.40
1:N:34:DT:O5'	6:A:1132:LYS:NZ	2.54	0.40
4:W:411:LEU:HD21	19:U:178:LEU:HD13	2.04	0.40
5:Z:426:VAL:CG1	5:Z:440:ILE:HD11	2.51	0.40
6:A:790:GLN:NE2	6:A:821:GLY:O	2.55	0.40
6:A:1123:ARG:NH2	6:A:1360:ASN:O	2.49	0.40
13:H:8:ASP:OD1	13:H:9:ILE:N	2.47	0.40
18:S:148:LEU:HD22	18:S:169:GLY:HA2	2.04	0.40
5:Z:424:ASP:HB2	5:Z:440:ILE:HD12	2.02	0.40
19:U:57:LEU:O	19:U:60:THR:HG22	2.22	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	
4	W	371/590 (63%)	356 (96%)	15 (4%)	0	100	100
5	Z	265/1087 (24%)	255 (96%)	10 (4%)	0	100	100
6	A	1405/1970 (71%)	1353 (96%)	52 (4%)	0	100	100
7	B	1130/1174 (96%)	1075 (95%)	55 (5%)	0	100	100
8	C	251/271 (93%)	241 (96%)	10 (4%)	0	100	100
9	D	122/142 (86%)	122 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	E	203/210 (97%)	200 (98%)	3 (2%)	0	100	100
11	F	75/127 (59%)	72 (96%)	3 (4%)	0	100	100
12	G	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
13	H	146/150 (97%)	142 (97%)	4 (3%)	0	100	100
14	I	112/125 (90%)	106 (95%)	6 (5%)	0	100	100
15	J	63/67 (94%)	61 (97%)	2 (3%)	0	100	100
16	K	113/117 (97%)	108 (96%)	5 (4%)	0	100	100
17	L	42/58 (72%)	39 (93%)	3 (7%)	0	100	100
18	S	120/301 (40%)	111 (92%)	9 (8%)	0	100	100
19	U	192/528 (36%)	187 (97%)	5 (3%)	0	100	100
All	All	4779/7089 (67%)	4593 (96%)	186 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	
4	W	338/513 (66%)	333 (98%)	5 (2%)	57	74
5	Z	243/940 (26%)	242 (100%)	1 (0%)	84	85
6	A	1246/1749 (71%)	1241 (100%)	5 (0%)	84	85
7	B	994/1027 (97%)	991 (100%)	3 (0%)	86	87
8	C	232/248 (94%)	230 (99%)	2 (1%)	70	79
9	D	114/126 (90%)	114 (100%)	0	100	100
10	E	190/192 (99%)	188 (99%)	2 (1%)	65	77
11	F	67/111 (60%)	67 (100%)	0	100	100
12	G	152/153 (99%)	152 (100%)	0	100	100
13	H	129/131 (98%)	127 (98%)	2 (2%)	55	72
14	I	103/112 (92%)	103 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	J	54/56 (96%)	53 (98%)	1 (2%)	50	70
16	K	104/106 (98%)	103 (99%)	1 (1%)	68	78
17	L	41/55 (74%)	41 (100%)	0	100	100
18	S	105/266 (40%)	104 (99%)	1 (1%)	68	78
19	U	167/451 (37%)	165 (99%)	2 (1%)	63	76
All	All	4279/6236 (69%)	4254 (99%)	25 (1%)	76	83

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	W	205	LEU
4	W	256	SER
4	W	274	HIS
4	W	328	ILE
4	W	411	LEU
5	Z	718	LYS
6	A	48	GLU
6	A	495	ASP
6	A	703	GLN
6	A	1348	SER
6	A	1430	CYS
7	B	159	THR
7	B	509	VAL
7	B	687	VAL
8	C	26	THR
8	C	92	GLU
10	E	66	ASP
10	E	91	CYS
13	H	18	GLU
13	H	32	SER
15	J	65	LEU
16	K	77	THR
18	S	235	GLU
19	U	31	SER
19	U	149	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
4	W	489	GLN
5	Z	559	GLN
6	A	289	GLN
6	A	295	GLN
6	A	372	ASN
6	A	531	ASN
6	A	739	ASN
6	A	792	ASN
6	A	991	GLN
6	A	1032	GLN
6	A	1036	ASN
7	B	43	GLN
7	B	992	ASN
7	B	1009	GLN
7	B	1013	ASN
7	B	1025	ASN
8	C	25	ASN
8	C	66	HIS
8	C	223	ASN
9	D	48	ASN
9	D	55	GLN
10	E	22	HIS
10	E	174	GLN
10	E	189	GLN
12	G	28	GLN
13	H	131	ASN
14	I	32	ASN
14	I	46	GLN
16	K	76	GLN
19	U	80	GLN
19	U	114	ASN
19	U	145	ASN
19	U	164	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	P	13/22 (59%)	5 (38%)	1 (7%)

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	P	11	U
2	P	12	A
2	P	13	G
2	P	15	U
2	P	16	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	P	12	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

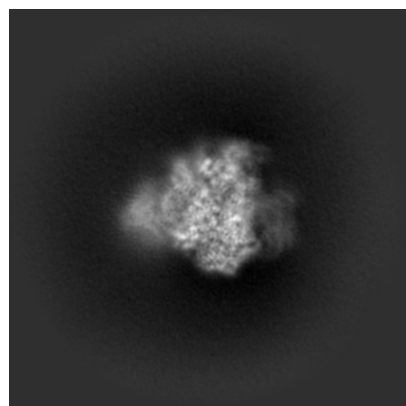
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42303. These allow visual inspection of the internal detail of the map and identification of artifacts.

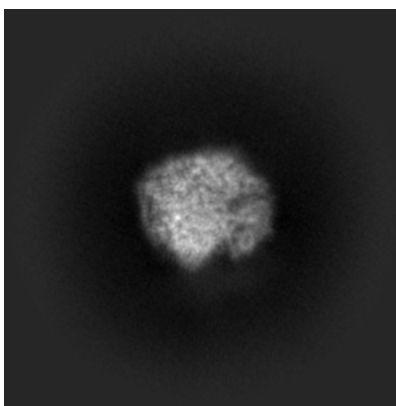
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

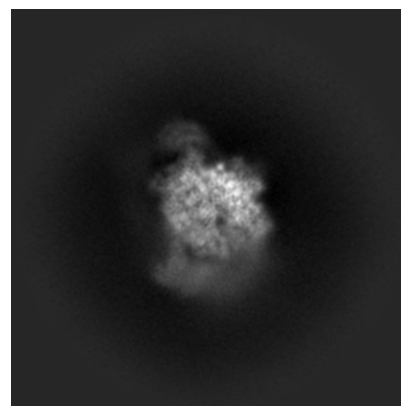
6.1.1 Primary map



X

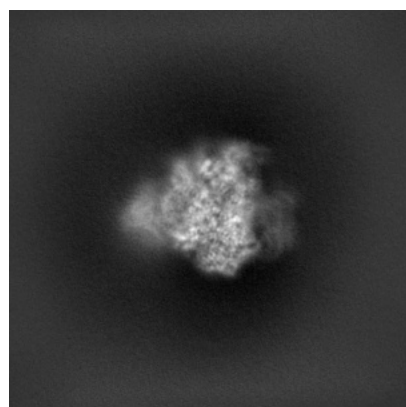


Y

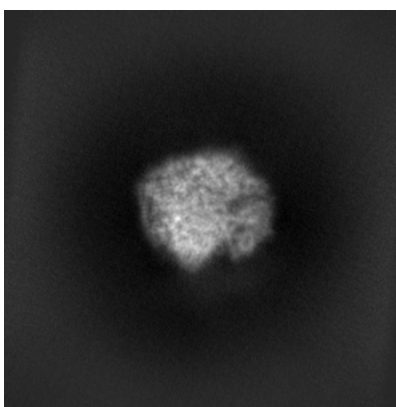


Z

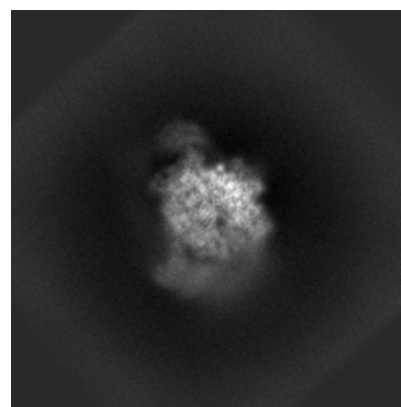
6.1.2 Raw map



X



Y

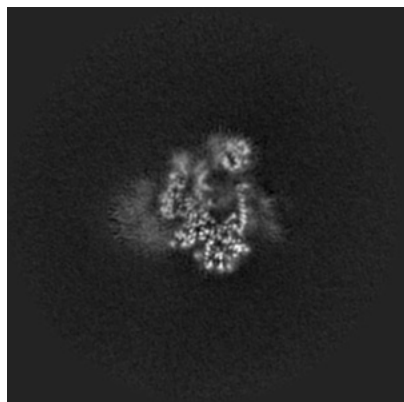


Z

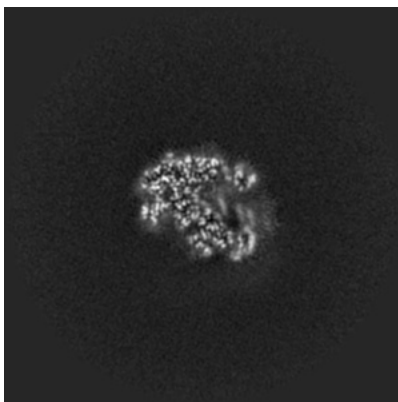
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

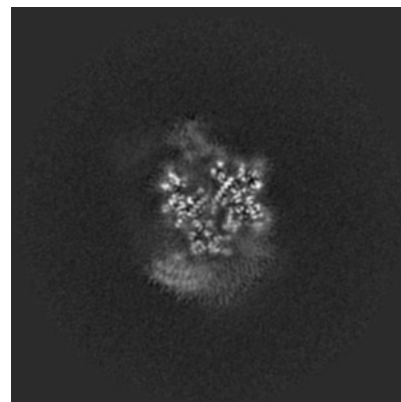
6.2.1 Primary map



X Index: 256

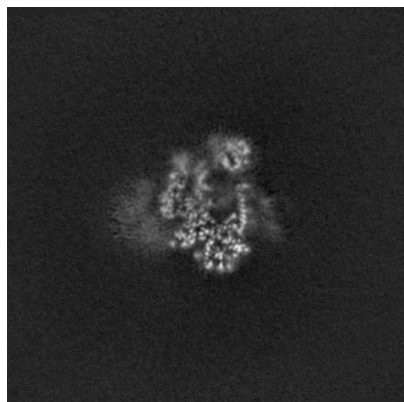


Y Index: 256

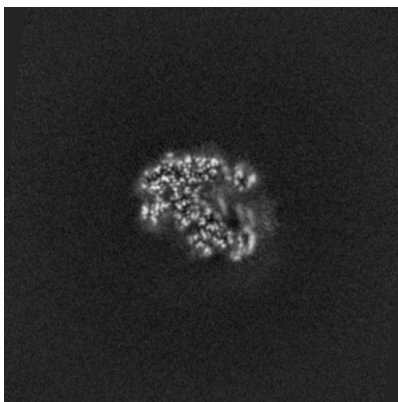


Z Index: 256

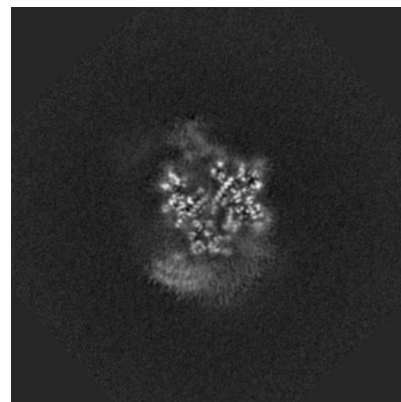
6.2.2 Raw map



X Index: 256



Y Index: 256

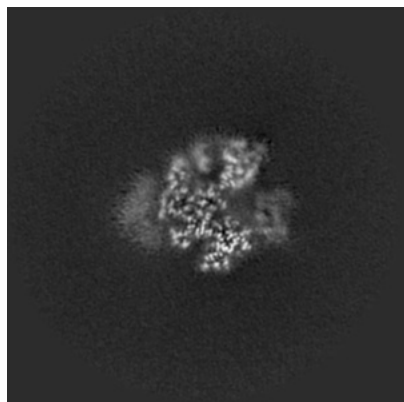


Z Index: 256

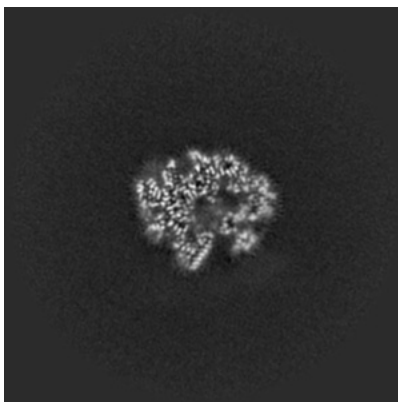
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

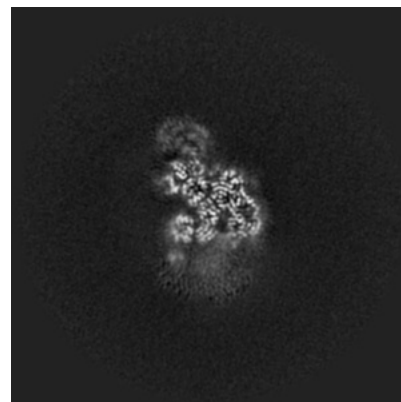
6.3.1 Primary map



X Index: 243

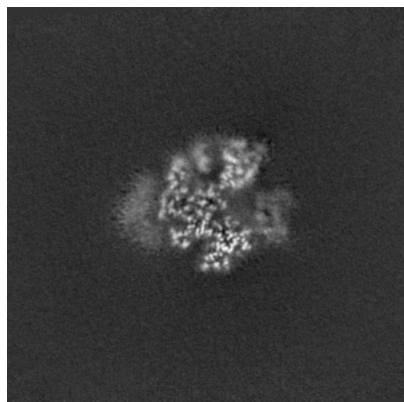


Y Index: 284

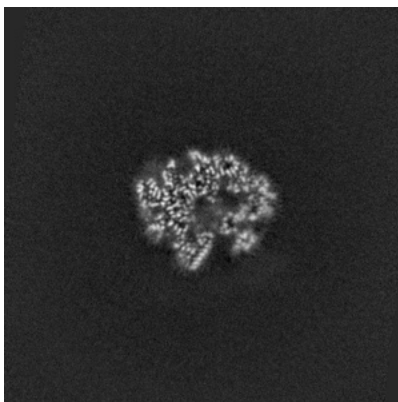


Z Index: 221

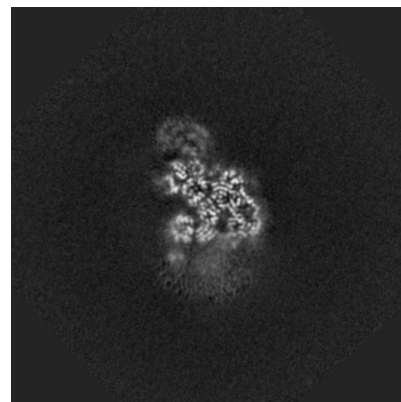
6.3.2 Raw map



X Index: 243



Y Index: 284

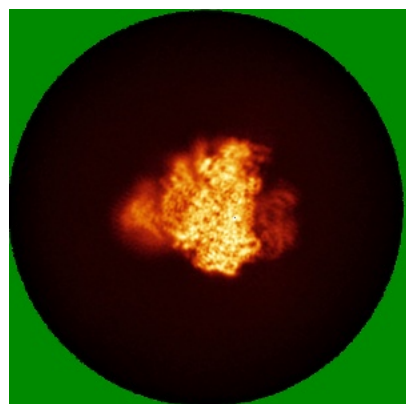


Z Index: 221

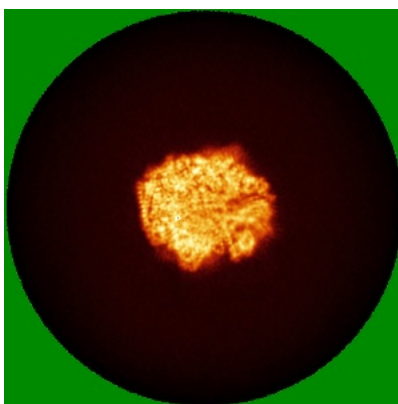
The images above show the largest variance slices of the map in three orthogonal directions.

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

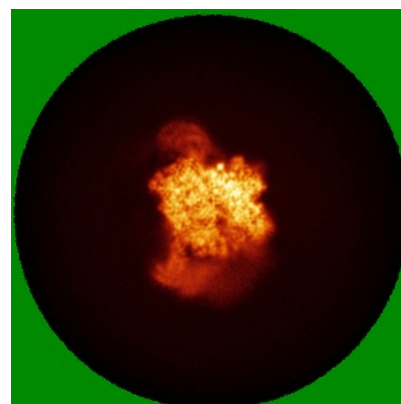
6.4.1 Primary map



X

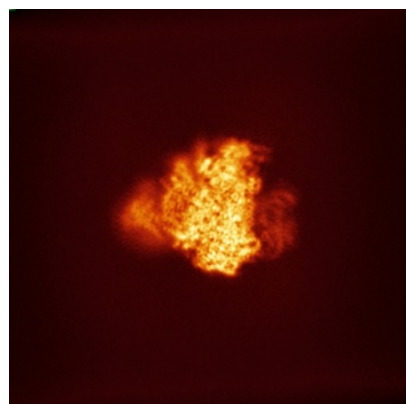


Y

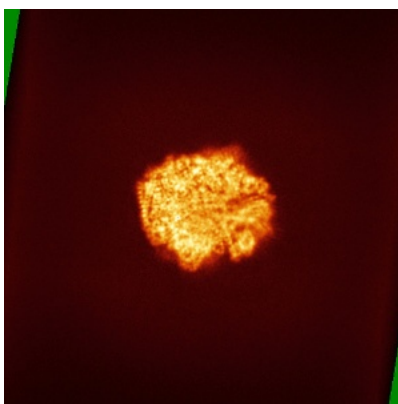


Z

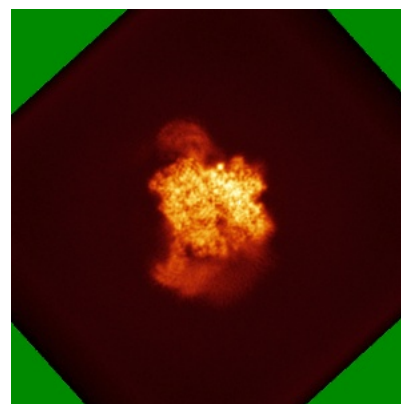
6.4.2 Raw map



X



Y

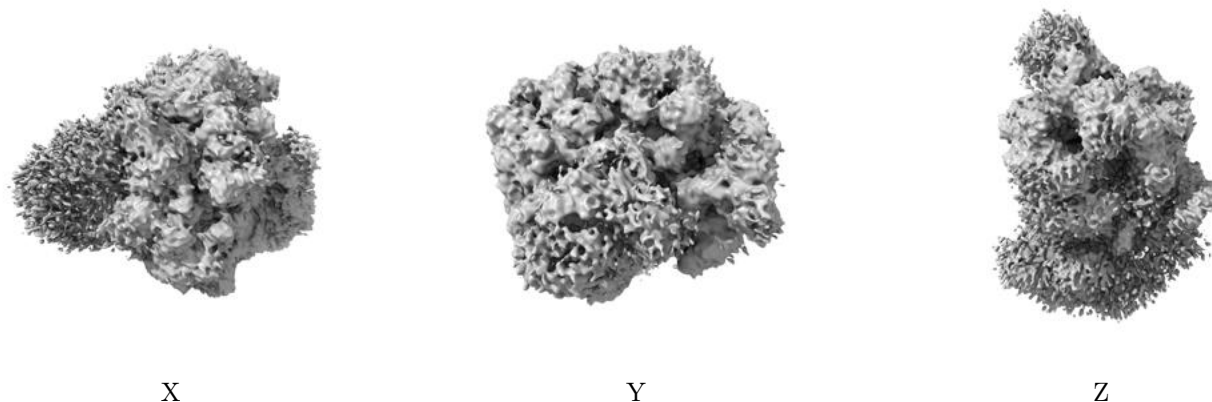


Z

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.

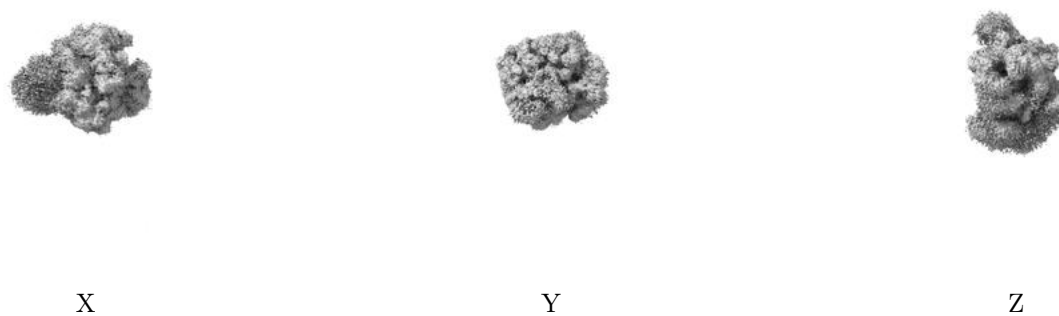
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

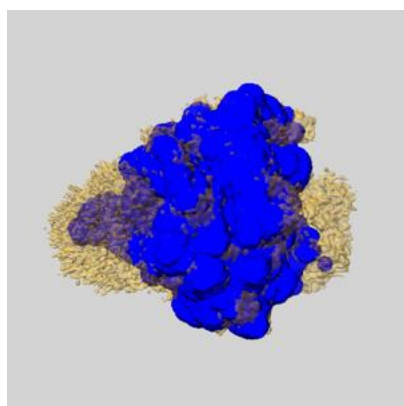
6.6 Mask visualisation [i](#)

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

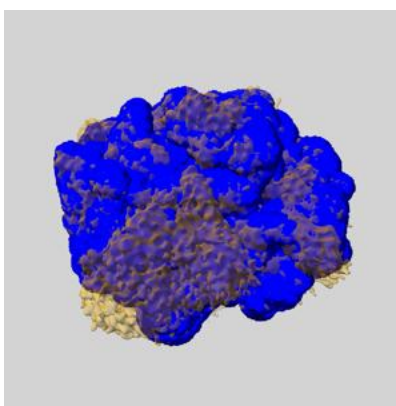
A mask typically either:

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

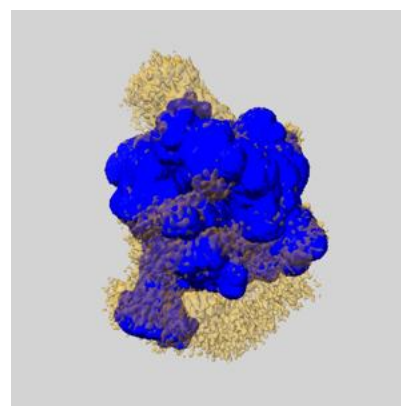
6.6.1 emd_42303_msk_1.map [i](#)



X



Y

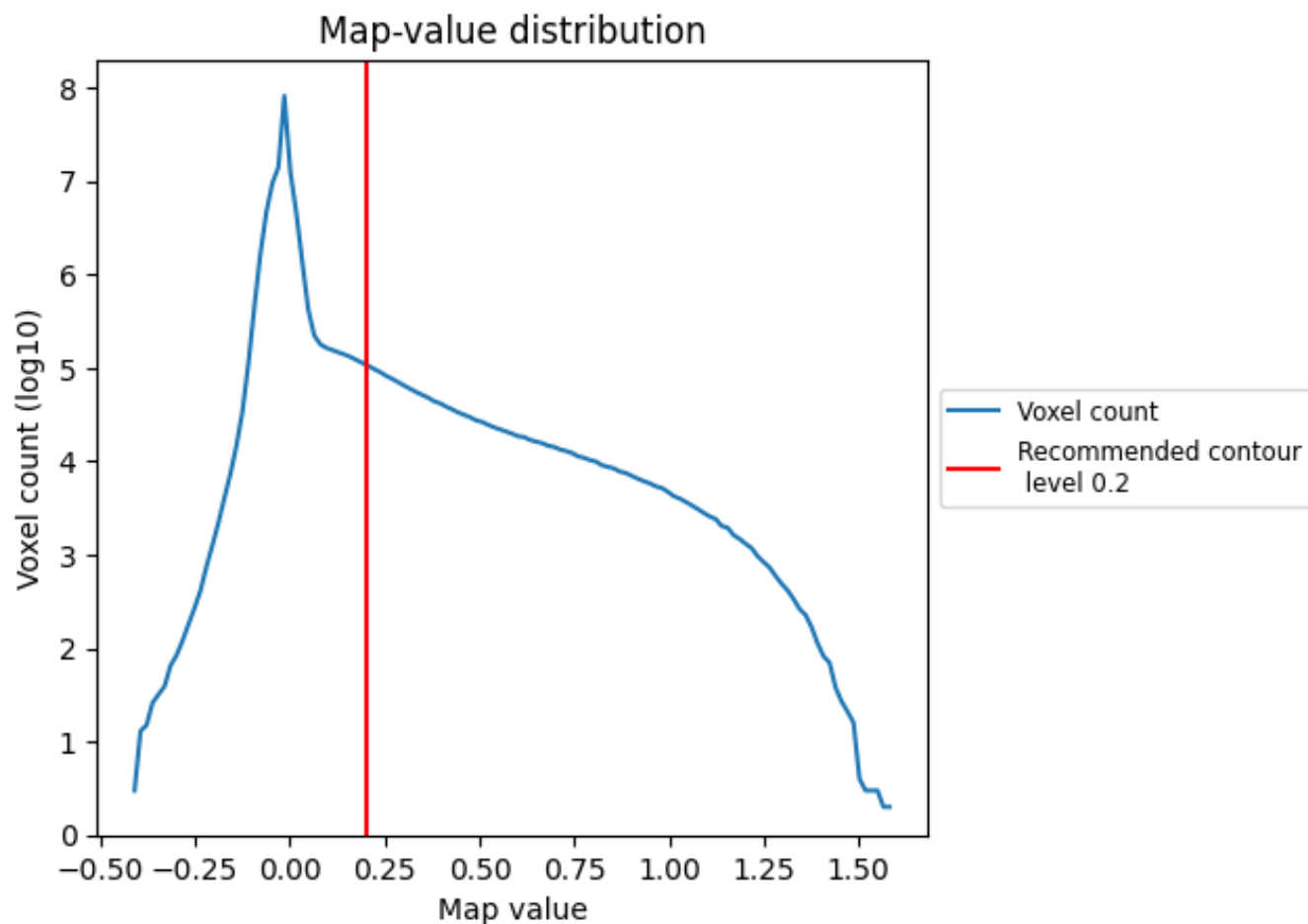


Z

7 Map analysis [i](#)

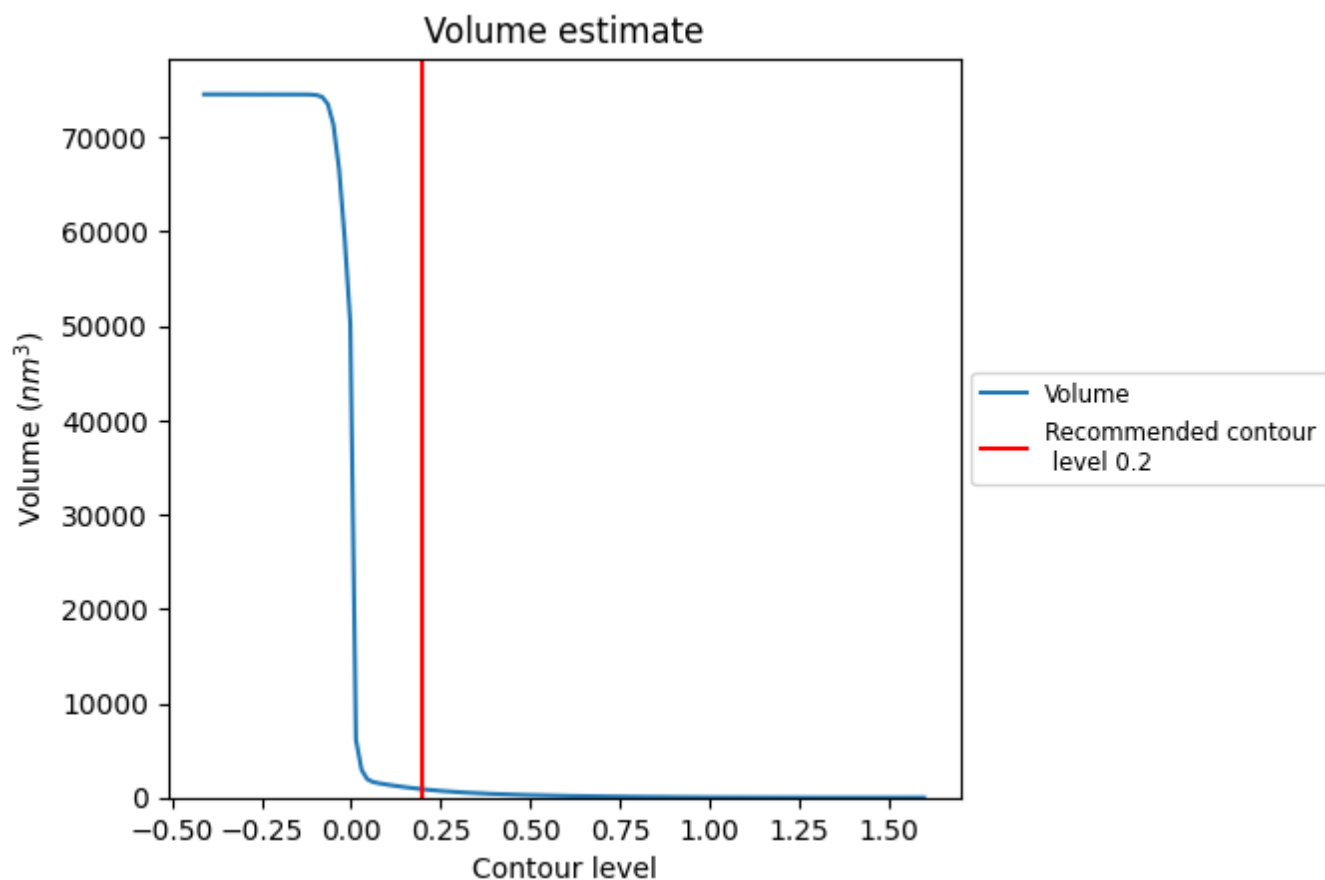
This section contains the results of statistical analysis of the map.

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.

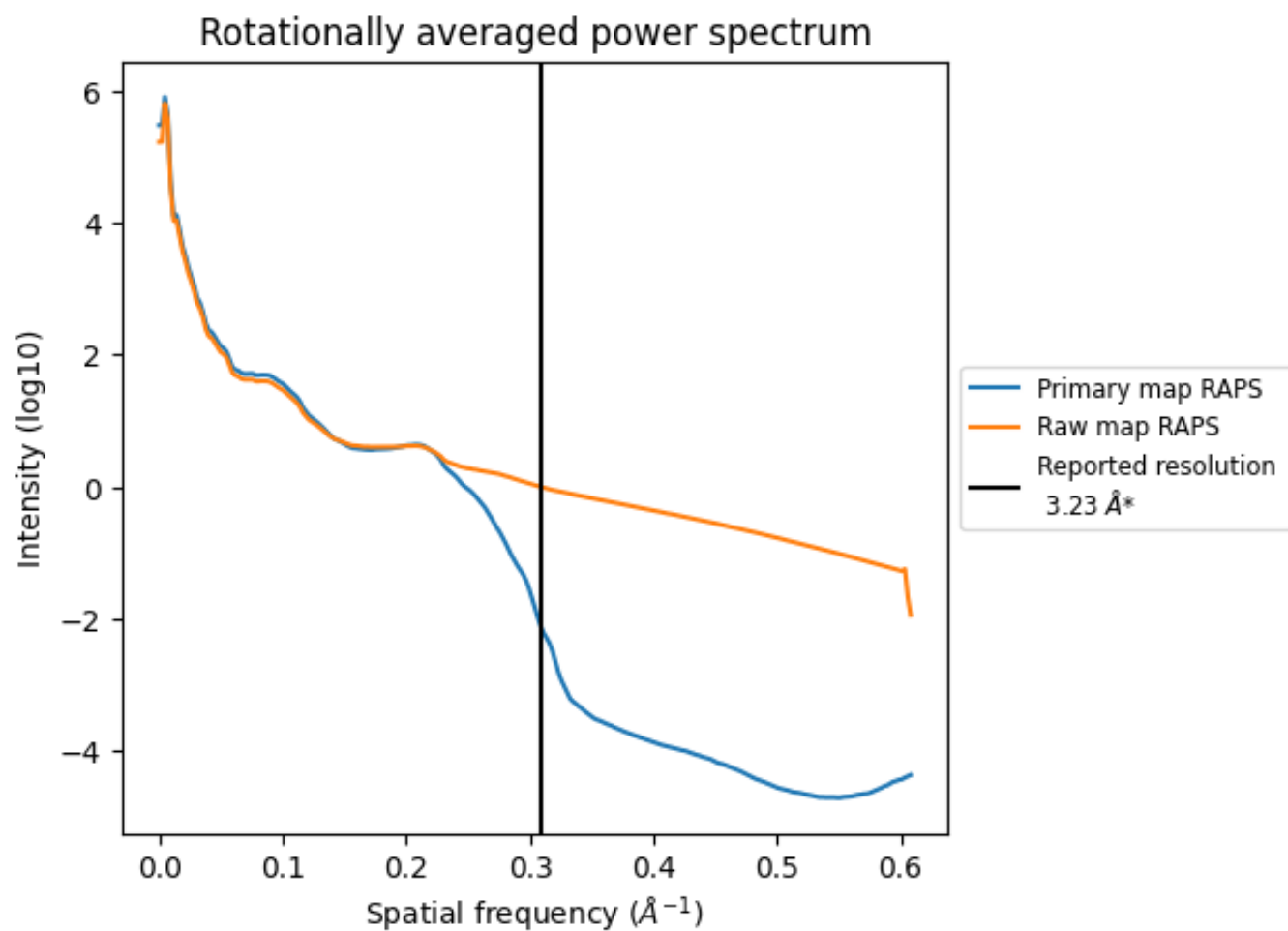
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 882 nm³; this corresponds to an approximate mass of 797 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 ⓘ

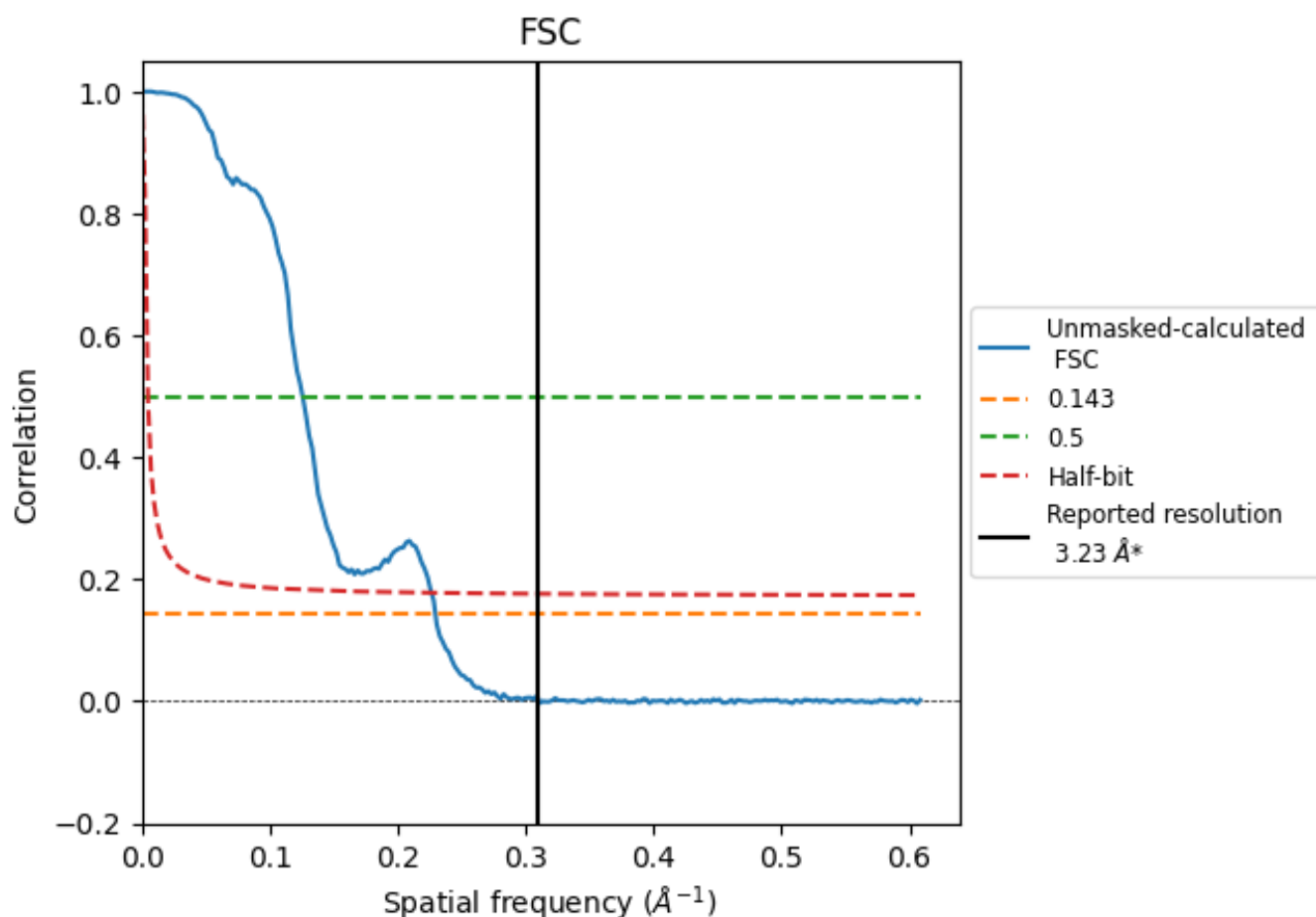


*Reported resolution corresponds to spatial frequency of $0.310 \text{ \AA}^{-1}$

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 0.310 Å⁻¹

8.2 Resolution estimates [i](#)

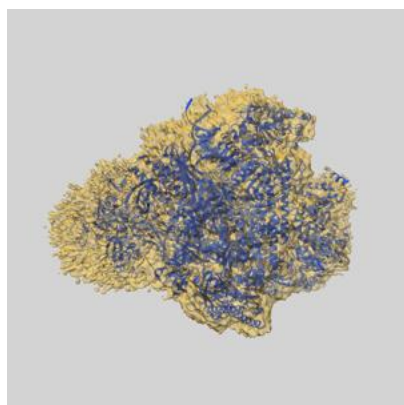
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.23	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.36	7.96	4.42

*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 4.36 differs from the reported value 3.23 by more than 10 %

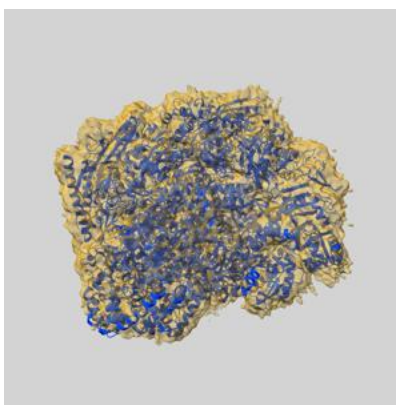
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42303 and PDB model 8UIS. Per-residue inclusion information can be found in section [3](#) on page [8](#).

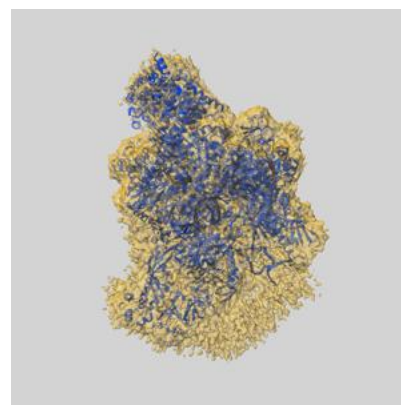
9.1 Map-model overlay [i](#)



X



Y



Z

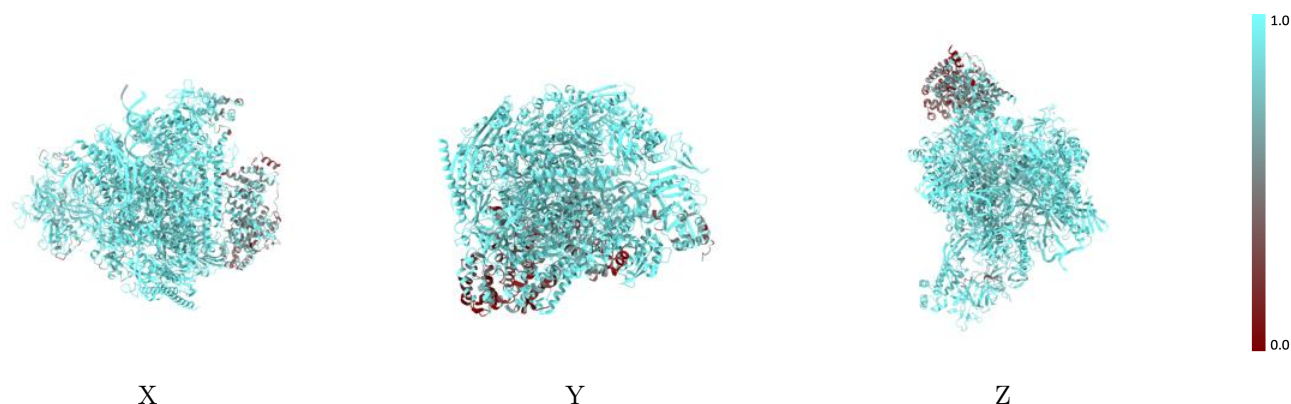
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



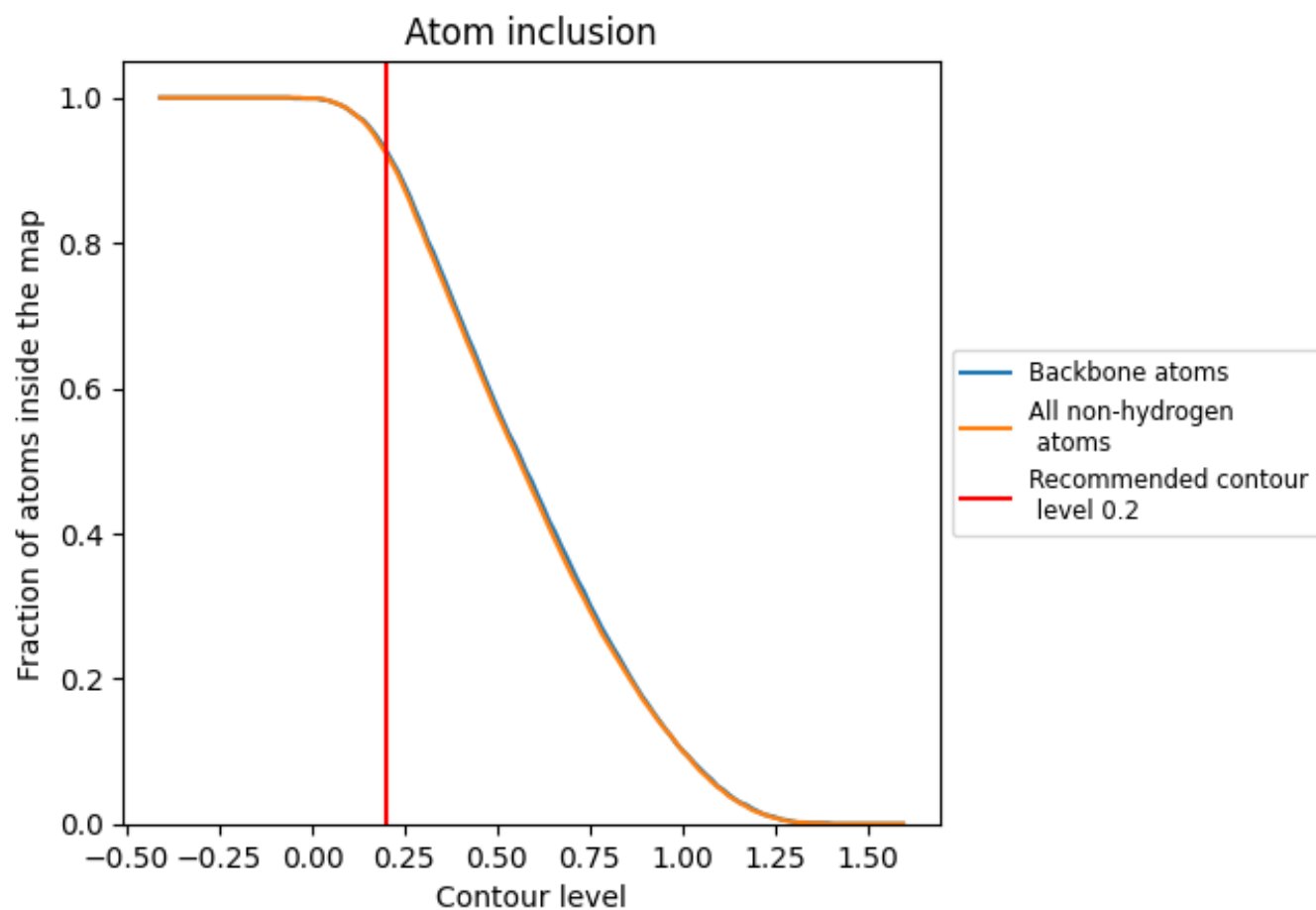
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion ⓘ



At the recommended contour level, 93% of all backbone atoms, 92% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9230	 0.3190
A	 0.9830	 0.3730
B	 0.9860	 0.4010
C	 0.9970	 0.4290
D	 0.9960	 0.2080
E	 0.9920	 0.3580
F	 0.9930	 0.4020
G	 0.9930	 0.2420
H	 0.9920	 0.4090
I	 0.9960	 0.3630
J	 0.9940	 0.4350
K	 0.9980	 0.4270
L	 1.0000	 0.4030
N	 0.9150	 0.1350
P	 0.9320	 0.2450
S	 0.8050	 0.1480
T	 0.9860	 0.2440
U	 0.5110	 0.0900
W	 0.6450	 0.1010
Z	 0.8270	 0.0940

