



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 05:26 PM UTC

PDB ID : 6TUT / pdb_00006tut
EMDB ID : EMD-10595
Title : Cryo-EM structure of the RNA Polymerase III-Maf1 complex
Authors : Vorlaender, M.K.; Hagen, W.J.H.; Mueller, C.W.
Deposited on : 2020-01-08
Resolution : 3.25 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:

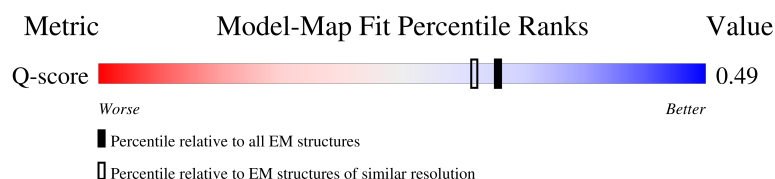
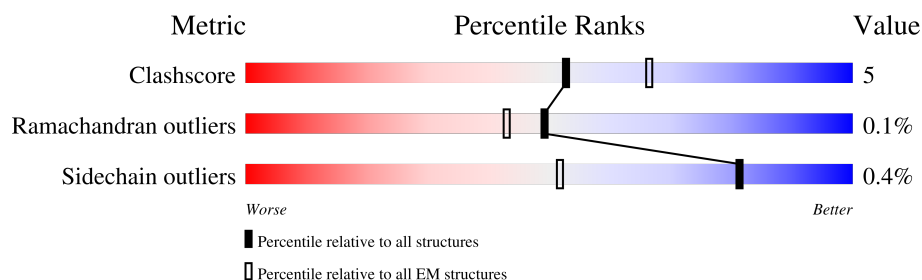
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14599 (2.75 - 3.75)

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	 7% 82% 13% 5%
2	B	1149	 6% 80% 15% 5%
3	C	335	 5% 85% 14%
4	D	161	 41% 56% 9% 35%

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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	R	267	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 40324 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	1390	Total	C	N	O	S	0	0
			10908	6880	1926	2046	56		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1097	Total	C	N	O	S	0	0
			8657	5481	1493	1623	60		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	334	Total	C	N	O	S	0	0
			2647	1676	453	510	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	104	Total	C	N	O	S	0	0
			857	553	138	161	5		

- 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	199	Total	C	N	O	S	0	0
			1594	1038	258	291	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	146	Total	C	N	O	S	0	0
			1161	726	195	235	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	43	Total	C	N	O	S	0	0
			332	210	51	65	6		

- 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	102	Total	C	N	O	S	0	0
			801	501	131	164	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	45	Total	C	N	O	S	0	0
			358	221	71	62	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	166	Total	C	N	O	S	0	0
			1345	862	225	257	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	125	Total	C	N	O	S	0	0
			968	610	173	181	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	551	Total	C	N	O	S	0	0
			4433	2819	763	833	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	196	Total	C	N	O	S	0	0
			1599	1036	258	299	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	79	Total	C	N	O	S	0	0
			503	319	89	94	1		

- Molecule 18 is a protein called Repressor of RNA polymerase III transcription MAF1, Repressor of RNA polymerase III transcription MAF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	142	Total	C	N	O	S	0	0
			1175	760	189	221	5		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-2	GLY	-	expression tag	UNP P41910
R	-1	ALA	-	expression tag	UNP P41910
R	0	MET	-	expression tag	UNP P41910
R	1	GLY	-	expression tag	UNP P41910

- Molecule 19 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
19	A	2	Total	Zn	0
			2	2	

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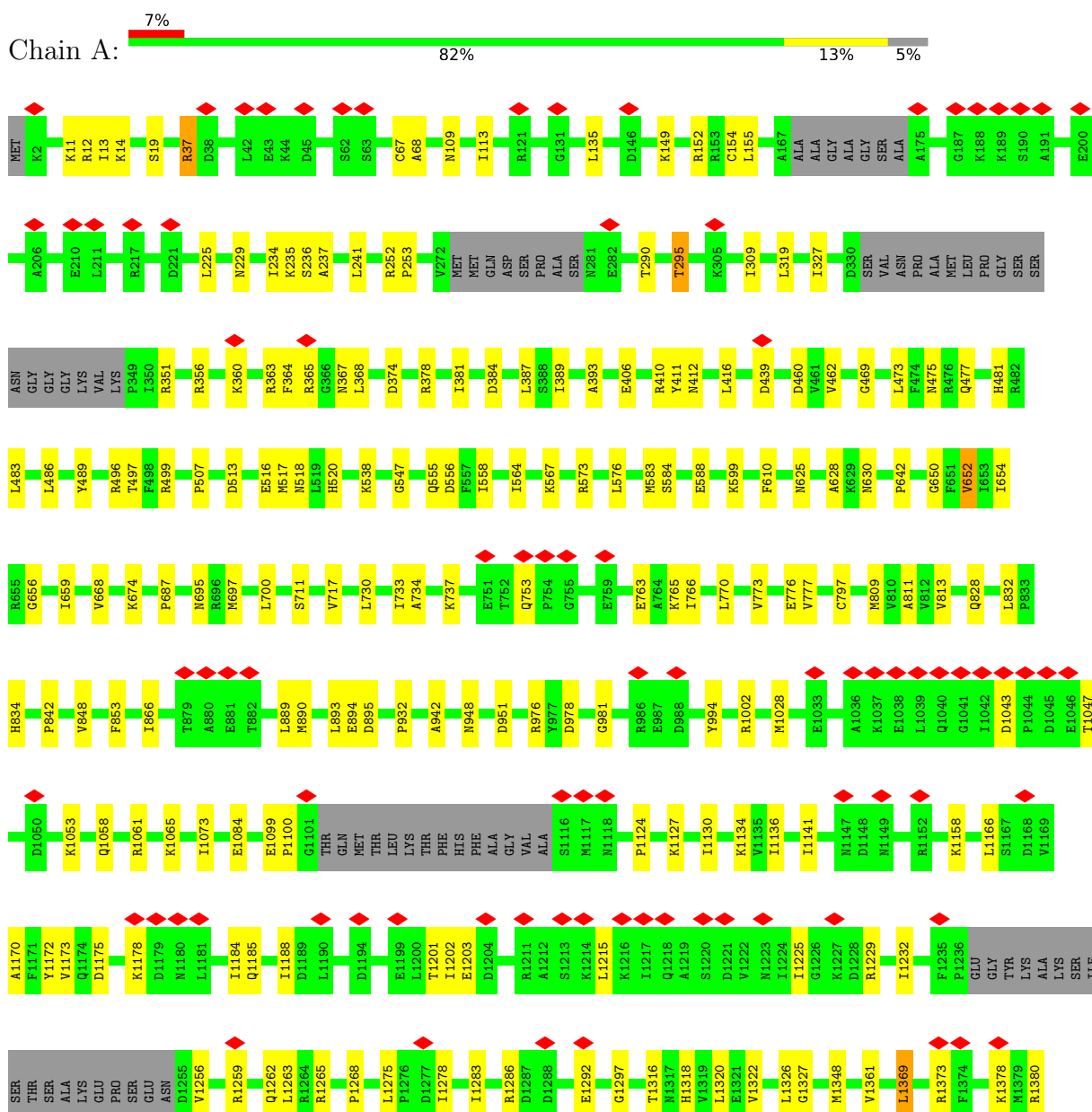
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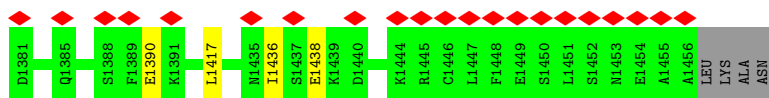
Mol	Chain	Residues	Atoms		AltConf
19	B	1	Total 1	Zn 1	0
19	I	1	Total 1	Zn 1	0
19	J	2	Total 2	Zn 2	0
19	L	1	Total 1	Zn 1	0

3 Residue-property plots

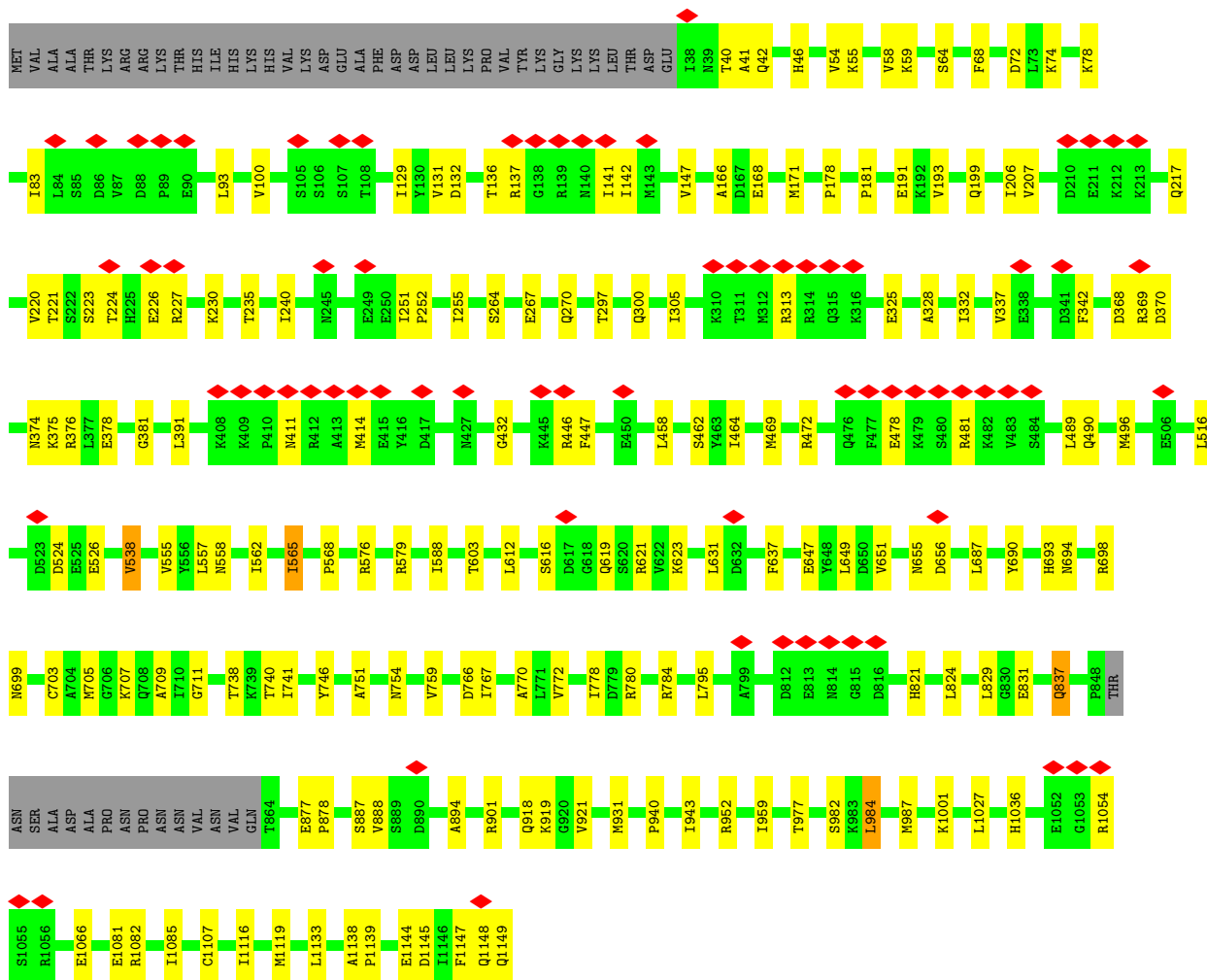
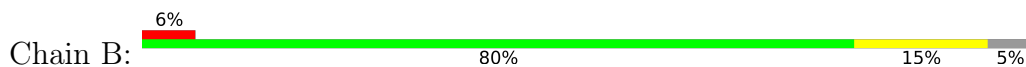
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

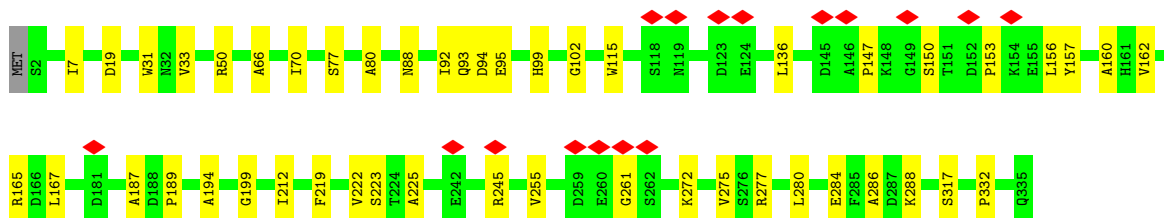
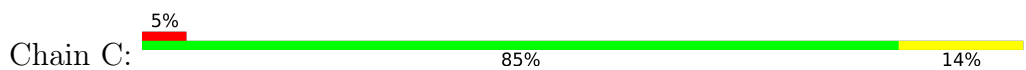




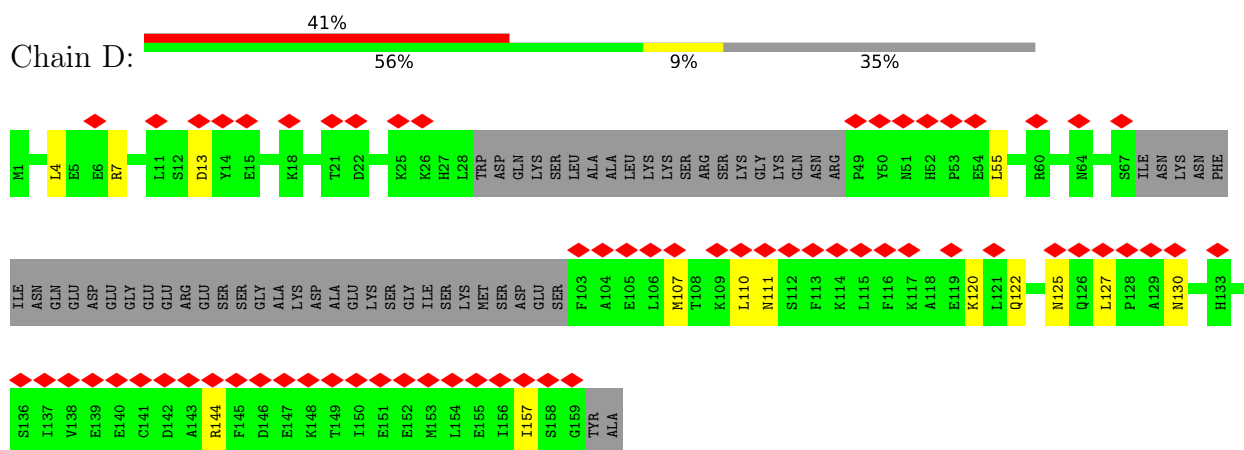
• Molecule 2: DNA-directed RNA polymerase III subunit RPC2



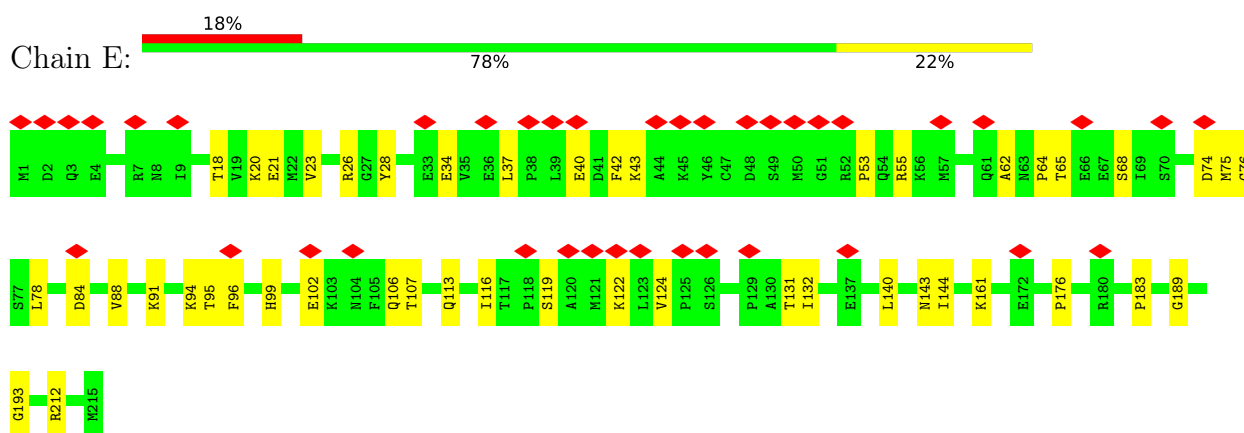
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1



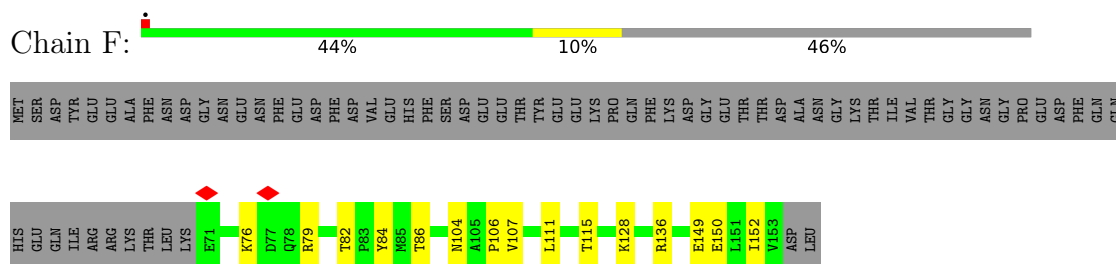
• Molecule 4: DNA-directed RNA polymerase III subunit RPC9



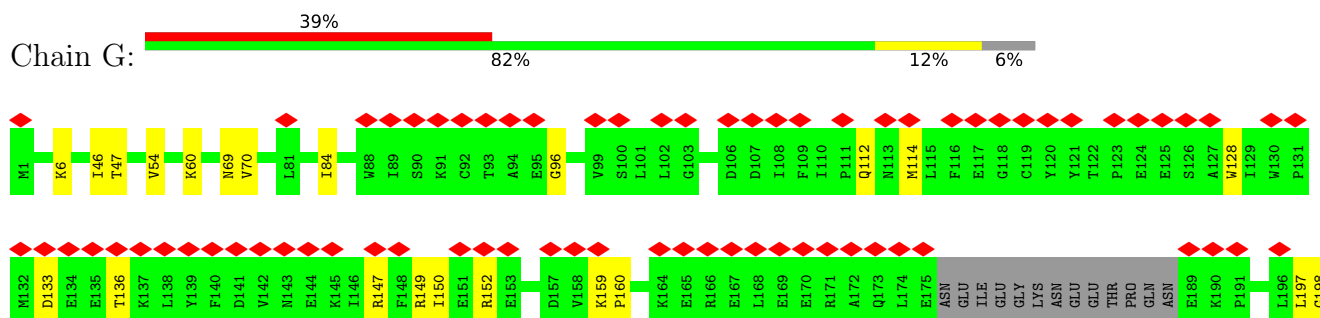
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

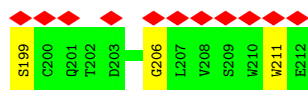


• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

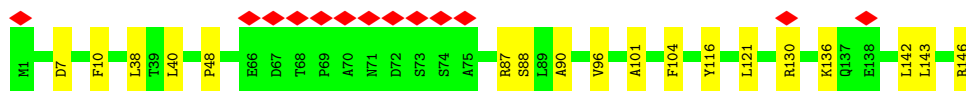
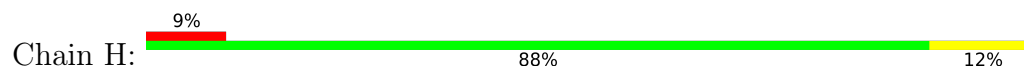


• Molecule 7: DNA-directed RNA polymerase III subunit RPC8

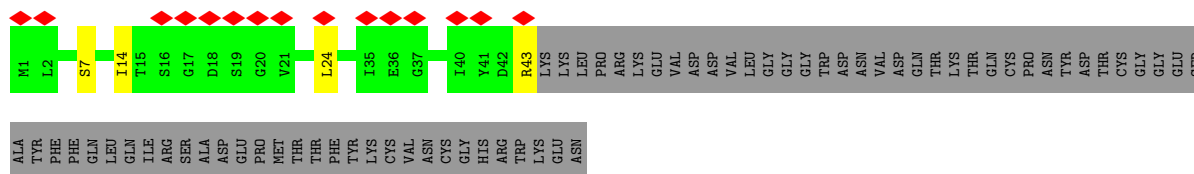




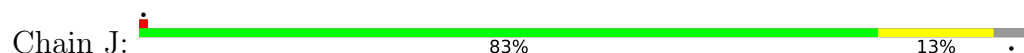
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



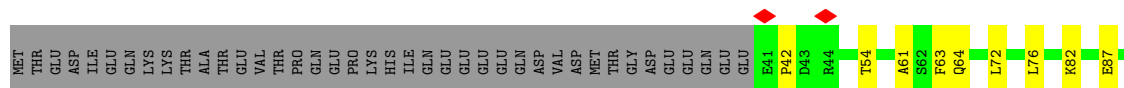
- Molecule 9: DNA-directed RNA polymerase III subunit RPC10



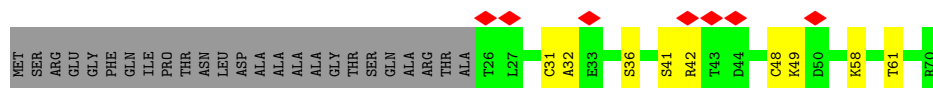
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



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

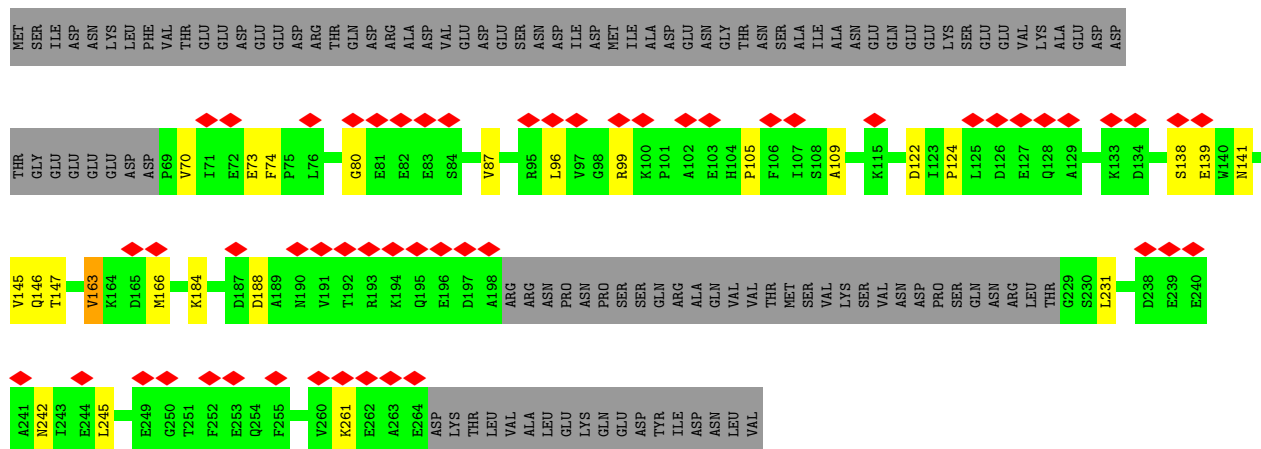


- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

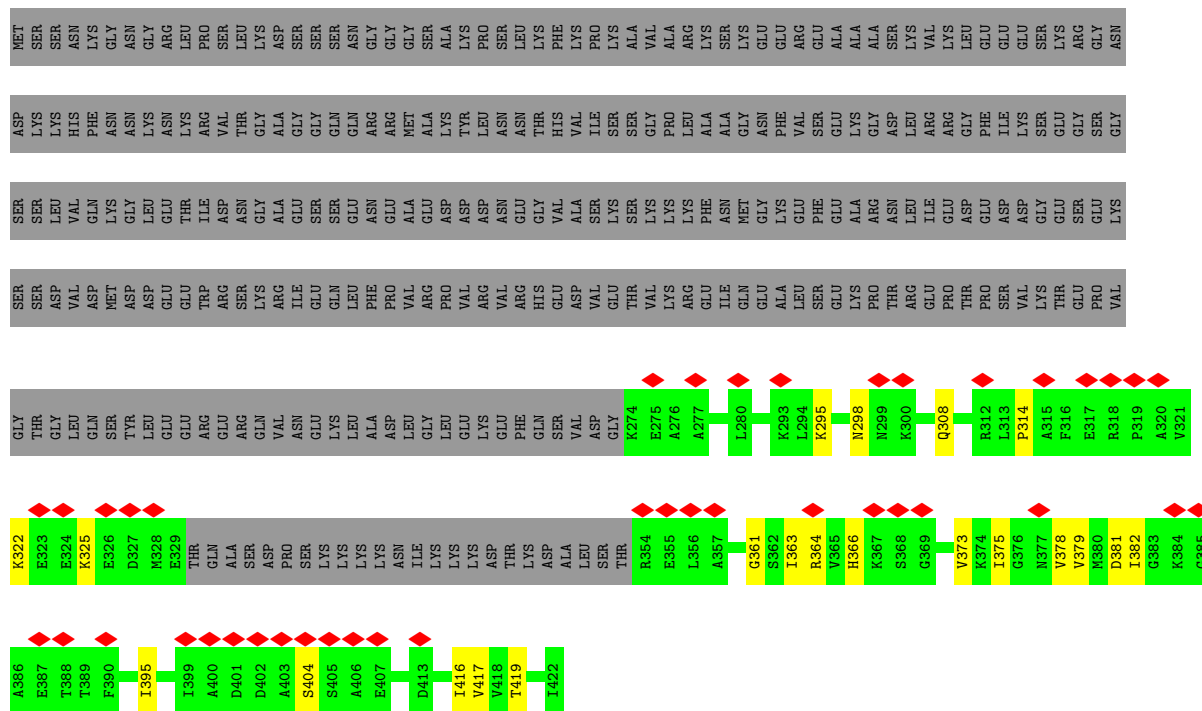


- Molecule 13: DNA-directed RNA polymerase III subunit RPC5

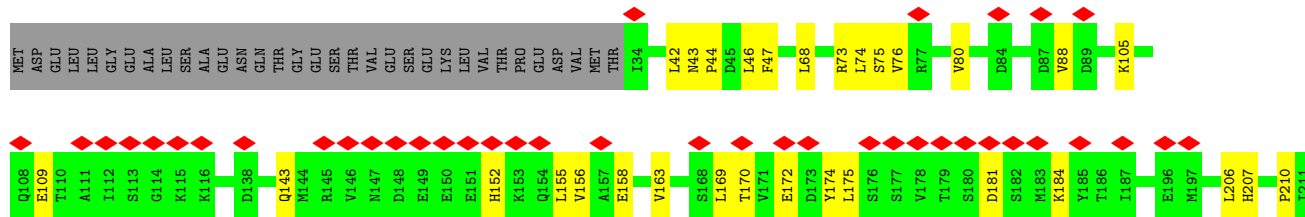




• Molecule 14: DNA-directed RNA polymerase III subunit RPC4



• Molecule 15: DNA-directed RNA polymerase III subunit RPC3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	117442	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 ($e^-/\text{\AA}^2$)	60.5	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.419	Depositor
Minimum map value	-0.239	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.075	Depositor
Map size (Å)	374.76, 374.76, 374.76	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.041, 1.041, 1.041	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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.44	0/11101	0.63	0/14993
2	B	0.48	0/8808	0.65	4/11879 (0.0%)
3	C	0.48	0/2703	0.65	2/3666 (0.1%)
4	D	0.18	0/870	0.45	0/1167
5	E	0.32	0/1795	0.57	0/2416
6	F	0.46	0/683	0.58	0/923
7	G	0.27	0/1634	0.47	0/2217
8	H	0.47	0/1181	0.68	0/1602
9	I	0.34	0/339	0.85	0/459
10	J	0.56	0/558	0.70	0/750
11	K	0.51	0/812	0.58	0/1096
12	L	0.41	0/360	0.74	2/478 (0.4%)
13	M	0.27	0/1377	0.55	0/1863
14	N	0.25	0/978	0.62	0/1310
15	O	0.27	0/4501	0.56	0/6072
16	P	0.24	0/1632	0.55	0/2206
17	Q	0.35	0/510	0.84	1/695 (0.1%)
18	R	0.27	0/1204	0.55	0/1633
All	All	0.41	0/41046	0.62	9/55425 (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	4
2	B	0	3
3	C	0	1
13	M	0	1
All	All	0	9

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Q	1092	PRO	N-CA-CB	6.36	110.26	103.52
12	L	49	LYS	CA-C-N	5.40	135.72	126.32
12	L	49	LYS	C-N-CA	5.40	135.72	126.32
2	B	637	PHE	CA-C-N	5.30	135.47	125.66
2	B	637	PHE	C-N-CA	5.30	135.47	125.66
3	C	286	ALA	CA-C-N	5.20	135.37	126.32
3	C	286	ALA	C-N-CA	5.20	135.37	126.32
2	B	837	GLN	CA-C-N	5.09	130.05	122.82
2	B	837	GLN	C-N-CA	5.09	130.05	122.82

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1043	ASP	Peptide
1	A	1178	LYS	Peptide
1	A	477	GLN	Peptide
1	A	932	PRO	Peptide
2	B	223	SER	Peptide
2	B	224	THR	Peptide
2	B	313	ARG	Peptide
3	C	223	SER	Peptide
13	M	105	PRO	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10908	0	11035	130	0
2	B	8657	0	8787	111	0
3	C	2647	0	2616	29	0
4	D	857	0	868	12	0
5	E	1759	0	1788	27	0
6	F	671	0	692	10	0
7	G	1594	0	1580	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	1161	0	1124	13	0
9	I	332	0	316	3	0
10	J	549	0	559	6	0
11	K	801	0	795	11	0
12	L	358	0	383	5	0
13	M	1345	0	1307	17	0
14	N	968	0	1014	15	0
15	O	4433	0	4600	51	0
16	P	1599	0	1579	15	0
17	Q	503	0	395	7	0
18	R	1175	0	1143	17	0
19	A	2	0	0	0	0
19	B	1	0	0	0	0
19	I	1	0	0	0	0
19	J	2	0	0	0	0
19	L	1	0	0	0	0
All	All	40324	0	40581	431	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 5.

All (431) 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)
15:O:530:GLU:HG3	15:O:534:ARG:HE	1.56	0.71
1:A:1185:GLN:HE21	1:A:1229:ARG:HD3	1.55	0.69
1:A:1316:THR:HG22	1:A:1318:HIS:H	1.59	0.68
1:A:483:LEU:HB3	1:A:507:PRO:HB3	1.77	0.66
1:A:497:THR:HG23	1:A:499:ARG:HD2	1.77	0.66
2:B:1001:LYS:O	3:C:277:ARG:NH2	2.29	0.65
18:R:30:ASP:O	18:R:334:ALA:HA	1.97	0.65
15:O:293:SER:HB2	15:O:316:LEU:HD13	1.77	0.64
1:A:583:MET:HB3	1:A:700:LEU:HB2	1.78	0.64
2:B:516:LEU:HD11	2:B:740:THR:HG23	1.79	0.64
16:P:260:CYS:SG	16:P:261:TYR:N	2.71	0.63
1:A:890:MET:HE3	1:A:894:GLU:HG2	1.80	0.62
2:B:538:VAL:HG12	2:B:565:ILE:HG23	1.80	0.62
1:A:12:ARG:NH2	2:B:1144:GLU:OE2	2.32	0.62
2:B:754:ASN:O	10:J:48:ARG:NH2	2.33	0.62
15:O:569:LYS:HG2	15:O:572:HIS:HD2	1.65	0.62
1:A:584:SER:HB2	1:A:588:GLU:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:478:GLU:HA	2:B:481:ARG:HH22	1.64	0.62
1:A:374:ASP:O	2:B:1082:ARG:NH1	2.33	0.62
2:B:772:VAL:HB	2:B:943:ILE:HB	1.81	0.62
15:O:210:PRO:HG2	15:O:213:ASP:HB2	1.81	0.62
2:B:496:MET:HE3	2:B:651:VAL:HG22	1.81	0.61
1:A:109:ASN:ND2	15:O:571:THR:OG1	2.34	0.61
15:O:152:HIS:HA	15:O:155:LEU:HB2	1.83	0.61
15:O:376:LEU:HD11	15:O:448:HIS:HA	1.82	0.61
2:B:1107:CYS:HB2	2:B:1116:ILE:HD11	1.82	0.61
1:A:652:VAL:HG11	1:A:668:VAL:HG11	1.83	0.61
2:B:931:MET:HE3	2:B:940:PRO:HG2	1.83	0.61
2:B:698:ARG:HD2	2:B:952:ARG:HB3	1.83	0.61
1:A:393:ALA:HB3	1:A:499:ARG:HB2	1.82	0.61
11:K:64:GLN:HE21	11:K:100:LEU:HD11	1.64	0.60
18:R:329:LYS:HG3	18:R:330:ARG:HG3	1.83	0.60
11:K:54:THR:HG22	11:K:61:ALA:HA	1.84	0.60
1:A:460:ASP:OD1	1:A:460:ASP:N	2.35	0.60
8:H:87:ARG:NH1	8:H:88:SER:O	2.35	0.60
1:A:1084:GLU:HB3	6:F:86:THR:HG23	1.84	0.60
2:B:411:ASN:HB3	2:B:414:MET:HB2	1.84	0.59
15:O:541:ILE:HD13	15:O:548:ILE:HD11	1.85	0.59
1:A:135:LEU:HD21	1:A:1378:LYS:HD2	1.84	0.59
1:A:555:GLN:NE2	2:B:767:ILE:O	2.35	0.59
2:B:136:THR:HG22	2:B:141:ILE:HG22	1.84	0.59
6:F:82:THR:O	6:F:136:ARG:NH1	2.34	0.59
2:B:829:LEU:O	12:L:58:LYS:NZ	2.36	0.59
7:G:152:ARG:HB3	7:G:197:LEU:HD12	1.85	0.59
2:B:207:VAL:HG22	2:B:217:GLN:HE21	1.67	0.58
12:L:31:CYS:SG	12:L:32:ALA:N	2.76	0.58
1:A:412:ASN:HB3	6:F:115:THR:HB	1.85	0.58
14:N:382:ILE:HD11	14:N:416:ILE:HD12	1.84	0.58
15:O:266:ASP:HB3	15:O:271:LEU:HA	1.84	0.58
2:B:837:GLN:HB3	2:B:878:PRO:HB3	1.84	0.58
5:E:28:TYR:HA	5:E:64:PRO:HA	1.86	0.58
13:M:87:VAL:HG23	14:N:395:ILE:HG13	1.85	0.58
2:B:297:THR:HG23	2:B:300:GLN:H	1.69	0.58
3:C:19:ASP:O	11:K:82:LYS:NZ	2.37	0.58
17:Q:47:ILE:HG21	17:Q:52:ARG:HH21	1.67	0.58
1:A:381:ILE:HD13	1:A:517:MET:HE3	1.86	0.58
1:A:832:LEU:HG	1:A:834:HIS:HD2	1.68	0.58
3:C:88:ASN:ND2	3:C:94:ASP:OD1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:549:GLN:HB3	15:O:565:LEU:HB2	1.85	0.58
3:C:157:TYR:HB2	3:C:160:ALA:HB2	1.86	0.57
15:O:240:GLN:O	15:O:244:ASN:ND2	2.37	0.57
2:B:526:GLU:OE1	2:B:558:ASN:ND2	2.34	0.57
1:A:473:LEU:HB2	1:A:520:HIS:HB2	1.86	0.57
1:A:630:ASN:HD22	1:A:650:GLY:HA2	1.69	0.57
2:B:616:SER:HB3	2:B:621:ARG:HH21	1.68	0.57
14:N:363:ILE:HG12	14:N:373:VAL:HG22	1.85	0.57
1:A:410:ARG:HG3	6:F:104:ASN:HD21	1.69	0.57
2:B:199:GLN:NE2	2:B:378:GLU:OE1	2.37	0.57
1:A:1201:THR:HG23	1:A:1203:GLU:H	1.69	0.57
1:A:378:ARG:HH11	1:A:518:ASN:HD21	1.51	0.57
2:B:252:PRO:HD2	2:B:255:ILE:HD11	1.86	0.57
1:A:567:LYS:HD2	8:H:121:LEU:HD23	1.87	0.57
4:D:107:MET:O	4:D:111:ASN:ND2	2.38	0.57
16:P:222:LEU:HD22	16:P:237:PRO:HB3	1.86	0.56
1:A:951:ASP:OD2	1:A:1065:LYS:NZ	2.39	0.56
7:G:150:ILE:HA	7:G:198:GLY:HA2	1.87	0.56
15:O:376:LEU:HD13	15:O:452:LEU:HD22	1.86	0.56
2:B:375:LYS:O	2:B:376:ARG:NH1	2.37	0.56
15:O:143:GLN:HE22	15:O:317:ARG:HD2	1.71	0.56
18:R:29:CYS:HB2	18:R:336:LEU:HD23	1.88	0.56
15:O:493:GLU:OE2	15:O:512:ARG:NH2	2.39	0.55
1:A:497:THR:O	1:A:499:ARG:NH1	2.35	0.55
5:E:99:HIS:HA	5:E:102:GLU:HG2	1.89	0.55
18:R:326:TYR:HA	18:R:333:VAL:HG12	1.88	0.55
3:C:255:VAL:HG22	3:C:272:LYS:HB3	1.89	0.55
13:M:70:VAL:HA	14:N:366:HIS:HA	1.89	0.55
8:H:40:LEU:HD11	8:H:142:LEU:HD21	1.88	0.55
10:J:36:LEU:HD11	10:J:51:LEU:HD12	1.89	0.55
2:B:738:THR:HG23	2:B:977:THR:HA	1.87	0.55
2:B:251:ILE:HG12	2:B:305:ILE:HG22	1.89	0.55
15:O:642:SER:OG	17:Q:51:GLU:OE1	2.24	0.55
1:A:483:LEU:HD13	1:A:486:LEU:HD21	1.89	0.54
2:B:369:ARG:O	2:B:375:LYS:NZ	2.39	0.54
2:B:703:CYS:O	2:B:707:LYS:NZ	2.39	0.54
1:A:573:ARG:HH21	11:K:87:GLU:HB2	1.72	0.54
15:O:239:SER:HB2	15:O:243:MET:HE1	1.89	0.54
2:B:462:SER:OG	2:B:709:ALA:O	2.25	0.54
4:D:127:LEU:HD12	4:D:157:ILE:HG23	1.89	0.54
9:I:7:SER:O	13:M:146:GLN:NE2	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:104:ARG:HE	11:K:106:GLN:HE21	1.55	0.54
1:A:13:ILE:HG13	2:B:1119:MET:HE1	1.89	0.54
7:G:133:ASP:H	7:G:136:THR:HA	1.73	0.54
1:A:777:VAL:HG12	1:A:811:ALA:HB1	1.89	0.54
1:A:1175:ASP:HB3	1:A:1184:ILE:HD13	1.90	0.54
15:O:643:ARG:NH1	17:Q:46:PRO:O	2.36	0.54
13:M:138:SER:OG	13:M:139:GLU:OE1	2.27	0.54
1:A:538:LYS:HB3	1:A:687:PRO:HB2	1.90	0.53
2:B:619:GLN:HE22	2:B:623:LYS:HD2	1.71	0.53
1:A:295:THR:HB	1:A:319:LEU:HD13	1.88	0.53
2:B:576:ARG:NH1	2:B:656:ASP:OD2	2.40	0.53
2:B:694:ASN:HD22	2:B:699:ASN:HD21	1.55	0.53
8:H:7:ASP:O	8:H:130:ARG:NH1	2.38	0.53
14:N:308:GLN:HB3	14:N:417:VAL:HG12	1.90	0.53
15:O:260:SER:HA	15:O:263:LEU:HD13	1.91	0.53
1:A:14:LYS:HD3	2:B:1144:GLU:HB3	1.89	0.53
16:P:253:LEU:HD13	16:P:261:TYR:HB3	1.90	0.53
15:O:206:LEU:HD11	15:O:256:PRO:HG2	1.90	0.53
2:B:137:ARG:HB3	2:B:142:ILE:HD13	1.91	0.53
15:O:43:ASN:HD22	15:O:44:PRO:HD2	1.74	0.53
2:B:741:ILE:HB	2:B:746:TYR:HB3	1.89	0.53
5:E:18:THR:OG1	5:E:140:LEU:O	2.24	0.53
15:O:43:ASN:HB3	15:O:46:LEU:HB3	1.90	0.53
15:O:163:VAL:HG12	15:O:169:LEU:HD21	1.91	0.53
1:A:309:ILE:HG13	15:O:566:PHE:HZ	1.74	0.52
5:E:74:ASP:O	5:E:106:GLN:NE2	2.42	0.52
13:M:96:LEU:HD23	13:M:99:ARG:HA	1.90	0.52
13:M:147:THR:HG21	13:M:184:LYS:HG3	1.91	0.52
15:O:522:ILE:O	15:O:526:ALA:N	2.42	0.52
3:C:33:VAL:HG21	11:K:126:ASP:HB3	1.91	0.52
5:E:176:PRO:HB2	5:E:212:ARG:HD2	1.91	0.52
13:M:124:PRO:HA	13:M:145:VAL:HA	1.92	0.52
2:B:738:THR:HG22	2:B:740:THR:H	1.74	0.52
3:C:284:GLU:O	3:C:288:LYS:NZ	2.38	0.52
15:O:73:ARG:NH2	15:O:109:GLU:OE2	2.42	0.52
4:D:122:GLN:NE2	7:G:84:ILE:O	2.43	0.52
9:I:14:ILE:HA	9:I:24:LEU:HA	1.92	0.52
5:E:161:LYS:NZ	5:E:193:GLY:O	2.43	0.52
15:O:289:LYS:HD3	15:O:323:SER:HB3	1.92	0.51
1:A:1322:VAL:HG13	1:A:1326:LEU:HD12	1.93	0.51
2:B:54:VAL:HG23	2:B:55:LYS:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:705:MET:HE3	2:B:1027:LEU:HD21	1.91	0.51
5:E:95:THR:O	5:E:99:HIS:ND1	2.36	0.51
1:A:889:LEU:HD21	1:A:1130:ILE:HD12	1.92	0.51
5:E:88:VAL:HG23	5:E:116:ILE:HD12	1.91	0.51
16:P:97:ILE:HG21	16:P:150:LEU:HG	1.93	0.51
1:A:866:ILE:HA	2:B:489:LEU:HD21	1.91	0.51
2:B:579:ARG:NH2	2:B:647:GLU:OE2	2.43	0.51
4:D:130:ASN:HD22	7:G:211:TRP:HB3	1.74	0.51
8:H:96:VAL:HG22	8:H:143:LEU:HG	1.93	0.51
1:A:1215:LEU:HD12	1:A:1263:LEU:HG	1.93	0.51
2:B:565:ILE:HD12	2:B:568:PRO:HA	1.91	0.51
5:E:68:SER:OG	5:E:75:MET:SD	2.67	0.51
14:N:314:PRO:HG3	14:N:325:LYS:HG3	1.91	0.51
1:A:1188:ILE:HD11	1:A:1202:ILE:HG22	1.91	0.51
1:A:1373:ARG:NH2	1:A:1390:GLU:OE1	2.43	0.51
1:A:481:HIS:HB3	1:A:1099:GLU:HG3	1.93	0.51
2:B:579:ARG:NH1	2:B:588:ILE:O	2.40	0.51
12:L:41:SER:OG	12:L:42:ARG:N	2.44	0.51
3:C:153:PRO:HA	3:C:156:LEU:HB2	1.91	0.51
2:B:83:ILE:HB	2:B:93:LEU:HB3	1.93	0.50
14:N:322:LYS:HZ2	14:N:379:VAL:H	1.59	0.50
1:A:1047:THR:O	1:A:1053:LYS:NZ	2.44	0.50
2:B:168:GLU:HG3	2:B:178:PRO:HG3	1.94	0.50
2:B:766:ASP:HB3	2:B:772:VAL:HG23	1.93	0.50
15:O:158:GLU:OE1	15:O:174:TYR:OH	2.30	0.50
15:O:181:ASP:HA	15:O:184:LYS:HB3	1.92	0.50
15:O:328:ASP:HB3	15:O:331:THR:HG23	1.92	0.50
8:H:48:PRO:O	8:H:146:ARG:NH2	2.36	0.50
1:A:558:ILE:HG22	1:A:797:CYS:HB3	1.92	0.50
1:A:654:ILE:HG12	1:A:659:ILE:HG12	1.93	0.50
1:A:1136:ILE:HG12	1:A:1318:HIS:HD2	1.76	0.50
2:B:795:LEU:HB2	2:B:894:ALA:HB3	1.94	0.50
16:P:307:LYS:HA	17:Q:40:PRO:HA	1.93	0.50
1:A:1275:LEU:HB2	1:A:1278:ILE:HD12	1.93	0.50
2:B:328:ALA:HA	2:B:337:VAL:HG12	1.94	0.50
15:O:42:LEU:HB3	15:O:47:PHE:HB2	1.92	0.50
2:B:235:THR:HG22	2:B:240:ILE:HG12	1.94	0.50
2:B:831:GLU:HB3	12:L:61:THR:HB	1.94	0.50
1:A:976:ARG:HB2	1:A:1002:ARG:HH12	1.77	0.49
2:B:368:ASP:O	2:B:374:ASN:ND2	2.43	0.49
15:O:80:VAL:HG11	15:O:88:VAL:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ASN:HB3	15:O:544:ASN:HD21	1.78	0.49
5:E:62:ALA:HB3	5:E:78:LEU:HB3	1.94	0.49
15:O:105:LYS:NZ	15:O:207:HIS:O	2.42	0.49
18:R:27:GLY:HA3	18:R:337:TYR:O	2.12	0.49
1:A:154:CYS:SG	1:A:155:LEU:N	2.85	0.49
1:A:599:LYS:HD3	8:H:90:ALA:HB1	1.95	0.49
16:P:144:THR:O	18:R:249:HIS:ND1	2.45	0.49
1:A:1028:MET:HG2	1:A:1047:THR:HG21	1.94	0.49
15:O:620:LEU:HD12	15:O:621:PRO:HD2	1.95	0.49
1:A:1286:ARG:HE	1:A:1292:GLU:HB2	1.77	0.49
4:D:130:ASN:ND2	7:G:211:TRP:O	2.46	0.49
16:P:256:VAL:HG22	16:P:257:THR:HG23	1.94	0.49
2:B:166:ALA:HB3	2:B:171:MET:HE2	1.94	0.49
2:B:558:ASN:HD21	2:B:603:THR:HG22	1.77	0.48
3:C:80:ALA:HB3	3:C:102:GLY:HA2	1.94	0.48
15:O:170:THR:OG1	15:O:276:PRO:O	2.30	0.48
1:A:976:ARG:NH1	1:A:994:TYR:O	2.45	0.48
3:C:147:PRO:O	3:C:150:SER:OG	2.29	0.48
1:A:363:ARG:HD3	1:A:367:ASN:HD22	1.78	0.48
1:A:1173:VAL:HG21	1:A:1268:PRO:HB3	1.94	0.48
2:B:226:GLU:O	2:B:227:ARG:NE	2.45	0.48
13:M:166:MET:HE1	14:N:295:LYS:HA	1.94	0.48
1:A:828:GLN:H	2:B:655:ASN:ND2	2.12	0.48
1:A:1124:PRO:HA	1:A:1127:LYS:HB2	1.96	0.48
2:B:40:THR:HG23	2:B:42:GLN:HG3	1.94	0.48
2:B:370:ASP:OD2	2:B:490:GLN:NE2	2.47	0.48
8:H:7:ASP:OD1	8:H:7:ASP:N	2.47	0.48
15:O:75:SER:OG	15:O:76:VAL:N	2.46	0.48
18:R:327:ASN:HB3	18:R:332:ARG:H	1.78	0.48
1:A:225:LEU:HD21	15:O:542:ARG:HA	1.96	0.48
1:A:753:GLN:HE22	1:A:765:LYS:HE2	1.77	0.48
16:P:114:THR:HB	16:P:116:LEU:HD23	1.95	0.48
1:A:942:ALA:HB2	1:A:1073:ILE:HD12	1.96	0.47
2:B:132:ASP:OD1	2:B:132:ASP:N	2.45	0.47
2:B:221:THR:HG21	2:B:332:ILE:HA	1.95	0.47
7:G:112:GLN:HE22	7:G:128:TRP:HH2	1.60	0.47
5:E:84:ASP:O	5:E:113:GLN:NE2	2.47	0.47
15:O:323:SER:HA	15:O:359:LEU:HD11	1.96	0.47
1:A:469:GLY:HA2	1:A:489:TYR:HB3	1.95	0.47
7:G:96:GLY:O	7:G:128:TRP:NE1	2.45	0.47
1:A:1172:TYR:HB3	9:I:43:ARG:HD3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:141:ASN:ND2	13:M:188:ASP:OD2	2.45	0.47
3:C:66:ALA:O	3:C:70:ILE:HG12	2.13	0.47
1:A:67:CYS:SG	1:A:68:ALA:N	2.88	0.47
1:A:351:ARG:HH11	1:A:356:ARG:HG2	1.79	0.47
1:A:730:LEU:HD13	1:A:776:GLU:HB3	1.97	0.47
2:B:612:LEU:HD12	2:B:649:LEU:HD12	1.97	0.47
1:A:770:LEU:HD11	1:A:842:PRO:HB3	1.96	0.47
1:A:893:LEU:HD21	1:A:1361:VAL:HG21	1.96	0.47
2:B:711:GLY:HA3	2:B:751:ALA:HA	1.97	0.47
1:A:1436:ILE:HG13	7:G:54:VAL:HG21	1.97	0.47
2:B:1036:HIS:CD2	2:B:1054:ARG:HE	2.33	0.46
1:A:236:SER:HB3	1:A:252:ARG:HH21	1.80	0.46
2:B:391:LEU:HD21	2:B:432:GLY:HA3	1.98	0.46
2:B:780:ARG:NH2	10:J:8:PHE:O	2.48	0.46
1:A:37:ARG:HH11	18:R:274:THR:HB	1.80	0.46
1:A:733:ILE:HG22	1:A:737:LYS:HE2	1.96	0.46
2:B:959:ILE:HG23	2:B:984:LEU:HD23	1.96	0.46
7:G:147:ARG:O	7:G:206:GLY:N	2.49	0.46
14:N:361:GLY:HA3	14:N:375:ILE:HG22	1.96	0.46
18:R:25:ILE:HD11	18:R:338:LEU:HD23	1.96	0.46
1:A:234:ILE:HD12	1:A:253:PRO:HG2	1.96	0.46
1:A:1170:ALA:HA	1:A:1188:ILE:HA	1.95	0.46
2:B:472:ARG:HH22	2:B:707:LYS:HE3	1.78	0.46
2:B:918:GLN:HG2	2:B:952:ARG:HH11	1.81	0.46
2:B:1133:LEU:HD22	2:B:1139:PRO:HD2	1.98	0.46
5:E:53:PRO:HB2	5:E:55:ARG:HG3	1.98	0.46
8:H:101:ALA:HB3	8:H:136:LYS:HA	1.98	0.46
11:K:63:PHE:HB2	11:K:103:ILE:HG22	1.98	0.46
2:B:1147:PHE:O	2:B:1149:GLN:NE2	2.48	0.46
1:A:360:LYS:HB3	1:A:365:ARG:HH21	1.79	0.46
1:A:1158:LYS:HB2	1:A:1283:ILE:HD11	1.96	0.46
6:F:84:TYR:HD1	6:F:152:ILE:HB	1.80	0.46
8:H:101:ALA:HB2	8:H:116:TYR:HE1	1.81	0.46
1:A:406:GLU:OE2	1:A:412:ASN:ND2	2.48	0.46
2:B:131:VAL:O	2:B:147:VAL:N	2.48	0.46
2:B:264:SER:HB3	2:B:267:GLU:HG2	1.97	0.46
13:M:245:LEU:HD23	14:N:404:SER:HB3	1.98	0.46
2:B:64:SER:HB3	2:B:381:GLY:H	1.80	0.46
3:C:165:ARG:HB3	3:C:189:PRO:HB2	1.98	0.46
3:C:332:PRO:HG3	11:K:42:PRO:HB2	1.98	0.46
18:R:257:THR:OG1	18:R:258:ASP:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:778:ILE:O	2:B:784:ARG:NH2	2.49	0.45
5:E:20:LYS:NZ	5:E:34:GLU:O	2.40	0.45
5:E:21:GLU:OE1	5:E:143:ASN:ND2	2.49	0.45
13:M:74:PHE:HB2	14:N:363:ILE:HB	1.99	0.45
3:C:245:ARG:NH1	3:C:261:GLY:O	2.36	0.45
15:O:319:THR:HB	15:O:359:LEU:HD23	1.98	0.45
12:L:36:SER:OG	12:L:48:CYS:SG	2.74	0.45
13:M:109:ALA:HB3	13:M:122:ASP:HB2	1.97	0.45
2:B:68:PHE:HA	2:B:72:ASP:HB2	1.97	0.45
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.97	0.45
5:E:119:SER:OG	5:E:122:LYS:NZ	2.44	0.45
18:R:263:SER:O	18:R:266:THR:OG1	2.32	0.45
1:A:1327:GLY:HA2	5:E:183:PRO:HD2	1.98	0.45
2:B:267:GLU:HA	2:B:270:GLN:HB2	1.99	0.45
10:J:65:PRO:HB2	10:J:67:GLU:HG3	1.99	0.45
15:O:356:THR:HB	15:O:359:LEU:HB2	1.99	0.45
2:B:690:TYR:HB3	2:B:693:HIS:HD2	1.82	0.45
3:C:77:SER:OG	3:C:219:PHE:O	2.33	0.45
1:A:556:ASP:HB3	2:B:767:ILE:HD12	1.99	0.45
1:A:717:VAL:HG13	1:A:809:MET:HB3	1.98	0.45
1:A:763:GLU:HA	1:A:766:ILE:HG22	1.99	0.45
4:D:110:LEU:O	4:D:120:LYS:NZ	2.49	0.45
8:H:90:ALA:HB2	8:H:96:VAL:HG21	1.98	0.45
15:O:326:ILE:HB	15:O:653:MET:HG2	1.99	0.45
2:B:901:ARG:HD2	3:C:93:GLN:HG2	1.99	0.45
6:F:79:ARG:NH2	6:F:150:GLU:OE2	2.32	0.45
16:P:106:TRP:O	16:P:109:THR:OG1	2.32	0.45
4:D:144:ARG:NH2	17:Q:1114:ARG:O	2.46	0.44
5:E:96:PHE:HA	5:E:99:HIS:CE1	2.52	0.44
15:O:172:GLU:HA	15:O:175:LEU:HB2	1.98	0.44
1:A:711:SER:OG	2:B:759:VAL:O	2.33	0.44
3:C:70:ILE:HB	3:C:317:SER:HB2	2.00	0.44
7:G:46:ILE:HG22	7:G:47:THR:HG23	1.98	0.44
16:P:141:LYS:HB2	16:P:145:ARG:HH21	1.83	0.44
18:R:268:ILE:HA	18:R:271:PHE:HB3	1.99	0.44
2:B:1147:PHE:HZ	7:G:60:LYS:HG3	1.82	0.44
5:E:65:THR:HG23	5:E:68:SER:H	1.83	0.44
16:P:95:SER:O	16:P:99:ALA:N	2.50	0.44
1:A:628:ALA:HB3	1:A:652:VAL:HG13	1.99	0.44
2:B:524:ASP:OD1	2:B:603:THR:OG1	2.32	0.44
7:G:54:VAL:HG12	7:G:70:VAL:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:322:LYS:HG3	14:N:378:VAL:HG23	1.99	0.44
3:C:92:ILE:HD13	3:C:194:ALA:HB1	2.00	0.44
6:F:76:LYS:HA	6:F:79:ARG:HG3	2.00	0.44
1:A:813:VAL:HB	1:A:848:VAL:HG23	2.00	0.44
1:A:1166:LEU:HD23	1:A:1268:PRO:HA	1.99	0.44
1:A:1184:ILE:HB	1:A:1232:ILE:HB	1.99	0.44
2:B:555:VAL:HG23	2:B:562:ILE:HB	2.00	0.44
2:B:784:ARG:HH12	3:C:99:HIS:CD2	2.36	0.44
5:E:91:LYS:HA	5:E:94:LYS:HE3	1.99	0.44
17:Q:75:MET:SD	17:Q:75:MET:N	2.91	0.44
1:A:547:GLY:O	1:A:674:LYS:NZ	2.50	0.44
1:A:1369:LEU:HD13	1:A:1369:LEU:HA	1.86	0.44
7:G:159:LYS:HD2	7:G:160:PRO:HD2	1.99	0.44
1:A:1318:HIS:CE1	1:A:1320:LEU:HB2	2.53	0.43
2:B:887:SER:OG	2:B:888:VAL:N	2.51	0.43
13:M:80:GLY:H	13:M:261:LYS:HE2	1.83	0.43
14:N:381:ASP:OD1	14:N:419:THR:OG1	2.34	0.43
5:E:76:GLY:H	5:E:106:GLN:HG2	1.83	0.43
16:P:306:ASP:OD1	16:P:306:ASP:N	2.49	0.43
16:P:172:ILE:HG22	16:P:174:PHE:H	1.83	0.43
1:A:475:ASN:HD22	2:B:1066:GLU:HG2	1.83	0.43
2:B:1081:GLU:HA	2:B:1085:ILE:HB	2.00	0.43
18:R:248:ASP:OD1	18:R:248:ASP:N	2.51	0.43
18:R:266:THR:O	18:R:269:SER:OG	2.31	0.43
1:A:113:ILE:HD13	1:A:241:LEU:HD23	2.01	0.43
1:A:406:GLU:HG2	1:A:416:LEU:HD21	2.01	0.43
3:C:115:TRP:HH2	3:C:212:ILE:HG23	1.83	0.43
1:A:11:LYS:NZ	2:B:1145:ASP:OD1	2.48	0.43
1:A:410:ARG:HH12	6:F:106:PRO:HA	1.83	0.43
2:B:74:LYS:HZ1	2:B:78:LYS:HE2	1.83	0.43
1:A:378:ARG:NE	1:A:516:GLU:OE1	2.52	0.43
5:E:37:LEU:HB3	5:E:42:PHE:HB2	2.00	0.43
5:E:107:THR:OG1	5:E:131:THR:O	2.35	0.43
6:F:107:VAL:HG21	6:F:111:LEU:HD23	2.01	0.43
1:A:19:SER:O	2:B:1138:ALA:N	2.49	0.43
1:A:384:ASP:HB3	1:A:387:LEU:HD22	2.01	0.43
1:A:513:ASP:HB2	2:B:919:LYS:HG3	2.01	0.43
1:A:1100:PRO:HB2	1:A:1348:MET:HG2	2.01	0.43
1:A:573:ARG:NH2	11:K:87:GLU:HB2	2.34	0.42
1:A:1436:ILE:HG22	1:A:1438:GLU:H	1.84	0.42
2:B:901:ARG:NH2	3:C:95:GLU:OE1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1256:VAL:HG23	1:A:1259:ARG:HH21	1.85	0.42
1:A:1058:GLN:HB3	8:H:104:PHE:HD2	1.84	0.42
2:B:982:SER:HB3	2:B:987:MET:HE3	1.99	0.42
11:K:76:LEU:HD21	11:K:121:LEU:HD23	2.01	0.42
15:O:152:HIS:HB3	15:O:156:VAL:HG13	2.01	0.42
16:P:135:LYS:HB3	16:P:151:TYR:HE1	1.84	0.42
18:R:264:LEU:HA	18:R:301:LEU:HD13	2.01	0.42
1:A:410:ARG:NH1	1:A:411:TYR:OH	2.52	0.42
13:M:163:VAL:HG13	14:N:298:ASN:HA	2.02	0.42
1:A:351:ARG:HE	1:A:356:ARG:HG2	1.84	0.42
15:O:68:LEU:HD22	15:O:74:LEU:HD12	2.01	0.42
15:O:631:ASN:HA	15:O:634:GLU:HB3	2.01	0.42
2:B:40:THR:OG1	2:B:41:ALA:N	2.51	0.42
2:B:446:ARG:HH21	2:B:447:PHE:HE1	1.67	0.42
15:O:497:ALA:HB2	15:O:505:MET:HB2	2.01	0.42
1:A:717:VAL:HG12	1:A:853:PHE:HB2	2.01	0.42
2:B:193:VAL:HG11	2:B:469:MET:HG3	2.01	0.42
2:B:337:VAL:HG21	2:B:342:PHE:HD1	1.85	0.42
3:C:7:ILE:HD13	3:C:275:VAL:HG11	2.02	0.42
5:E:23:VAL:HG12	5:E:26:ARG:HD2	2.02	0.42
1:A:948:ASN:O	1:A:1061:ARG:NH2	2.52	0.42
15:O:552:PRO:HB3	15:O:557:ARG:HG3	2.02	0.42
15:O:623:GLU:O	15:O:627:LEU:N	2.43	0.42
16:P:129:GLU:OE2	16:P:132:ARG:NH2	2.52	0.42
1:A:496:ARG:NH1	2:B:877:GLU:OE2	2.52	0.42
1:A:978:ASP:OD1	1:A:981:GLY:N	2.53	0.42
1:A:1278:ILE:HA	1:A:1297:GLY:HA3	2.02	0.42
2:B:206:ILE:HD11	2:B:369:ARG:HG2	2.02	0.42
3:C:136:LEU:HB2	3:C:167:LEU:HD23	2.01	0.42
5:E:40:GLU:HA	5:E:43:LYS:HB2	2.02	0.42
8:H:10:PHE:HD2	8:H:38:LEU:HD22	1.85	0.42
15:O:585:MET:HB2	15:O:644:LEU:HD22	2.01	0.42
1:A:364:PHE:HD1	1:A:368:LEU:HD12	1.85	0.42
1:A:866:ILE:HG12	2:B:489:LEU:HG	2.02	0.42
2:B:58:VAL:HG11	2:B:181:PRO:HB2	2.02	0.42
13:M:73:GLU:HG3	14:N:364:ARG:HG2	2.01	0.42
1:A:384:ASP:HB2	1:A:499:ARG:HB3	2.02	0.41
5:E:144:ILE:H	5:E:144:ILE:HG13	1.64	0.41
1:A:564:ILE:HB	1:A:610:PHE:HE2	1.85	0.41
1:A:697:MET:HE2	1:A:697:MET:HB3	1.90	0.41
1:A:895:ASP:OD1	1:A:1380:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:50:ARG:NH1	3:C:187:ALA:O	2.52	0.41
4:D:55:LEU:HD11	7:G:47:THR:HG22	2.02	0.41
7:G:149:ARG:O	7:G:199:SER:N	2.52	0.41
1:A:625:ASN:OD1	1:A:656:GLY:N	2.49	0.41
1:A:1417:LEU:HA	1:A:1417:LEU:HD23	1.86	0.41
2:B:464:ILE:HG13	2:B:687:LEU:HD11	2.01	0.41
2:B:766:ASP:HA	2:B:770:ALA:HB3	2.02	0.41
1:A:149:LYS:O	1:A:152:ARG:NH1	2.52	0.41
1:A:1225:ILE:HB	1:A:1229:ARG:HB3	2.01	0.41
2:B:526:GLU:HB2	2:B:557:LEU:HD21	2.03	0.41
3:C:245:ARG:HH22	3:C:261:GLY:HA2	1.86	0.41
7:G:114:MET:HB3	7:G:199:SER:HA	2.02	0.41
13:M:242:ASN:OD1	13:M:242:ASN:N	2.50	0.41
1:A:1134:LYS:O	1:A:1318:HIS:NE2	2.52	0.41
1:A:1141:ILE:HG12	1:A:1316:THR:HG23	2.02	0.41
2:B:46:HIS:ND1	2:B:631:LEU:HD21	2.36	0.41
5:E:26:ARG:HH22	5:E:189:GLY:HA3	1.85	0.41
1:A:416:LEU:HD22	1:A:462:VAL:HG21	2.02	0.41
1:A:1175:ASP:N	1:A:1175:ASP:OD1	2.53	0.41
15:O:454:ASN:HA	15:O:457:LEU:HB2	2.02	0.41
18:R:330:ARG:HE	18:R:332:ARG:HD2	1.85	0.41
1:A:235:LYS:O	1:A:237:ALA:N	2.47	0.41
10:J:1:MET:HA	10:J:56:LEU:HB2	2.02	0.41
1:A:389:ILE:HG23	1:A:695:ASN:HD21	1.85	0.41
2:B:220:VAL:HG22	2:B:230:LYS:HG3	2.03	0.41
2:B:821:HIS:ND1	2:B:824:LEU:HD22	2.35	0.41
4:D:4:LEU:HD12	7:G:6:LYS:HG2	2.01	0.41
1:A:734:ALA:HB2	1:A:773:VAL:HG11	2.03	0.41
3:C:199:GLY:HA3	10:J:67:GLU:HB3	2.03	0.41
4:D:7:ARG:NH2	17:Q:1118:LYS:O	2.54	0.41
15:O:589:LEU:HD11	15:O:641:LEU:HD22	2.03	0.41
2:B:191:GLU:HG3	2:B:458:LEU:HB3	2.03	0.40
6:F:128:LYS:HD2	6:F:149:GLU:HA	2.02	0.40
1:A:378:ARG:HH11	1:A:518:ASN:ND2	2.19	0.40
1:A:1262:GLN:OE1	1:A:1265:ARG:NH2	2.55	0.40
3:C:222:VAL:HG11	3:C:225:ALA:HB2	2.03	0.40
2:B:325:GLU:HB2	13:M:231:LEU:HD21	2.03	0.40
4:D:122:GLN:HE22	7:G:84:ILE:N	2.18	0.40
2:B:55:LYS:HB3	2:B:59:LYS:HD3	2.03	0.40
2:B:1148:GLN:O	7:G:69:ASN:ND2	2.55	0.40
3:C:277:ARG:HB2	3:C:280:LEU:HD12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:VAL:HG12	2:B:129:ILE:HG12	2.03	0.40
3:C:31:TRP:HH2	11:K:127:LEU:HD12	1.86	0.40
4:D:13:ASP:N	4:D:125:ASN:OD1	2.49	0.40
18:R:270:LYS:HA	18:R:273:ASN:HB2	2.03	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	1378/1460 (94%)	1269 (92%)	107 (8%)	2 (0%)	48	76
2	B	1093/1149 (95%)	1007 (92%)	86 (8%)	0	100	100
3	C	332/335 (99%)	306 (92%)	26 (8%)	0	100	100
4	D	98/161 (61%)	96 (98%)	2 (2%)	0	100	100
5	E	213/215 (99%)	197 (92%)	16 (8%)	0	100	100
6	F	81/155 (52%)	77 (95%)	4 (5%)	0	100	100
7	G	195/212 (92%)	181 (93%)	14 (7%)	0	100	100
8	H	144/146 (99%)	125 (87%)	19 (13%)	0	100	100
9	I	41/110 (37%)	31 (76%)	10 (24%)	0	100	100
10	J	65/70 (93%)	60 (92%)	5 (8%)	0	100	100
11	K	100/142 (70%)	98 (98%)	2 (2%)	0	100	100
12	L	43/70 (61%)	35 (81%)	8 (19%)	0	100	100
13	M	162/282 (57%)	151 (93%)	11 (7%)	0	100	100
14	N	121/422 (29%)	106 (88%)	15 (12%)	0	100	100
15	O	547/654 (84%)	513 (94%)	34 (6%)	0	100	100
16	P	188/317 (59%)	164 (87%)	24 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Q	73/251 (29%)	60 (82%)	10 (14%)	3 (4%)	2	13
18	R	138/267 (52%)	126 (91%)	12 (9%)	0	100	100
All	All	5012/6418 (78%)	4602 (92%)	405 (8%)	5 (0%)	49	76

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	Q	1080	ASP
1	A	642	PRO
17	Q	1084	ASN
17	Q	49	ASN
1	A	439	ASP

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	1206/1257 (96%)	1199 (99%)	7 (1%)	78	81
2	B	959/1006 (95%)	955 (100%)	4 (0%)	84	84
3	C	295/296 (100%)	294 (100%)	1 (0%)	86	86
4	D	97/145 (67%)	97 (100%)	0	100	100
5	E	197/197 (100%)	197 (100%)	0	100	100
6	F	73/137 (53%)	73 (100%)	0	100	100
7	G	173/190 (91%)	173 (100%)	0	100	100
8	H	128/128 (100%)	128 (100%)	0	100	100
9	I	39/98 (40%)	39 (100%)	0	100	100
10	J	62/65 (95%)	61 (98%)	1 (2%)	55	70
11	K	92/130 (71%)	91 (99%)	1 (1%)	65	75
12	L	40/57 (70%)	40 (100%)	0	100	100
13	M	142/249 (57%)	141 (99%)	1 (1%)	76	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	105/360 (29%)	105 (100%)	0	100	100
15	O	506/593 (85%)	506 (100%)	0	100	100
16	P	179/285 (63%)	179 (100%)	0	100	100
17	Q	35/212 (16%)	35 (100%)	0	100	100
18	R	134/243 (55%)	133 (99%)	1 (1%)	76	79
All	All	4462/5648 (79%)	4446 (100%)	16 (0%)	81	84

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ARG
1	A	290	THR
1	A	295	THR
1	A	327	ILE
1	A	576	LEU
1	A	652	VAL
1	A	1369	LEU
2	B	538	VAL
2	B	565	ILE
2	B	921	VAL
2	B	984	LEU
3	C	162	VAL
10	J	54	VAL
11	K	72	LEU
13	M	163	VAL
18	R	270	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	134	ASN
1	A	147	GLN
1	A	229	ASN
1	A	281	ASN
1	A	328	ASN
1	A	367	ASN
1	A	386	ASN
1	A	488	HIS

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Mol	Chain	Res	Type
1	A	518	ASN
1	A	520	HIS
1	A	578	GLN
1	A	630	ASN
1	A	675	HIS
1	A	695	ASN
1	A	805	ASN
1	A	808	GLN
1	A	815	GLN
1	A	834	HIS
1	A	899	GLN
1	A	931	GLN
1	A	1174	GLN
1	A	1185	GLN
1	A	1233	ASN
1	A	1261	GLN
2	B	144	HIS
2	B	217	GLN
2	B	225	HIS
2	B	244	HIS
2	B	315	GLN
2	B	334	HIS
2	B	397	ASN
2	B	428	ASN
2	B	490	GLN
2	B	619	GLN
2	B	655	ASN
2	B	699	ASN
2	B	774	ASN
2	B	903	ASN
2	B	928	GLN
2	B	947	HIS
2	B	1029	HIS
2	B	1036	HIS
2	B	1077	GLN
2	B	1148	GLN
3	C	32	ASN
3	C	53	ASN
3	C	200	GLN
3	C	330	ASN
4	D	27	HIS
4	D	61	ASN

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Mol	Chain	Res	Type
4	D	111	ASN
4	D	122	GLN
5	E	61	GLN
5	E	106	GLN
5	E	146	HIS
6	F	104	ASN
7	G	28	HIS
7	G	32	ASN
7	G	41	ASN
7	G	112	GLN
7	G	201	GLN
8	H	35	GLN
8	H	71	ASN
11	K	64	GLN
11	K	74	ASN
11	K	83	ASN
11	K	95	HIS
11	K	102	ASN
11	K	106	GLN
14	N	289	HIS
14	N	392	GLN
15	O	43	ASN
15	O	143	GLN
15	O	202	GLN
15	O	229	ASN
15	O	369	HIS
15	O	448	HIS
15	O	544	ASN
15	O	584	ASN
17	Q	60	ASN
18	R	17	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
17	Q	2
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Q	75:MET	C	1076:SER	N	22.36
1	Q	1096:LEU	C	1104:ASP	N	12.78
1	B	489:LEU	C	490:GLN	N	1.19

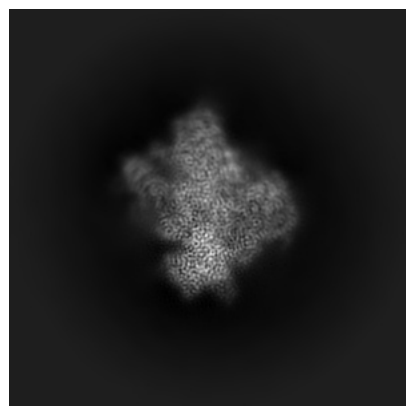
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10595. These allow visual inspection of the internal detail of the map and identification of artifacts.

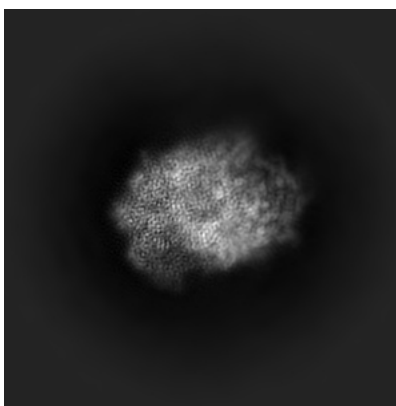
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

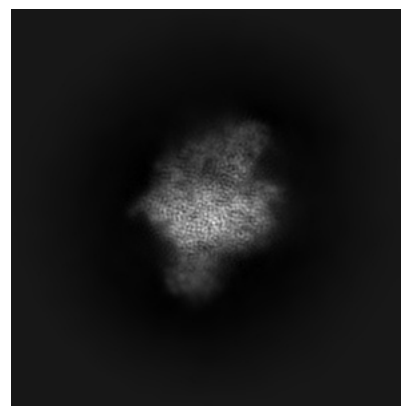
6.1.1 Primary map



X

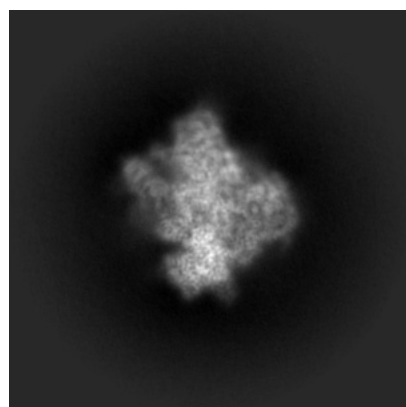


Y

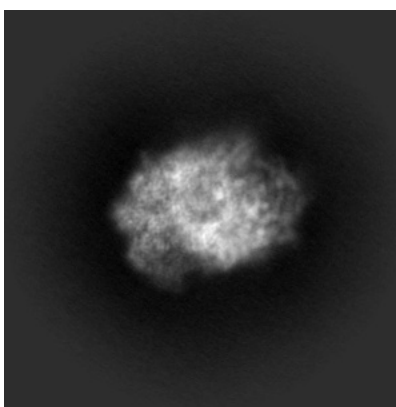


Z

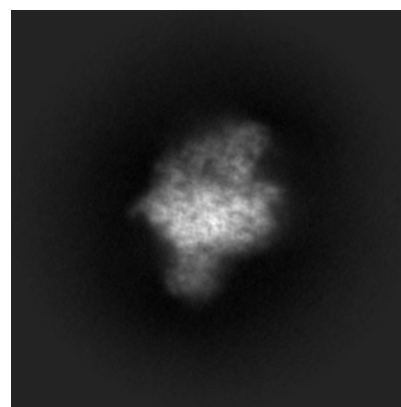
6.1.2 Raw map



X



Y

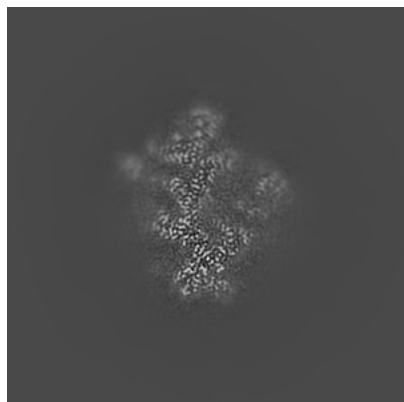


Z

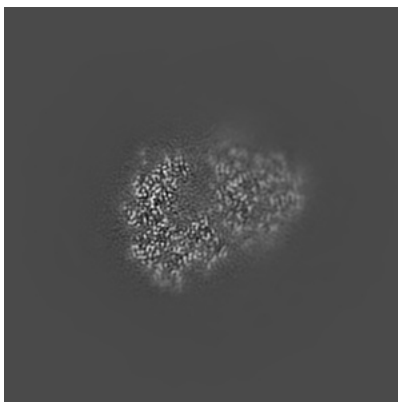
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

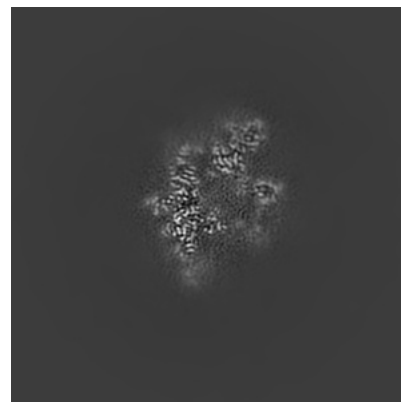
6.2.1 Primary map



X Index: 180

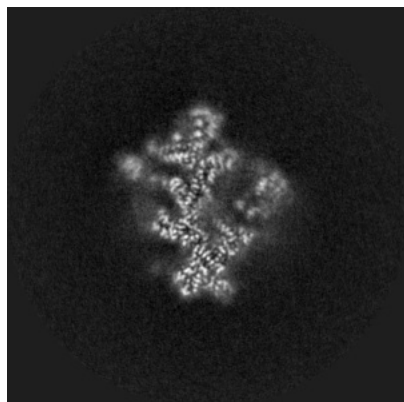


Y Index: 180

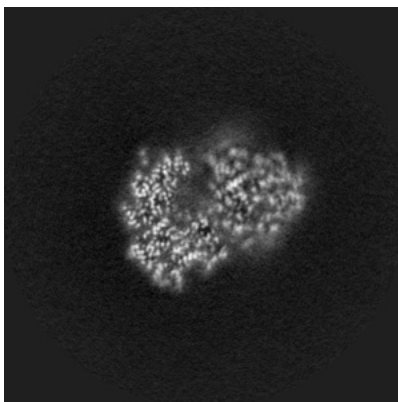


Z Index: 180

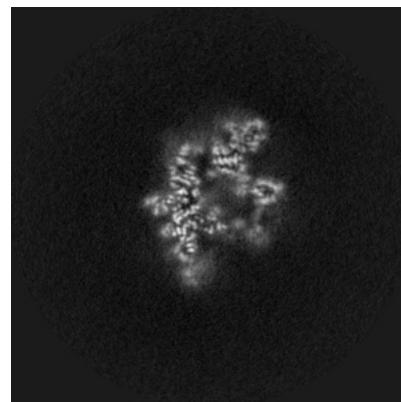
6.2.2 Raw map



X Index: 180



Y Index: 180

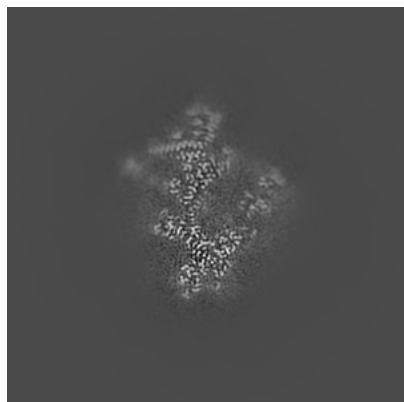


Z Index: 180

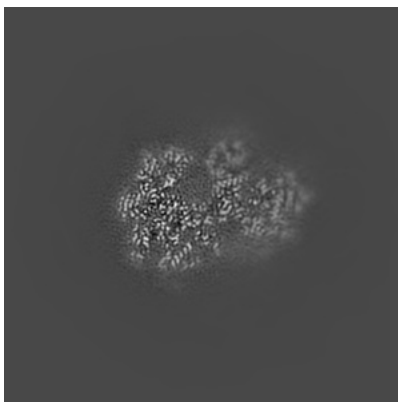
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

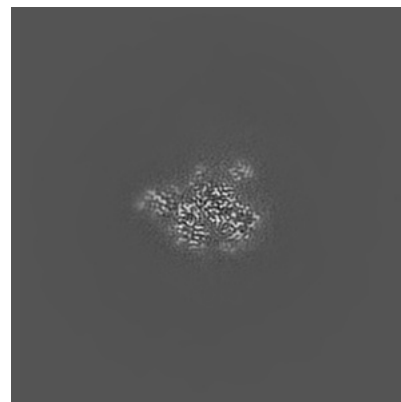
6.3.1 Primary map



X Index: 183

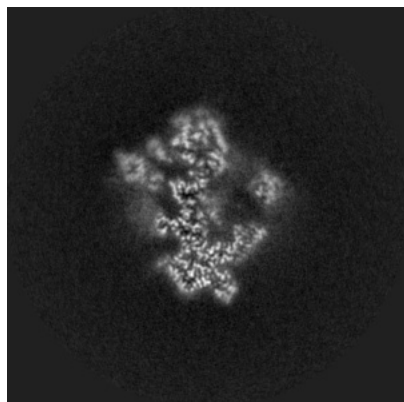


Y Index: 170

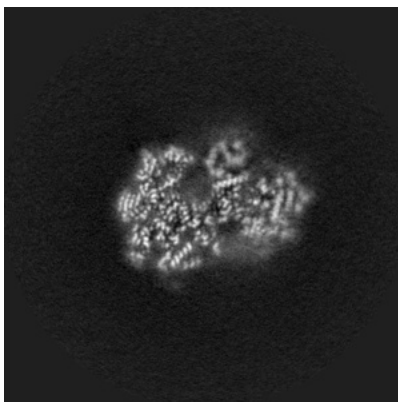


Z Index: 135

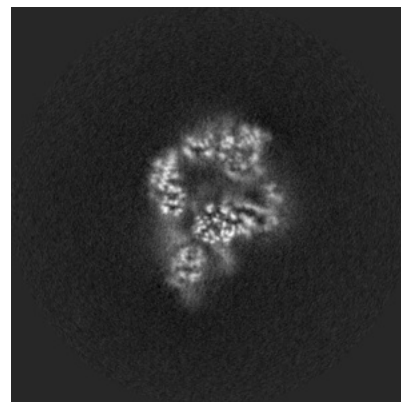
6.3.2 Raw map



X Index: 174



Y Index: 170

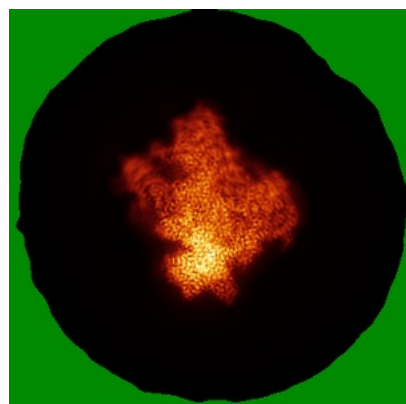


Z Index: 195

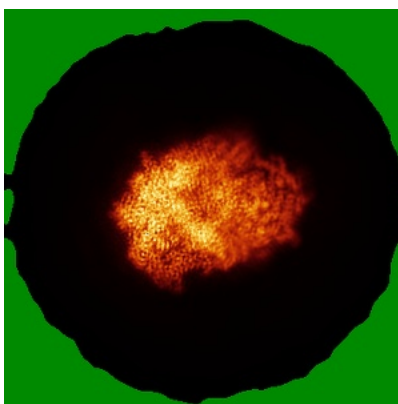
The images above show the largest variance slices of the map in three orthogonal directions.

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

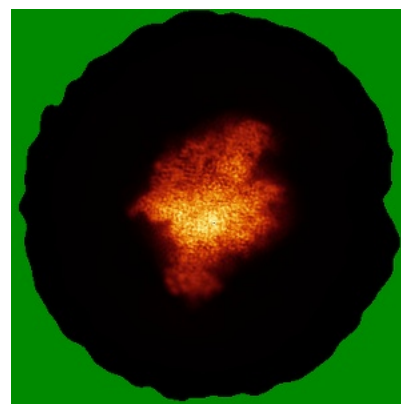
6.4.1 Primary map



X

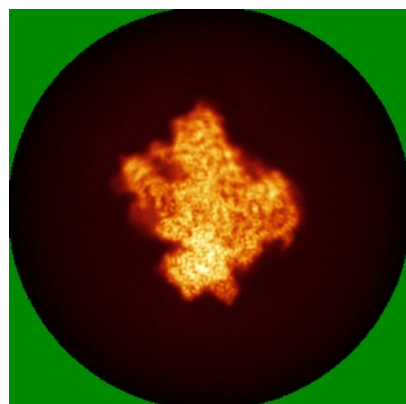


Y

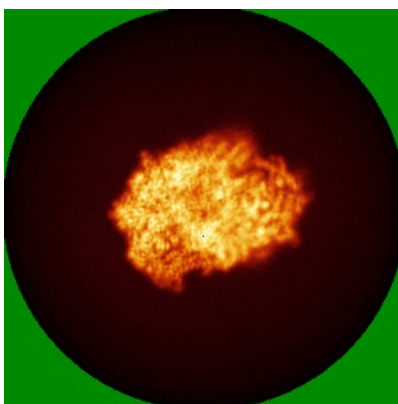


Z

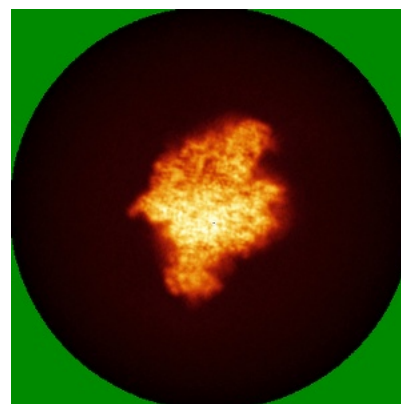
6.4.2 Raw map



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.

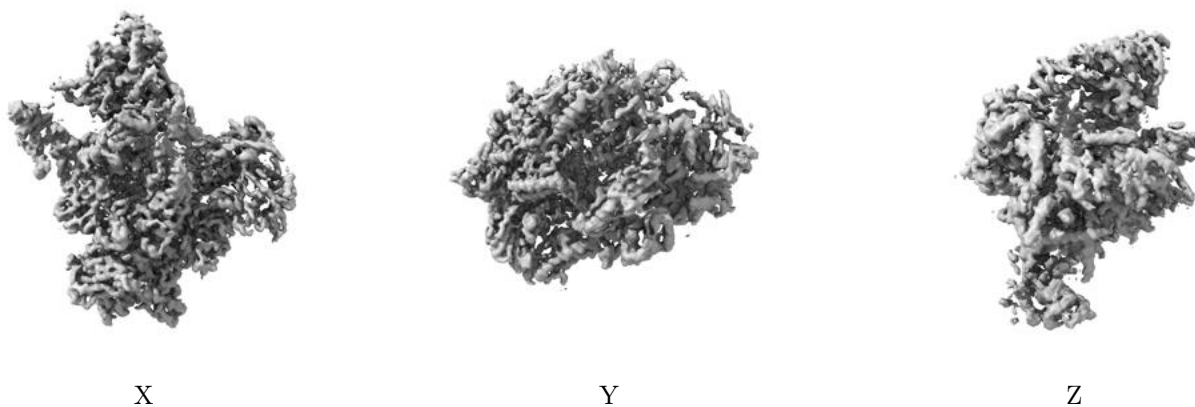
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.075. 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.

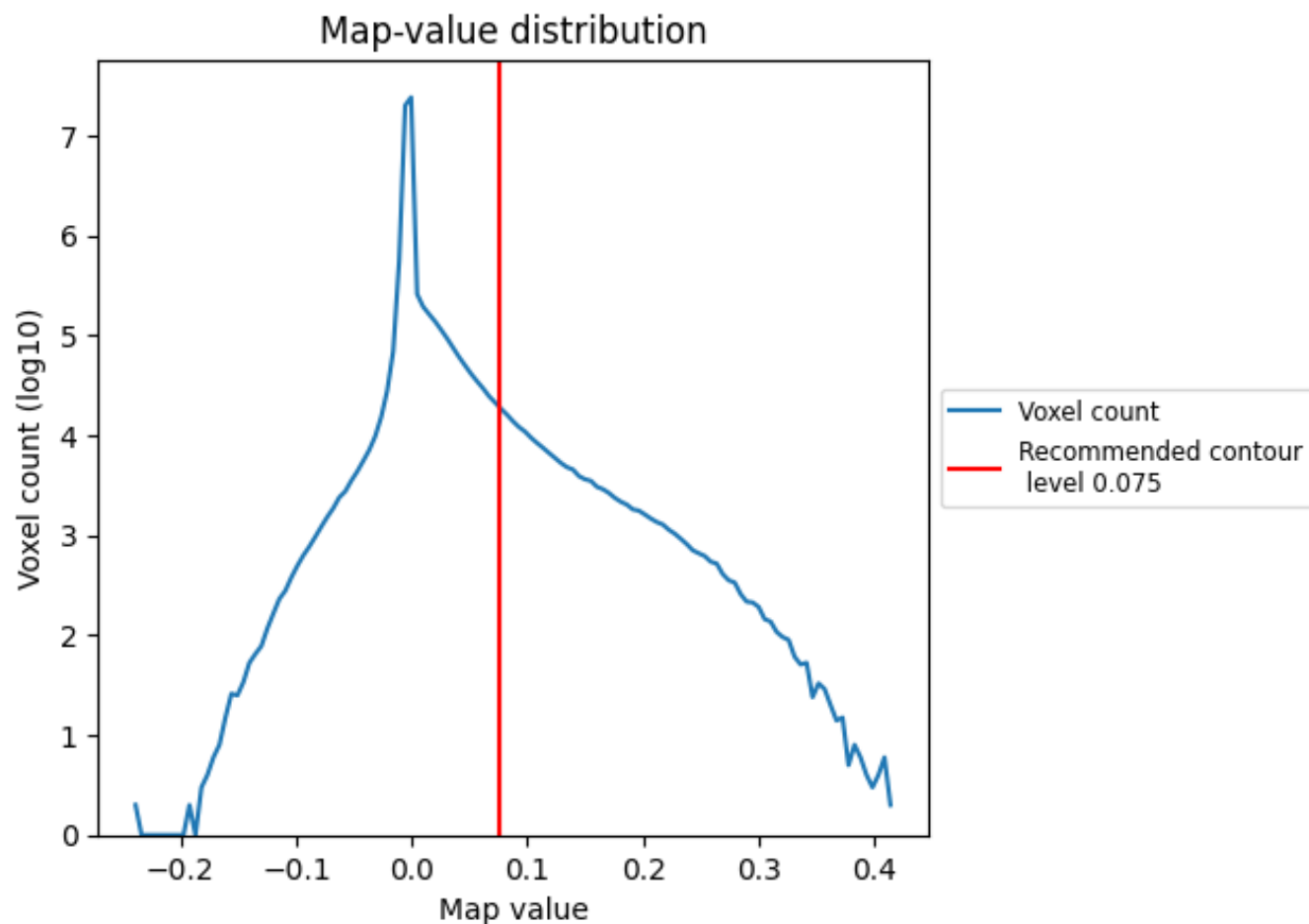
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

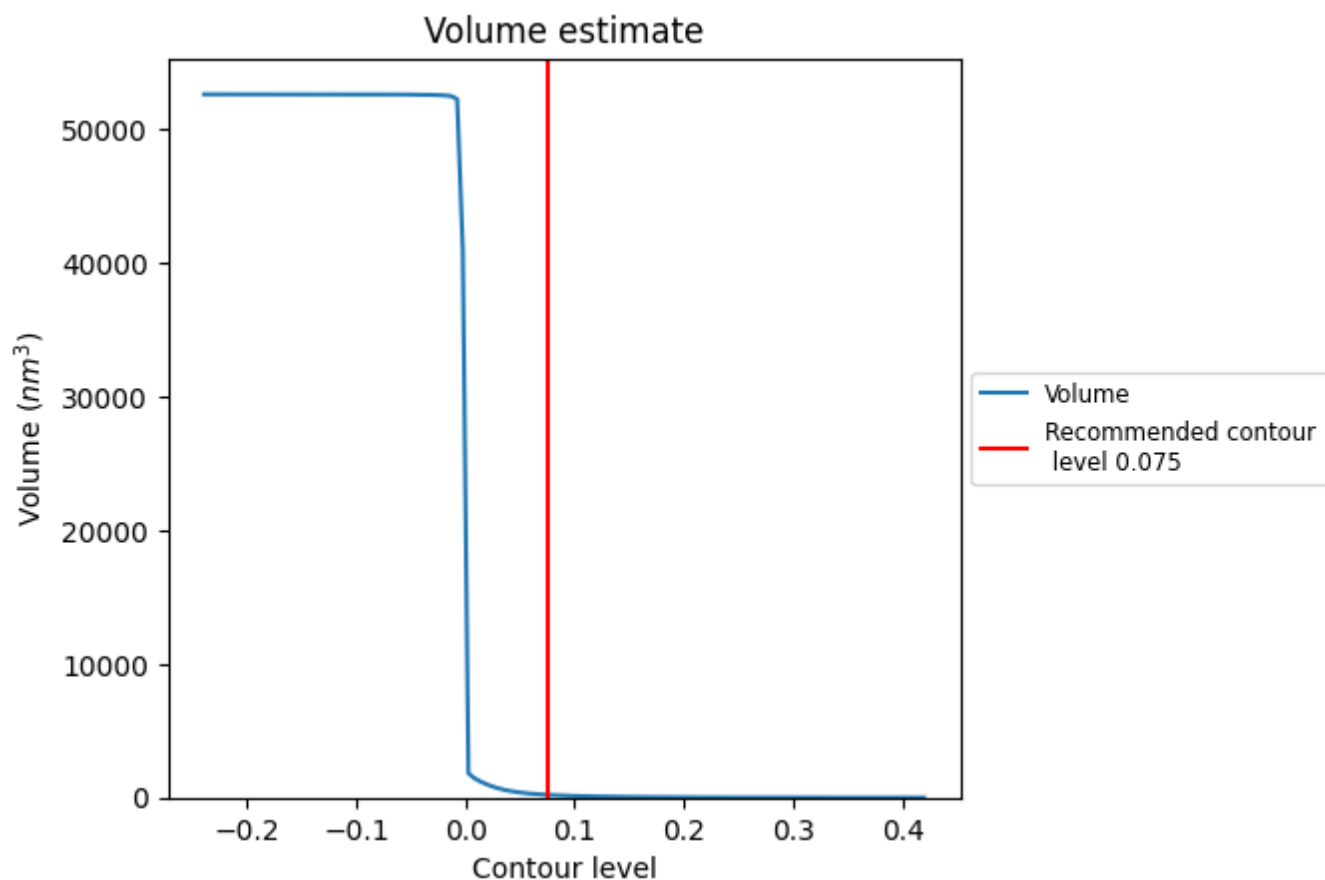
This section contains the results of statistical analysis of the map.

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.

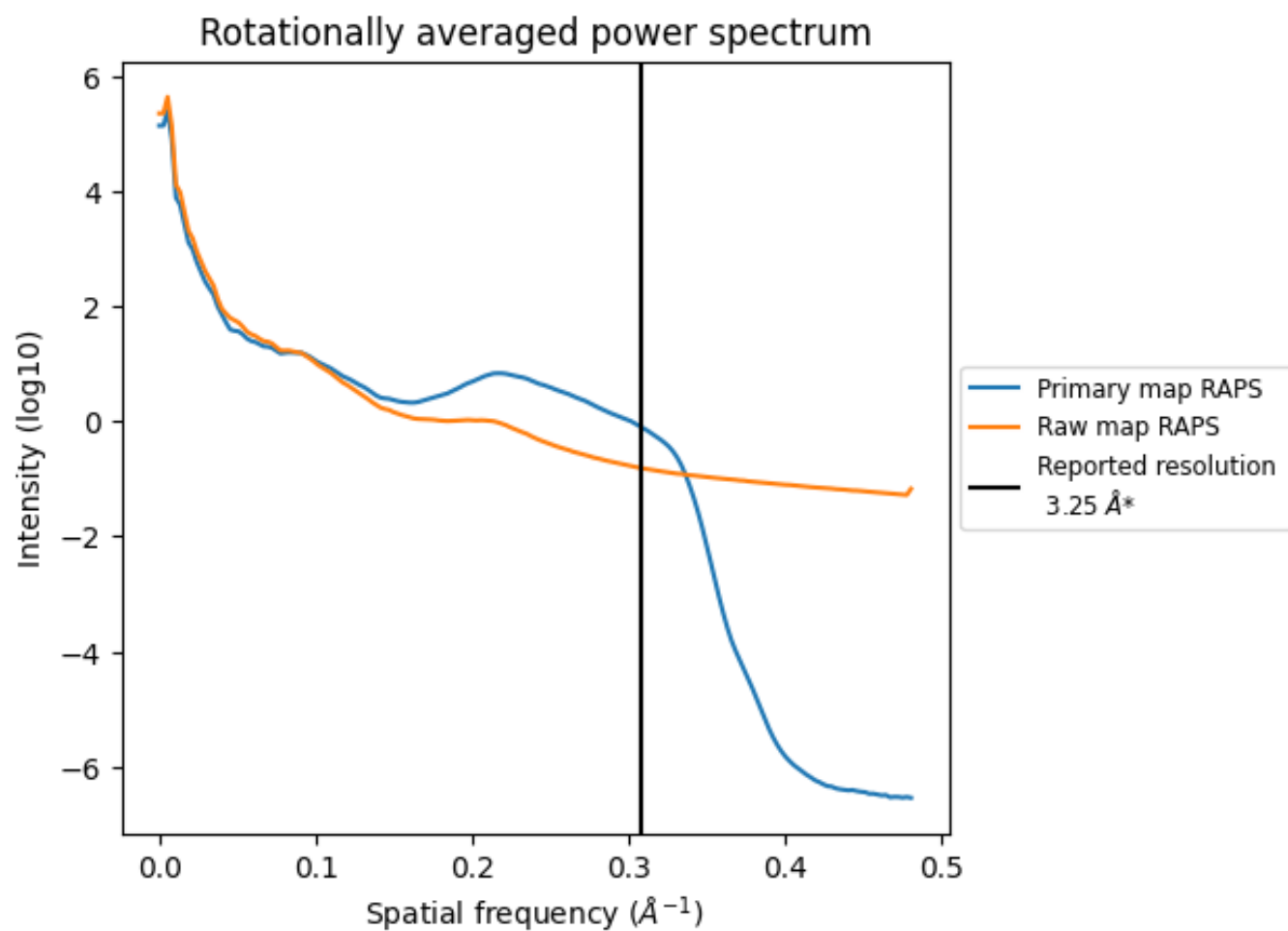
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 202 nm³; this corresponds to an approximate mass of 182 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 ⓘ

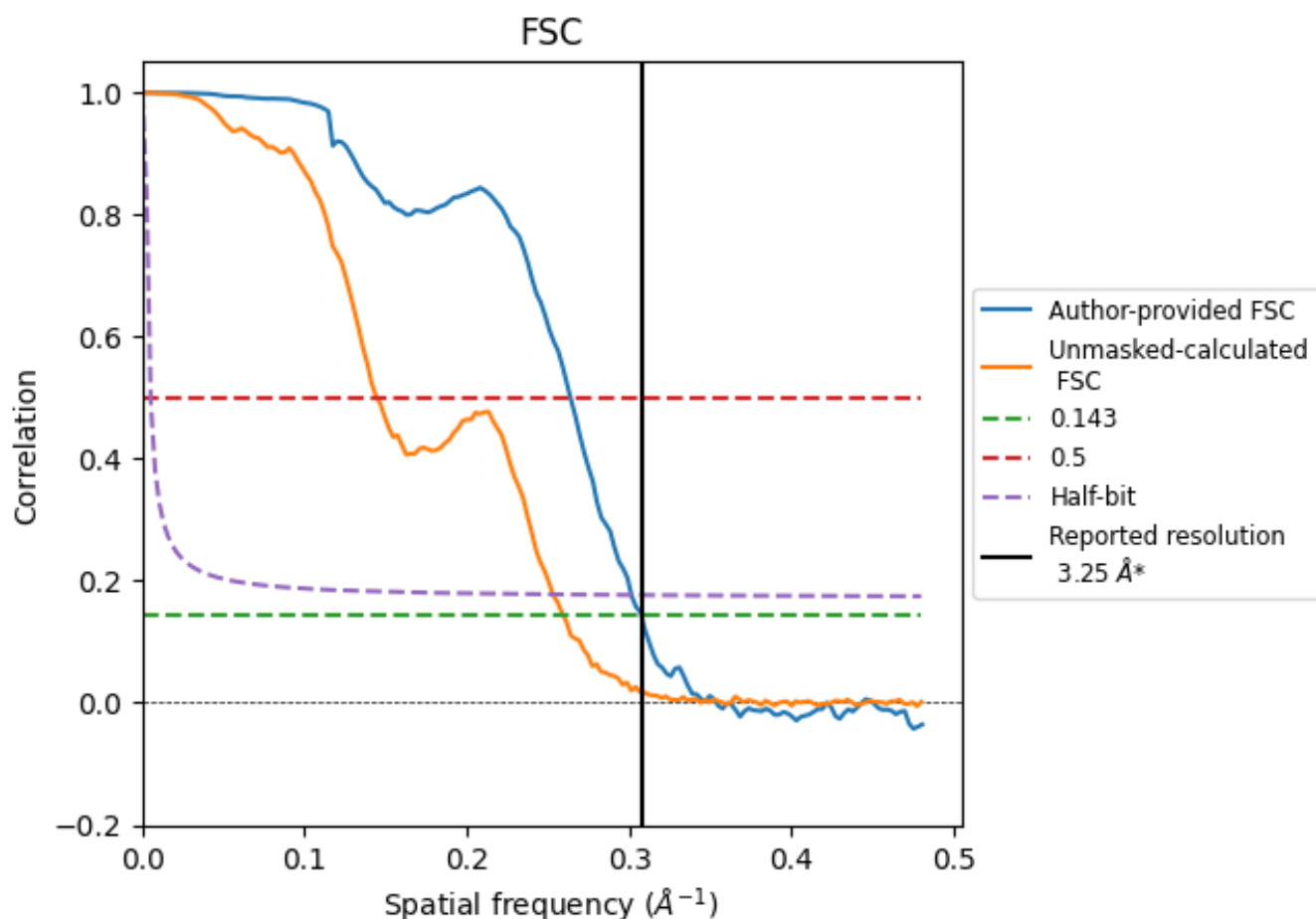


*Reported resolution corresponds to spatial frequency of $0.308 \text{ \AA}^{-1}$

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 0.308 Å⁻¹

8.2 Resolution estimates [i](#)

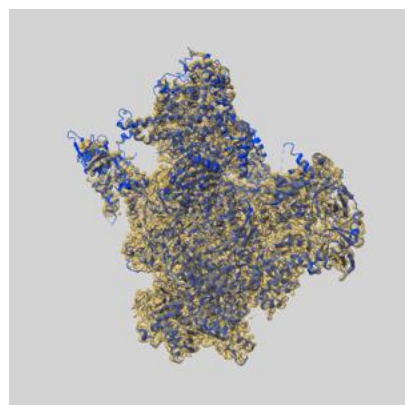
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.25	-	-
Author-provided FSC curve	3.25	3.79	3.32
Unmasked-calculated*	3.85	6.91	3.95

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.85 differs from the reported value 3.25 by more than 10 %

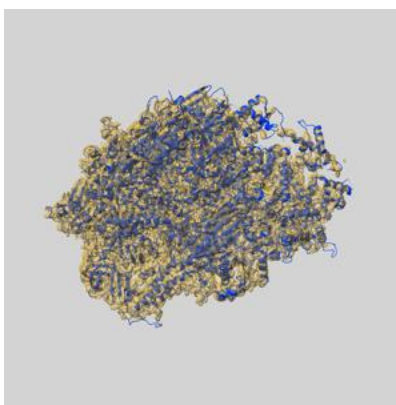
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10595 and PDB model 6TUT. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

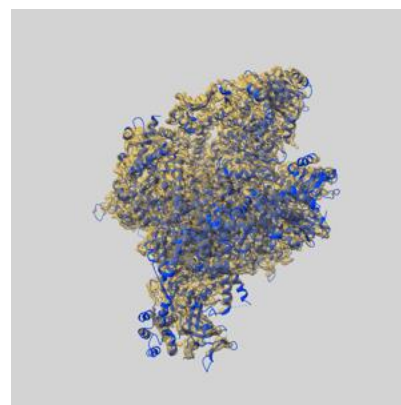
9.1 Map-model overlay [i](#)



X



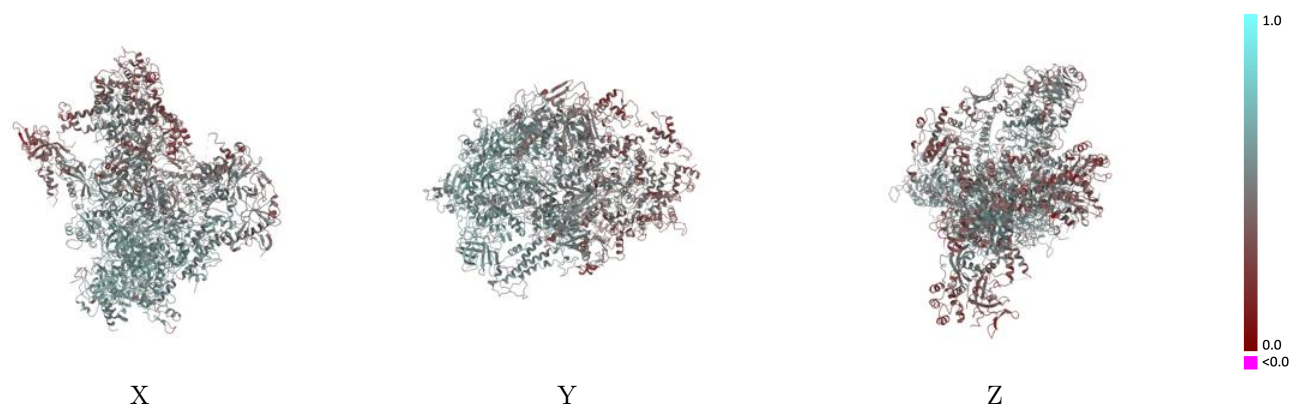
Y



Z

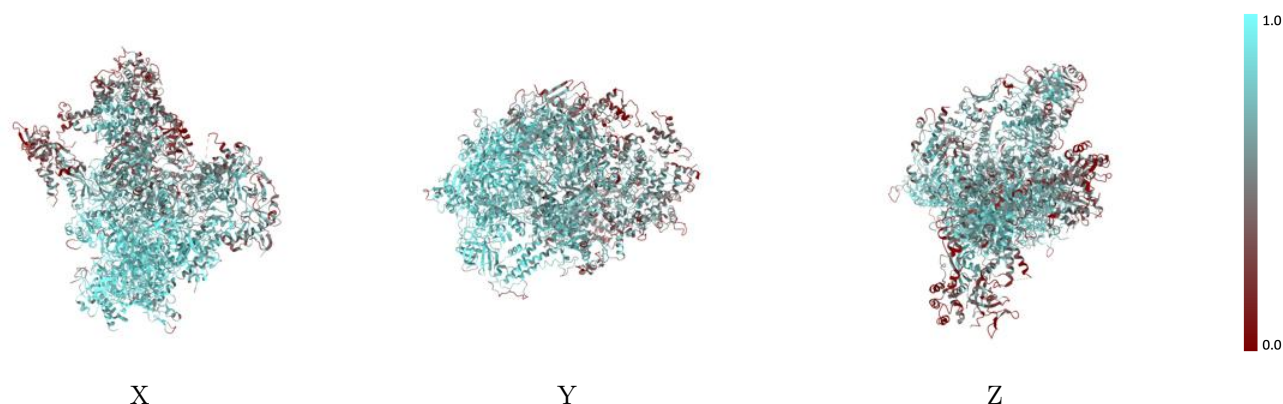
The images above show the 3D surface view of the map at the recommended contour level 0.075 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



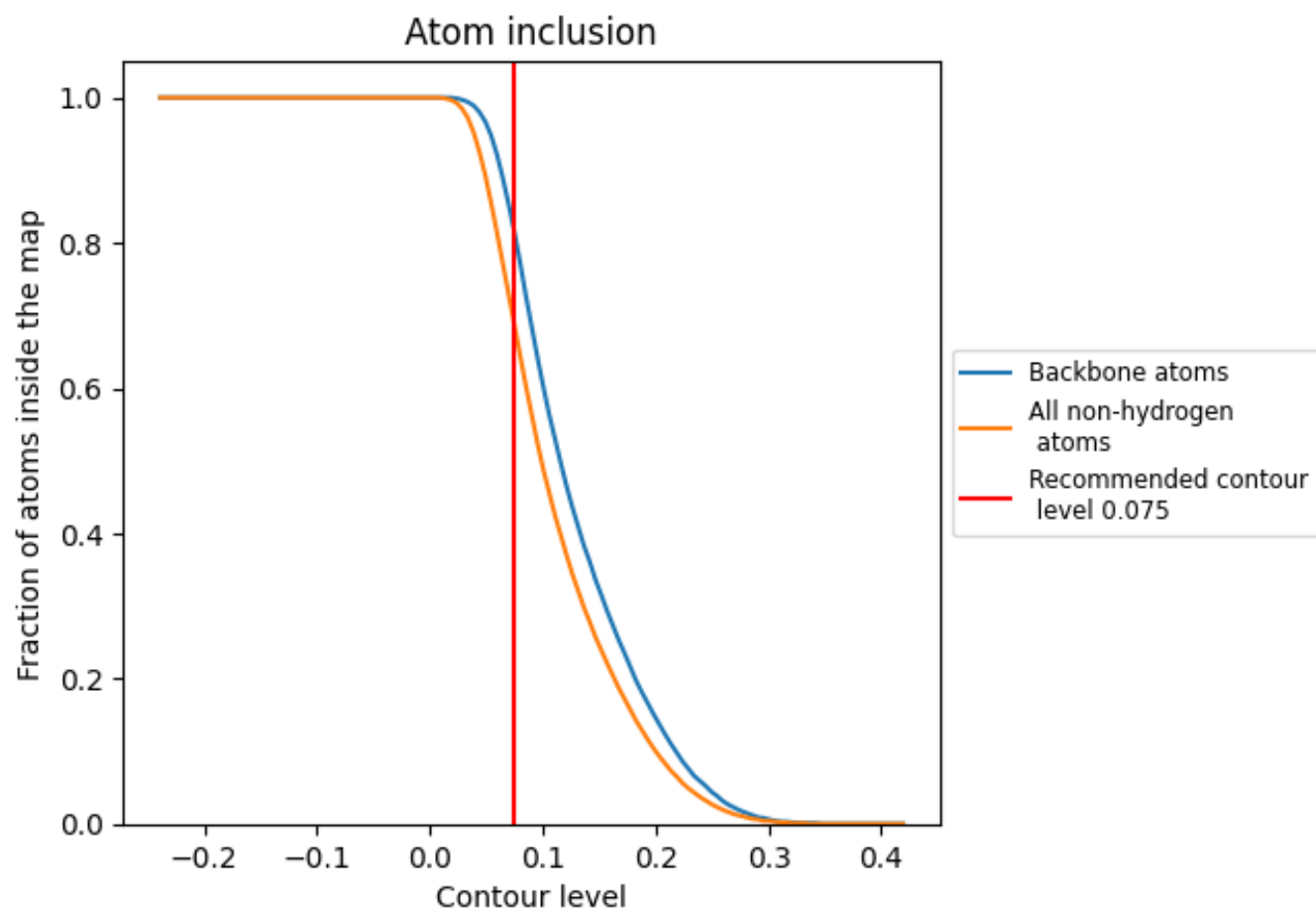
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.075).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 69% 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 (0.075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6860	 0.4900
A	 0.7660	 0.5280
B	 0.7990	 0.5480
C	 0.8440	 0.5590
D	 0.2940	 0.3260
E	 0.6280	 0.4320
F	 0.8530	 0.5610
G	 0.4770	 0.3950
H	 0.7740	 0.5360
I	 0.5610	 0.4210
J	 0.8800	 0.5730
K	 0.8710	 0.5860
L	 0.7510	 0.5170
M	 0.5030	 0.4300
N	 0.5010	 0.4390
O	 0.5510	 0.4070
P	 0.3280	 0.3190
Q	 0.5770	 0.4160
R	 0.4480	 0.3990

