



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 11:28 PM UTC

PDB ID : 7NVU / pdb_00007nvu
EMDB ID : EMD-12613
Title : RNA polymerase II core pre-initiation complex with open promoter DNA
Authors : Aibara, S.; Schilbach, S.; Cramer, P.
Deposited on : 2021-03-16
Resolution : 2.50 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:

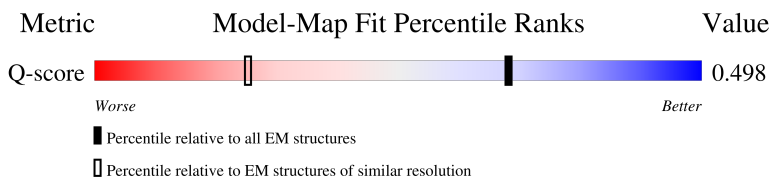
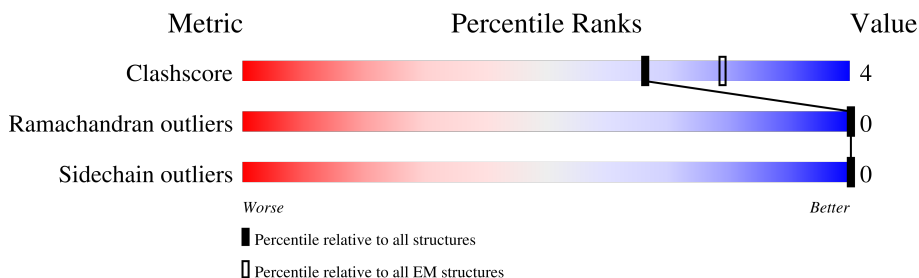
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 2.50 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.



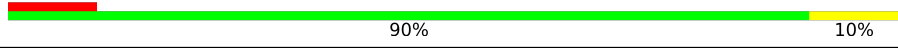
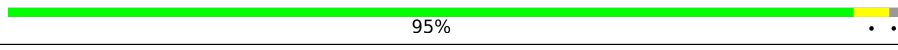
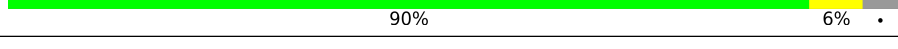
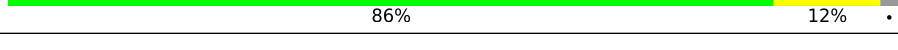
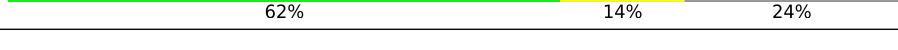
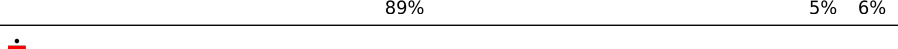
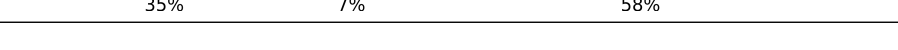
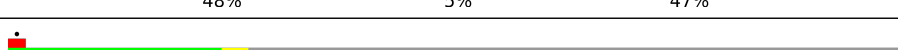
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7115 (2.00 - 3.00)

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	1970	
2	B	1174	
3	C	275	
4	D	142	

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Mol	Chain	Length	Quality of chain
5	E	210	
6	F	127	
7	G	172	
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	M	316	
14	N	106	
15	O	339	
16	Q	517	
17	R	249	
18	T	106	
19	U	376	
20	V	109	
21	W	439	
22	X	291	

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 44240 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 RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1423	Total	C	N	O	S	0	0
			11274	7092	2016	2094	72		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1136	Total	C	N	O	S	0	0
			9076	5739	1597	1676	64		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	257	Total	C	N	O	S	0	0
			2059	1294	351	408	6		

- Molecule 4 is a protein called RPOL4c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	128	Total	C	N	O	S	0	0
			1050	656	178	212	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	209	Total	C	N	O	S	0	0
			1721	1089	300	324	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	79	Total	C	N	O	S	0	0
			636	406	108	117	5		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1351	875	219	249	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	114	Total	C	N	O	S	0	0
			928	571	166	180	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	64	Total	C	N	O	S	0	0
			507	328	86	87	6		

- Molecule 11 is a protein called RNA_pol_L_2 domain-containing protein.

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

- Molecule 12 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	44	Total	C	N	O	S	0	0
			373	231	72	64	6		

- Molecule 13 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	298	Total	C	N	O	S	0	0
			2301	1435	409	439	18		

- Molecule 14 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	44	Total	C	N	O	P	0	0
			914	431	178	262	43		

- Molecule 15 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	179	Total	C	N	O	S	0	0
			1422	923	251	241	7		

- Molecule 16 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	138	Total	C	N	O	S	0	0
			1138	719	208	208	3		

- Molecule 17 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	222	Total	C	N	O	S	0	0
			1788	1127	320	338	3		

- Molecule 18 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	46	Total	C	N	O	P	0	0
			911	431	160	274	46		

- Molecule 19 is a protein called Transcription initiation factor IIA subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	113	Total	C	N	O	S	0	0
			930	585	152	189	4		

- Molecule 20 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	99	Total	C	N	O	S	0	0
			806	510	142	151	3		

- Molecule 21 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	187	Total	C	N	O	S	0	0
			1535	964	275	285	11		

- Molecule 22 is a protein called Transcription initiation factor IIE subunit beta.

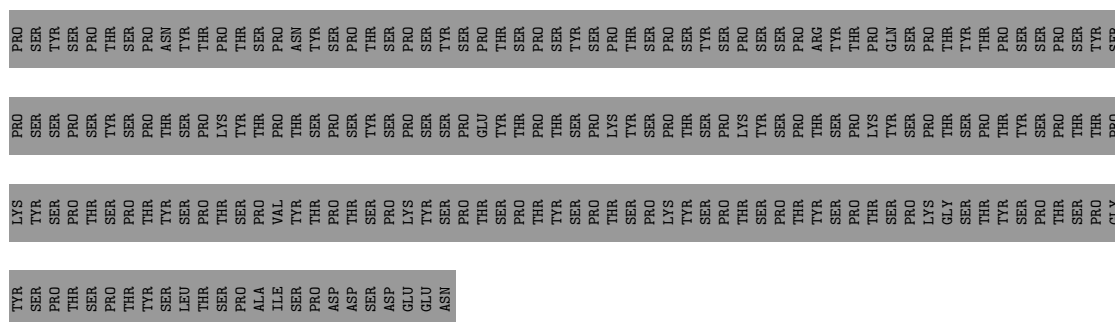
Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	171	Total	C	N	O	S	0	0
			1403	895	243	261	4		

- Molecule 23 is ZINC ION (CCD ID: ZN) (formula: Zn).

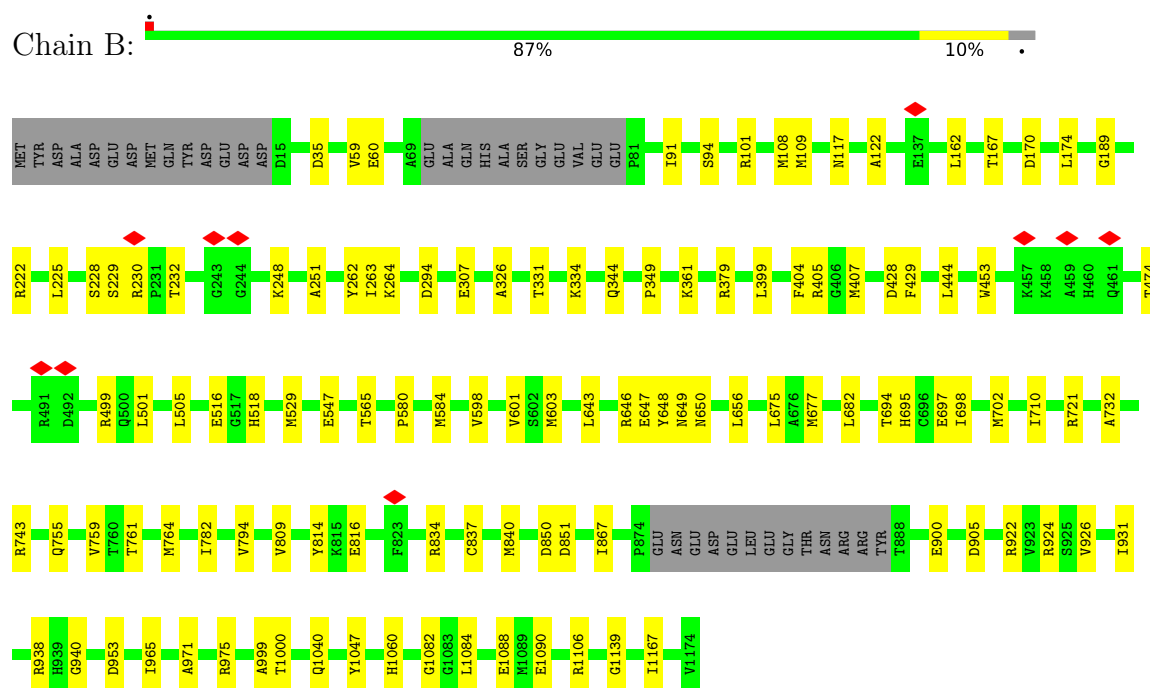
Mol	Chain	Residues	Atoms		AltConf
23	A	2	Total	Zn	0
			2	2	
23	B	1	Total	Zn	0
			1	1	
23	C	1	Total	Zn	0
			1	1	
23	I	2	Total	Zn	0
			2	2	
23	J	1	Total	Zn	0
			1	1	
23	L	1	Total	Zn	0
			1	1	
23	M	1	Total	Zn	0
			1	1	
23	W	1	Total	Zn	0
			1	1	

- Molecule 24 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

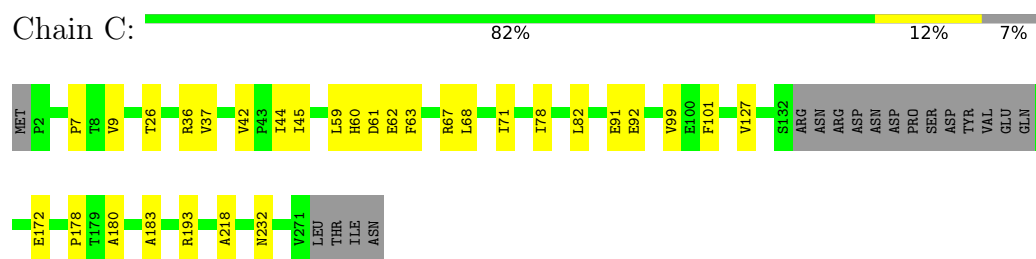
Mol	Chain	Residues	Atoms		AltConf
24	A	1	Total	Mg	0
			1	1	



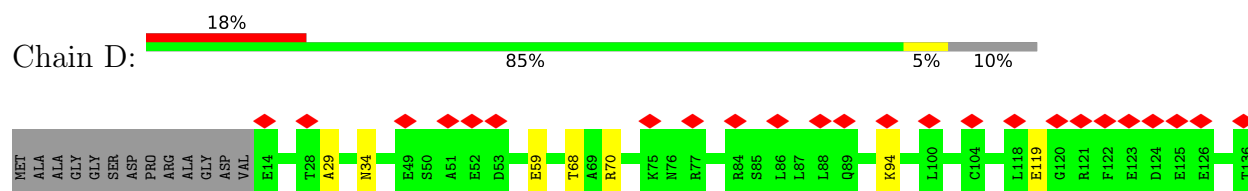
- Molecule 2: DNA-directed RNA polymerase subunit beta



- Molecule 3: DNA-directed RNA polymerase II subunit RPB3



- Molecule 4: RPOL4c domain-containing protein





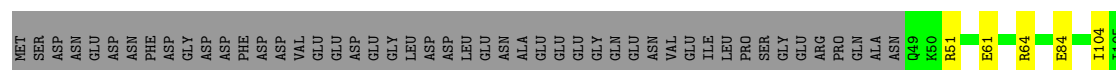
- Molecule 5: DNA-directed RNA polymerase II subunit E

Chain E: 86% 14%



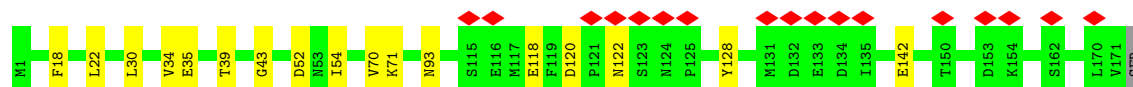
- Molecule 6: DNA-directed RNA polymerase II subunit F

Chain F: 55% 7% 38%



- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G: 10% 90% 10%



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

Chain H: 95%



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

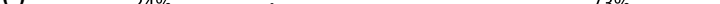
Chain I: 77% 14% 9%

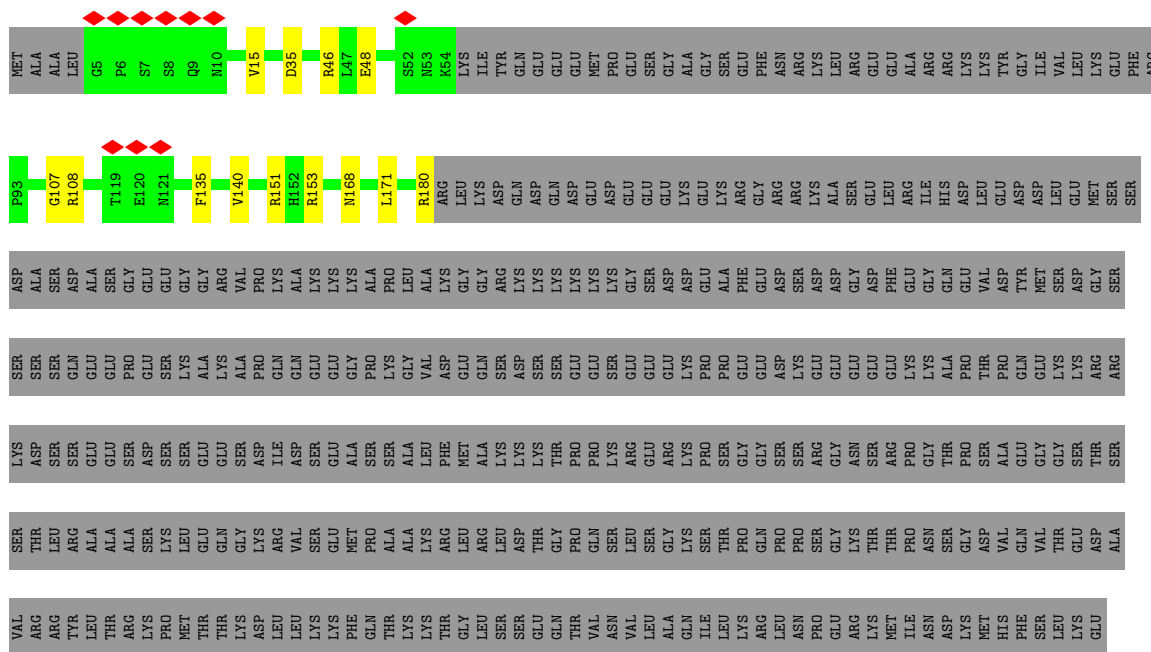


- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

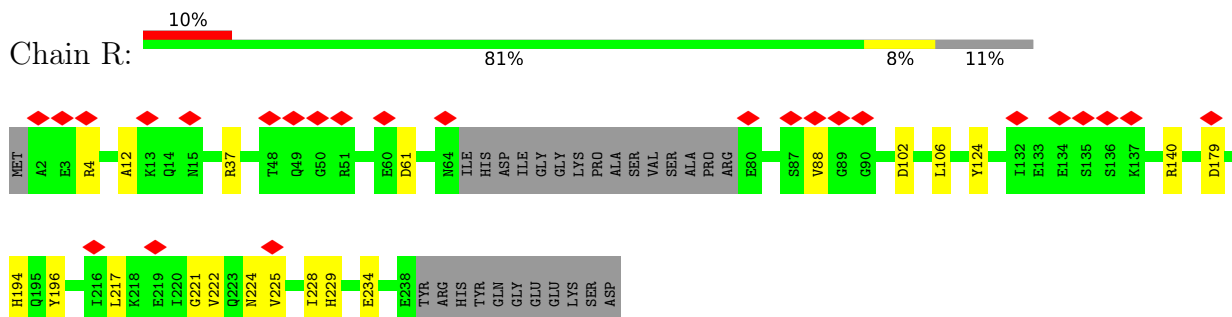
Chain J: 90% 6%



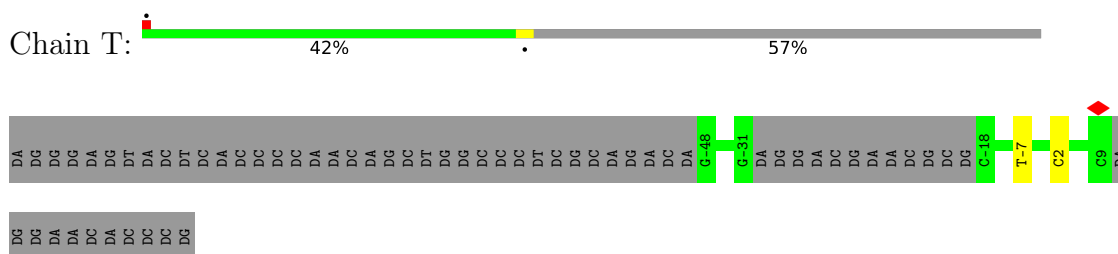
- Chain Q:  24% 73%



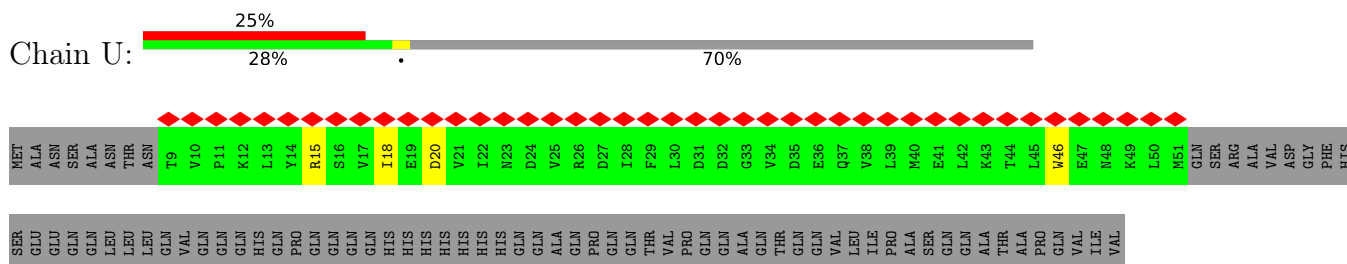
- Molecule 17: General transcription factor IIF subunit 2



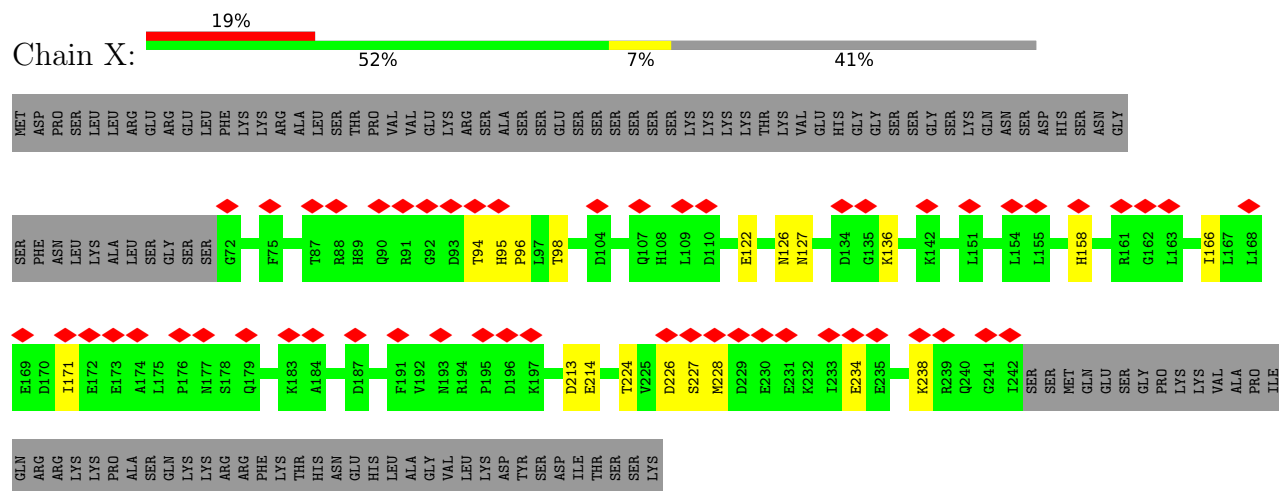
- Molecule 18: Template DNA



- Molecule 19: Transcription initiation factor IIA subunit 1



Chain X:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	255110	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 ($e^-/\text{\AA}^2$)	43	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	77.338	Depositor
Minimum map value	-43.445	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.981	Depositor
Recommended contour level	3	Depositor
Map size (Å)	472.49997, 472.49997, 472.49997	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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	A	0.15	0/11479	0.27	0/15496
2	B	0.16	0/9257	0.28	0/12493
3	C	0.17	0/2102	0.29	0/2857
4	D	0.07	0/1064	0.18	0/1428
5	E	0.12	0/1752	0.23	0/2366
6	F	0.16	0/646	0.28	0/871
7	G	0.10	0/1382	0.21	0/1874
8	H	0.14	0/1207	0.25	0/1628
9	I	0.12	0/949	0.25	0/1284
10	J	0.18	0/516	0.27	0/696
11	K	0.16	0/939	0.24	0/1271
12	L	0.16	0/378	0.30	0/500
13	M	0.12	0/2337	0.24	0/3154
14	N	0.15	0/1027	0.38	0/1585
15	O	0.11	0/1448	0.26	0/1948
16	Q	0.08	0/1167	0.21	0/1576
17	R	0.09	0/1817	0.21	0/2445
18	T	0.16	0/1016	0.40	0/1560
19	U	0.08	0/945	0.23	0/1274
20	V	0.11	0/816	0.24	0/1105
21	W	0.09	0/1560	0.23	0/2097
22	X	0.08	0/1427	0.23	0/1916
All	All	0.14	0/45231	0.26	0/61424

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	538	VAL	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	11274	0	11406	125	0
2	B	9076	0	9116	77	0
3	C	2059	0	2007	28	0
4	D	1050	0	1033	5	0
5	E	1721	0	1737	18	0
6	F	636	0	665	8	0
7	G	1351	0	1358	14	0
8	H	1186	0	1147	5	0
9	I	928	0	859	13	0
10	J	507	0	523	3	0
11	K	920	0	942	11	0
12	L	373	0	378	6	0
13	M	2301	0	2316	12	0
14	N	914	0	495	4	0
15	O	1422	0	1514	11	0
16	Q	1138	0	1103	8	0
17	R	1788	0	1819	13	0
18	T	911	0	505	2	0
19	U	930	0	888	6	0
20	V	806	0	818	5	0
21	W	1535	0	1540	13	0
22	X	1403	0	1428	11	0
23	A	2	0	0	0	0
23	B	1	0	0	0	0
23	C	1	0	0	0	0
23	I	2	0	0	0	0
23	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	L	1	0	0	0	0
23	M	1	0	0	0	0
23	W	1	0	0	0	0
24	A	1	0	0	0	0
All	All	44240	0	43597	345	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 (345) 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)
3:C:67:ARG:NH2	10:J:3:ILE:O	1.90	1.03
8:H:8:ASP:OD2	8:H:32:SER:OG	1.89	0.91
2:B:529:MET:HE1	2:B:698:ILE:HD12	1.62	0.81
1:A:1471:PHE:CD1	6:F:106:ILE:HD11	2.16	0.80
1:A:1208:SER:O	1:A:1260:ARG:NH1	2.15	0.80
2:B:60:GLU:OE2	17:R:140:ARG:NH1	2.14	0.80
1:A:430:ARG:NH2	13:M:26:ASP:OD2	2.14	0.79
5:E:51:GLY:O	5:E:54:ARG:NH1	2.16	0.79
5:E:3:ASP:OD2	5:E:49:SER:OG	2.01	0.79
1:A:863:ARG:NH2	1:A:1129:ASN:OD1	2.15	0.79
1:A:1178:ASP:OD2	1:A:1260:ARG:NH2	2.17	0.78
1:A:535:MET:O	1:A:669:TYR:OH	2.02	0.78
1:A:33:ARG:NH1	2:B:1139:GLY:O	2.19	0.76
1:A:1115:LYS:NZ	1:A:1338:THR:O	2.19	0.76
17:R:224:ASN:ND2	17:R:234:GLU:OE2	2.19	0.75
2:B:474:THR:OG1	2:B:732:ALA:O	2.04	0.75
15:O:188:ARG:NH2	19:U:321:SER:OG	2.20	0.75
2:B:721:ARG:NH1	2:B:940:GLY:O	2.20	0.75
15:O:206:GLU:OE1	15:O:236:LYS:NZ	2.20	0.74
1:A:1416:ARG:NH1	1:A:1434:GLU:OE2	2.19	0.74
1:A:902:GLU:OE1	1:A:985:ARG:NH2	2.20	0.74
2:B:59:VAL:HG21	2:B:91:ILE:HD11	1.68	0.73
2:B:344:GLN:O	2:B:361:LYS:NZ	2.21	0.73
2:B:501:LEU:HD12	2:B:505:LEU:HD12	1.72	0.72
16:Q:35:ASP:OD1	16:Q:108:ARG:NH2	2.22	0.72
2:B:529:MET:HE2	2:B:702:MET:HG3	1.72	0.71
22:X:234:GLU:OE1	22:X:238:LYS:NZ	2.22	0.71
1:A:463:THR:OG1	2:B:1090:GLU:OE2	2.07	0.71
3:C:67:ARG:NH1	3:C:149:LEU:O	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:107:GLY:O	16:Q:151:ARG:NH1	2.24	0.71
1:A:1440:MET:SD	2:B:1167:ILE:HD11	2.32	0.69
1:A:119:VAL:HG21	1:A:147:LEU:CD2	2.23	0.69
1:A:809:HIS:CE1	2:B:675:LEU:HD22	2.29	0.68
2:B:101:ARG:NH2	13:M:171:GLU:O	2.25	0.68
7:G:120:ASP:OD1	7:G:122:ASN:ND2	2.27	0.68
5:E:55:ARG:NH1	5:E:107:GLN:OE1	2.26	0.68
17:R:37:ARG:NH1	17:R:61:ASP:OD2	2.28	0.67
2:B:228:SER:OG	2:B:405:ARG:NH2	2.28	0.66
2:B:294:ASP:OD2	2:B:379:ARG:NH1	2.28	0.66
3:C:180:ALA:O	10:J:42:ARG:NH2	2.30	0.65
1:A:321:GLU:OE1	1:A:341:GLN:NE2	2.29	0.64
2:B:407:MET:HE1	2:B:444:LEU:HG	1.79	0.64
1:A:287:ASN:OD1	1:A:288:ASN:N	2.30	0.64
1:A:119:VAL:HG21	1:A:147:LEU:HD22	1.79	0.64
1:A:617:PRO:O	8:H:124:ARG:NH2	2.31	0.64
3:C:59:LEU:HD13	3:C:63:PHE:CE2	2.33	0.64
2:B:794:VAL:HG13	2:B:965:ILE:HG23	1.79	0.63
1:A:274:ASP:OD1	1:A:342:ARG:NH2	2.30	0.63
1:A:1166:LEU:O	1:A:1170:THR:OG1	2.11	0.62
4:D:34:ASN:O	4:D:68:THR:OG1	2.18	0.62
2:B:675:LEU:HD21	2:B:697:GLU:HG2	1.82	0.61
17:R:4:ARG:NH2	17:R:102:ASP:OD2	2.33	0.61
21:W:42:CYS:SG	21:W:75:ARG:NH2	2.73	0.61
5:E:79:GLU:OE2	5:E:86:THR:OG1	2.15	0.61
1:A:233:CYS:SG	1:A:244:ARG:NH1	2.73	0.61
7:G:30:LEU:HD22	7:G:70:VAL:HG11	1.82	0.61
1:A:479:TRP:CD1	2:B:931:ILE:HD12	2.35	0.60
3:C:9:VAL:HG11	11:K:105:PHE:CD1	2.37	0.60
11:K:64:PRO:HG3	11:K:72:ILE:HD12	1.83	0.60
13:M:128:ILE:HG23	13:M:183:VAL:HG11	1.82	0.60
19:U:366:ILE:HD11	20:V:48:LEU:HG	1.83	0.60
1:A:1253:GLU:N	1:A:1253:GLU:OE1	2.35	0.60
2:B:264:LYS:NZ	2:B:326:ALA:O	2.35	0.60
1:A:45:GLU:OE2	1:A:53:LYS:NZ	2.32	0.60
2:B:926:VAL:HG21	3:C:62:GLU:HG3	1.84	0.59
21:W:70:LYS:O	21:W:73:LYS:NZ	2.35	0.59
7:G:54:ILE:HD13	7:G:70:VAL:HG13	1.84	0.59
15:O:186:ARG:NH1	15:O:244:LEU:O	2.35	0.59
1:A:668:PHE:CE1	1:A:672:ILE:HD11	2.37	0.59
5:E:101:ARG:NH2	5:E:128:GLU:OE2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:118:GLU:OE1	7:G:118:GLU:N	2.35	0.59
1:A:458:PHE:HE2	1:A:484:LEU:HD11	1.68	0.59
2:B:428:ASP:OD1	2:B:429:PHE:N	2.35	0.59
2:B:677:MET:H	2:B:682:LEU:HD22	1.68	0.59
21:W:125:ALA:O	21:W:128:LYS:NZ	2.36	0.59
1:A:1242:ASP:HA	1:A:1262:MET:HE2	1.85	0.58
2:B:816:GLU:HB2	2:B:867:ILE:HD13	1.84	0.58
4:D:59:GLU:N	4:D:59:GLU:OE1	2.35	0.58
3:C:59:LEU:HD13	3:C:63:PHE:CD2	2.38	0.58
21:W:108:ASP:OD1	21:W:109:HIS:N	2.37	0.58
16:Q:15:VAL:O	16:Q:135:PHE:N	2.36	0.57
2:B:407:MET:HE1	2:B:444:LEU:CD2	2.34	0.57
1:A:790:GLN:NE2	1:A:791:GLN:O	2.37	0.57
2:B:643:LEU:HD11	2:B:656:LEU:HD11	1.86	0.57
3:C:172:GLU:OE2	12:L:58:ARG:NH2	2.38	0.56
1:A:813:ASP:OD1	9:I:100:HIS:NE2	2.37	0.56
4:D:119:GLU:N	4:D:119:GLU:OE1	2.38	0.56
7:G:93:ASN:O	7:G:128:TYR:OH	2.14	0.56
1:A:334:ARG:NH2	13:M:67:VAL:O	2.39	0.56
1:A:114:CYS:O	1:A:115:SER:OG	2.16	0.56
1:A:1242:ASP:O	1:A:1262:MET:N	2.39	0.56
3:C:9:VAL:HG11	11:K:105:PHE:HD1	1.69	0.56
1:A:924:TYR:OH	1:A:953:GLU:OE2	2.24	0.56
21:W:126:SER:OG	21:W:138:ASP:OD1	2.23	0.56
2:B:761:THR:HG23	2:B:1000:THR:HA	1.87	0.56
5:E:2:ASP:OD1	5:E:4:GLU:N	2.39	0.55
7:G:52:ASP:N	7:G:71:LYS:O	2.40	0.55
1:A:78:MET:SD	13:M:46:ILE:HD12	2.47	0.54
1:A:1414:ILE:O	1:A:1414:ILE:HG22	2.07	0.54
5:E:31:ASP:OD1	5:E:32:GLU:N	2.40	0.54
1:A:46:THR:HG23	1:A:58:MET:CG	2.37	0.54
1:A:362:SER:HB2	2:B:1084:LEU:HD12	1.90	0.54
1:A:521:VAL:HG13	1:A:535:MET:HE1	1.89	0.54
3:C:78:ILE:HG21	3:C:127:VAL:CG2	2.39	0.53
9:I:50:ASN:O	9:I:51:SER:OG	2.22	0.53
9:I:60:HIS:O	9:I:60:HIS:ND1	2.41	0.53
22:X:166:ILE:HG21	22:X:171:ILE:HD11	1.89	0.53
19:U:310:GLU:OE2	19:U:312:GLU:HB2	2.09	0.52
1:A:552:ASP:O	8:H:24:ARG:NH1	2.42	0.52
15:O:297:LYS:NZ	15:O:323:GLU:OE2	2.42	0.52
1:A:1030:SER:OG	5:E:162:ARG:NE	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:307:GLU:OE2	16:Q:168:ASN:ND2	2.42	0.52
13:M:128:ILE:HG23	13:M:183:VAL:CG1	2.38	0.52
15:O:206:GLU:HB3	15:O:207:PRO:HD3	1.90	0.52
1:A:621:ILE:HG23	1:A:621:ILE:O	2.10	0.52
7:G:39:THR:O	7:G:43:GLY:N	2.40	0.52
17:R:217:LEU:O	17:R:221:GLY:N	2.42	0.52
1:A:875:TYR:OH	6:F:61:GLU:OE2	2.19	0.52
1:A:106:VAL:O	1:A:110:VAL:HG12	2.09	0.52
9:I:27:LYS:N	9:I:36:LEU:O	2.38	0.52
2:B:764:MET:HE1	2:B:938:ARG:HH12	1.75	0.52
1:A:1468:THR:HG23	6:F:64:ARG:HB2	1.92	0.52
1:A:68:THR:O	1:A:68:THR:HG23	2.10	0.51
2:B:764:MET:HE1	2:B:938:ARG:NH1	2.25	0.51
1:A:65:ILE:O	1:A:78:MET:HE2	2.10	0.51
22:X:226:ASP:OD1	22:X:227:SER:N	2.44	0.51
5:E:6:GLU:OE2	5:E:55:ARG:NH2	2.43	0.51
1:A:184:CYS:O	1:A:184:CYS:SG	2.68	0.51
2:B:837:CYS:SG	2:B:840:MET:HE2	2.50	0.51
5:E:41:LYS:O	5:E:45:GLY:N	2.38	0.51
1:A:1236:ASN:O	1:A:1240:GLY:N	2.44	0.51
16:Q:153:ARG:NH1	16:Q:180:ARG:O	2.43	0.51
1:A:322:LEU:O	1:A:327:ARG:NH1	2.42	0.51
14:N:0:DC:H2'	14:N:1:DT:H72	1.93	0.51
2:B:809:VAL:HG21	3:C:60:HIS:CE1	2.45	0.51
4:D:29:ALA:O	4:D:94:LYS:NZ	2.34	0.51
1:A:786:ALA:O	1:A:787:VAL:HG13	2.11	0.51
22:X:95:HIS:ND1	22:X:96:PRO:O	2.43	0.51
2:B:399:LEU:HB3	2:B:453:TRP:CZ2	2.47	0.50
1:A:1171:ALA:N	1:A:1215:GLU:O	2.41	0.50
5:E:71:GLN:HB2	5:E:99:ILE:HD12	1.93	0.50
11:K:57:LEU:N	11:K:76:GLN:O	2.44	0.50
2:B:761:THR:N	2:B:764:MET:HE3	2.27	0.50
2:B:850:ASP:OD1	2:B:851:ASP:N	2.44	0.50
7:G:18:PHE:HA	7:G:22:LEU:HD12	1.92	0.50
20:V:62:LEU:HA	20:V:76:LEU:HD23	1.93	0.50
1:A:686:THR:OG1	2:B:782:ILE:O	2.23	0.50
1:A:1484:MET:SD	1:A:1484:MET:N	2.84	0.50
1:A:477:LEU:HB2	1:A:483:ARG:NH2	2.27	0.50
3:C:68:LEU:HA	3:C:71:ILE:HD12	1.94	0.49
22:X:158:HIS:NE2	22:X:166:ILE:HD11	2.27	0.49
1:A:1182:GLN:O	1:A:1190:GLN:NE2	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1186:VAL:HG12	1:A:1187:ALA:N	2.26	0.49
2:B:953:ASP:OD1	3:C:36:ARG:NH2	2.42	0.49
1:A:1185:VAL:HG12	1:A:1186:VAL:HG23	1.92	0.49
21:W:148:MET:SD	21:W:149:THR:N	2.85	0.49
1:A:1129:ASN:O	1:A:1130:ILE:C	2.55	0.49
15:O:280:PHE:HE1	15:O:296:ILE:HD12	1.78	0.49
20:V:57:ASN:OD1	20:V:58:PHE:N	2.46	0.49
1:A:1248:ASN:ND2	1:A:1254:LYS:O	2.44	0.49
1:A:908:THR:O	1:A:908:THR:HG22	2.12	0.48
15:O:196:ARG:NH1	18:T:-7:DT:O3'	2.46	0.48
22:X:224:THR:O	22:X:228:MET:HE2	2.13	0.48
1:A:478:PRO:O	1:A:479:TRP:CG	2.66	0.48
1:A:556:GLU:OE2	1:A:583:ARG:NH1	2.46	0.48
2:B:404:PHE:HA	2:B:407:MET:HE3	1.94	0.48
11:K:81:TYR:OH	11:K:89:ASN:OD1	2.28	0.48
3:C:78:ILE:HG21	3:C:127:VAL:HG22	1.95	0.48
1:A:668:PHE:CZ	1:A:672:ILE:HD11	2.49	0.48
1:A:823:VAL:HG11	1:A:831:LEU:HD22	1.96	0.48
1:A:893:GLU:OE1	5:E:197:SER:OG	2.21	0.48
2:B:814:TYR:OH	2:B:900:GLU:OE1	2.27	0.48
21:W:184:ILE:HD12	21:W:187:ILE:HD13	1.95	0.48
1:A:1286:ARG:NH2	2:B:251:ALA:O	2.46	0.48
2:B:407:MET:HE1	2:B:444:LEU:CG	2.43	0.48
2:B:565:THR:HG21	2:B:580:PRO:HG3	1.95	0.48
11:K:105:PHE:CE2	11:K:109:ILE:HD11	2.48	0.48
1:A:687:ILE:HD12	1:A:765:ASN:HB2	1.95	0.48
1:A:1216:LEU:HD12	1:A:1228:MET:SD	2.54	0.48
9:I:26:PRO:CB	9:I:53:ILE:HD12	2.44	0.48
13:M:80:LEU:HD12	13:M:80:LEU:O	2.14	0.47
15:O:203:ARG:NE	20:V:65:TYR:OH	2.45	0.47
1:A:595:ILE:HD11	1:A:675:VAL:HG11	1.95	0.47
2:B:248:LYS:HE3	16:Q:171:LEU:HD21	1.96	0.47
3:C:45:ILE:CD1	3:C:82:LEU:HD12	2.45	0.47
1:A:46:THR:HG22	1:A:47:THR:HG23	1.97	0.47
2:B:167:THR:HG23	2:B:170:ASP:H	1.80	0.47
2:B:710:ILE:HA	2:B:764:MET:HE2	1.97	0.47
1:A:460:ARG:HB2	1:A:501:MET:HE3	1.97	0.47
1:A:1179:PRO:O	9:I:33:ARG:NH1	2.47	0.47
13:M:30:GLY:HA2	13:M:45:VAL:HG22	1.97	0.47
17:R:194:HIS:ND1	17:R:196:TYR:O	2.45	0.47
1:A:46:THR:HG23	1:A:58:MET:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:ILE:HA	1:A:482:PHE:O	2.15	0.47
3:C:60:HIS:CE1	3:C:63:PHE:HB2	2.50	0.47
3:C:193:ARG:NH2	3:C:218:ALA:O	2.47	0.47
14:N:38:DT:H2'	14:N:39:DT:H72	1.97	0.47
1:A:1263:ASN:OD1	1:A:1264:SER:N	2.48	0.46
15:O:191:GLU:OE2	15:O:203:ARG:NH2	2.49	0.46
1:A:823:VAL:CG1	1:A:831:LEU:HD22	2.45	0.46
1:A:883:ILE:O	1:A:883:ILE:HG22	2.14	0.46
2:B:516:GLU:N	2:B:516:GLU:OE1	2.49	0.46
2:B:794:VAL:CG1	2:B:965:ILE:HG23	2.44	0.46
11:K:105:PHE:CD2	11:K:109:ILE:HD11	2.51	0.46
21:W:144:LEU:HD22	21:W:155:THR:H	1.79	0.46
21:W:154:CYS:O	21:W:158:HIS:N	2.41	0.46
1:A:706:ILE:HD11	1:A:787:VAL:CG1	2.46	0.46
2:B:905:ASP:OD1	2:B:924:ARG:NH1	2.46	0.46
3:C:7:PRO:O	11:K:104:ARG:NH1	2.47	0.46
12:L:22:CYS:SG	12:L:24:THR:OG1	2.71	0.46
22:X:122:GLU:OE1	22:X:126:ASN:ND2	2.48	0.46
1:A:1186:VAL:HG12	1:A:1187:ALA:H	1.80	0.46
2:B:229:SER:O	2:B:230:ARG:C	2.59	0.46
17:R:88:VAL:HG12	17:R:88:VAL:O	2.14	0.46
19:U:20:ASP:OD2	20:V:51:ARG:NH2	2.49	0.46
1:A:587:THR:OG1	8:H:119:GLY:O	2.26	0.46
6:F:51:ARG:NH2	6:F:122:GLU:OE1	2.47	0.46
1:A:530:SER:O	1:A:531:ASN:OD1	2.33	0.46
5:E:29:THR:HG23	5:E:31:ASP:OD1	2.16	0.46
2:B:743:ARG:O	2:B:922:ARG:NH1	2.49	0.46
3:C:7:PRO:HB3	3:C:26:THR:CG2	2.46	0.46
12:L:32:ASP:N	12:L:32:ASP:OD1	2.47	0.45
1:A:481:THR:O	1:A:483:ARG:NE	2.49	0.45
1:A:514:GLU:OE2	1:A:1468:THR:HG21	2.15	0.45
3:C:101:PHE:N	3:C:163:ALA:O	2.46	0.45
1:A:1475:LEU:CD2	7:G:22:LEU:HD11	2.47	0.45
2:B:262:TYR:O	2:B:263:ILE:HD13	2.17	0.45
17:R:228:ILE:HG23	17:R:229:HIS:N	2.32	0.45
1:A:862:ARG:NH1	2:B:1088:GLU:OE1	2.50	0.45
1:A:1347:LEU:HB3	5:E:137:ILE:HD13	2.00	0.44
2:B:499:ARG:NH1	2:B:518:HIS:O	2.49	0.44
1:A:686:THR:HG21	2:B:1040:GLN:O	2.17	0.44
1:A:1228:MET:SD	1:A:1255:LEU:HD12	2.57	0.44
1:A:26:LEU:HD13	1:A:31:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:185:ILE:HD12	5:E:209:VAL:CG2	2.47	0.44
1:A:422:ASP:OD1	1:A:422:ASP:N	2.49	0.44
1:A:1234:LYS:NZ	1:A:1298:LEU:O	2.49	0.44
2:B:225:LEU:HD22	2:B:349:PRO:HB2	1.99	0.44
1:A:61:ARG:O	1:A:73:THR:OG1	2.32	0.44
1:A:508:SER:OG	1:A:511:THR:HG22	2.17	0.44
2:B:109:MET:HE2	2:B:174:LEU:HD22	1.99	0.44
6:F:51:ARG:NH2	6:F:117:ASP:O	2.41	0.44
17:R:222:VAL:O	17:R:234:GLU:N	2.45	0.44
21:W:137:THR:HG22	21:W:138:ASP:N	2.33	0.44
19:U:18:ILE:HD11	19:U:46:TRP:CZ3	2.53	0.44
2:B:35:ASP:OD2	2:B:646:ARG:NH2	2.45	0.44
2:B:222:ARG:HB3	2:B:232:THR:HG21	2.00	0.44
1:A:1261:ILE:HG22	1:A:1262:MET:N	2.33	0.44
22:X:98:THR:HG22	22:X:136:LYS:HG2	1.99	0.44
8:H:74:GLU:N	8:H:74:GLU:OE1	2.51	0.43
10:J:9:THR:OG1	10:J:47:ARG:NH2	2.45	0.43
1:A:962:ASP:HB3	1:A:1043:ILE:HG23	2.00	0.43
9:I:79:PRO:O	9:I:95:VAL:HG23	2.18	0.43
1:A:542:LEU:HD23	1:A:774:ALA:HA	2.00	0.43
1:A:1473:LEU:HD22	6:F:104:ILE:HG21	2.00	0.43
1:A:908:THR:HG23	1:A:916:PHE:CE1	2.53	0.43
4:D:70:ARG:NH1	7:G:142:GLU:OE2	2.51	0.43
1:A:458:PHE:CE2	1:A:484:LEU:HD21	2.53	0.43
14:N:-1:DG:N2	18:T:2:DC:O2	2.52	0.43
22:X:126:ASN:OD1	22:X:127:ASN:N	2.51	0.43
7:G:30:LEU:O	7:G:34:VAL:HG22	2.18	0.43
1:A:64:VAL:HG12	1:A:64:VAL:O	2.19	0.43
3:C:91:GLU:O	3:C:92:GLU:C	2.62	0.43
17:R:179:ASP:OD1	17:R:179:ASP:N	2.52	0.43
1:A:1201:ASP:OD1	1:A:1201:ASP:N	2.52	0.42
3:C:44:ILE:HG21	3:C:178:PRO:HB3	2.01	0.42
13:M:31:ASP:OD1	13:M:33:ILE:HD11	2.19	0.42
2:B:759:VAL:HG12	2:B:999:ALA:HB2	2.00	0.42
5:E:111:THR:HG23	5:E:114:ALA:H	1.84	0.42
15:O:297:LYS:HB3	15:O:298:PRO:HD3	2.00	0.42
21:W:157:CYS:SG	21:W:159:THR:HG22	2.58	0.42
22:X:213:ASP:OD2	22:X:214:GLU:N	2.52	0.42
1:A:365:THR:HG22	1:A:482:PHE:CE2	2.54	0.42
1:A:457:ILE:HD11	1:A:515:ILE:HG23	2.01	0.42
1:A:906:LEU:HD13	1:A:966:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:27:LYS:O	9:I:36:LEU:N	2.46	0.42
13:M:273:GLU:O	13:M:277:ILE:HD12	2.20	0.42
1:A:1130:ILE:HD13	1:A:1411:LEU:HD22	2.02	0.42
1:A:1338:THR:OG1	1:A:1340:GLY:O	2.30	0.42
2:B:647:GLU:O	2:B:648:TYR:CG	2.72	0.42
11:K:24:ASP:OD2	11:K:74:ARG:NH2	2.52	0.42
2:B:851:ASP:OD2	12:L:17:TYR:OH	2.38	0.42
9:I:69:ILE:HG22	9:I:71:ASP:H	1.85	0.42
9:I:96:PHE:CD2	9:I:110:LEU:HD13	2.55	0.42
13:M:275:GLY:O	13:M:279:GLY:N	2.52	0.42
3:C:99:VAL:HG21	3:C:127:VAL:HG21	2.02	0.42
2:B:117:ASN:HA	2:B:189:GLY:HA3	2.02	0.42
3:C:183:ALA:HB3	3:C:232:ASN:HB3	2.02	0.42
1:A:1284:PHE:CE2	1:A:1288:ILE:HD11	2.55	0.41
2:B:649:ASN:O	2:B:650:ASN:HB2	2.20	0.41
1:A:863:ARG:HB3	1:A:1414:ILE:HG22	2.01	0.41
1:A:1344:MET:CE	5:E:137:ILE:HD11	2.50	0.41
3:C:63:PHE:O	3:C:67:ARG:HG3	2.20	0.41
9:I:49:ASP:OD1	9:I:49:ASP:N	2.51	0.41
21:W:40:ASN:ND2	21:W:42:CYS:O	2.53	0.41
1:A:491:PRO:HG3	1:A:535:MET:HE2	2.01	0.41
1:A:495:ASP:OD1	1:A:495:ASP:C	2.62	0.41
11:K:17:LYS:O	11:K:36:ASN:ND2	2.53	0.41
1:A:910:LYS:N	1:A:911:PRO:HD2	2.35	0.41
1:A:1475:LEU:HD23	7:G:22:LEU:HD11	2.02	0.41
2:B:547:GLU:OE1	17:R:124:TYR:OH	2.37	0.41
19:U:15:ARG:HA	19:U:18:ILE:HD12	2.02	0.41
1:A:865:ILE:HD13	1:A:1092:ALA:HB3	2.02	0.41
2:B:108:MET:O	2:B:162:LEU:HD12	2.21	0.41
2:B:834:ARG:HA	2:B:840:MET:HE3	2.02	0.41
2:B:1060:HIS:NE2	2:B:1082:GLY:O	2.41	0.41
3:C:61:ASP:OD2	12:L:48:ARG:NH1	2.50	0.41
7:G:34:VAL:HG23	7:G:35:GLU:N	2.35	0.41
1:A:359:VAL:HG12	2:B:1106:ARG:O	2.20	0.41
2:B:94:SER:O	2:B:122:ALA:HB1	2.21	0.41
13:M:15:CYS:HB3	13:M:18:HIS:HB2	2.02	0.41
1:A:154:CYS:SG	1:A:183:GLY:O	2.79	0.41
1:A:1454:VAL:HG12	1:A:1458:ILE:HD12	2.03	0.41
2:B:755:GLN:O	2:B:1047:TYR:OH	2.37	0.41
7:G:22:LEU:HD23	7:G:22:LEU:C	2.46	0.41
9:I:115:THR:O	9:I:115:THR:HG22	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:36:DT:H2"	14:N:37:DC:C6	2.56	0.41
1:A:547:LYS:O	1:A:553:VAL:HG21	2.21	0.41
2:B:331:THR:HG23	2:B:334:LYS:H	1.85	0.41
2:B:598:VAL:CG2	2:B:601:VAL:HG23	2.50	0.41
3:C:36:ARG:HD3	11:K:41:THR:OG1	2.21	0.41
3:C:37:VAL:O	3:C:42:VAL:HG23	2.20	0.41
16:Q:46:ARG:NH2	16:Q:48:GLU:OE2	2.54	0.41
17:R:12:ALA:HB2	17:R:106:LEU:HD23	2.02	0.41
21:W:107:LEU:HD21	21:W:184:ILE:HD11	2.03	0.41
1:A:365:THR:HG22	1:A:482:PHE:CD2	2.56	0.41
1:A:653:VAL:HG11	1:A:669:TYR:OH	2.20	0.41
1:A:693:ILE:HG22	1:A:694:ALA:N	2.35	0.41
5:E:44:PHE:CZ	5:E:58:LEU:HD23	2.56	0.41
9:I:69:ILE:O	9:I:72:VAL:HG22	2.20	0.41
12:L:15:MET:HE1	12:L:46:LYS:HE3	2.02	0.41
15:O:187:ALA:HB3	15:O:190:ALA:HB3	2.03	0.41
16:Q:140:VAL:HG23	16:Q:140:VAL:O	2.21	0.41
6:F:84:GLU:HG2	6:F:84:GLU:O	2.20	0.41
6:F:106:ILE:CG2	6:F:118:TRP:HB2	2.51	0.40
1:A:36:VAL:HG11	1:A:73:THR:HG21	2.03	0.40
2:B:501:LEU:HD12	2:B:505:LEU:CD1	2.48	0.40
17:R:225:VAL:O	17:R:225:VAL:HG13	2.21	0.40
1:A:495:ASP:OD1	1:A:497:ASP:OD1	2.40	0.40
1:A:628:VAL:HA	1:A:638:GLY:HA3	2.03	0.40
1:A:1184:THR:HG21	1:A:1258:ARG:HE	1.86	0.40
2:B:971:ALA:O	2:B:975:ARG:HG3	2.21	0.40
22:X:94:THR:HG22	22:X:94:THR:O	2.22	0.40
2:B:584:MET:HE1	2:B:603:MET:HB3	2.03	0.40
2:B:694:THR:HG22	2:B:695:HIS:CE1	2.57	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	1413/1970 (72%)	1374 (97%)	39 (3%)	0	100	100
2	B	1130/1174 (96%)	1091 (96%)	39 (4%)	0	100	100
3	C	253/275 (92%)	248 (98%)	5 (2%)	0	100	100
4	D	126/142 (89%)	124 (98%)	2 (2%)	0	100	100
5	E	207/210 (99%)	203 (98%)	4 (2%)	0	100	100
6	F	77/127 (61%)	77 (100%)	0	0	100	100
7	G	169/172 (98%)	168 (99%)	1 (1%)	0	100	100
8	H	146/150 (97%)	142 (97%)	4 (3%)	0	100	100
9	I	112/125 (90%)	106 (95%)	6 (5%)	0	100	100
10	J	62/67 (92%)	61 (98%)	1 (2%)	0	100	100
11	K	113/117 (97%)	110 (97%)	3 (3%)	0	100	100
12	L	42/58 (72%)	38 (90%)	4 (10%)	0	100	100
13	M	294/316 (93%)	289 (98%)	5 (2%)	0	100	100
15	O	177/339 (52%)	176 (99%)	1 (1%)	0	100	100
16	Q	134/517 (26%)	130 (97%)	4 (3%)	0	100	100
17	R	218/249 (88%)	215 (99%)	3 (1%)	0	100	100
19	U	109/376 (29%)	101 (93%)	8 (7%)	0	100	100
20	V	97/109 (89%)	95 (98%)	2 (2%)	0	100	100
21	W	185/439 (42%)	185 (100%)	0	0	100	100
22	X	169/291 (58%)	166 (98%)	3 (2%)	0	100	100
All	All	5233/7223 (72%)	5099 (97%)	134 (3%)	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	
1	A	1254/1749 (72%)	1254 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	994/1027 (97%)	994 (100%)	0	100	100
3	C	234/252 (93%)	234 (100%)	0	100	100
4	D	118/126 (94%)	118 (100%)	0	100	100
5	E	191/192 (100%)	191 (100%)	0	100	100
6	F	69/111 (62%)	69 (100%)	0	100	100
7	G	152/153 (99%)	152 (100%)	0	100	100
8	H	129/131 (98%)	129 (100%)	0	100	100
9	I	103/112 (92%)	103 (100%)	0	100	100
10	J	53/56 (95%)	53 (100%)	0	100	100
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	41/55 (74%)	41 (100%)	0	100	100
13	M	253/268 (94%)	253 (100%)	0	100	100
15	O	154/293 (53%)	154 (100%)	0	100	100
16	Q	121/448 (27%)	121 (100%)	0	100	100
17	R	196/218 (90%)	196 (100%)	0	100	100
19	U	105/324 (32%)	105 (100%)	0	100	100
20	V	90/98 (92%)	90 (100%)	0	100	100
21	W	169/373 (45%)	169 (100%)	0	100	100
22	X	154/261 (59%)	154 (100%)	0	100	100
All	All	4684/6353 (74%)	4684 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	673	GLN
1	A	792	ASN
1	A	905	ASN
1	A	926	ASN
1	A	947	HIS
1	A	1182	GLN
1	A	1194	ASN
1	A	1303	GLN
2	B	164	ASN

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Mol	Chain	Res	Type
2	B	197	GLN
2	B	1071	ASN
2	B	1129	ASN
2	B	1160	GLN
3	C	260	GLN
4	D	102	ASN
7	G	122	ASN
7	G	139	GLN
9	I	98	GLN
13	M	129	ASN
15	O	278	GLN
16	Q	129	GLN
16	Q	145	ASN
17	R	64	ASN
17	R	91	GLN
17	R	152	ASN
22	X	160	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

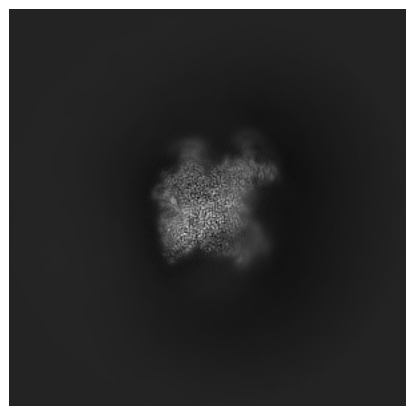
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12613. These allow visual inspection of the internal detail of the map and identification of artifacts.

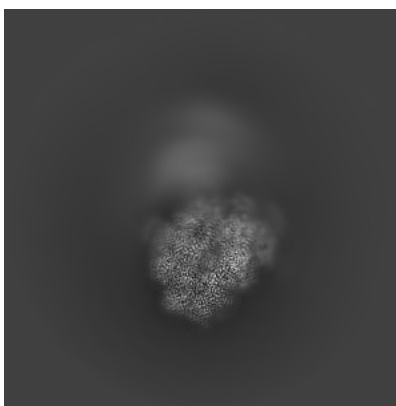
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

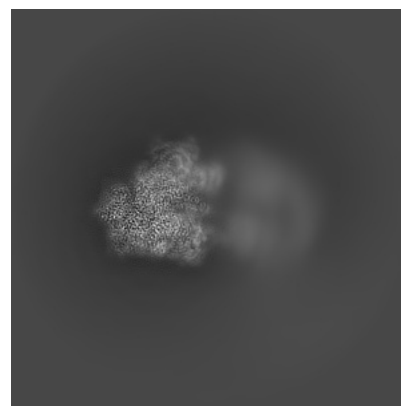
6.1.1 Primary map



X

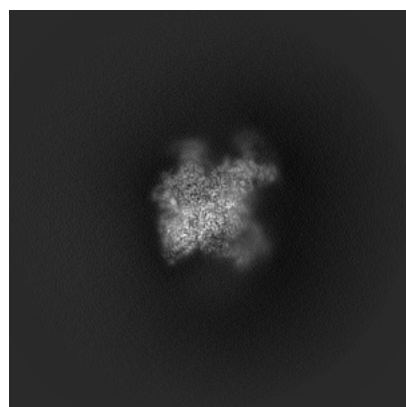


Y

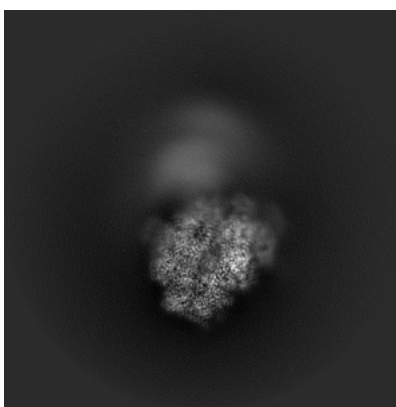


Z

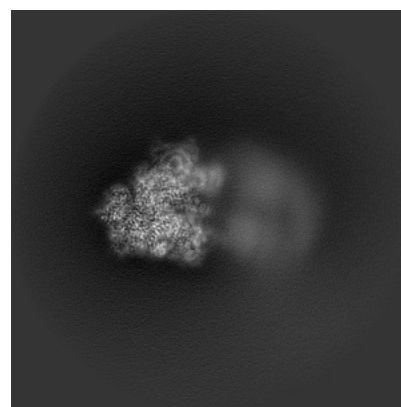
6.1.2 Raw map



X



Y

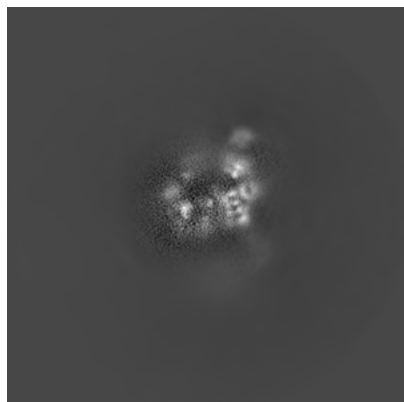


Z

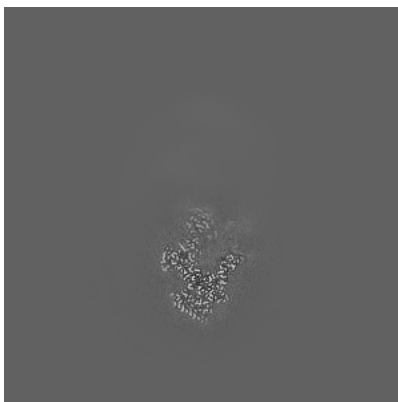
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

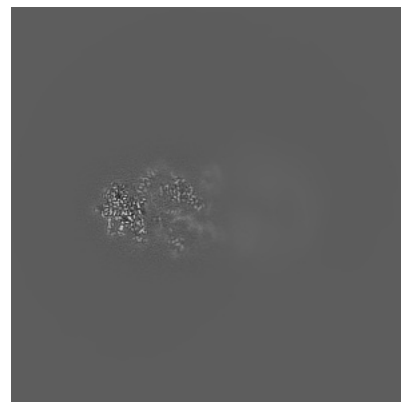
6.2.1 Primary map



X Index: 225



Y Index: 225

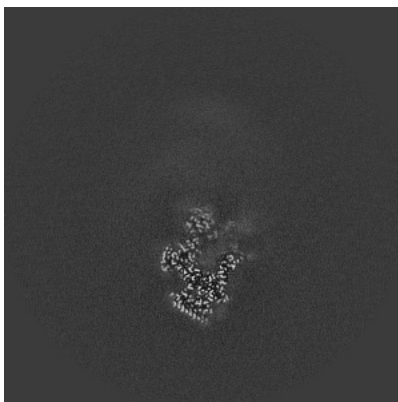


Z Index: 225

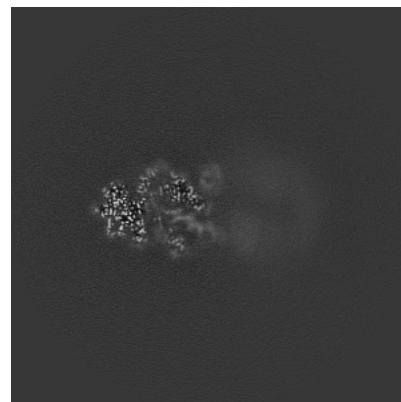
6.2.2 Raw map



X Index: 225



Y Index: 225

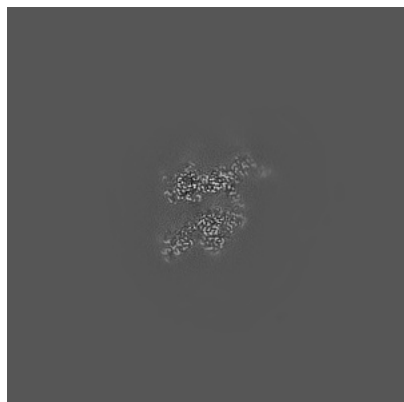


Z Index: 225

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

6.3 Largest variance slices [i](#)

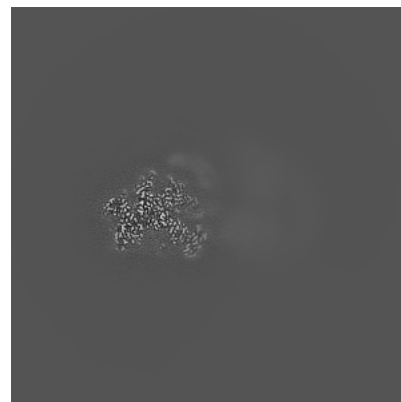
6.3.1 Primary map



X Index: 158

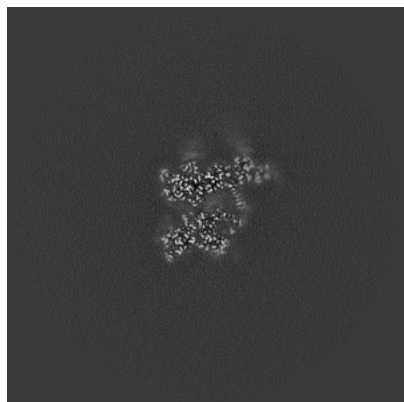


Y Index: 216

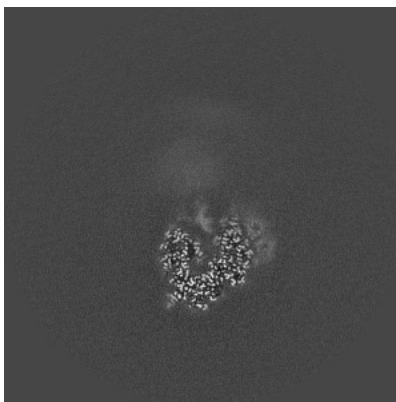


Z Index: 204

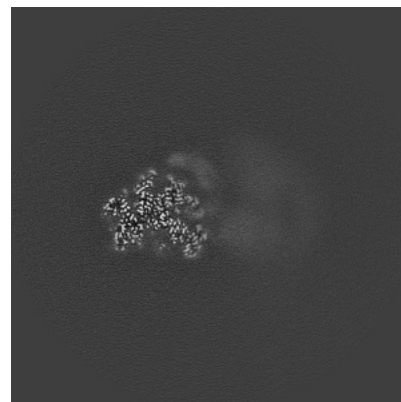
6.3.2 Raw map



X Index: 162



Y Index: 205

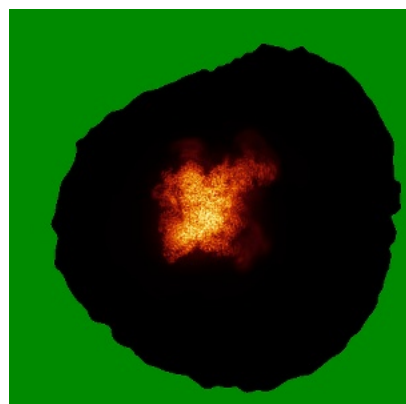


Z Index: 204

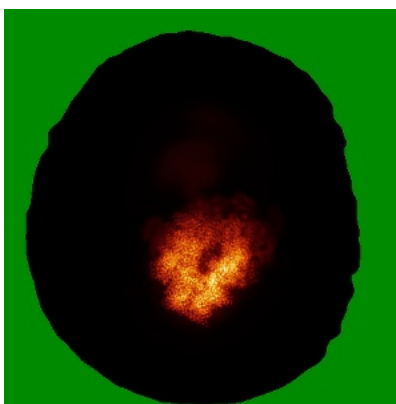
The images above show the largest variance slices of the map in three orthogonal directions.

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

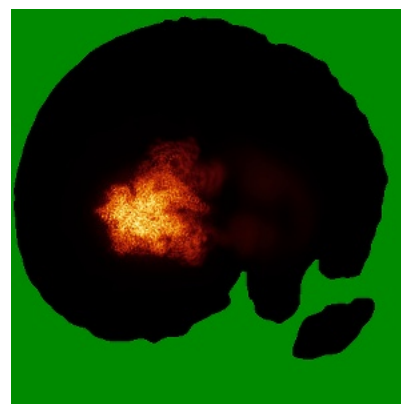
6.4.1 Primary map



X

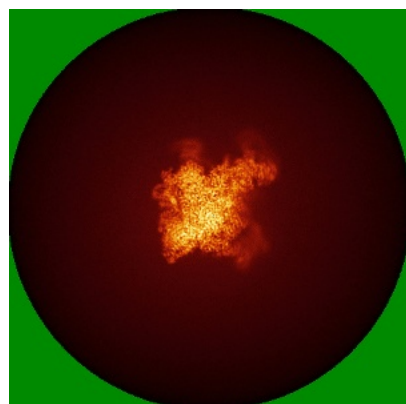


Y

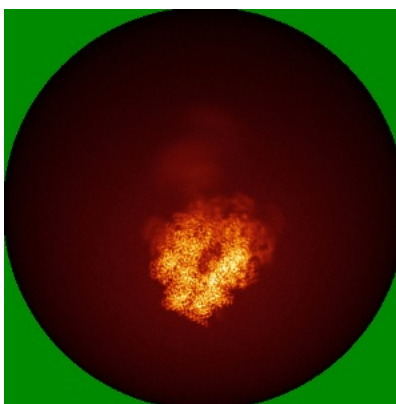


Z

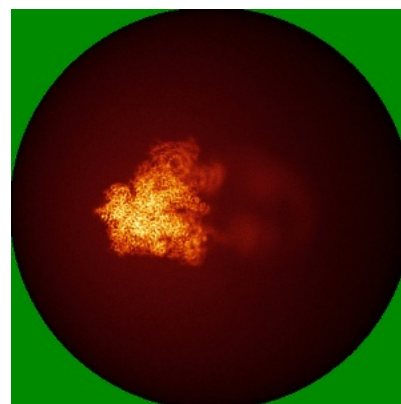
6.4.2 Raw map



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.

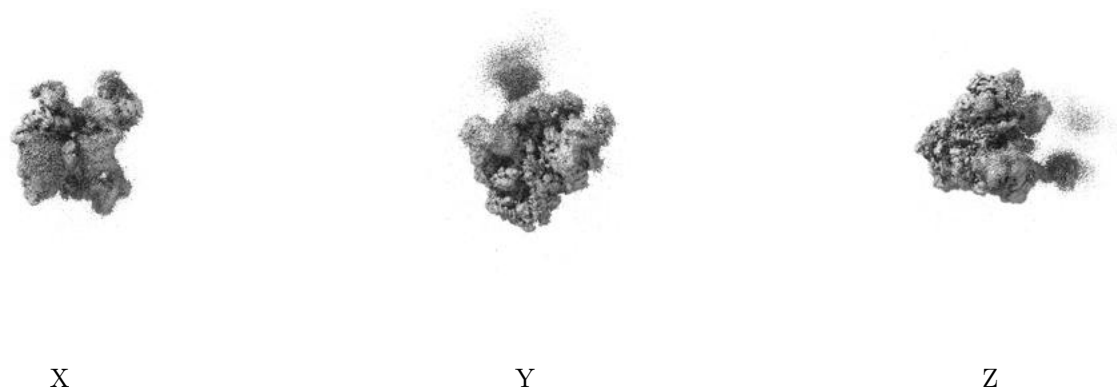
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.0. 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.

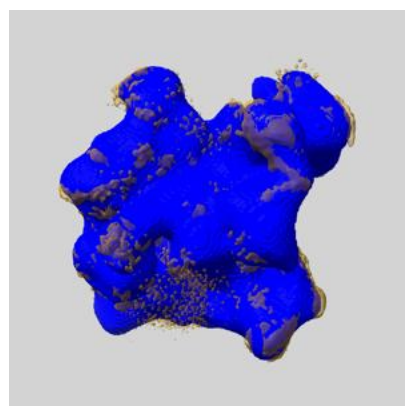
6.6 Mask visualisation [i](#)

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

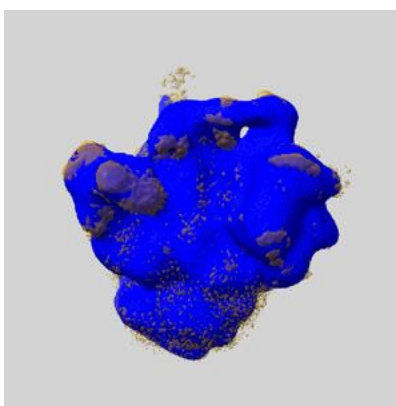
A mask typically either:

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

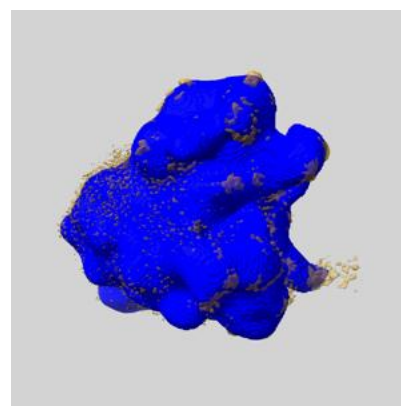
6.6.1 emd_12613_msk_1.map [i](#)



X



Y

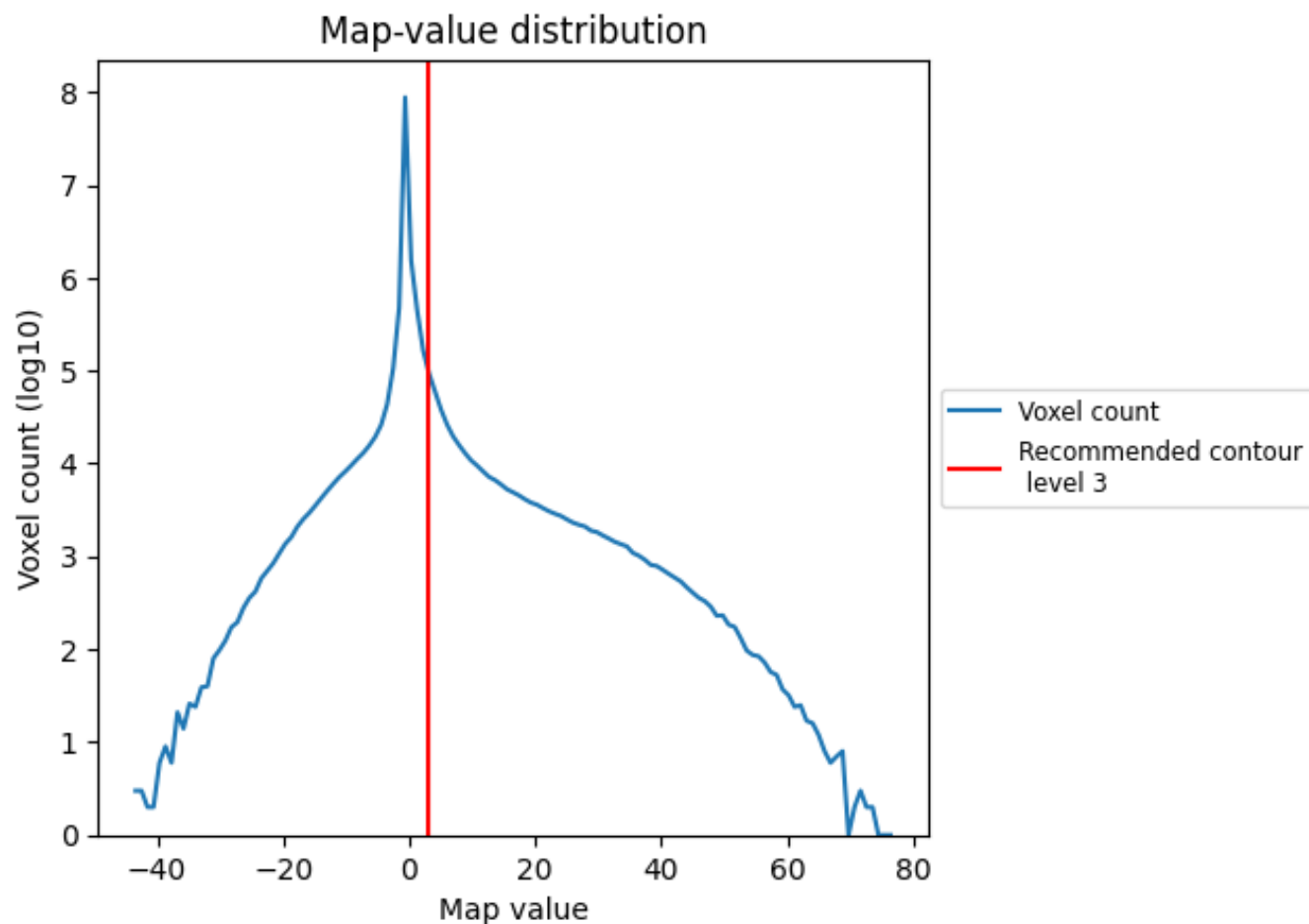


Z

7 Map analysis [i](#)

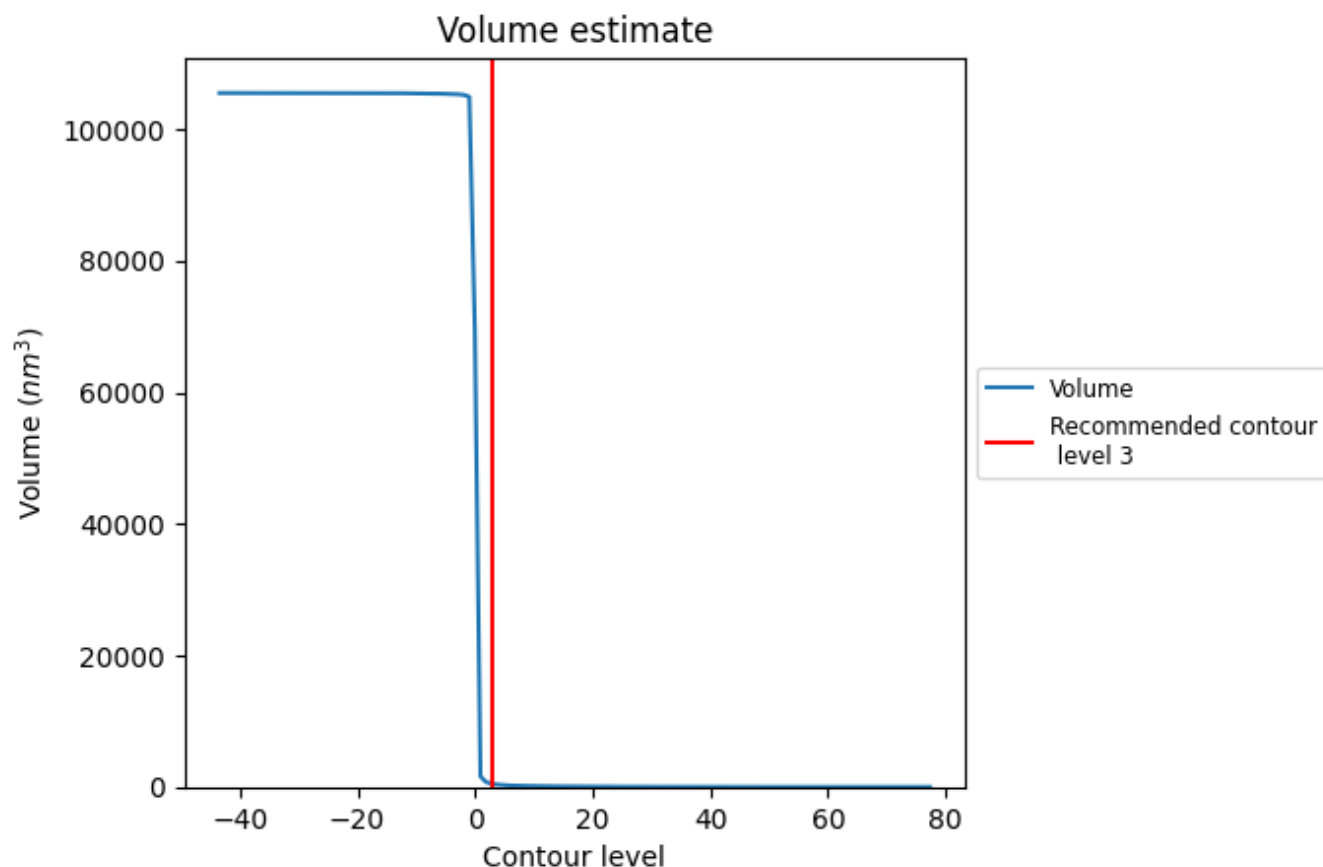
This section contains the results of statistical analysis of the map.

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.

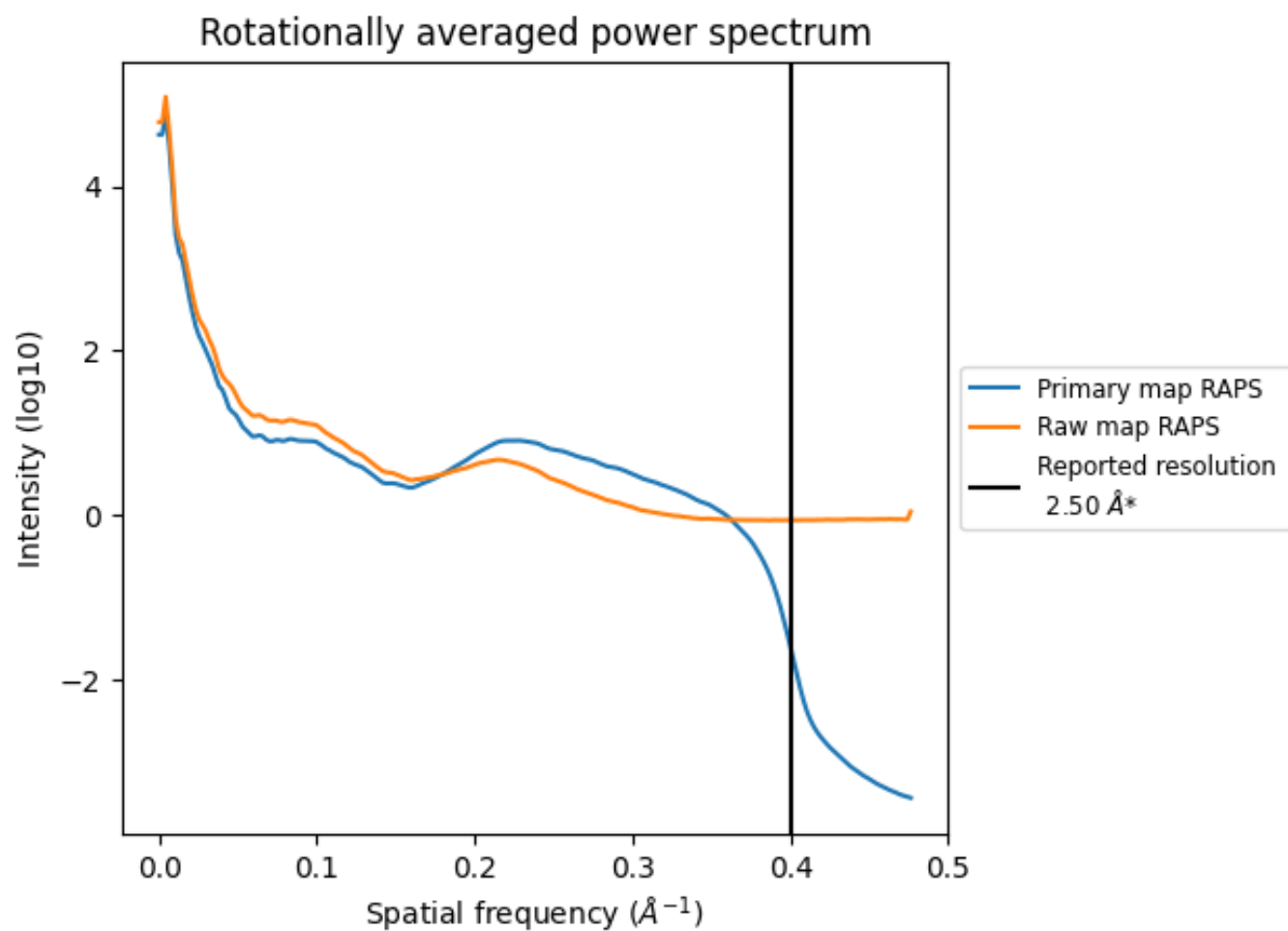
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 472 nm^3 ; this corresponds to an approximate mass of 426 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 ⓘ

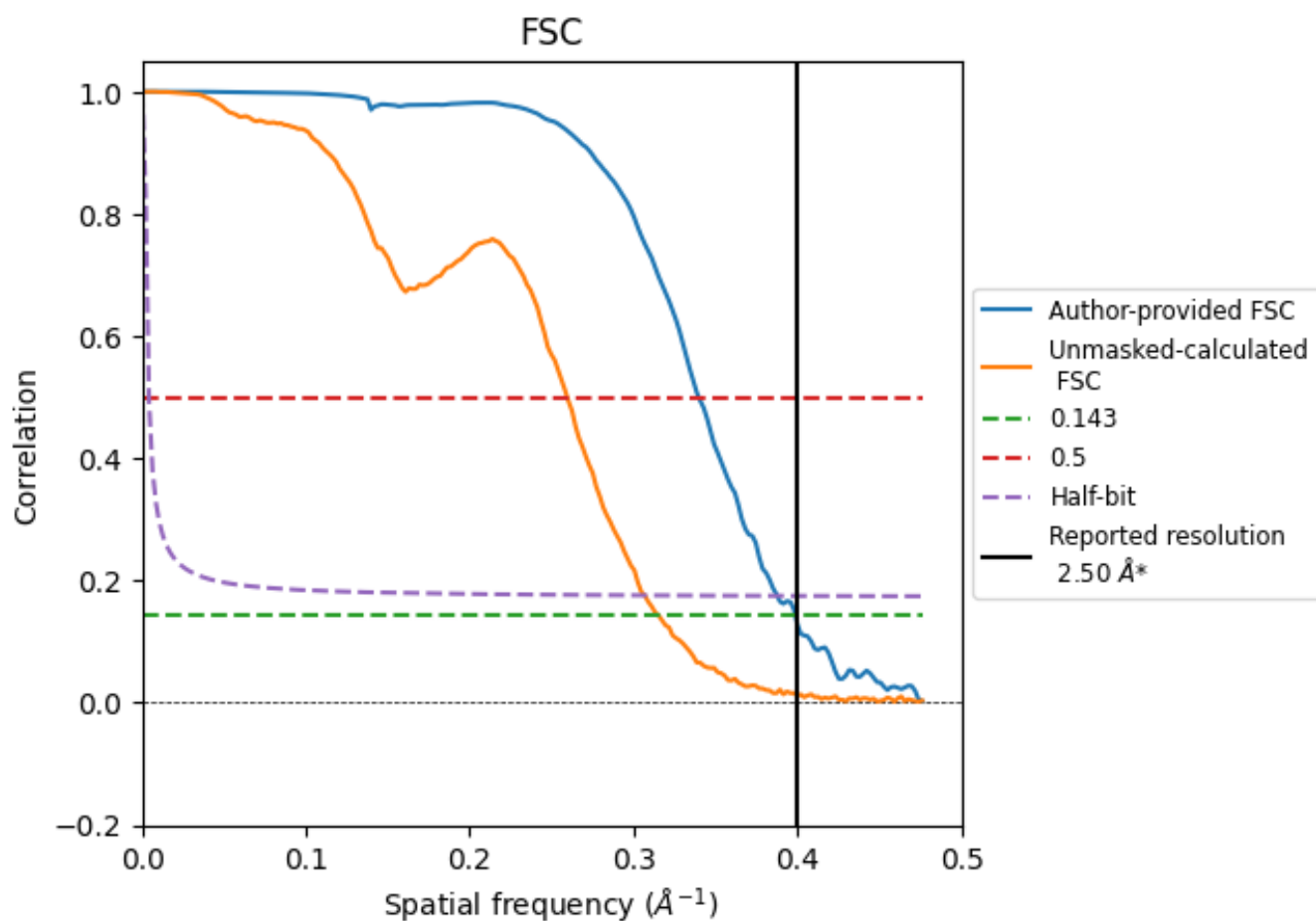


*Reported resolution corresponds to spatial frequency of 0.400 $\text{\AA}^{-1}$

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 0.400 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

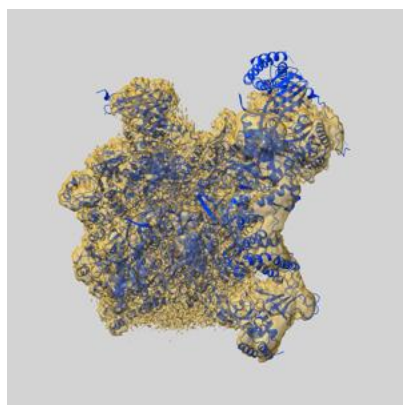
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.51	2.94	2.58
Unmasked-calculated*	3.17	3.85	3.26

*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 3.17 differs from the reported value 2.5 by more than 10 %

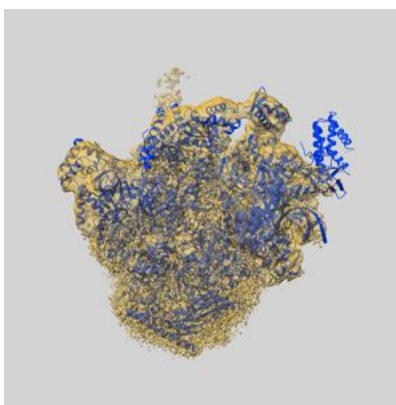
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12613 and PDB model 7NVU. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

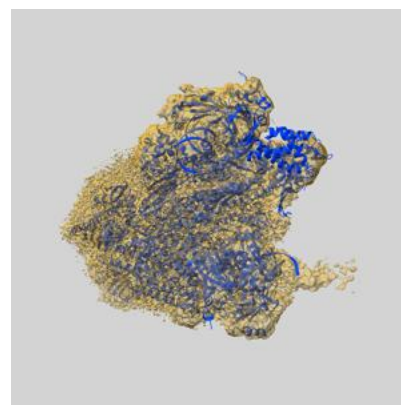
9.1 Map-model overlay [i](#)



X



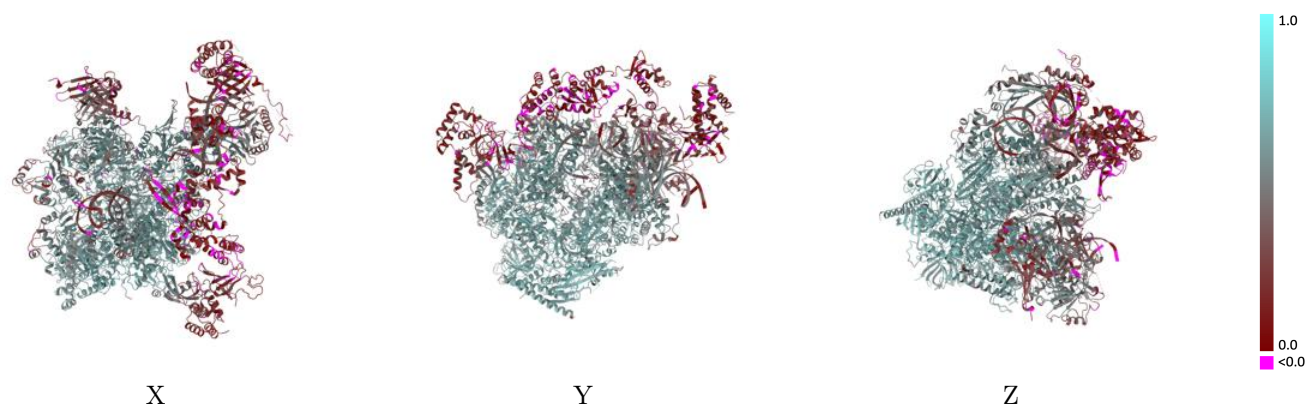
Y



Z

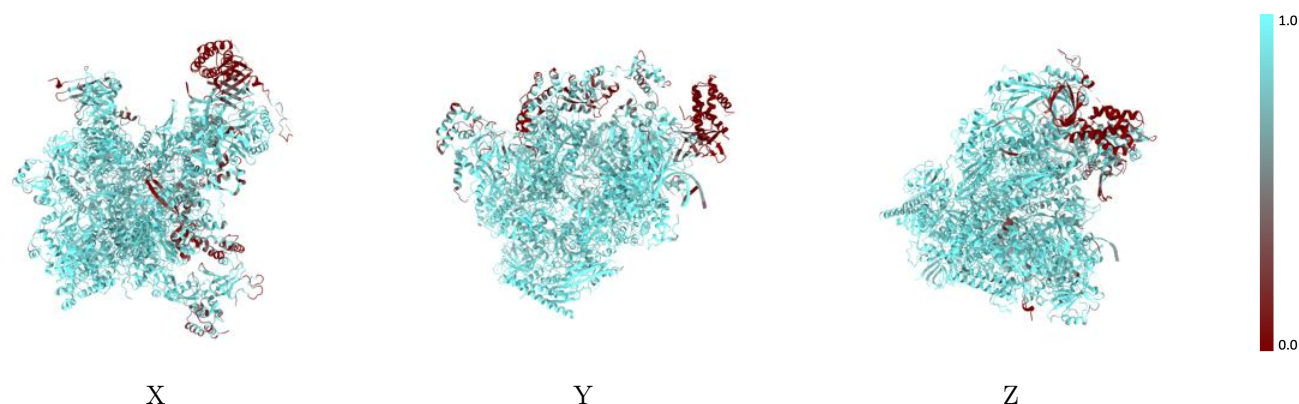
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



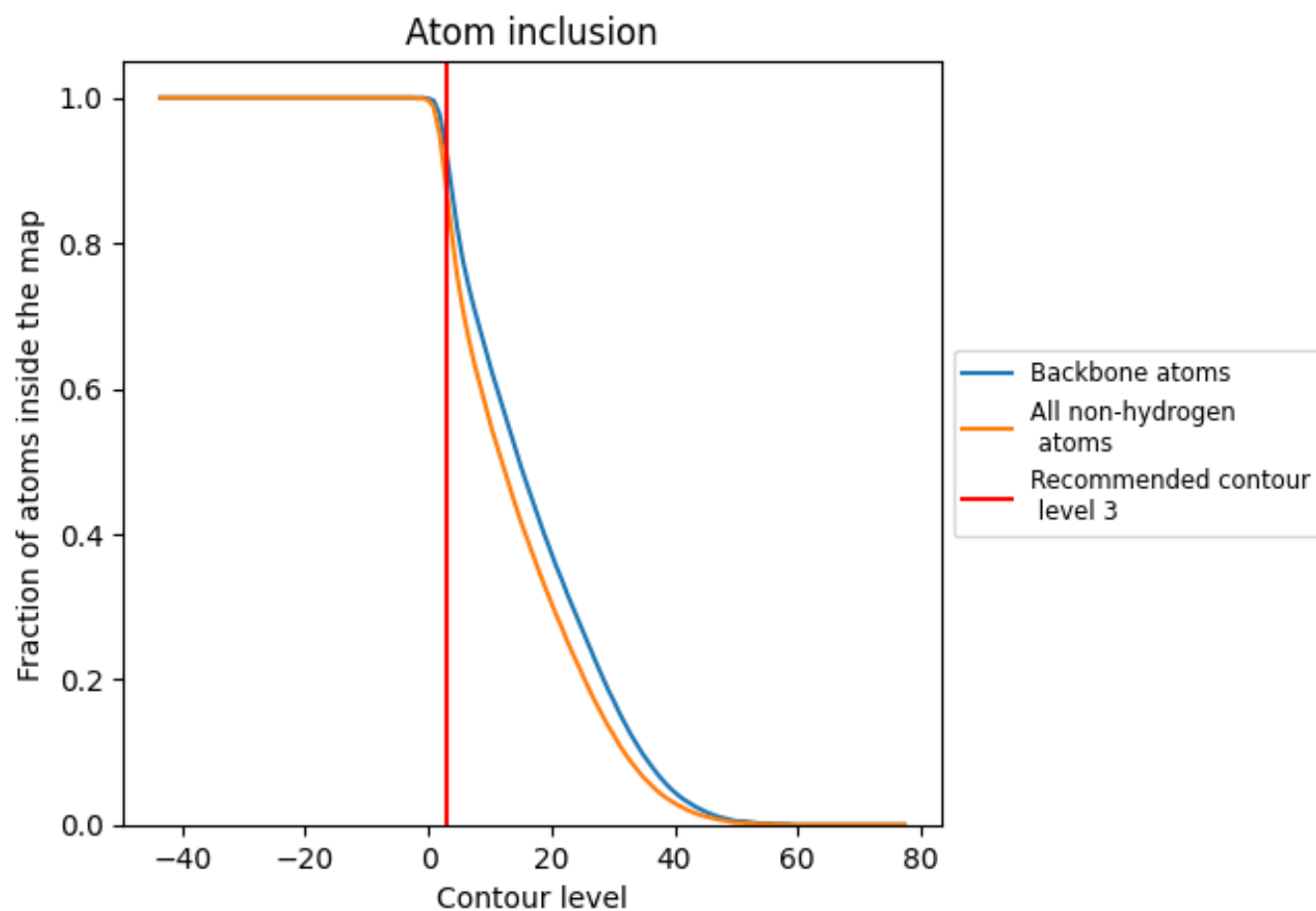
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 87% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8730	 0.4980
A	 0.9610	 0.6000
B	 0.9600	 0.6170
C	 0.9720	 0.6430
D	 0.6550	 0.2040
E	 0.9490	 0.5570
F	 0.9660	 0.6290
G	 0.8190	 0.3100
H	 0.9600	 0.6090
I	 0.9320	 0.5190
J	 0.9880	 0.6630
K	 0.9850	 0.6500
L	 0.9440	 0.5630
M	 0.9480	 0.5600
N	 0.9140	 0.3470
O	 0.9010	 0.4090
Q	 0.8020	 0.3410
R	 0.7510	 0.2870
T	 0.8970	 0.3650
U	 0.1680	 0.1570
V	 0.1420	 0.1640
W	 0.5100	 0.0760
X	 0.6040	 0.1170

