



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 12:10 AM UTC

PDB ID : 7OBB / pdb_00007obb
EMDB ID : EMD-12797
Title : Cryo-EM structure of human RNA Polymerase I Open Complex
Authors : Misiaszek, A.D.; Girbig, M.; Mueller, C.W.
Deposited on : 2021-04-21
Resolution : 3.30 Å(reported)
Based on initial model : 7AEI

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

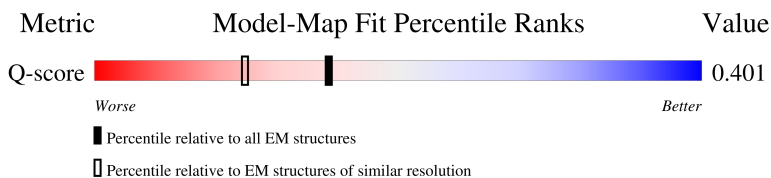
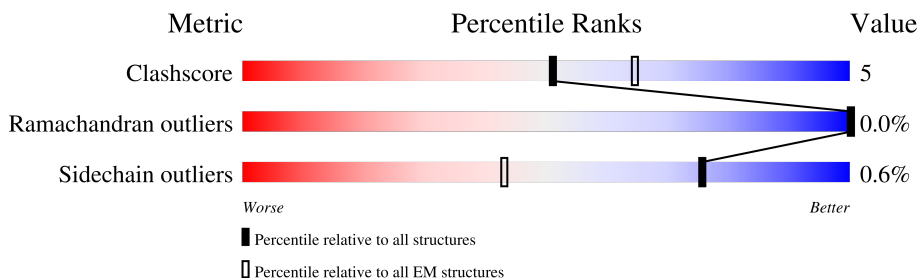
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

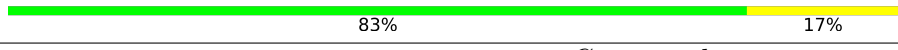
The reported resolution of this entry is 3.30 Å.

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	15087 (2.80 - 3.80)

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	1720	
2	B	1135	
3	C	346	
4	E	210	

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Mol	Chain	Length	Quality of chain
5	F	127	
6	G	338	
7	H	150	
8	I	126	
9	J	67	
10	K	133	
11	L	58	
12	M	419	
13	N	510	
14	T	43	
15	S	43	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 33048 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 I subunit RPA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1510	Total	C	N	O	S	0	0
			12050	7664	2114	2192	80		

- Molecule 2 is a protein called DNA-directed RNA polymerase I subunit RPA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1130	Total	C	N	O	S	0	0
			8962	5740	1527	1622	73		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	309	Total	C	N	O	S	0	0
			2474	1561	440	462	11		

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	210	Total	C	N	O	S	0	0
			1728	1094	301	324	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	44	PHE	SER	conflict	UNP P19388

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	77	Total	C	N	O	S	0	0
			619	398	105	111	5		

- Molecule 6 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	153	Total	C	N	O	S	0	0
			1183	749	209	218	7		

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 8 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	104	Total	C	N	O	S	0	0
			809	494	145	159	11		

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	107	Total	C	N	O	S	0	0
			856	531	153	165	7		

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	46	Total	C	N	O	S	0	0
			388	241	75	66	6		

- Molecule 12 is a protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	105	Total	C	N	O	S	0	0
			837	522	154	155	6		

- Molecule 13 is a protein called DNA-directed RNA polymerase I subunit RPA34.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	149	Total	C	N	O	S	0	0
			1083	684	193	201	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	9	Total	C	N	O	P	0	0
			185	89	34	53	9		

- Molecule 15 is a DNA chain called DNA non-template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	8	Total	C	N	O	P	0	0
			163	79	26	50	8		

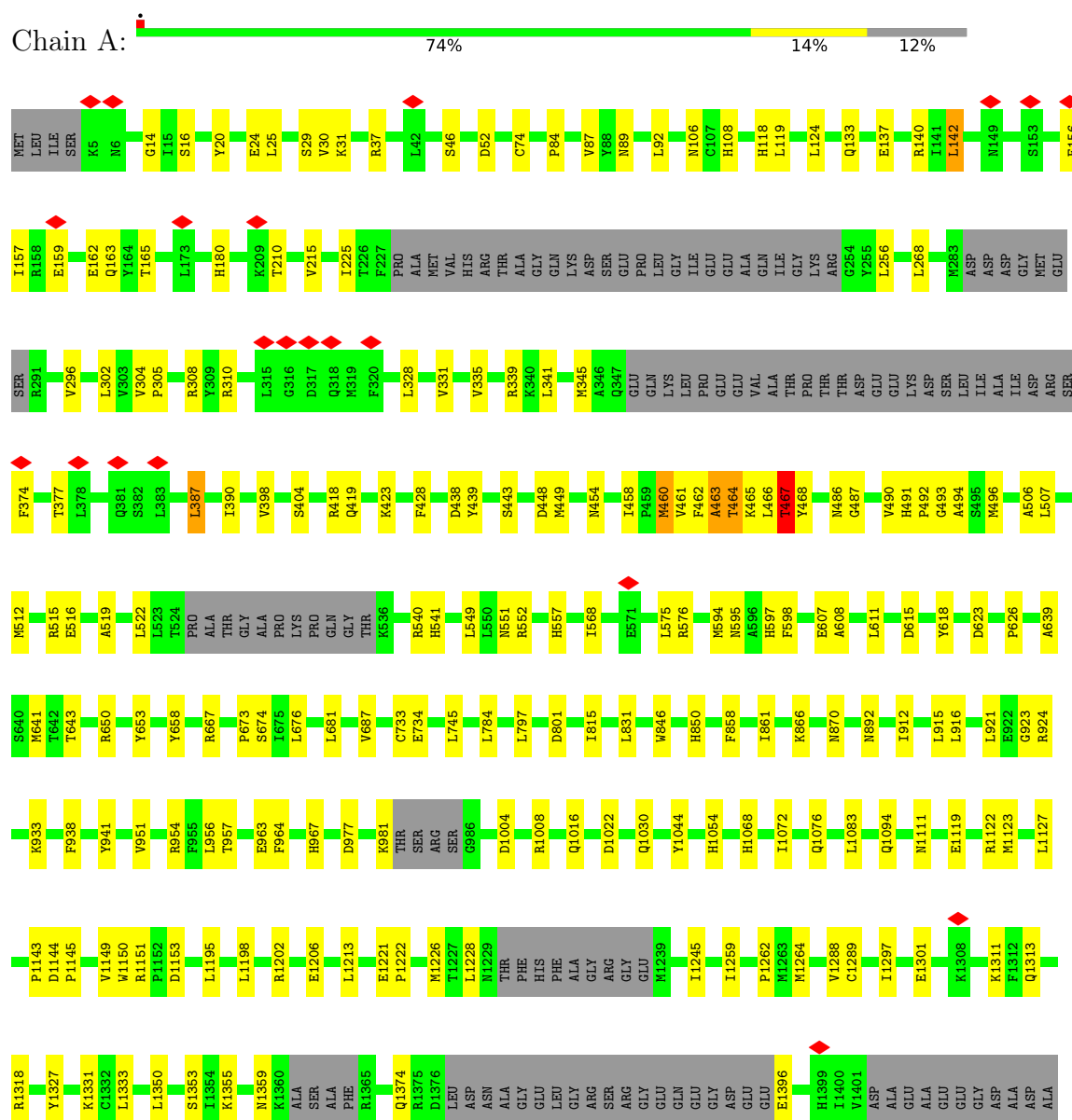
- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

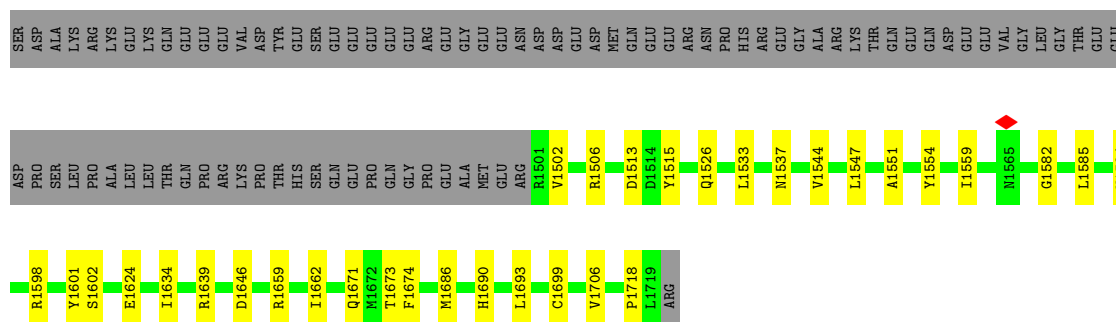
Mol	Chain	Residues	Atoms		AltConf
16	A	2	Total	Zn	0
			2	2	
16	B	1	Total	Zn	0
			1	1	
16	I	2	Total	Zn	0
			2	2	
16	J	1	Total	Zn	0
			1	1	
16	L	1	Total	Zn	0
			1	1	

3 Residue-property plots

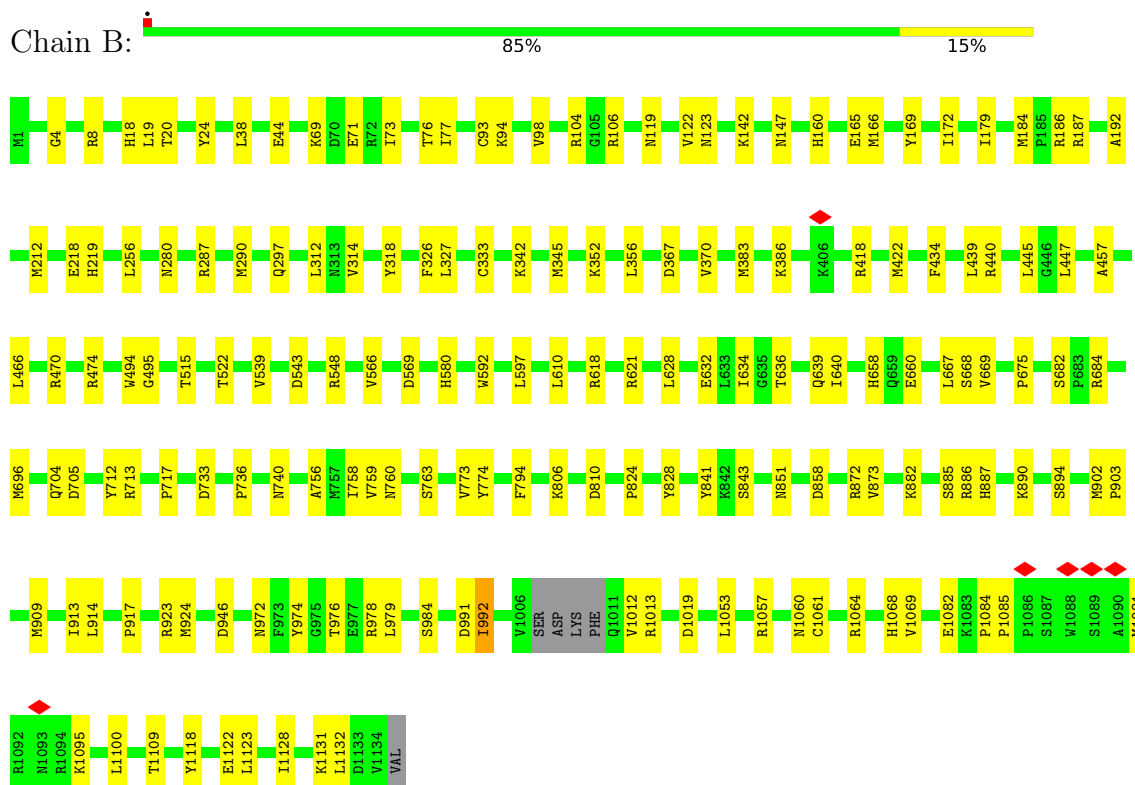
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 I subunit RPA1

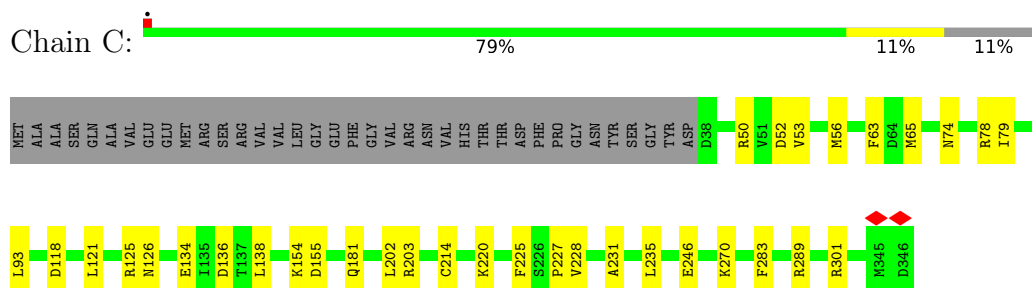




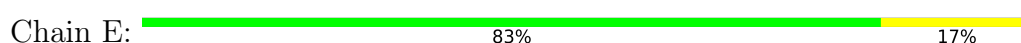
• Molecule 2: DNA-directed RNA polymerase I subunit RPA2

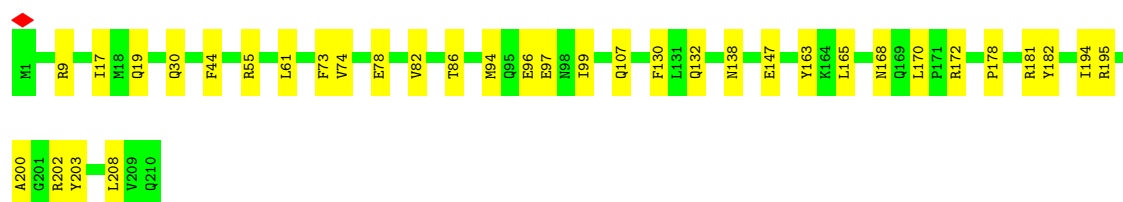


• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

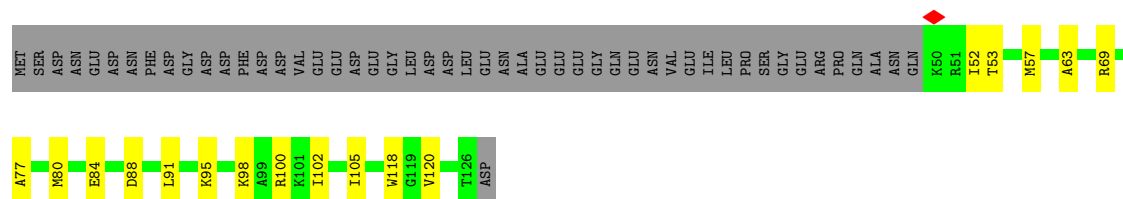


• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

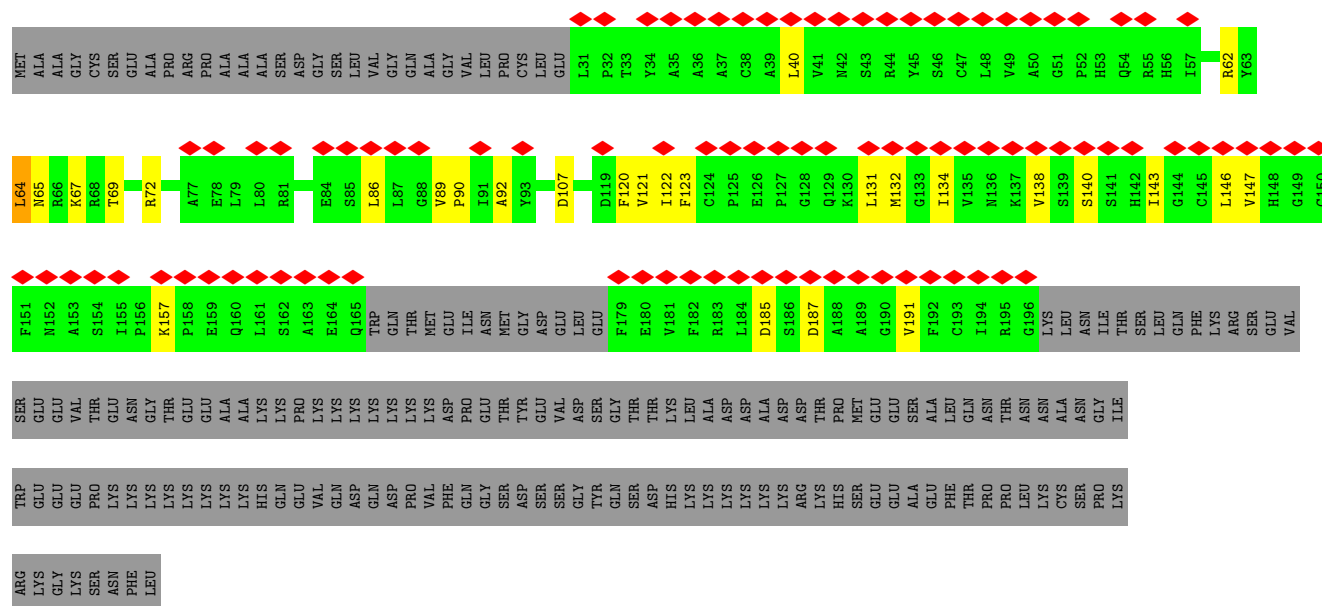
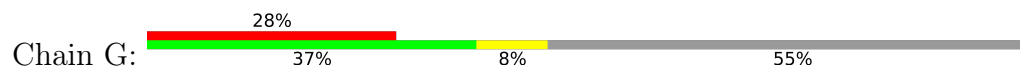




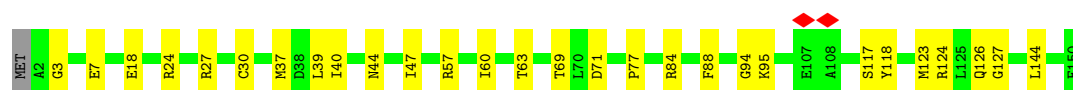
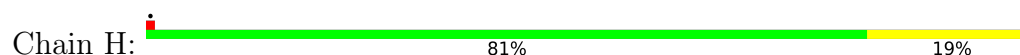
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2



- Molecule 6: DNA-directed RNA polymerase I subunit RPA43



- Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC3



- Molecule 8: DNA-directed RNA polymerase I subunit RPA12



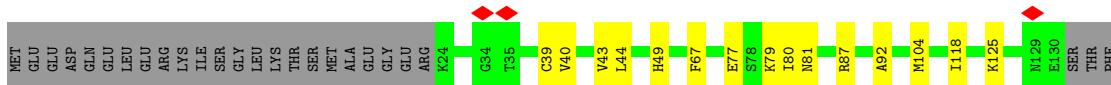
- Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 79% 16% .



- Molecule 10: DNA-directed RNA polymerases I and III subunit RPAC2

Chain K:  69% 11% 20%

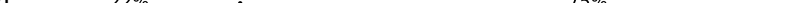


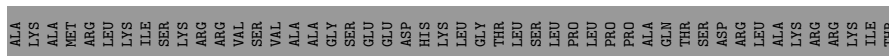
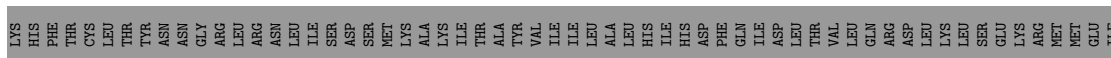
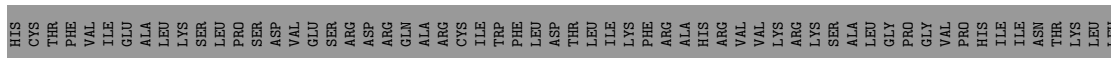
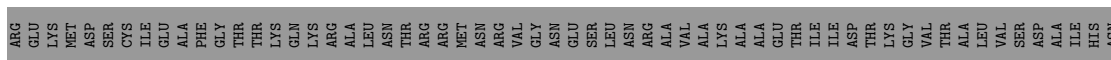
- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L: 67% 12% 21%



- Molecule 12: DNA-directed RNA polymerase I subunit RPA49

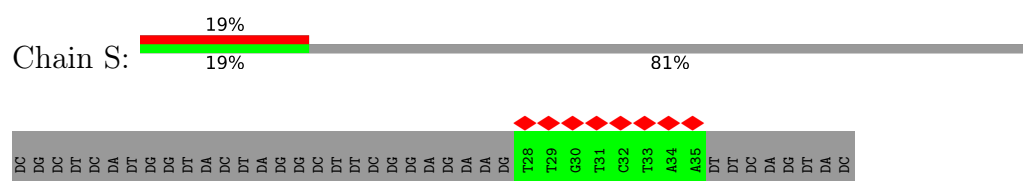
Chain M:  22% 75%



- Molecule 13: DNA-directed RNA polymerase I subunit RPA34

- Molecule 14: DNA template strand

- Molecule 15: DNA non-template strand



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	175912	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 ($e^-/\text{\AA}^2$)	41.2	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2250	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.026	Depositor
Minimum map value	-0.009	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00386	Depositor
Map size (Å)	236.73601, 236.73601, 236.73601	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.39	0/12296	0.68	8/16600 (0.0%)
2	B	0.47	0/9181	0.65	2/12426 (0.0%)
3	C	0.43	0/2522	0.64	2/3418 (0.1%)
4	E	0.30	0/1759	0.60	0/2376
5	F	0.31	0/629	0.65	0/850
6	G	0.27	0/1207	0.65	0/1634
7	H	0.37	0/1219	0.56	0/1644
8	I	0.32	0/823	0.64	1/1107 (0.1%)
9	J	0.55	0/516	0.70	0/696
10	K	0.44	0/871	0.61	0/1174
11	L	0.42	0/394	0.62	0/524
12	M	0.24	0/852	0.52	0/1146
13	N	0.28	0/1118	0.58	0/1532
14	T	0.23	0/207	0.44	0/317
15	S	0.23	0/181	0.46	0/277
All	All	0.40	0/33775	0.65	13/45721 (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	3
2	B	0	1
6	G	0	1
13	N	0	2
All	All	0	7

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	464	THR	N-CA-C	-8.47	102.71	113.72
1	A	133	GLN	N-CA-C	-6.26	105.80	113.50
2	B	69	LYS	CA-C-N	5.52	132.08	121.54
2	B	69	LYS	C-N-CA	5.52	132.08	121.54
1	A	467	THR	N-CA-C	5.35	117.63	108.90
1	A	815	ILE	N-CA-C	-5.20	107.76	112.96
1	A	463	ALA	N-CA-C	5.19	119.48	113.20
1	A	465	LYS	N-CA-C	5.17	120.44	113.72
3	C	154	LYS	CA-C-N	5.12	131.33	121.54
3	C	154	LYS	C-N-CA	5.12	131.33	121.54
1	A	1374	GLN	CA-C-N	5.12	131.31	121.54
1	A	1374	GLN	C-N-CA	5.12	131.31	121.54
8	I	108	GLY	N-CA-C	5.05	121.46	112.22

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	387	LEU	Mainchain
1	A	458	ILE	Mainchain
1	A	491	HIS	Peptide
2	B	457	ALA	Peptide
6	G	86	LEU	Peptide
13	N	154	GLY	Mainchain,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	12050	0	12184	161	0
2	B	8962	0	8945	105	0
3	C	2474	0	2469	24	0
4	E	1728	0	1749	25	0
5	F	619	0	655	11	0
6	G	1183	0	1172	16	0
7	H	1197	0	1156	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	I	809	0	752	14	0
9	J	507	0	524	8	0
10	K	856	0	840	12	0
11	L	388	0	393	5	0
12	M	837	0	819	11	0
13	N	1083	0	1079	10	0
14	T	185	0	103	1	0
15	S	163	0	93	0	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
All	All	33048	0	32933	362	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 (362) 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)
1:A:463:ALA:HB2	1:A:568:ILE:HD12	1.65	0.77
1:A:1353:SER:OG	1:A:1547:LEU:HD21	1.84	0.76
2:B:312:LEU:HD21	2:B:327:LEU:HB3	1.72	0.72
1:A:468:TYR:N	1:A:540:ARG:O	2.24	0.69
1:A:1559:ILE:HA	1:A:1582:GLY:HA3	1.76	0.67
1:A:1353:SER:HB2	1:A:1547:LEU:HD11	1.76	0.66
2:B:882:LYS:HD3	2:B:890:LYS:HD3	1.77	0.66
1:A:468:TYR:HB2	1:A:598:PHE:CE2	2.31	0.65
2:B:4:GLY:H	2:B:8:ARG:HD3	1.59	0.65
2:B:759:VAL:HG22	2:B:913:ILE:HG12	1.78	0.65
1:A:468:TYR:HB2	1:A:598:PHE:CZ	2.31	0.65
1:A:1072:ILE:HG22	1:A:1076:GLN:HE22	1.62	0.64
1:A:374:PHE:N	1:A:377:THR:HG1	1.95	0.63
7:H:124:ARG:NH1	7:H:126:GLN:OE1	2.30	0.63
2:B:192:ALA:HB1	2:B:356:LEU:HD22	1.79	0.63
1:A:557:HIS:HB3	1:A:1221:GLU:HG2	1.79	0.63
1:A:1111:ASN:HD22	4:E:61:LEU:HD22	1.64	0.63
2:B:1057:ARG:NH1	2:B:1061:CYS:SG	2.72	0.62
3:C:227:PRO:HG2	3:C:228:VAL:HG23	1.81	0.62
2:B:909:MET:HE3	9:J:44:CYS:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1123:LEU:HB3	2:B:1128:ILE:HB	1.81	0.61
2:B:160:HIS:ND1	2:B:705:ASP:OD2	2.34	0.61
1:A:463:ALA:CB	1:A:568:ILE:HD12	2.29	0.61
1:A:1350:LEU:HA	1:A:1547:LEU:HD13	1.83	0.61
2:B:704:GLN:OE1	2:B:851:ASN:ND2	2.34	0.61
1:A:1662:ILE:HG12	1:A:1671:GLN:HG2	1.83	0.61
2:B:383:MET:HB3	2:B:445:LEU:HD22	1.83	0.60
1:A:304:VAL:HG12	1:A:328:LEU:HD13	1.83	0.60
3:C:235:LEU:HB2	3:C:301:ARG:HD3	1.82	0.60
1:A:1222:PRO:HB2	1:A:1634:ILE:HD13	1.83	0.60
1:A:490:VAL:HG12	1:A:492:PRO:HD3	1.82	0.60
2:B:494:TRP:NE1	2:B:660:GLU:OE2	2.33	0.60
4:E:170:LEU:O	4:E:172:ARG:NH1	2.35	0.59
1:A:305:PRO:O	1:A:310:ARG:NH1	2.35	0.59
1:A:418:ARG:NH1	14:T:15:DA:OP1	2.35	0.59
1:A:1288:VAL:HG11	1:A:1333:LEU:HD11	1.84	0.59
1:A:507:LEU:HD12	1:A:515:ARG:HG2	1.84	0.59
2:B:758:ILE:HB	2:B:914:LEU:HB2	1.85	0.59
1:A:84:PRO:HB3	1:A:339:ARG:HE	1.68	0.59
1:A:1396:GLU:O	2:B:440:ARG:NH2	2.35	0.59
6:G:131:LEU:HD13	6:G:147:VAL:HG11	1.86	0.58
3:C:82:ALA:HB1	3:C:220:LYS:HB3	1.84	0.58
3:C:138:LEU:HB2	3:C:214:CYS:HB2	1.83	0.58
1:A:1353:SER:CB	1:A:1547:LEU:HD11	2.32	0.58
2:B:1060:ASN:OD1	2:B:1064:ARG:NH2	2.37	0.57
2:B:979:LEU:HD13	2:B:992:ILE:HB	1.86	0.57
3:C:134:GLU:O	3:C:181:GLN:NE2	2.36	0.57
2:B:592:TRP:O	2:B:618:ARG:NH2	2.38	0.57
1:A:92:LEU:HD23	1:A:1686:MET:HE2	1.87	0.57
1:A:454:ASN:ND2	1:A:615:ASP:OD2	2.38	0.57
1:A:443:SER:HB2	1:A:462:PHE:CZ	2.41	0.56
2:B:1069:VAL:HG11	2:B:1132:LEU:HD12	1.87	0.56
1:A:302:LEU:HD12	1:A:331:VAL:HG11	1.87	0.56
1:A:1506:ARG:NH2	1:A:1513:ASP:O	2.39	0.56
3:C:202:LEU:O	3:C:203:ARG:NH1	2.38	0.56
4:E:19:GLN:OE1	4:E:138:ASN:ND2	2.38	0.56
1:A:443:SER:HB2	1:A:462:PHE:HZ	1.70	0.56
12:M:79:LEU:HD23	12:M:108:ASN:HB2	1.88	0.56
7:H:30:CYS:HB2	7:H:39:LEU:HB3	1.88	0.56
1:A:137:GLU:OE2	1:A:140:ARG:NH1	2.38	0.55
2:B:73:ILE:HG12	2:B:122:VAL:HG12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1318:ARG:HD2	1:A:1526:GLN:HE21	1.71	0.55
5:F:84:GLU:OE1	5:F:95:LYS:NZ	2.39	0.55
1:A:460:MET:O	1:A:460:MET:HG3	2.07	0.55
3:C:56:MET:O	10:K:125:LYS:NZ	2.37	0.55
1:A:639:ALA:O	1:A:643:THR:OG1	2.24	0.55
4:E:170:LEU:HD23	4:E:208:LEU:HG	1.88	0.55
1:A:1297:ILE:HD13	1:A:1544:VAL:HG12	1.88	0.55
12:M:27:GLN:HB3	12:M:108:ASN:HA	1.88	0.55
1:A:14:GLY:HA2	1:A:1693:LEU:HD23	1.88	0.55
1:A:964:PHE:HE2	2:B:667:LEU:HD21	1.71	0.55
2:B:978:ARG:HD2	2:B:991:ASP:HB3	1.87	0.55
1:A:341:LEU:HG	1:A:345:MET:HE2	1.89	0.55
2:B:71:GLU:HG2	2:B:123:ASN:HD21	1.72	0.55
4:E:178:PRO:O	4:E:182:TYR:HB2	2.07	0.54
7:H:3:GLY:H	7:H:84:ARG:HH22	1.55	0.54
1:A:159:GLU:O	1:A:163:GLN:HB2	2.06	0.54
1:A:404:SER:H	1:A:419:GLN:HE22	1.54	0.54
1:A:956:LEU:HD23	1:A:957:THR:HG23	1.89	0.54
2:B:515:THR:HA	2:B:668:SER:HA	1.90	0.54
1:A:866:LYS:O	1:A:870:ASN:ND2	2.40	0.54
2:B:903:PRO:HB2	2:B:979:LEU:HD23	1.90	0.54
2:B:1118:TYR:O	2:B:1122:GLU:HB2	2.07	0.54
1:A:977:ASP:OD2	8:I:100:ARG:NH2	2.41	0.53
1:A:1123:MET:HG2	1:A:1127:LEU:HD12	1.90	0.53
1:A:468:TYR:HD2	1:A:540:ARG:HE	1.55	0.53
4:E:96:GLU:HG3	4:E:97:GLU:HG3	1.90	0.53
2:B:186:ARG:NH2	2:B:636:THR:OG1	2.42	0.53
2:B:543:ASP:HB2	12:M:81:CYS:HB2	1.91	0.53
13:N:75:GLY:O	13:N:78:HIS:ND1	2.42	0.53
1:A:302:LEU:HD11	1:A:398:VAL:HG22	1.90	0.53
1:A:108:HIS:HB3	1:A:268:LEU:HA	1.91	0.53
2:B:984:SER:O	3:C:74:ASN:ND2	2.42	0.53
2:B:367:ASP:OD1	2:B:474:ARG:NH2	2.39	0.52
2:B:713:ARG:NH2	9:J:1:MET:SD	2.82	0.52
1:A:1151:ARG:NH1	1:A:1153:ASP:OD2	2.41	0.52
1:A:1202:ARG:NH2	1:A:1206:GLU:OE2	2.42	0.52
7:H:18:GLU:OE2	7:H:27:ARG:NH1	2.43	0.52
2:B:93:CYS:SG	2:B:94:LYS:N	2.83	0.52
2:B:991:ASP:N	2:B:991:ASP:OD1	2.41	0.52
7:H:94:GLY:HA3	7:H:118:TYR:HA	1.91	0.52
2:B:19:LEU:HD12	2:B:20:THR:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:15:SER:OG	12:M:30:ASN:O	2.28	0.52
1:A:37:ARG:O	1:A:46:SER:OG	2.28	0.52
1:A:1004:ASP:HA	1:A:1151:ARG:HH12	1.75	0.52
5:F:57:MET:HE1	5:F:120:VAL:HG13	1.92	0.52
11:L:28:ILE:HD13	11:L:34:ILE:HG22	1.90	0.52
1:A:933:LYS:NZ	1:A:938:PHE:O	2.40	0.52
1:A:74:CYS:O	1:A:308:ARG:NH1	2.43	0.51
1:A:84:PRO:HD3	1:A:335:VAL:HG13	1.90	0.51
2:B:974:TYR:OH	3:C:289:ARG:NH1	2.43	0.51
1:A:106:ASN:HD21	1:A:210:THR:HG21	1.74	0.51
2:B:1012:VAL:O	2:B:1013:ARG:NH1	2.39	0.51
3:C:63:PHE:HE2	3:C:65:MET:HE3	1.75	0.51
4:E:17:ILE:HG21	4:E:74:VAL:HG11	1.93	0.51
13:N:82:VAL:HG22	13:N:117:ILE:HG12	1.92	0.51
1:A:981:LYS:HD2	1:A:1228:LEU:HB2	1.93	0.51
2:B:280:ASN:HD22	8:I:55:VAL:HG21	1.76	0.51
1:A:31:LYS:NZ	1:A:52:ASP:OD2	2.39	0.51
5:F:98:LYS:O	5:F:100:ARG:NH1	2.44	0.51
3:C:246:GLU:HG2	3:C:270:LYS:HD2	1.92	0.51
1:A:215:VAL:HG12	1:A:225:ILE:HG22	1.93	0.51
6:G:120:PHE:HB3	6:G:122:ILE:HG23	1.92	0.51
8:I:11:SER:O	12:M:66:ARG:NH2	2.44	0.51
2:B:142:LYS:NZ	2:B:165:GLU:O	2.43	0.50
2:B:333:CYS:O	2:B:342:LYS:NZ	2.43	0.50
12:M:62:ALA:HB3	12:M:69:TYR:HB2	1.93	0.50
1:A:180:HIS:HE1	1:A:1690:HIS:CD2	2.30	0.50
1:A:1537:ASN:HD21	8:I:29:LEU:HD21	1.76	0.50
2:B:773:VAL:HG13	2:B:873:VAL:HB	1.93	0.50
1:A:487:GLY:HA3	1:A:515:ARG:HH11	1.75	0.50
2:B:418:ARG:HG2	2:B:422:MET:HE2	1.93	0.50
2:B:104:ARG:NH2	2:B:169:TYR:OH	2.44	0.50
3:C:50:ARG:NH1	3:C:52:ASP:OD2	2.45	0.50
3:C:78:ARG:HH12	10:K:49:HIS:HB2	1.76	0.50
6:G:69:THR:HA	6:G:72:ARG:HG2	1.92	0.50
2:B:212:MET:HE1	2:B:345:MET:HE2	1.93	0.50
2:B:684:ARG:HD2	2:B:923:ARG:HB3	1.93	0.50
1:A:1016:GLN:NE2	1:A:1646:ASP:OD2	2.37	0.50
2:B:978:ARG:HG3	3:C:283:PHE:HD2	1.76	0.50
1:A:967:HIS:HE1	2:B:682:SER:H	1.60	0.49
7:H:63:THR:HG21	7:H:69:THR:HG23	1.93	0.49
2:B:810:ASP:OD2	11:L:17:TYR:OH	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:GLU:HA	1:A:165:THR:HG22	1.94	0.49
2:B:76:THR:HG23	2:B:119:ASN:HB3	1.94	0.49
3:C:79:ILE:HG23	3:C:83:GLU:HB2	1.94	0.49
6:G:140:SER:HA	6:G:157:LYS:HD3	1.95	0.49
4:E:94:MET:HG2	4:E:99:ILE:HD11	1.94	0.49
2:B:696:MET:HG3	2:B:712:TYR:HB3	1.95	0.49
9:J:35:LEU:HD11	9:J:50:LEU:HB2	1.94	0.49
1:A:87:VAL:HG21	1:A:398:VAL:HG21	1.94	0.49
1:A:1022:ASP:OD2	1:A:1639:ARG:NH2	2.40	0.49
4:E:82:VAL:HG13	4:E:86:THR:HB	1.94	0.49
1:A:916:LEU:HD22	1:A:951:VAL:HG11	1.94	0.49
1:A:1083:LEU:HD13	1:A:1598:ARG:HH22	1.77	0.49
2:B:634:ILE:HG21	2:B:639:GLN:HB3	1.94	0.49
10:K:43:VAL:HG22	10:K:81:ASN:HD22	1.78	0.49
10:K:44:LEU:HD22	10:K:80:ILE:HD11	1.95	0.49
1:A:443:SER:HB3	1:A:575:LEU:HG	1.94	0.48
7:H:77:PRO:HD2	10:K:87:ARG:HH22	1.78	0.48
10:K:40:VAL:HG12	10:K:92:ALA:HB3	1.96	0.48
1:A:846:TRP:HE1	1:A:858:PHE:HE1	1.61	0.48
2:B:756:ALA:HB1	2:B:894:SER:HB2	1.95	0.48
7:H:37:MET:HG2	7:H:127:GLY:HA3	1.95	0.48
1:A:29:SER:OG	1:A:30:VAL:N	2.47	0.48
1:A:1153:ASP:OD1	1:A:1153:ASP:N	2.45	0.48
1:A:486:ASN:O	1:A:515:ARG:NH1	2.46	0.48
1:A:305:PRO:HG2	1:A:310:ARG:HH11	1.78	0.48
1:A:1289:CYS:HA	1:A:1551:ALA:HA	1.95	0.48
2:B:312:LEU:HD23	2:B:326:PHE:HD2	1.77	0.48
2:B:972:ASN:ND2	2:B:976:THR:OG1	2.40	0.48
1:A:850:HIS:ND1	1:A:941:TYR:OH	2.35	0.48
4:E:165:LEU:HD21	4:E:170:LEU:HD13	1.96	0.48
9:J:10:CYS:SG	9:J:42:ARG:NH2	2.82	0.48
1:A:1143:PRO:O	4:E:202:ARG:NH1	2.41	0.48
2:B:794:PHE:HA	2:B:828:TYR:HA	1.96	0.48
1:A:1331:LYS:HE2	1:A:1554:TYR:CG	2.49	0.47
1:A:658:TYR:HB2	10:K:67:PHE:HZ	1.78	0.47
1:A:1327:TYR:HE2	1:A:1333:LEU:HB2	1.78	0.47
6:G:89:VAL:HG13	6:G:123:PHE:HB3	1.95	0.47
1:A:439:TYR:HB2	2:B:1057:ARG:HH12	1.78	0.47
1:A:912:ILE:HD11	2:B:924:MET:HG2	1.96	0.47
1:A:745:LEU:HD23	7:H:117:SER:HB3	1.96	0.47
1:A:89:ASN:ND2	1:A:296:VAL:O	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:674:SER:OG	7:H:118:TYR:O	2.32	0.47
1:A:1718:PRO:HD3	5:F:105:ILE:HG12	1.97	0.47
2:B:539:VAL:HG22	2:B:566:VAL:HG22	1.97	0.47
3:C:78:ARG:NH1	10:K:49:HIS:HB2	2.30	0.47
2:B:106:ARG:HB2	11:L:43:ILE:HD11	1.95	0.47
2:B:166:MET:HE1	2:B:466:LEU:HD23	1.96	0.47
13:N:78:HIS:CD2	13:N:79:ARG:HE	2.32	0.47
1:A:1226:MET:HE3	1:A:1245:ILE:HG13	1.97	0.47
2:B:909:MET:HG3	9:J:42:ARG:HD2	1.97	0.47
10:K:77:GLU:OE1	10:K:79:LYS:NZ	2.49	0.47
12:M:7:PRO:HB2	13:N:63:LEU:HB2	1.97	0.46
2:B:806:LYS:HD3	2:B:824:PRO:HD2	1.98	0.46
1:A:118:HIS:NE2	1:A:156:GLU:O	2.49	0.46
2:B:740:ASN:HB2	9:J:47:ARG:HD3	1.97	0.46
3:C:228:VAL:HG11	3:C:231:ALA:HB2	1.97	0.46
5:F:88:ASP:HB3	5:F:91:LEU:HD13	1.98	0.46
12:M:40:ARG:HB2	12:M:63:GLU:HB2	1.97	0.46
1:A:745:LEU:O	7:H:117:SER:OG	2.27	0.46
3:C:86:THR:OG1	3:C:225:PHE:O	2.33	0.46
1:A:1145:PRO:HG3	4:E:202:ARG:HB2	1.97	0.46
3:C:93:LEU:HB3	11:L:52:LEU:HD11	1.98	0.46
7:H:88:PHE:HD2	7:H:144:LEU:HB3	1.81	0.46
5:F:53:THR:OG1	5:F:118:TRP:NE1	2.49	0.46
7:H:24:ARG:O	7:H:44:ASN:ND2	2.49	0.46
6:G:64:LEU:O	6:G:67:LYS:NZ	2.44	0.46
6:G:92:ALA:HB3	6:G:121:VAL:HB	1.98	0.46
8:I:85:ARG:HH12	8:I:124:GLU:HG3	1.81	0.46
1:A:551:ASN:HB3	1:A:595:ASN:HB2	1.98	0.46
1:A:1301:GLU:HB3	8:I:55:VAL:HG13	1.97	0.46
2:B:439:LEU:HD21	2:B:445:LEU:HD12	1.98	0.46
6:G:90:PRO:HA	6:G:122:ILE:HA	1.97	0.46
1:A:1008:ARG:NH2	4:E:163:TYR:O	2.47	0.45
1:A:1094:GLN:HE21	4:E:30:GLN:NE2	2.14	0.45
2:B:979:LEU:HB2	2:B:992:ILE:HD13	1.97	0.45
1:A:438:ASP:O	2:B:1057:ARG:NH2	2.49	0.45
4:E:107:GLN:HA	4:E:132:GLN:HB2	1.98	0.45
1:A:641:MET:HE1	1:A:784:LEU:HD11	1.98	0.45
13:N:83:LEU:HB2	13:N:116:ARG:HB3	1.99	0.45
6:G:134:ILE:H	6:G:146:LEU:H	1.64	0.45
1:A:341:LEU:HD22	1:A:390:ILE:HD12	1.98	0.45
1:A:428:PHE:HB3	1:A:1673:THR:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:TYR:O	1:A:540:ARG:HG3	2.17	0.45
1:A:374:PHE:N	1:A:377:THR:OG1	2.50	0.45
2:B:18:HIS:NE2	2:B:733:ASP:OD2	2.41	0.45
5:F:77:ALA:HA	6:G:62:ARG:HA	1.99	0.45
13:N:98:SER:OG	13:N:100:GLU:OE1	2.34	0.45
6:G:138:VAL:HG23	6:G:143:ILE:HG12	1.98	0.45
1:A:468:TYR:HB2	1:A:598:PHE:HZ	1.82	0.45
3:C:125:ARG:HG2	3:C:136:ASP:HB3	1.97	0.45
4:E:168:ASN:HA	4:E:172:ARG:HH22	1.82	0.45
1:A:1054:HIS:HB3	1:A:1198:LEU:HD22	1.99	0.44
2:B:370:VAL:HG21	2:B:640:ILE:HD12	1.99	0.44
4:E:73:PHE:HD2	4:E:99:ILE:HD13	1.81	0.44
1:A:1022:ASP:HB3	4:E:200:ALA:HB2	1.99	0.44
1:A:1350:LEU:HD12	1:A:1547:LEU:HD12	1.99	0.44
1:A:1502:VAL:HG12	1:A:1515:TYR:HD2	1.83	0.44
2:B:256:LEU:O	2:B:297:GLN:NE2	2.50	0.44
2:B:580:HIS:CD2	2:B:628:LEU:HD21	2.52	0.44
2:B:858:ASP:OD1	2:B:858:ASP:N	2.51	0.44
1:A:16:SER:HB2	1:A:1690:HIS:HB3	1.99	0.44
2:B:38:LEU:HD22	2:B:470:ARG:HD3	2.00	0.44
2:B:1091:MET:HB3	6:G:185:ASP:HB2	1.99	0.44
8:I:115:CYS:SG	8:I:116:THR:N	2.91	0.44
1:A:519:ALA:HA	1:A:522:LEU:HD23	1.98	0.44
1:A:608:ALA:HB2	2:B:1053:LEU:HD21	1.99	0.44
4:E:9:ARG:HE	4:E:132:GLN:HE22	1.65	0.44
1:A:733:CYS:SG	1:A:734:GLU:N	2.91	0.44
1:A:1311:LYS:NZ	8:I:33:GLN:O	2.40	0.44
2:B:495:GLY:HA3	2:B:621:ARG:NH1	2.33	0.44
8:I:100:ARG:HD3	8:I:102:MET:HE3	2.00	0.44
1:A:951:VAL:HG13	1:A:963:GLU:HB3	2.00	0.44
2:B:774:TYR:CE1	2:B:872:ARG:HG2	2.53	0.44
4:E:130:PHE:HE1	4:E:181:ARG:HG3	1.82	0.44
1:A:449:MET:HE3	1:A:449:MET:HB3	1.79	0.44
2:B:179:ILE:HD11	2:B:434:PHE:HE1	1.82	0.44
6:G:132:MET:HE2	6:G:134:ILE:HD11	1.98	0.44
1:A:1350:LEU:HD12	1:A:1547:LEU:CD1	2.48	0.44
5:F:69:ARG:HD3	5:F:102:ILE:HG23	1.99	0.44
8:I:13:PHE:O	8:I:21:SER:OG	2.29	0.44
1:A:1659:ARG:HA	1:A:1674:PHE:HE2	1.83	0.43
2:B:98:VAL:O	2:B:147:ASN:ND2	2.42	0.43
2:B:1118:TYR:O	2:B:1122:GLU:CB	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:103:ARG:NH2	8:I:125:ASP:O	2.51	0.43
11:L:19:CYS:SG	11:L:20:GLY:N	2.91	0.43
13:N:45:ILE:HG12	13:N:115:LEU:HB2	1.99	0.43
1:A:549:LEU:N	1:A:597:HIS:O	2.46	0.43
1:A:1355:LYS:O	1:A:1359:ASN:ND2	2.51	0.43
1:A:1699:CYS:HB2	1:A:1706:VAL:HG12	1.99	0.43
2:B:885:SER:OG	2:B:886:ARG:N	2.48	0.43
7:H:63:THR:HB	7:H:71:ASP:HB3	2.00	0.43
1:A:681:LEU:HD11	7:H:47:ILE:HG13	1.99	0.43
1:A:1094:GLN:HE21	4:E:30:GLN:HE21	1.66	0.43
3:C:53:VAL:HG21	10:K:118:ILE:HD13	2.01	0.43
8:I:38:CYS:SG	8:I:39:ILE:N	2.91	0.43
1:A:745:LEU:HD21	7:H:95:LYS:HB2	1.99	0.43
1:A:831:LEU:HD21	1:A:861:ILE:HD11	1.99	0.43
1:A:1119:GLU:HG2	1:A:1122:ARG:HH21	1.83	0.43
1:A:512:MET:HE3	1:A:516:GLU:HB3	1.99	0.43
1:A:611:LEU:HD23	5:F:63:ALA:HB2	2.00	0.43
1:A:921:LEU:N	1:A:924:ARG:O	2.41	0.43
12:M:44:TYR:HB3	13:N:24:ALA:HB1	1.99	0.43
2:B:668:SER:OG	2:B:669:VAL:N	2.51	0.43
1:A:1264:MET:HA	1:A:1602:SER:HA	2.00	0.43
1:A:1585:LEU:HA	1:A:1585:LEU:HD13	1.84	0.43
7:H:7:GLU:OE2	7:H:57:ARG:NE	2.52	0.43
1:A:486:ASN:ND2	1:A:493:GLY:O	2.43	0.43
2:B:184:MET:HE3	2:B:447:LEU:HD22	2.01	0.43
1:A:467:THR:HA	1:A:541:HIS:HA	2.01	0.43
1:A:801:ASP:HB2	1:A:892:ASN:OD1	2.19	0.43
2:B:287:ARG:HG3	2:B:290:MET:HE3	2.01	0.43
2:B:548:ARG:NH2	2:B:569:ASP:OD2	2.52	0.43
1:A:1149:VAL:HG12	1:A:1150:TRP:CD1	2.54	0.42
4:E:55:ARG:HD2	4:E:78:GLU:HA	2.01	0.42
13:N:156:PRO:HA	13:N:157:PRO:HD3	1.94	0.42
1:A:119:LEU:HD13	1:A:142:LEU:HD22	2.00	0.42
1:A:618:TYR:CZ	1:A:626:PRO:HB3	2.54	0.42
1:A:1313:GLN:HE21	1:A:1533:LEU:HD13	1.84	0.42
1:A:512:MET:HA	1:A:515:ARG:HE	1.84	0.42
1:A:597:HIS:HB3	2:B:1057:ARG:HD2	2.00	0.42
2:B:717:PRO:HG2	2:B:736:PRO:HG2	2.00	0.42
4:E:147:GLU:HB2	4:E:194:ILE:HB	2.01	0.42
1:A:24:GLU:HG3	2:B:1100:LEU:HD13	2.00	0.42
1:A:496:MET:HG3	1:A:506:ALA:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:797:LEU:HB2	2:B:917:PRO:HB3	2.01	0.42
4:E:44:PHE:HD1	4:E:44:PHE:HA	1.72	0.42
1:A:673:PRO:HB2	1:A:676:LEU:HD23	2.02	0.42
1:A:552:ARG:HB2	1:A:594:MET:HE2	2.02	0.42
1:A:607:GLU:HG3	5:F:63:ALA:HB1	2.01	0.42
1:A:653:TYR:HD1	1:A:687:VAL:HG22	1.85	0.42
1:A:667:ARG:NE	10:K:39:CYS:SG	2.75	0.42
1:A:866:LYS:NZ	1:A:923:GLY:O	2.52	0.42
2:B:760:ASN:HB3	2:B:763:SER:HB3	2.02	0.42
2:B:172:ILE:HG13	2:B:434:PHE:HB3	2.02	0.42
6:G:107:ASP:OD1	6:G:107:ASP:N	2.53	0.42
2:B:44:GLU:OE1	2:B:522:THR:OG1	2.37	0.42
2:B:219:HIS:HD2	2:B:386:LYS:HE3	1.84	0.42
1:A:468:TYR:HB2	1:A:598:PHE:HE2	1.82	0.41
2:B:946:ASP:OD1	2:B:946:ASP:N	2.51	0.41
1:A:16:SER:O	2:B:1131:LYS:N	2.54	0.41
1:A:225:ILE:HG23	1:A:256:LEU:HB2	2.02	0.41
1:A:1044:TYR:HD1	1:A:1195:LEU:HD22	1.84	0.41
1:A:387:LEU:HA	1:A:387:LEU:HD23	1.86	0.41
1:A:650:ARG:HH22	7:H:77:PRO:HG3	1.85	0.41
2:B:632:GLU:OE1	2:B:658:HIS:NE2	2.46	0.41
1:A:1068:HIS:NE2	1:A:1144:ASP:O	2.41	0.41
9:J:25:LEU:HD23	9:J:25:LEU:HA	1.88	0.41
8:I:89:ARG:NH2	8:I:118:CYS:O	2.53	0.41
4:E:195:ARG:HD2	4:E:203:TYR:HD2	1.85	0.41
12:M:79:LEU:HD13	12:M:81:CYS:HB3	2.03	0.41
3:C:118:ASP:HB3	3:C:121:LEU:HD23	2.02	0.41
1:A:1004:ASP:OD1	1:A:1004:ASP:N	2.53	0.41
1:A:1350:LEU:CD1	1:A:1547:LEU:HD12	2.51	0.41
2:B:675:PRO:O	2:B:887:HIS:NE2	2.53	0.41
2:B:841:TYR:CZ	2:B:843:SER:HB3	2.56	0.41
1:A:20:TYR:CE2	1:A:25:LEU:HD21	2.55	0.41
3:C:126:ASN:N	3:C:126:ASN:OD1	2.53	0.41
10:K:104:MET:HE2	10:K:104:MET:HB3	1.85	0.41
2:B:314:VAL:HB	2:B:318:TYR:HD2	1.86	0.40
2:B:1084:PRO:HA	2:B:1085:PRO:HD3	1.89	0.40
5:F:80:MET:HE2	6:G:65:ASN:HD21	1.86	0.40
7:H:60:ILE:HD11	7:H:123:MET:HE1	2.03	0.40
2:B:597:LEU:HD13	2:B:610:LEU:HD12	2.03	0.40
2:B:902:MET:HE1	2:B:914:LEU:HG	2.03	0.40
6:G:187:ASP:HB3	6:G:191:VAL:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:21:GLN:NE2	13:N:31:SER:OG	2.38	0.40
1:A:1213:LEU:HD23	1:A:1213:LEU:HA	1.82	0.40
1:A:448:ASP:HB2	1:A:576:ARG:HB3	2.03	0.40
1:A:494:ALA:HB3	1:A:541:HIS:ND1	2.35	0.40
1:A:623:ASP:O	1:A:1030:GLN:NE2	2.54	0.40
1:A:1601:TYR:OH	1:A:1624:GLU:OE2	2.27	0.40
2:B:187:ARG:NH2	2:B:218:GLU:OE2	2.48	0.40
2:B:1019:ASP:N	2:B:1019:ASP:OD1	2.44	0.40
2:B:1068:HIS:CD2	2:B:1109:THR:HG22	2.55	0.40
2:B:1082:GLU:OE1	2:B:1095:LYS:NZ	2.41	0.40
1:A:1259:ILE:HD11	1:A:1262:PRO:HB3	2.04	0.40
2:B:24:TYR:CZ	9:J:58:LYS:HE2	2.57	0.40
2:B:192:ALA:HB2	2:B:352:LYS:HE2	2.03	0.40
3:C:203:ARG:HA	3:C:203:ARG:HD3	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1490/1720 (87%)	1363 (92%)	127 (8%)	0	100	100
2	B	1126/1135 (99%)	1045 (93%)	81 (7%)	0	100	100
3	C	307/346 (89%)	290 (94%)	16 (5%)	1 (0%)	36	65
4	E	208/210 (99%)	191 (92%)	17 (8%)	0	100	100
5	F	75/127 (59%)	73 (97%)	2 (3%)	0	100	100
6	G	149/338 (44%)	126 (85%)	23 (15%)	0	100	100
7	H	147/150 (98%)	137 (93%)	10 (7%)	0	100	100
8	I	100/126 (79%)	94 (94%)	6 (6%)	0	100	100
9	J	62/67 (92%)	58 (94%)	4 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	K	105/133 (79%)	98 (93%)	7 (7%)	0	100	100
11	L	44/58 (76%)	39 (89%)	5 (11%)	0	100	100
12	M	101/419 (24%)	92 (91%)	9 (9%)	0	100	100
13	N	147/510 (29%)	139 (95%)	8 (5%)	0	100	100
All	All	4061/5339 (76%)	3745 (92%)	315 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	155	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	1331/1504 (88%)	1319 (99%)	12 (1%)	70	78
2	B	987/992 (100%)	985 (100%)	2 (0%)	87	88
3	C	272/302 (90%)	272 (100%)	0	100	100
4	E	192/192 (100%)	192 (100%)	0	100	100
5	F	67/111 (60%)	66 (98%)	1 (2%)	57	72
6	G	128/288 (44%)	126 (98%)	2 (2%)	55	72
7	H	130/131 (99%)	129 (99%)	1 (1%)	73	79
8	I	93/111 (84%)	92 (99%)	1 (1%)	65	76
9	J	53/56 (95%)	51 (96%)	2 (4%)	29	57
10	K	96/119 (81%)	96 (100%)	0	100	100
11	L	43/55 (78%)	43 (100%)	0	100	100
12	M	91/366 (25%)	90 (99%)	1 (1%)	65	76
13	N	118/427 (28%)	117 (99%)	1 (1%)	73	79
All	All	3601/4654 (77%)	3578 (99%)	23 (1%)	76	81

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	LEU
1	A	142	LEU
1	A	157	ILE
1	A	423	LYS
1	A	460	MET
1	A	461	VAL
1	A	464	THR
1	A	466	LEU
1	A	467	THR
1	A	915	LEU
1	A	954	ARG
1	A	1594	VAL
2	B	77	ILE
2	B	992	ILE
5	F	52	ILE
6	G	40	LEU
6	G	64	LEU
7	H	40	ILE
8	I	55	VAL
9	J	53	VAL
9	J	59	LEU
12	M	91	ILE
13	N	21	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	69	GLN
1	A	80	HIS
1	A	143	ASN
1	A	180	HIS
1	A	318	GLN
1	A	586	ASN
1	A	595	ASN
1	A	597	HIS
1	A	686	GLN
1	A	704	ASN
1	A	753	HIS
1	A	813	GLN
1	A	859	ASN

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Mol	Chain	Res	Type
1	A	908	ASN
1	A	911	GLN
1	A	1054	HIS
1	A	1076	GLN
1	A	1097	GLN
1	A	1111	ASN
1	A	1309	GLN
1	A	1313	GLN
1	A	1359	ASN
1	A	1503	GLN
1	A	1526	GLN
1	A	1537	ASN
1	A	1579	ASN
1	A	1584	ASN
1	A	1640	HIS
1	A	1671	GLN
1	A	1690	HIS
2	B	188	ASN
2	B	219	HIS
2	B	223	ASN
2	B	231	ASN
2	B	266	GLN
2	B	280	ASN
2	B	313	ASN
2	B	365	ASN
2	B	672	ASN
2	B	685	ASN
2	B	690	GLN
2	B	715	GLN
2	B	740	ASN
2	B	846	ASN
2	B	1068	HIS
3	C	96	ASN
3	C	102	GLN
3	C	160	ASN
3	C	166	HIS
3	C	305	HIS
4	E	30	GLN
4	E	142	HIS
4	E	148	HIS
4	E	168	ASN
4	E	210	GLN

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Mol	Chain	Res	Type
6	G	42	ASN
6	G	65	ASN
6	G	113	HIS
6	G	129	GLN
6	G	148	HIS
7	H	44	ASN
9	J	52	HIS
10	K	31	GLN
10	K	81	ASN
10	K	108	GLN
10	K	109	HIS
12	M	21	GLN
12	M	34	GLN
12	M	108	ASN
12	M	110	GLN
13	N	131	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 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](#)

There are no chain breaks in this entry.

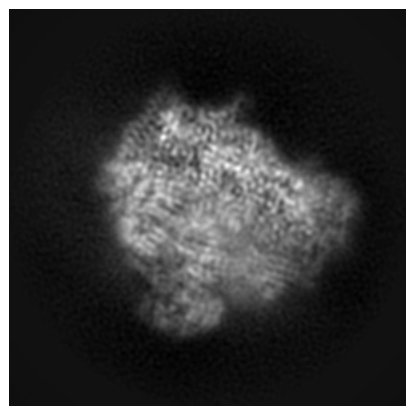
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12797. These allow visual inspection of the internal detail of the map and identification of artifacts.

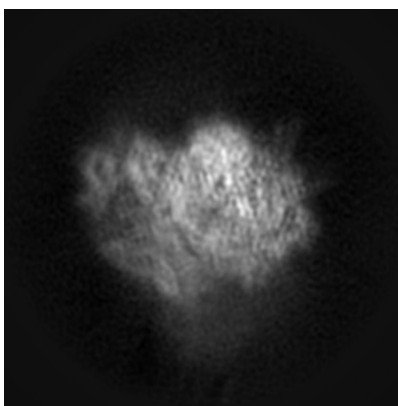
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

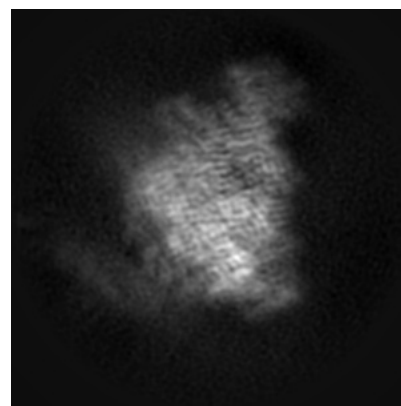
6.1.1 Primary map



X

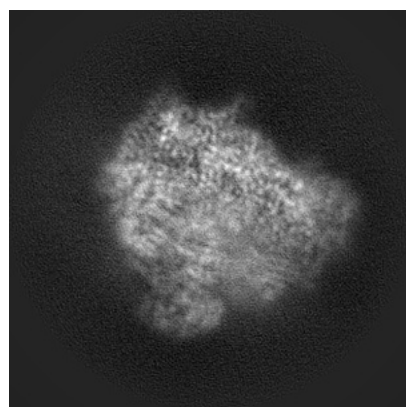


Y

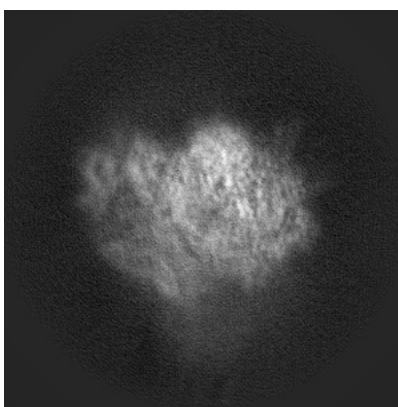


Z

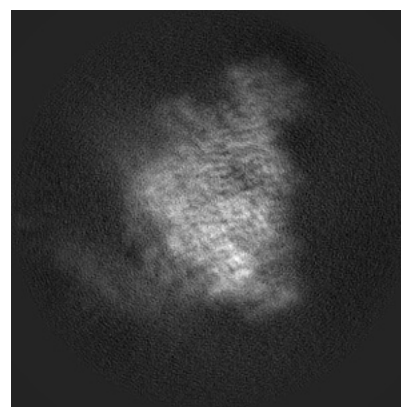
6.1.2 Raw map



X



Y

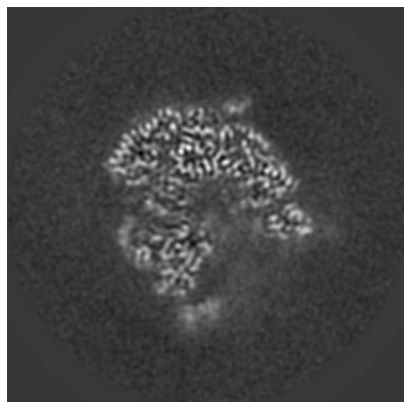


Z

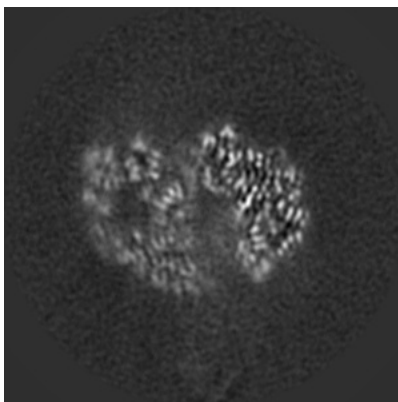
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

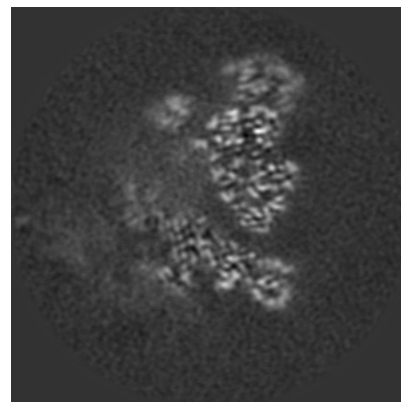
6.2.1 Primary map



X Index: 144

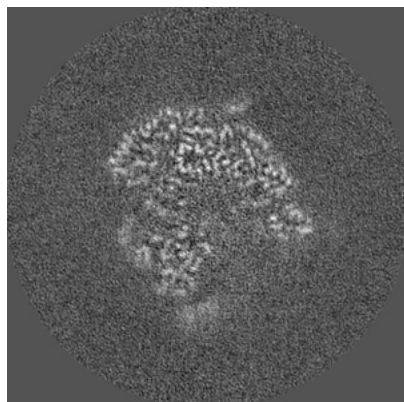


Y Index: 144

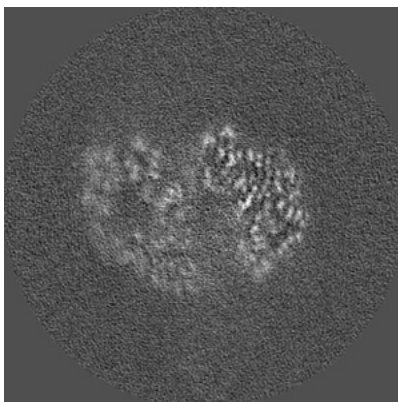


Z Index: 144

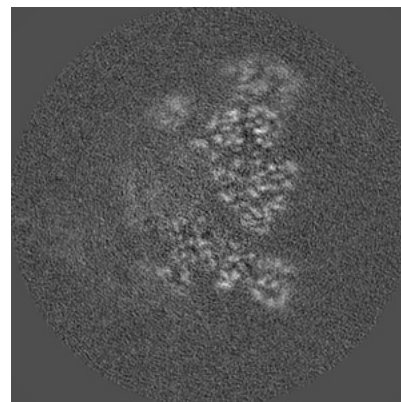
6.2.2 Raw map



X Index: 144



Y Index: 144

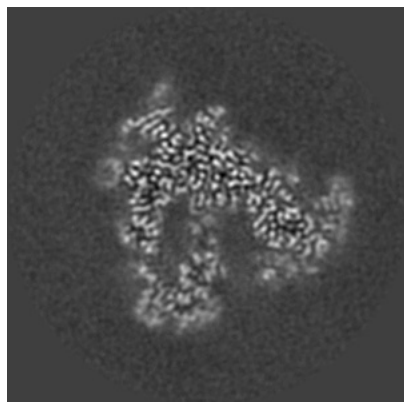


Z Index: 144

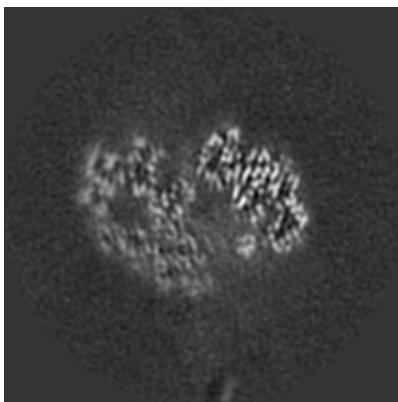
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

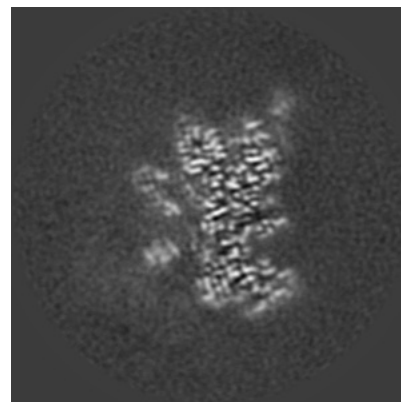
6.3.1 Primary map



X Index: 165

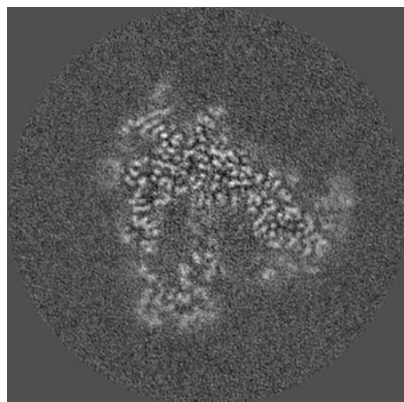


Y Index: 139

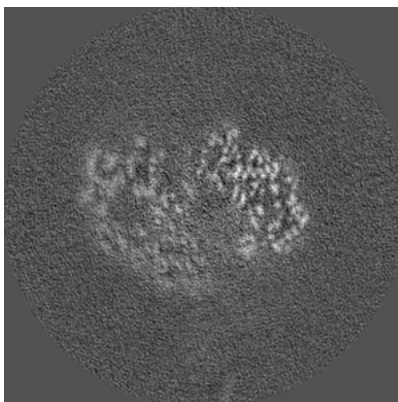


Z Index: 171

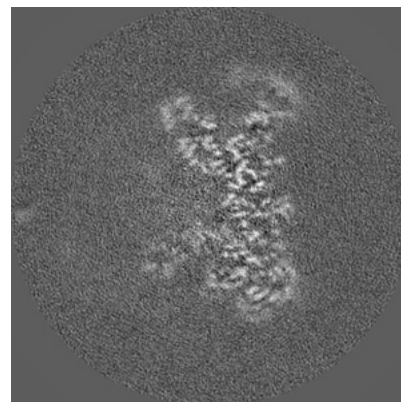
6.3.2 Raw map



X Index: 165



Y Index: 140

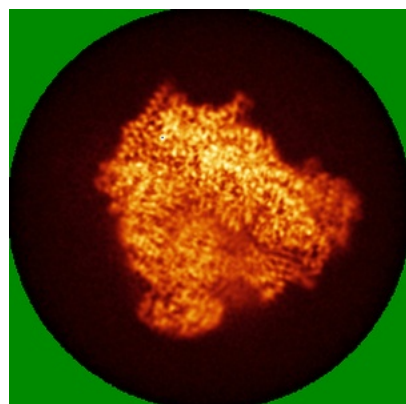


Z Index: 161

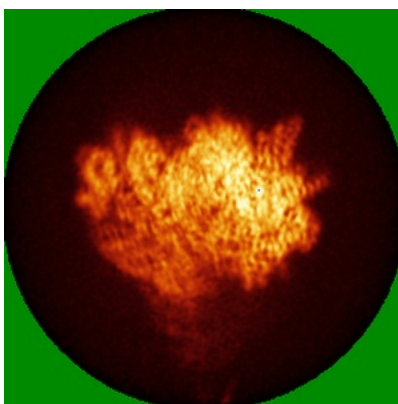
The images above show the largest variance slices of the map in three orthogonal directions.

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

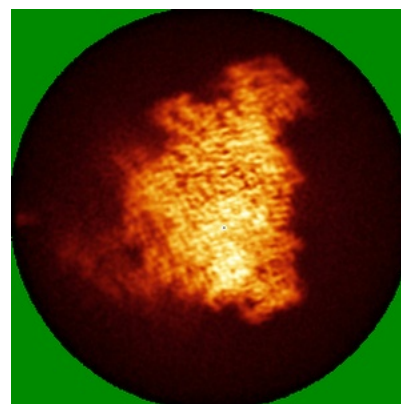
6.4.1 Primary map



X

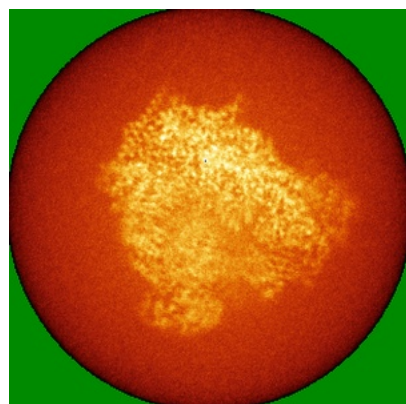


Y

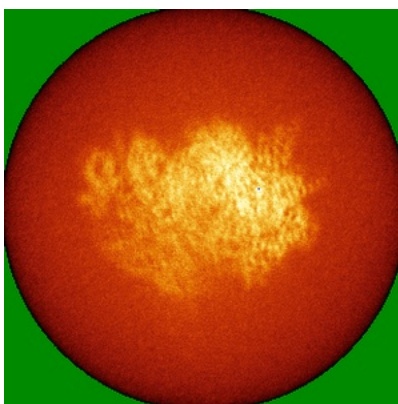


Z

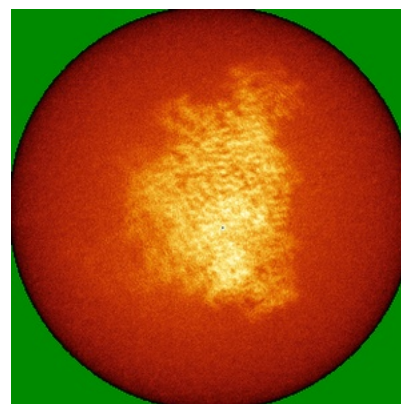
6.4.2 Raw map



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.

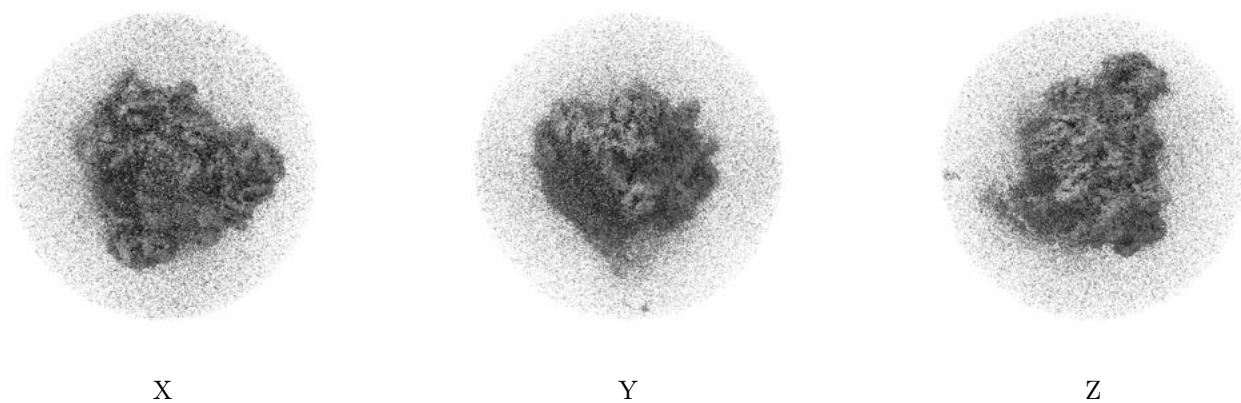
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00386. 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.

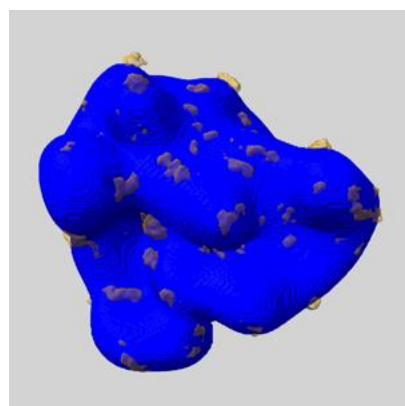
6.6 Mask visualisation [i](#)

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

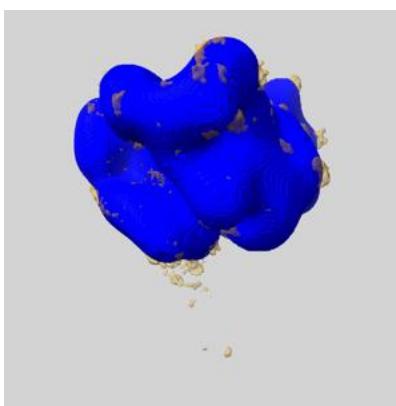
A mask typically either:

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

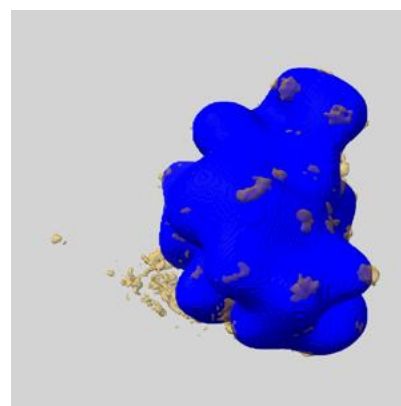
6.6.1 emd_12797_msk_1.map [i](#)



X



Y

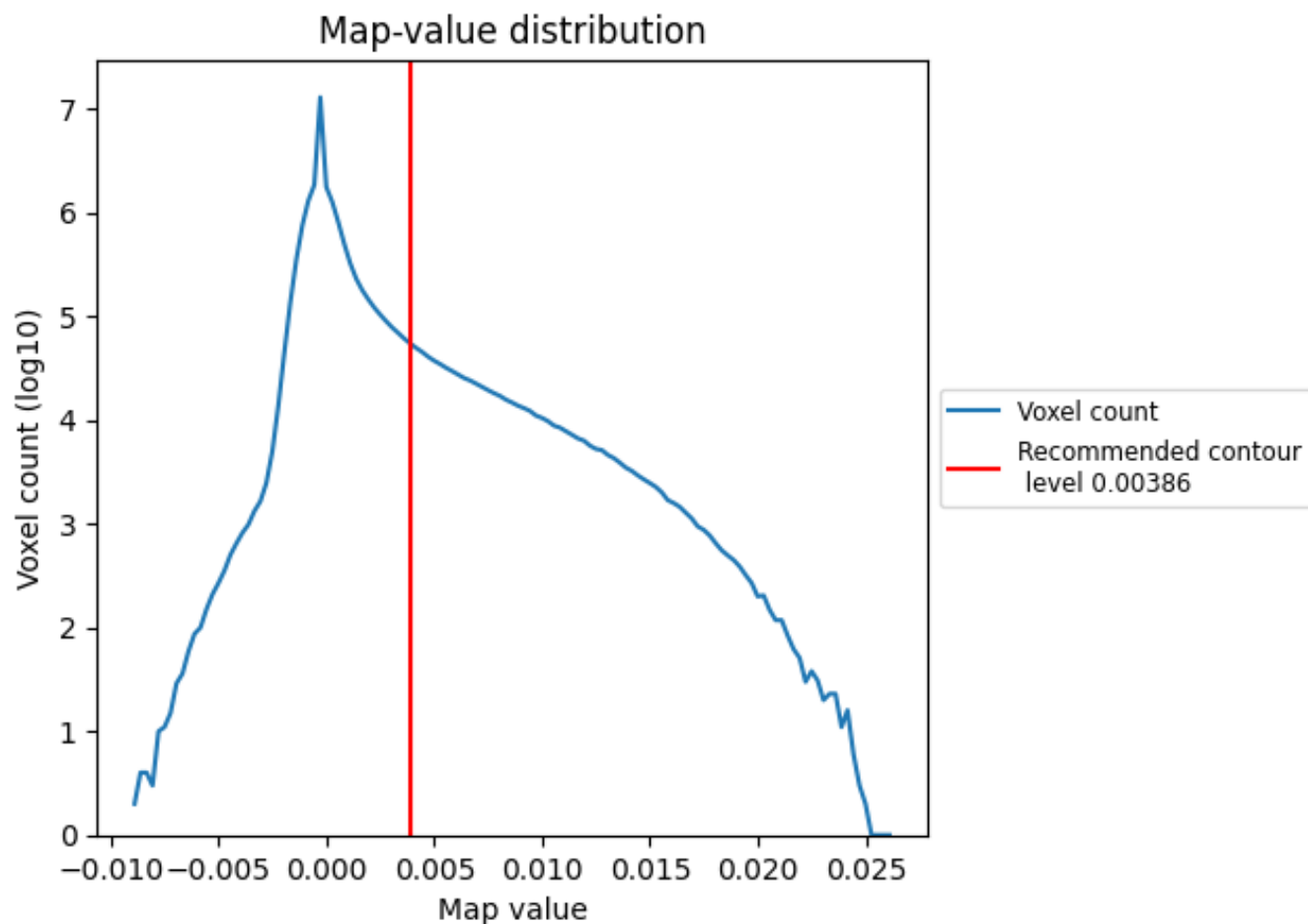


Z

7 Map analysis [i](#)

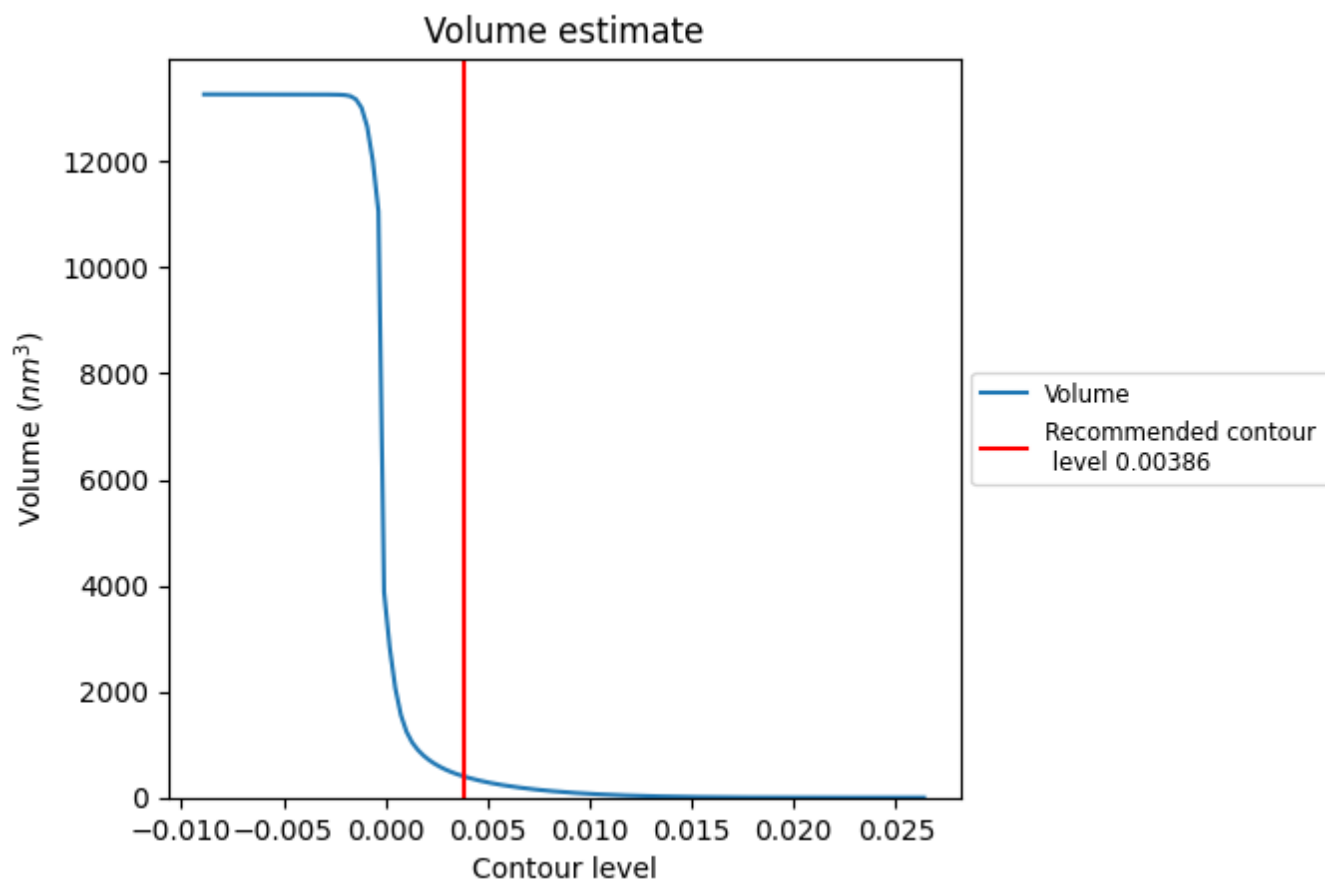
This section contains the results of statistical analysis of the map.

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.

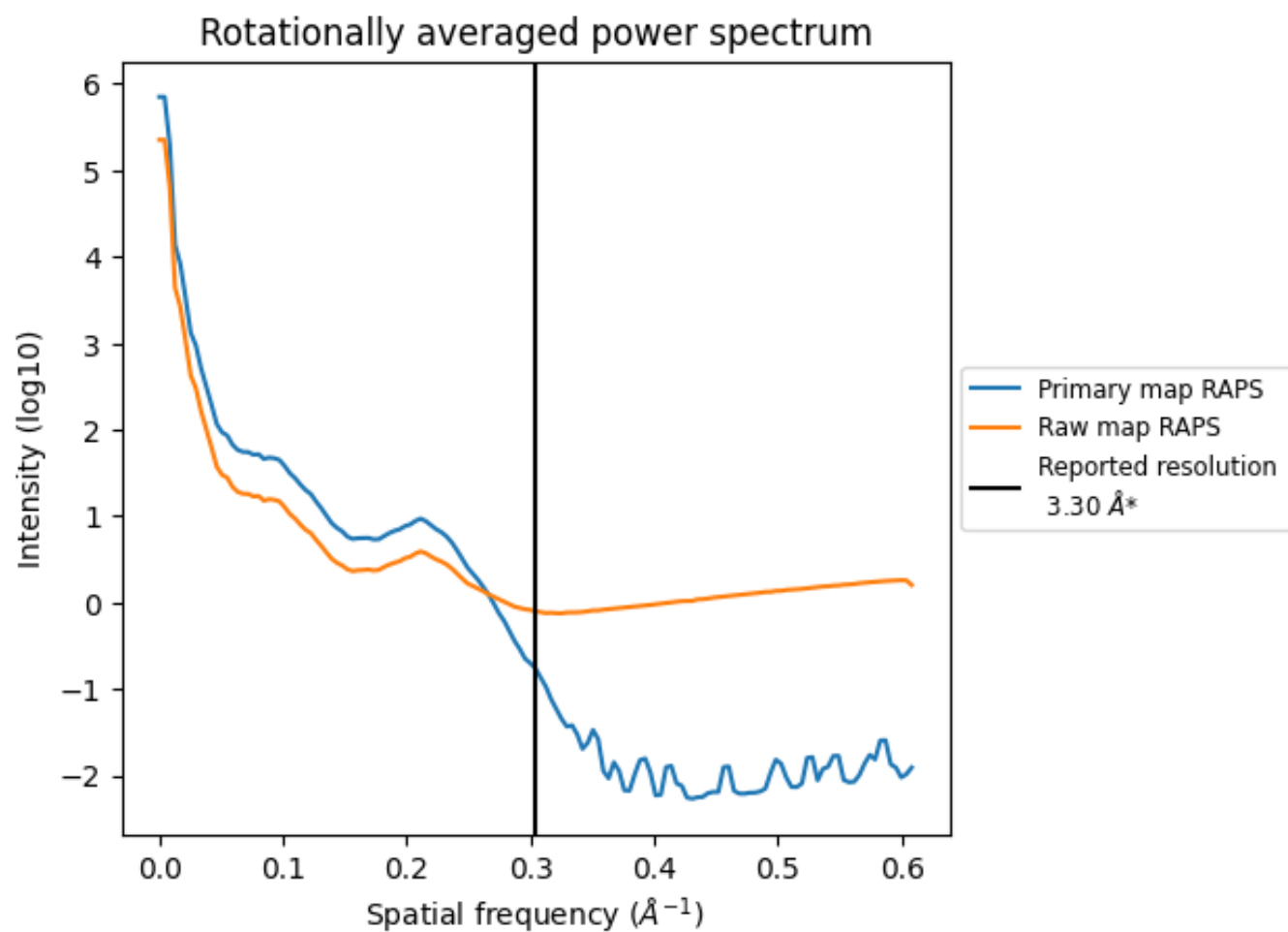
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 397 nm³; this corresponds to an approximate mass of 359 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 ⓘ

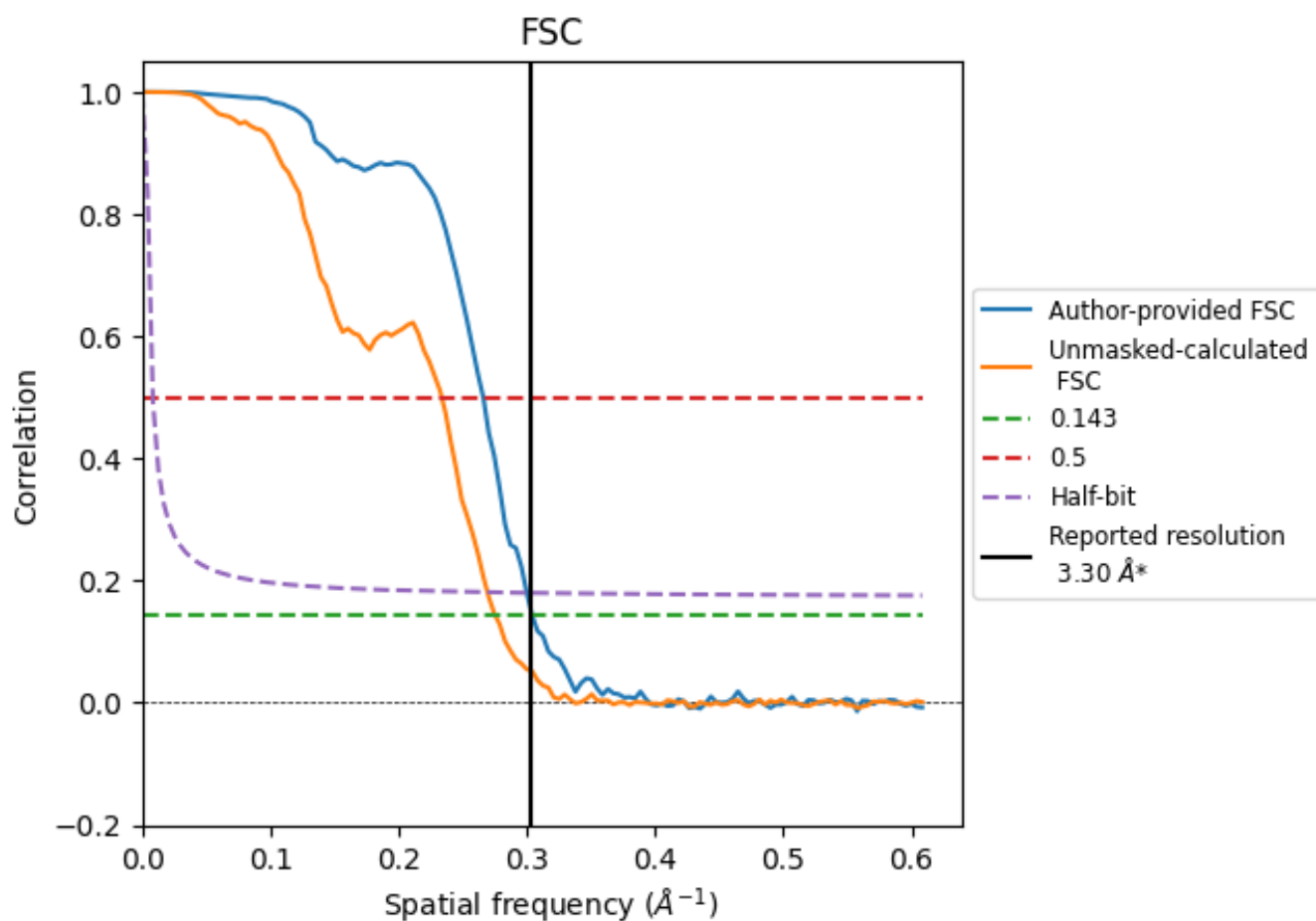


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

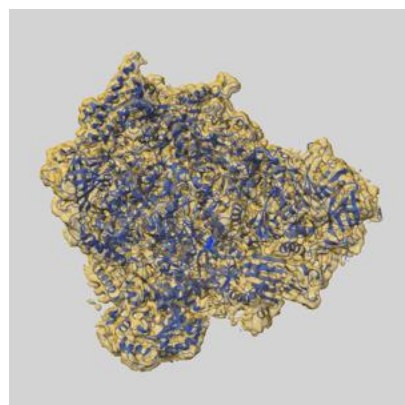
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.29	3.76	3.33
Unmasked-calculated*	3.63	4.28	3.71

*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 3.63 differs from the reported value 3.3 by more than 10 %

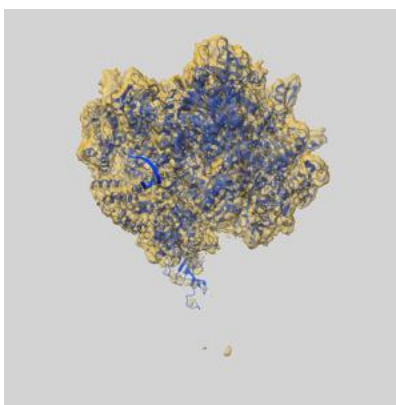
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12797 and PDB model 7OBB. Per-residue inclusion information can be found in section [3](#) on page [7](#).

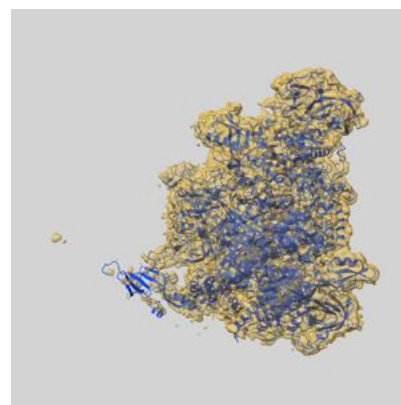
9.1 Map-model overlay [i](#)



X



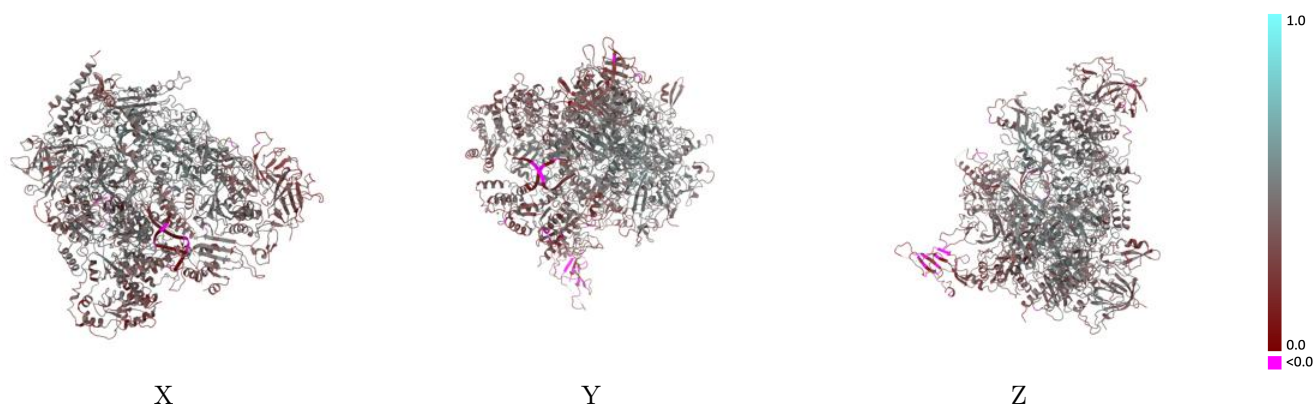
Y



Z

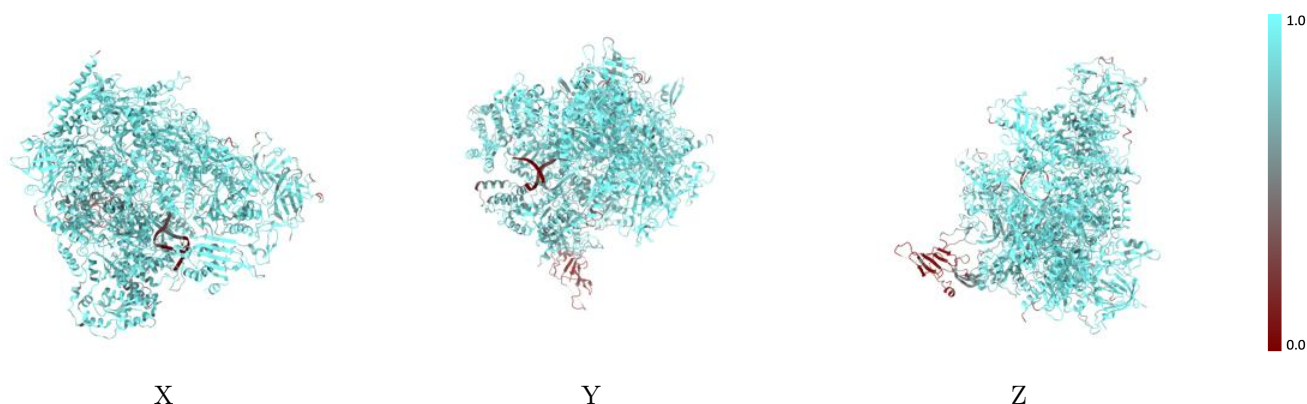
The images above show the 3D surface view of the map at the recommended contour level 0.00386 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



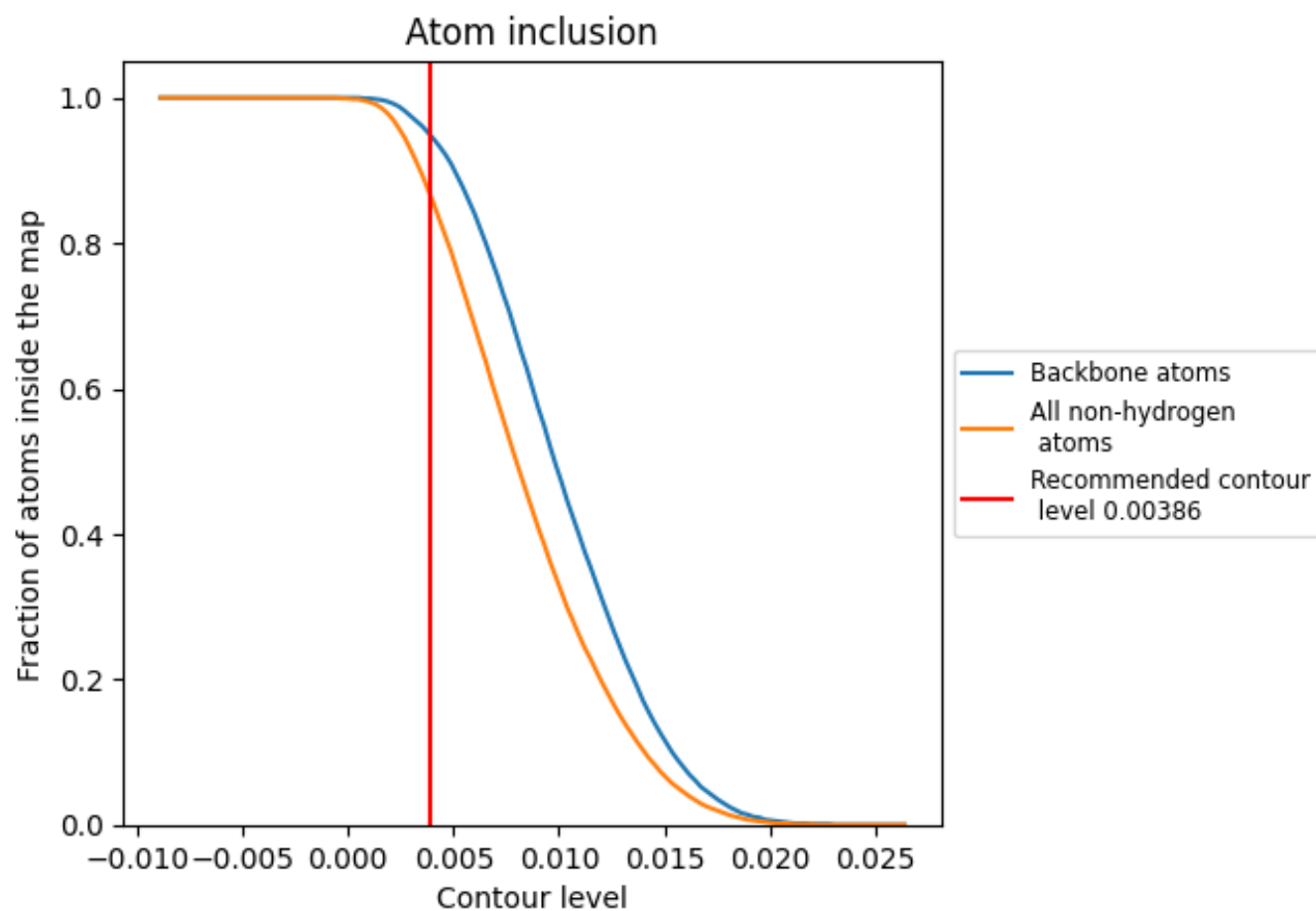
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00386).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% 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 (0.00386) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8690	 0.4010
A	 0.8790	 0.3990
B	 0.9270	 0.4490
C	 0.9170	 0.4150
E	 0.9020	 0.3860
F	 0.8500	 0.3840
G	 0.3400	 0.2120
H	 0.9010	 0.4040
I	 0.8780	 0.4170
J	 0.9640	 0.4710
K	 0.8970	 0.4130
L	 0.9490	 0.4510
M	 0.8240	 0.3160
N	 0.7910	 0.3290
S	 0.1720	 0.0780
T	 0.4160	 0.0890

