



Full wwPDB EM Validation Report ⓘ

Aug 10, 2026 – 01:25 pm BST

PDB ID : 28JC / pdb_000028jc
EMDB ID : EMD-56542
Title : RNA polymerase II bound to RPAP2 and Gdown1
Authors : Schmitzova, J.; Zhan, Y.; Dienemann, C.
Deposited on : 2026-02-03
Resolution : 2.94 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:

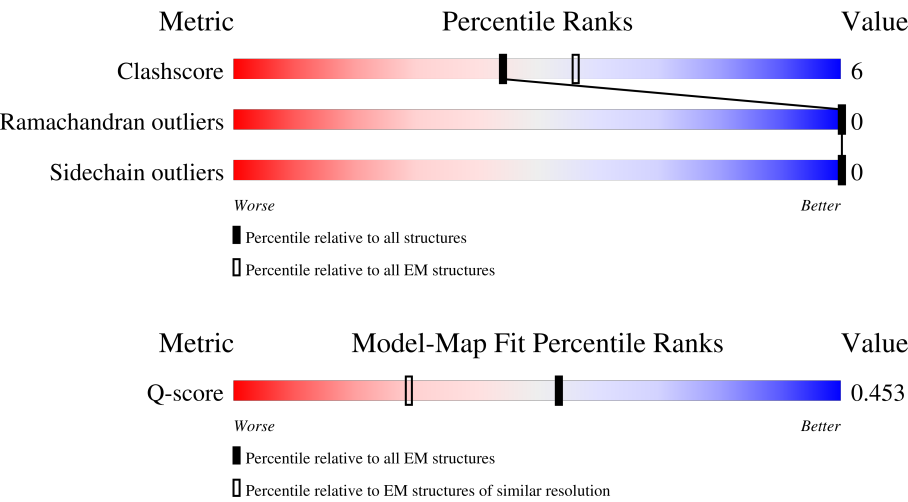
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.94 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.



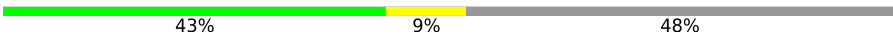
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13068 (2.44 - 3.44)

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	D	142	
2	E	210	
3	F	127	
4	G	172	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	H	150	 83% 16% .
6	I	125	 79% 12% 9%
7	J	67	 64% 33% .
8	K	117	 81% 17% .
9	L	58	 53% 22% 24%
10	M	368	 31% 5% 64%
11	A	1970	 43% 9% 48%
12	B	1174	 69% 18% 14%
13	C	275	 78% 19% .
14	N	612	 21% . 75%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 29492 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 II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	129	Total	C	N	O	S	0	0
			1063	665	179	215	4		

- Molecule 2 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	209	Total	C	N	O	S	0	0
			1715	1083	300	324	8		

- Molecule 3 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	79	Total	C	N	O	S	0	0
			636	407	108	116	5		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	114	Total	C	N	O	S	0	0
			927	571	166	179	11		

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	65	Total	C	N	O	S	0	0
			515	334	87	88	6		

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

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

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	44	Total	C	N	O	S	0	0
			372	231	72	63	6		

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit GRINL1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	132	Total	C	N	O	S	0	0
			1082	685	199	191	7		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	1029	Total	C	N	O	S	0	0
			8206	5168	1447	1547	44		

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	B	1015	Total	C	N	O	S	0	0
			8128	5158	1412	1508	50		

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	C	265	Total	C	N	O	S	0	0
			2135	1340	367	422	6		

- Molecule 14 is a protein called Putative RNA polymerase II subunit B1 CTD phosphatase RPAP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	153	Total	C	N	O	S	0	0
			1250	794	212	237	7		

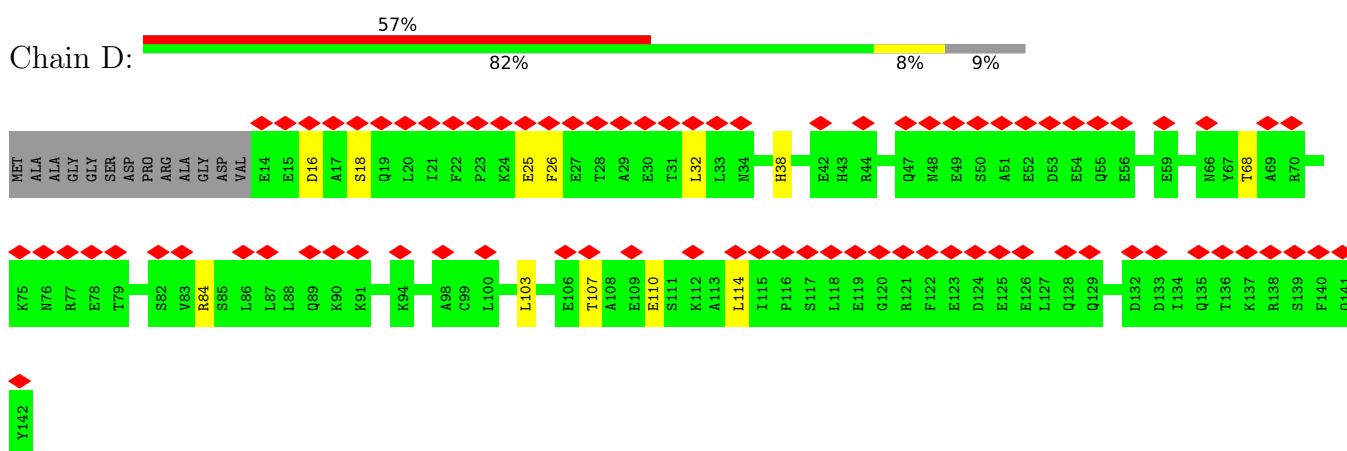
- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
15	I	2	Total	Zn	0
			2	2	
15	J	1	Total	Zn	0
			1	1	
15	L	1	Total	Zn	0
			1	1	
15	C	1	Total	Zn	0
			1	1	
15	N	1	Total	Zn	0
			1	1	

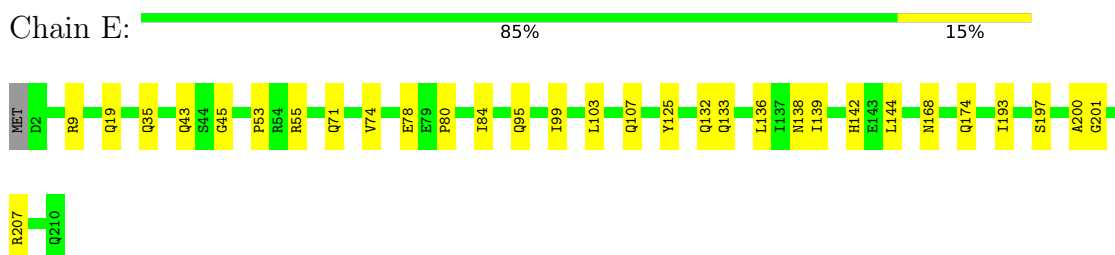
3 Residue-property plots

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.

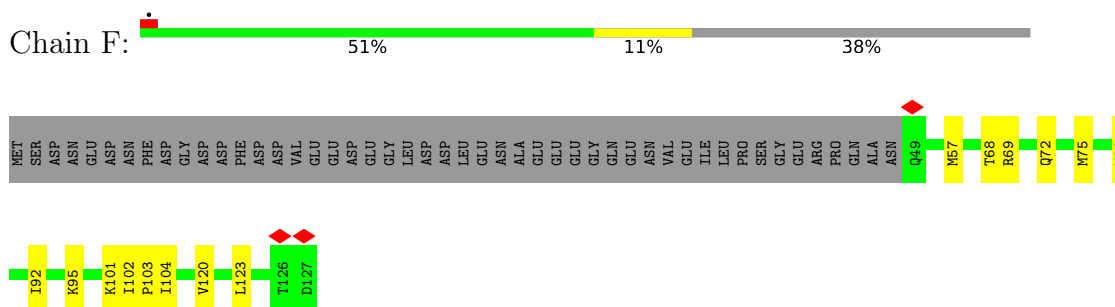
- Molecule 1: DNA-directed RNA polymerase II subunit RPB4



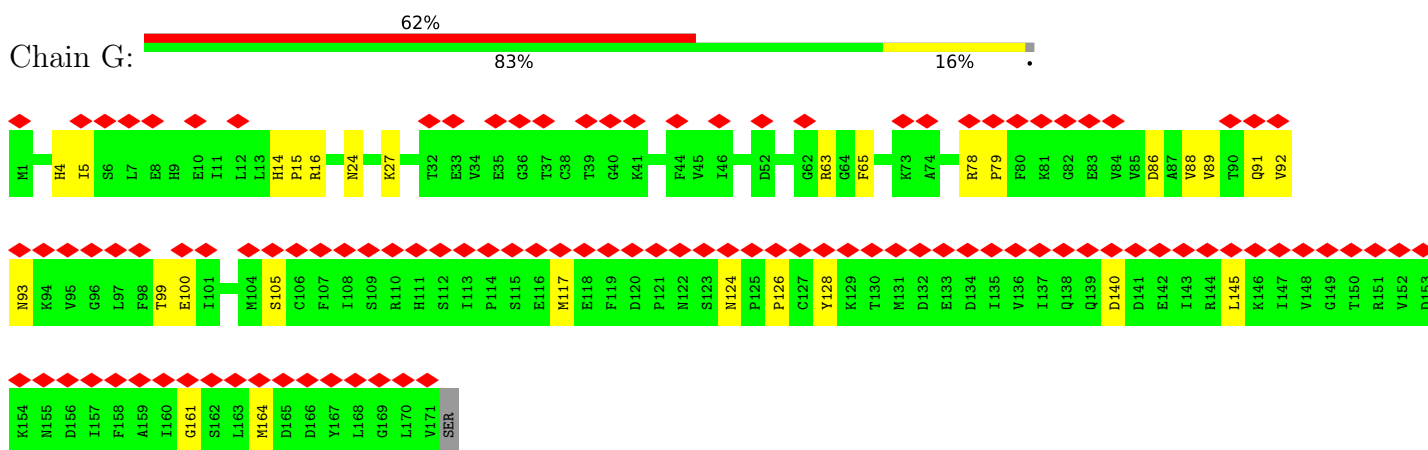
- Molecule 2: DNA-directed RNA polymerases I, II, and III subunit RPABC1



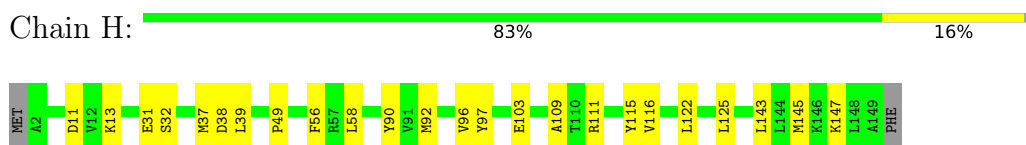
- Molecule 3: DNA-directed RNA polymerases I, II, and III subunit RPABC2



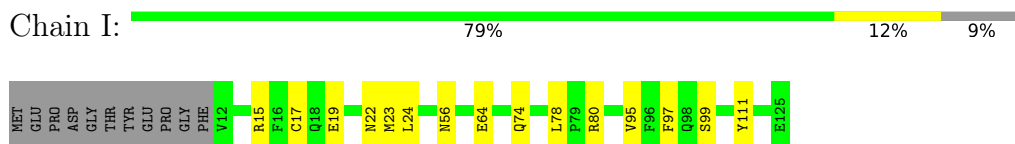
- Molecule 4: DNA-directed RNA polymerase II subunit RPB7



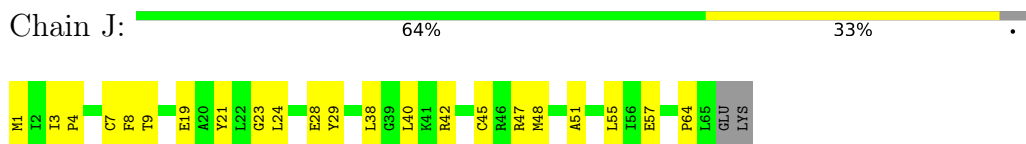
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC3



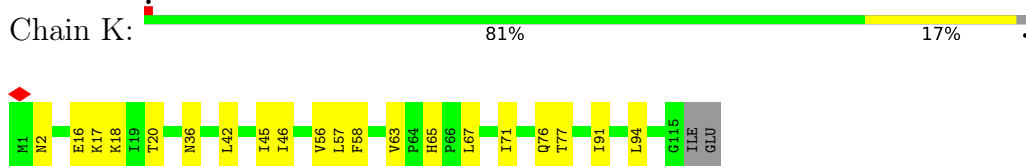
- Molecule 6: DNA-directed RNA polymerase II subunit RPB9



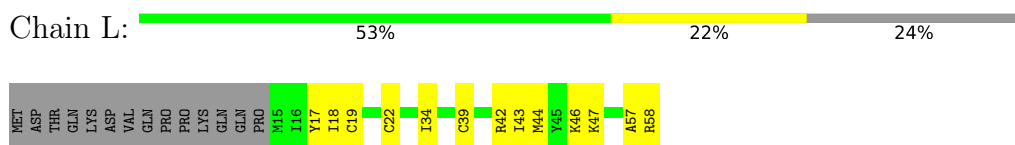
- Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- Molecule 8: DNA-directed RNA polymerase II subunit RPB11-a



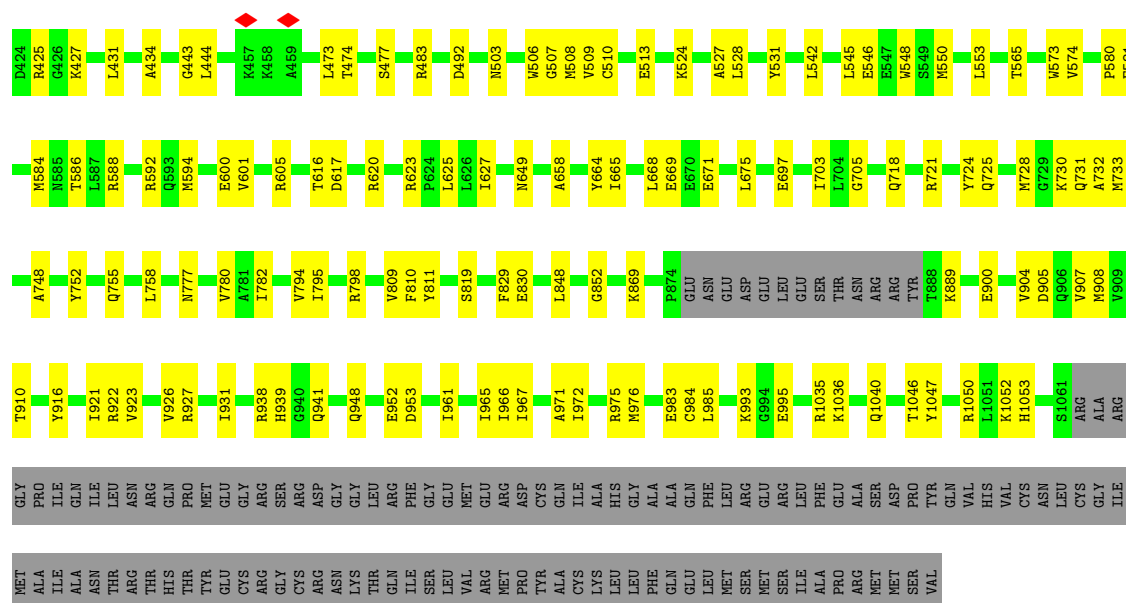
- Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC4



- Molecule 10: DNA-directed RNA polymerase II subunit GRINL1A

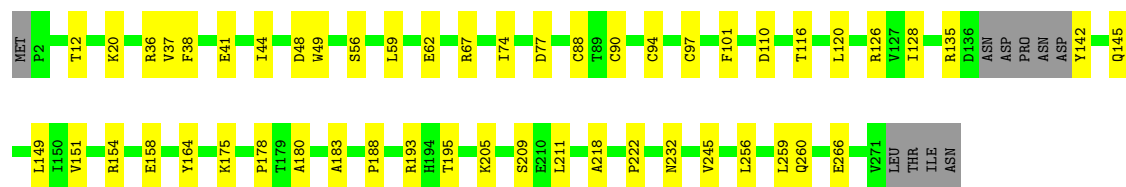
- Molecule 11: DNA-directed RNA polymerase II subunit RPB1





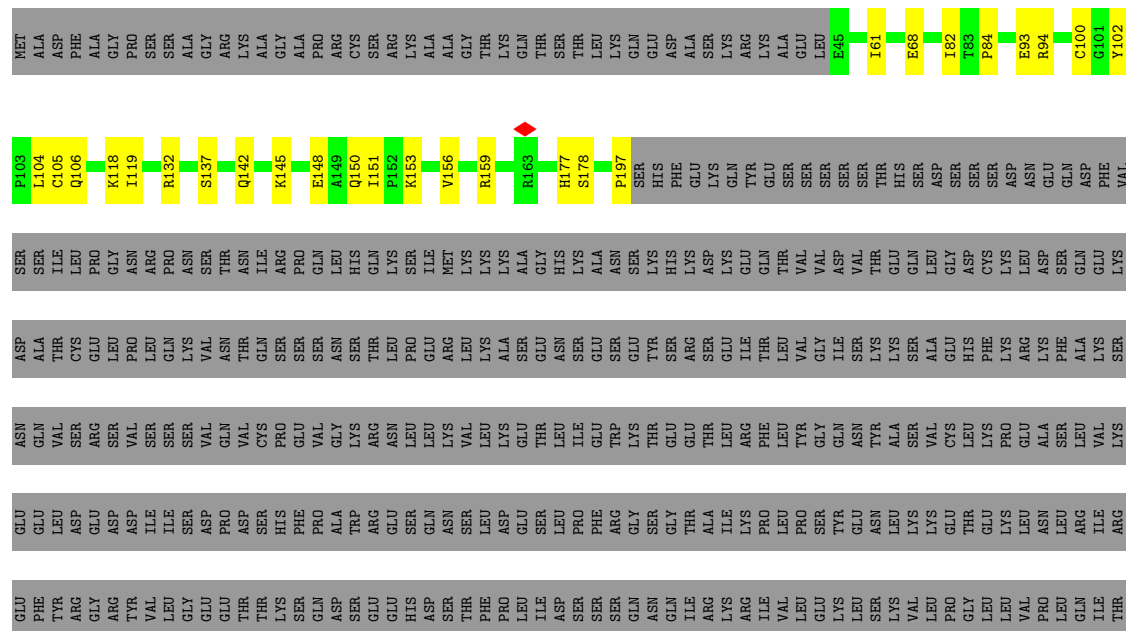
• Molecule 13: DNA-directed RNA polymerase II subunit RPB3

Chain C: 78% 19% .



• Molecule 14: Putative RNA polymerase II subunit B1 CTD phosphatase RPAP2

Chain N: 21% . 75%



LEU GLY ASP LEU ILE TYR THR GLN LEU LYS ASN LEU VAL ARG THR PHE ARG LEU THR ASN ARG ASN ILE ILE HIS LYS PRO ALA GLU TRP THR LEU ILE ALA MET VAL LEU SER LEU THR PRO ILE LEU GLY ILE GLN LYS HIS SER GLN GLY MET VAL PHE THR ARG PHE LEU

ASP THR LEU LEU GLU LEU HIS LEU LYS ASN ASP LEU GLU SER LEU THR ILE ILE PHE ARG THR SER CYS LEU PRO GLU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47505	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	39.91	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.055	Depositor
Minimum map value	-0.022	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00511	Depositor
Map size (Å)	294.0, 294.0, 294.0	wwPDB
Map dimensions	280, 280, 280	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: 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	D	0.12	0/1078	0.34	0/1446
2	E	0.16	0/1745	0.39	0/2358
3	F	0.22	0/646	0.64	0/873
4	G	0.12	0/1382	0.34	0/1874
5	H	0.16	0/1207	0.43	0/1628
6	I	0.16	0/948	0.44	0/1284
7	J	0.24	0/524	0.52	0/707
8	K	0.21	0/939	0.49	1/1271 (0.1%)
9	L	0.22	0/377	0.57	0/500
10	M	0.21	0/1095	0.55	0/1457
11	A	0.16	0/8351	0.41	1/11279 (0.0%)
12	B	0.18	0/8293	0.43	1/11203 (0.0%)
13	C	0.15	0/2179	0.36	0/2960
14	N	0.20	0/1275	0.58	0/1714
All	All	0.17	0/30039	0.43	3/40554 (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
4	G	0	1
6	I	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	649	ASN	N-CA-C	-6.96	105.72	114.56
8	K	16	GLU	CA-CB-CG	5.71	125.52	114.10
11	A	1185	VAL	N-CA-C	-5.11	108.52	113.53

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	G	124	ASN	Peptide
6	I	15	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1063	0	1042	7	0
2	E	1715	0	1733	22	0
3	F	636	0	667	8	0
4	G	1351	0	1358	16	0
5	H	1186	0	1147	15	0
6	I	927	0	859	10	0
7	J	515	0	534	19	0
8	K	920	0	942	14	0
9	L	372	0	378	9	0
10	M	1082	0	1150	14	0
11	A	8206	0	8239	110	0
12	B	8128	0	8162	135	0
13	C	2135	0	2079	35	0
14	N	1250	0	1246	16	0
15	C	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
15	N	1	0	0	0	0
All	All	29492	0	29536	380	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 6.

All (380) 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)
9:L:19:CYS:HB3	9:L:22:CYS:SG	2.14	0.86
14:N:100:CYS:SG	14:N:105:CYS:HB3	2.15	0.85
9:L:22:CYS:HB3	9:L:39:CYS:SG	2.32	0.70
11:A:1343:LEU:HD22	11:A:1368:VAL:HG11	1.72	0.69
13:C:56:SER:HB2	13:C:158:GLU:H	1.57	0.69
12:B:758:LEU:H	12:B:777:ASN:HD21	1.38	0.68
8:K:17:LYS:HE3	8:K:20:THR:HG22	1.76	0.68
13:C:49:TRP:HB3	13:C:164:TYR:HB2	1.75	0.67
3:F:102:ILE:HG22	3:F:104:ILE:H	1.60	0.67
12:B:984:CYS:SG	12:B:1046:THR:OG1	2.53	0.67
2:E:139:ILE:HD11	11:A:1369:LEU:HA	1.77	0.66
11:A:1246:ILE:HB	11:A:1258:ARG:HB2	1.77	0.66
3:F:80:MET:HG2	3:F:101:LYS:HE3	1.76	0.66
3:F:102:ILE:HB	3:F:120:VAL:HG21	1.78	0.65
3:F:57:MET:HG3	3:F:123:LEU:HD13	1.79	0.64
8:K:42:LEU:HD21	13:C:259:LEU:HD22	1.78	0.64
12:B:600:GLU:O	12:B:620:ARG:NH2	2.31	0.64
14:N:68:GLU:HB2	14:N:106:GLN:HE22	1.61	0.64
11:A:808:PRO:HB2	12:B:675:LEU:HD12	1.80	0.63
5:H:96:VAL:HG22	5:H:116:VAL:HG22	1.80	0.63
11:A:689:ILE:HG13	12:B:985:LEU:HD22	1.80	0.63
2:E:174:GLN:HE21	11:A:1410:HIS:HB3	1.65	0.62
3:F:92:ILE:HA	3:F:95:LYS:HG2	1.81	0.62
5:H:11:ASP:OD1	5:H:13:LYS:NZ	2.32	0.62
11:A:393:ILE:HG12	11:A:445:LYS:HG2	1.81	0.62
13:C:37:VAL:HG13	13:C:41:GLU:HB2	1.81	0.62
2:E:9:ARG:HG3	2:E:136:LEU:HD21	1.82	0.61
6:I:23:MET:SD	12:B:302:LYS:NZ	2.72	0.61
11:A:1261:ILE:HD11	14:N:119:ILE:HG21	1.83	0.61
7:J:19:GLU:OE1	10:M:33:ARG:NH2	2.33	0.61
12:B:91:ILE:HG22	12:B:126:VAL:HG23	1.81	0.61
12:B:748:ALA:HB3	12:B:811:TYR:HB2	1.82	0.60
11:A:630:VAL:HG21	11:A:652:LEU:HD21	1.83	0.60
11:A:732:THR:HG22	11:A:735:GLN:HE21	1.66	0.60
12:B:295:PRO:HA	12:B:298:MET:HB2	1.83	0.60
13:C:77:ASP:HB2	13:C:126:ARG:HH22	1.67	0.60
10:M:315:GLN:O	10:M:319:ASN:ND2	2.34	0.60
12:B:274:ARG:NH1	12:B:279:VAL:O	2.35	0.60
12:B:810:PHE:HB2	12:B:927:ARG:HD2	1.82	0.60
11:A:1288:ILE:HG22	11:A:1292:MET:HE2	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:265:GLN:HB3	12:B:324:ARG:HD3	1.84	0.59
13:C:183:ALA:HB3	13:C:232:ASN:HB3	1.82	0.59
11:A:487:SER:HA	11:A:538:VAL:HB	1.84	0.59
7:J:64:PRO:HD3	13:C:154:ARG:HD3	1.84	0.59
11:A:420:ILE:HB	11:A:445:LYS:HB2	1.84	0.59
12:B:592:ARG:HE	12:B:627:ILE:HD13	1.67	0.58
7:J:3:ILE:O	13:C:67:ARG:NH1	2.36	0.58
8:K:91:ILE:HG21	13:C:260:GLN:HB2	1.85	0.58
7:J:47:ARG:NH1	12:B:777:ASN:O	2.37	0.58
11:A:1182:GLN:O	11:A:1190:GLN:NE2	2.37	0.57
12:B:904:VAL:HG12	12:B:923:VAL:HG22	1.85	0.57
12:B:483:ARG:NH2	12:B:527:ALA:O	2.36	0.57
8:K:63:VAL:HG22	8:K:71:ILE:HG22	1.86	0.57
11:A:1099:ALA:HA	11:A:1102:MET:HE2	1.87	0.57
11:A:1130:ILE:HG12	11:A:1413:ALA:HB2	1.85	0.57
11:A:368:THR:HG21	12:B:931:ILE:HG22	1.86	0.57
13:C:193:ARG:NH1	13:C:218:ALA:O	2.35	0.57
4:G:88:VAL:HG13	4:G:140:ASP:HA	1.86	0.57
2:E:200:ALA:HB2	11:A:894:ASP:HB3	1.87	0.56
11:A:1020:LEU:HD21	11:A:1073:GLU:HA	1.87	0.56
11:A:1193:VAL:HG23	11:A:1246:ILE:HG21	1.87	0.56
12:B:509:VAL:HG11	12:B:524:LYS:HD2	1.87	0.56
12:B:513:GLU:OE2	12:B:730:LYS:NZ	2.33	0.56
14:N:148:GLU:O	14:N:153:LYS:NZ	2.39	0.56
12:B:273:PHE:HB3	12:B:284:ILE:HD12	1.88	0.56
2:E:80:PRO:HA	2:E:107:GLN:HB2	1.87	0.56
8:K:58:PHE:HB3	8:K:76:GLN:HB3	1.87	0.56
6:I:22:ASN:HA	12:B:281:ASP:HB2	1.88	0.56
10:M:251:THR:HG21	12:B:531:TYR:HE2	1.70	0.56
12:B:99:TRP:HD1	12:B:105:PRO:HG3	1.70	0.56
11:A:371:PRO:HB3	11:A:673:GLN:HE22	1.72	0.55
12:B:65:ILE:HD11	12:B:416:ARG:HD3	1.89	0.55
7:J:21:TYR:HB2	7:J:38:LEU:HD11	1.89	0.55
12:B:387:HIS:NE2	12:B:671:GLU:OE2	2.39	0.55
12:B:777:ASN:HA	12:B:1047:TYR:HA	1.89	0.55
13:C:205:LYS:HE2	13:C:211:LEU:HD23	1.88	0.55
5:H:31:GLU:HA	5:H:38:ASP:HA	1.89	0.54
5:H:56:PHE:HE2	5:H:58:LEU:HD23	1.72	0.54
12:B:601:VAL:HG22	12:B:616:THR:HG23	1.89	0.54
12:B:617:ASP:O	12:B:620:ARG:NH1	2.40	0.54
8:K:18:LYS:NZ	8:K:36:ASN:O	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:29:TYR:HE2	10:M:44:LEU:HD22	1.73	0.54
11:A:587:THR:H	11:A:590:GLN:HE21	1.55	0.54
6:I:17:CYS:HB3	6:I:24:LEU:HD21	1.88	0.54
11:A:948:ILE:HG12	11:A:1007:ILE:HG21	1.89	0.54
11:A:1144:LEU:HD23	11:A:1353:ASP:HA	1.89	0.54
12:B:1040:GLN:NE2	13:C:195:THR:OG1	2.41	0.54
11:A:873:VAL:HG22	11:A:879:VAL:HG22	1.89	0.54
12:B:222:ARG:HA	12:B:234:THR:HG22	1.89	0.54
5:H:90:TYR:HB3	5:H:145:MET:HG2	1.90	0.54
4:G:78:ARG:NH1	4:G:79:PRO:O	2.41	0.54
9:L:17:TYR:HB3	9:L:44:MET:HG2	1.89	0.54
11:A:604:ARG:NE	11:A:650:GLY:O	2.41	0.54
11:A:1007:ILE:HA	11:A:1010:VAL:HG12	1.90	0.54
12:B:545:LEU:HB3	12:B:550:MET:HG3	1.90	0.53
11:A:691:ASP:OD2	11:A:765:ASN:ND2	2.40	0.53
5:H:39:LEU:HD12	5:H:125:LEU:HD13	1.91	0.53
5:H:49:PRO:O	5:H:147:LYS:NZ	2.40	0.53
11:A:1176:TYR:HB2	11:A:1211:LEU:HD23	1.90	0.53
6:I:56:ASN:HB3	11:A:1173:THR:HB	1.89	0.53
10:M:302:GLN:HE22	12:B:90:GLN:HE22	1.57	0.53
11:A:1365:ILE:HG23	11:A:1369:LEU:HD12	1.89	0.53
12:B:111:ASN:ND2	12:B:175:ASN:O	2.40	0.53
12:B:546:GLU:HA	12:B:550:MET:HB2	1.91	0.53
12:B:830:GLU:OE2	12:B:889:LYS:NZ	2.42	0.53
12:B:953:ASP:OD1	13:C:36:ARG:NH2	2.42	0.53
3:F:75:MET:HE3	4:G:15:PRO:HG2	1.91	0.53
11:A:559:GLU:HG2	11:A:682:ILE:HD13	1.91	0.53
12:B:276:LEU:HD21	12:B:347:MET:HE1	1.90	0.53
12:B:795:ILE:HB	12:B:966:ILE:HB	1.91	0.53
11:A:1368:VAL:HG13	11:A:1369:LEU:HG	1.90	0.52
2:E:107:GLN:HA	2:E:132:GLN:HB2	1.90	0.52
11:A:902:GLU:OE2	11:A:982:ASN:ND2	2.42	0.52
12:B:508:MET:HE2	12:B:623:ARG:HG3	1.90	0.52
14:N:118:LYS:NZ	14:N:178:SER:OG	2.39	0.52
3:F:69:ARG:HH21	3:F:103:PRO:HD2	1.75	0.52
11:A:1403:ASP:HA	11:A:1406:THR:HG22	1.90	0.52
2:E:84:ILE:HG13	14:N:93:GLU:HG2	1.91	0.52
8:K:2:ASN:HD21	11:A:381:PRO:HB2	1.75	0.52
12:B:310:VAL:HG23	12:B:311:ILE:HD12	1.92	0.52
8:K:57:LEU:HB2	8:K:76:GLN:HG2	1.90	0.52
11:A:1234:LYS:NZ	11:A:1298:LEU:O	2.36	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:96:PRO:HG3	12:B:154:ILE:HG13	1.91	0.51
12:B:143:GLN:NE2	12:B:145:GLN:OE1	2.43	0.51
12:B:907:VAL:HG22	12:B:921:ILE:HG12	1.92	0.51
13:C:38:PHE:HE1	13:C:245:VAL:HA	1.75	0.51
11:A:362:SER:HB3	11:A:388:MET:HE3	1.93	0.51
12:B:407:MET:HE1	12:B:443:GLY:HA3	1.92	0.51
8:K:17:LYS:NZ	13:C:266:GLU:OE2	2.35	0.51
5:H:32:SER:HB3	5:H:37:MET:HB3	1.91	0.51
11:A:389:THR:O	11:A:507:GLN:NE2	2.44	0.51
8:K:45:ILE:HG22	8:K:46:ILE:HD13	1.93	0.51
11:A:1359:SER:OG	11:A:1360:ASN:N	2.43	0.51
10:M:231:TYR:HA	10:M:234:VAL:HG12	1.93	0.51
11:A:408:ARG:NE	11:A:412:GLN:OE1	2.39	0.50
12:B:625:LEU:HD13	12:B:675:LEU:HD21	1.93	0.50
12:B:725:GLN:HB2	12:B:939:HIS:HA	1.92	0.50
2:E:19:GLN:OE1	2:E:138:ASN:ND2	2.44	0.50
12:B:297:MET:HG3	12:B:373:LEU:HD13	1.93	0.50
12:B:905:ASP:OD2	12:B:922:ARG:NH2	2.45	0.50
14:N:94:ARG:NH1	14:N:100:CYS:O	2.44	0.50
11:A:575:PRO:HG3	11:A:594:LEU:HD11	1.92	0.50
12:B:237:VAL:HG12	12:B:372:LEU:HD13	1.92	0.50
7:J:1:MET:N	12:B:752:TYR:O	2.45	0.50
11:A:410:ASN:HD21	11:A:417:LYS:HA	1.75	0.50
12:B:900:GLU:OE1	12:B:927:ARG:NH1	2.45	0.50
11:A:1212:LEU:HD11	11:A:1289:GLU:HG3	1.93	0.50
13:C:59:LEU:HD12	13:C:151:VAL:HG23	1.92	0.50
12:B:809:VAL:HG12	12:B:926:VAL:HG22	1.94	0.50
9:L:17:TYR:HE1	9:L:46:LYS:HE3	1.77	0.49
12:B:492:ASP:OD1	12:B:492:ASP:N	2.45	0.49
4:G:164:MET:N	4:G:164:MET:SD	2.85	0.49
5:H:97:TYR:CZ	5:H:115:TYR:HB3	2.47	0.49
11:A:364:ARG:HE	11:A:500:GLU:HG2	1.78	0.49
2:E:71:GLN:HB2	2:E:99:ILE:HD12	1.95	0.49
4:G:117:MET:HE2	4:G:128:TYR:HB3	1.93	0.49
11:A:545:VAL:HG11	11:A:645:LEU:HD22	1.93	0.49
11:A:583:ARG:NH1	13:C:222:PRO:O	2.45	0.49
11:A:1212:LEU:HB2	11:A:1285:LEU:HD21	1.94	0.49
9:L:43:ILE:HD13	12:B:910:THR:HG21	1.95	0.49
12:B:938:ARG:NH2	12:B:983:GLU:OE2	2.43	0.49
1:D:16:ASP:OD2	1:D:18:SER:OG	2.31	0.49
12:B:34:PHE:HZ	12:B:528:LEU:HB3	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:46:SER:HB3	12:B:397:GLY:H	1.77	0.49
12:B:565:THR:HG21	12:B:580:PRO:HB3	1.94	0.49
2:E:107:GLN:HG2	2:E:132:GLN:HE21	1.78	0.49
11:A:1209:PRO:HA	11:A:1260:ARG:HH21	1.77	0.49
12:B:550:MET:HE1	12:B:574:VAL:HG13	1.94	0.49
2:E:55:ARG:HH12	2:E:107:GLN:HE21	1.61	0.48
11:A:1218:ARG:NH2	11:A:1252:ALA:O	2.45	0.48
13:C:90:CYS:SG	13:C:94:CYS:HB3	2.53	0.48
11:A:1248:ASN:HD21	11:A:1256:VAL:H	1.60	0.48
12:B:665:ILE:HG23	12:B:669:GLU:HB3	1.96	0.48
8:K:67:LEU:HB3	11:A:478:PRO:HG2	1.96	0.48
11:A:1181:PRO:HG3	11:A:1260:ARG:HH12	1.79	0.48
12:B:507:GLY:HA2	12:B:703:ILE:HA	1.96	0.48
6:I:19:GLU:OE2	6:I:19:GLU:N	2.47	0.48
7:J:57:GLU:OE1	7:J:57:GLU:N	2.47	0.48
7:J:9:THR:HG21	12:B:961:ILE:HG23	1.96	0.48
2:E:35:GLN:NE2	2:E:43:GLN:OE1	2.47	0.48
12:B:403:LEU:HD23	12:B:444:LEU:HD23	1.96	0.48
12:B:320:PHE:O	12:B:324:ARG:NH1	2.47	0.47
12:B:474:THR:OG1	12:B:732:ALA:O	2.32	0.47
12:B:477:SER:HB2	12:B:730:LYS:HA	1.96	0.47
4:G:24:ASN:HA	4:G:27:LYS:HG2	1.94	0.47
4:G:92:VAL:HB	4:G:126:PRO:HB2	1.96	0.47
12:B:324:ARG:HH21	14:N:197:PRO:HA	1.79	0.47
12:B:584:MET:HG3	12:B:605:ARG:HB2	1.96	0.47
10:M:233:GLU:O	10:M:237:MET:HB2	2.13	0.47
12:B:56:GLN:HE22	12:B:90:GLN:HA	1.79	0.47
12:B:993:LYS:HD3	12:B:995:GLU:HG2	1.95	0.47
13:C:116:THR:HG22	13:C:149:LEU:HA	1.95	0.47
1:D:32:LEU:HA	1:D:84:ARG:HH22	1.80	0.47
11:A:628:VAL:HA	11:A:638:GLY:HA3	1.97	0.47
11:A:856:GLU:HB3	11:A:1121:VAL:HG11	1.96	0.47
11:A:557:ARG:O	11:A:561:MET:HG2	2.15	0.47
11:A:806:THR:O	12:B:503:ASN:ND2	2.48	0.47
11:A:473:ARG:HH12	11:A:516:GLN:HE22	1.62	0.47
11:A:693:ILE:HD13	11:A:828:LEU:HD21	1.97	0.47
12:B:431:LEU:HA	12:B:434:ALA:HB3	1.97	0.47
12:B:819:SER:HA	12:B:916:TYR:HD2	1.80	0.47
6:I:64:GLU:OE1	6:I:64:GLU:N	2.47	0.47
7:J:40:LEU:HD22	7:J:45:CYS:HB3	1.97	0.47
11:A:695:ASP:OD1	11:A:698:THR:OG1	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1004:LEU:HD13	11:A:1062:GLY:HA2	1.95	0.47
12:B:239:MET:HB2	12:B:372:LEU:HD21	1.97	0.47
7:J:42:ARG:NH2	13:C:180:ALA:O	2.48	0.46
5:H:103:GLU:HB3	5:H:109:ALA:HB2	1.97	0.46
9:L:34:ILE:O	9:L:42:ARG:NH1	2.48	0.46
12:B:297:MET:HB2	12:B:377:LEU:HD11	1.97	0.46
14:N:142:GLN:NE2	14:N:177:HIS:O	2.49	0.46
11:A:390:PHE:HB2	11:A:505:LEU:HD21	1.97	0.46
11:A:757:GLN:HA	11:A:760:LEU:HG	1.96	0.46
12:B:752:TYR:HE1	12:B:809:VAL:HG13	1.81	0.46
11:A:1318:LYS:HE2	11:A:1332:GLN:HG2	1.98	0.46
11:A:469:MET:SD	11:A:469:MET:N	2.87	0.46
11:A:557:ARG:HG2	11:A:561:MET:HE2	1.98	0.46
12:B:288:ILE:HG22	12:B:289:ILE:HG13	1.98	0.46
11:A:803:LYS:O	11:A:812:LYS:NZ	2.44	0.46
11:A:827:TYR:OH	11:A:839:HIS:NE2	2.35	0.46
11:A:1192:TRP:HA	11:A:1195:VAL:HG22	1.97	0.46
2:E:55:ARG:HB2	2:E:78:GLU:HB3	1.98	0.46
4:G:145:LEU:HD12	4:G:161:GLY:HA3	1.97	0.46
12:B:506:TRP:NE1	12:B:697:GLU:OE2	2.42	0.46
12:B:724:TYR:CE1	12:B:941:GLN:HA	2.51	0.46
11:A:1170:THR:HA	11:A:1216:LEU:HA	1.96	0.46
12:B:37:LYS:NZ	12:B:664:TYR:OH	2.48	0.46
12:B:731:GLN:OE1	12:B:1053:HIS:NE2	2.48	0.46
8:K:65:HIS:HE1	8:K:67:LEU:HD12	1.81	0.45
11:A:870:SER:HB2	11:A:882:SER:HB3	1.97	0.45
11:A:1362:ILE:HG21	11:A:1378:LEU:HD13	1.98	0.45
4:G:89:VAL:HG22	4:G:99:THR:HG22	1.97	0.45
12:B:389:GLY:HA3	12:B:668:LEU:HG	1.98	0.45
1:D:107:THR:HG23	1:D:110:GLU:H	1.79	0.45
3:F:68:THR:O	3:F:72:GLN:HG3	2.17	0.45
8:K:56:VAL:HG22	8:K:77:THR:HG22	1.98	0.45
12:B:37:LYS:HD2	12:B:41:ARG:HG2	1.99	0.45
4:G:100:GLU:HA	4:G:105:SER:HA	1.98	0.45
6:I:80:ARG:HG2	6:I:95:VAL:HG22	1.99	0.45
11:A:1211:LEU:HD11	11:A:1258:ARG:HB3	1.99	0.45
12:B:123:PRO:HB3	12:B:148:PHE:HE1	1.81	0.45
12:B:623:ARG:NH1	12:B:697:GLU:OE1	2.44	0.45
14:N:84:PRO:HD3	14:N:151:ILE:HG12	1.98	0.45
5:H:122:LEU:HD12	11:A:621:ILE:HG13	1.99	0.45
11:A:682:ILE:HG23	12:B:1035:ARG:HD3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:917:GLU:OE2	11:A:921:ARG:NH1	2.50	0.45
12:B:331:THR:HG23	12:B:334:LYS:H	1.82	0.45
12:B:363:TYR:HB3	12:B:573:TRP:CD1	2.51	0.45
11:A:1005:HIS:HD1	11:A:1007:ILE:HG12	1.80	0.45
12:B:67:LEU:HB3	12:B:423:ILE:HG13	1.97	0.45
11:A:1178:ASP:OD1	11:A:1178:ASP:N	2.49	0.45
12:B:210:LYS:NZ	12:B:218:THR:OG1	2.49	0.45
12:B:780:VAL:HG22	12:B:965:ILE:HB	1.99	0.45
12:B:99:TRP:CD1	12:B:105:PRO:HG3	2.51	0.44
9:L:58:ARG:NH1	13:C:48:ASP:OD1	2.51	0.44
11:A:790:GLN:HA	11:A:822:PHE:HA	1.99	0.44
14:N:156:VAL:HA	14:N:159:ARG:HB3	1.99	0.44
10:M:248:LYS:HA	10:M:248:LYS:HD3	1.87	0.44
11:A:505:LEU:HD12	11:A:506:PRO:HD2	2.00	0.44
12:B:798:ARG:HD2	12:B:948:GLN:HB3	1.98	0.44
11:A:1032:GLN:HE21	11:A:1036:ASN:HD21	1.66	0.44
12:B:794:VAL:HB	12:B:965:ILE:HG23	2.00	0.44
12:B:971:ALA:O	12:B:976:MET:N	2.51	0.44
12:B:548:TRP:CZ3	12:B:586:THR:HG21	2.53	0.44
12:B:1035:ARG:NH1	12:B:1036:LYS:O	2.49	0.44
12:B:510:CYS:SG	12:B:705:GLY:N	2.85	0.44
12:B:733:MET:HE3	12:B:1050:ARG:HG2	2.00	0.44
2:E:168:ASN:OD1	2:E:168:ASN:N	2.50	0.44
11:A:1364:GLU:O	11:A:1368:VAL:HG12	2.18	0.44
13:C:12:THR:N	13:C:20:LYS:O	2.46	0.44
11:A:479:TRP:HB2	11:A:483:ARG:HH22	1.82	0.44
11:A:791:GLN:HE21	11:A:823:VAL:HG21	1.83	0.44
12:B:274:ARG:HD3	12:B:279:VAL:HA	1.99	0.44
12:B:908:MET:HE3	12:B:908:MET:HB3	1.86	0.44
11:A:767:LYS:HA	11:A:770:VAL:HG22	2.00	0.43
1:D:38:HIS:HB2	1:D:68:THR:HB	2.00	0.43
5:H:111:ARG:HD2	5:H:111:ARG:HA	1.78	0.43
11:A:1375:ARG:HG3	11:A:1406:THR:HG21	2.01	0.43
13:C:188:PRO:HB2	13:C:209:SER:HB3	1.99	0.43
4:G:63:ARG:HG3	4:G:65:PHE:H	1.83	0.43
11:A:508:SER:HB3	11:A:511:THR:HG22	2.00	0.43
11:A:554:PHE:HB3	11:A:585:LEU:HD22	2.00	0.43
12:B:782:ILE:HG12	12:B:967:ILE:HD11	2.00	0.43
2:E:95:GLN:OE1	2:E:125:TYR:OH	2.37	0.43
13:C:44:ILE:HG21	13:C:178:PRO:HB3	1.99	0.43
6:I:74:GLN:NE2	12:B:581:GLU:OE1	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:7:CYS:HA	7:J:48:MET:SD	2.58	0.43
7:J:28:GLU:HG2	10:M:50:LYS:HD2	2.01	0.43
12:B:224:CYS:HB3	12:B:232:THR:HA	2.00	0.43
12:B:553:LEU:HD23	12:B:553:LEU:HA	1.84	0.43
1:D:25:GLU:HG3	4:G:5:ILE:HG22	1.99	0.43
2:E:74:VAL:HA	2:E:103:LEU:HB3	2.00	0.43
10:M:21:LEU:HD11	10:M:69:ARG:HH11	1.83	0.43
10:M:21:LEU:O	10:M:25:ARG:NH1	2.52	0.43
10:M:331:LYS:HA	10:M:331:LYS:HD3	1.73	0.43
14:N:150:GLN:H	14:N:150:GLN:HG2	1.69	0.43
7:J:1:MET:HA	7:J:55:LEU:HB2	2.01	0.43
7:J:3:ILE:HD12	7:J:4:PRO:HD2	2.01	0.43
7:J:24:LEU:HD11	10:M:40:PHE:HZ	1.83	0.43
11:A:1410:HIS:CE1	11:A:1412:MET:HE1	2.54	0.43
14:N:132:ARG:NH1	14:N:137:SER:O	2.51	0.43
9:L:18:ILE:HD11	9:L:47:LYS:HE3	2.01	0.43
12:B:285:LEU:HD21	12:B:305:LEU:HD11	2.01	0.43
12:B:542:LEU:HD11	12:B:574:VAL:HG21	2.01	0.43
14:N:61:ILE:HB	14:N:82:ILE:HD11	2.01	0.43
1:D:103:LEU:HD13	1:D:114:LEU:HD13	1.99	0.43
11:A:1141:VAL:HB	11:A:1336:LEU:HB2	2.01	0.43
12:B:594:MET:HG3	12:B:658:ALA:HA	2.01	0.43
13:C:110:ASP:OD1	13:C:110:ASP:N	2.51	0.43
13:C:145:GLN:N	13:C:145:GLN:OE1	2.52	0.43
11:A:577:PRO:HG3	11:A:586:TRP:CZ2	2.54	0.42
11:A:1016:LEU:HD21	11:A:1072:ILE:HG21	2.01	0.42
12:B:50:PHE:HB2	12:B:397:GLY:HA2	2.00	0.42
11:A:1235:ILE:HG21	11:A:1245:CYS:SG	2.59	0.42
11:A:1361:ASP:OD1	11:A:1361:ASP:N	2.46	0.42
12:B:425:ARG:HH22	12:B:427:LYS:HD3	1.83	0.42
9:L:57:ALA:HB3	13:C:175:LYS:HZ2	1.84	0.42
11:A:389:THR:HG22	11:A:449:HIS:HD2	1.83	0.42
11:A:803:LYS:N	12:B:671:GLU:OE1	2.44	0.42
12:B:93:LEU:HD12	12:B:124:LEU:HD13	2.02	0.42
12:B:403:LEU:O	12:B:407:MET:HG2	2.18	0.42
12:B:473:LEU:HD22	12:B:1052:LYS:HD3	2.02	0.42
14:N:145:LYS:HD3	14:N:145:LYS:HA	1.94	0.42
11:A:901:VAL:HA	11:A:980:PRO:HA	2.01	0.42
13:C:135:ARG:HD3	13:C:142:TYR:HA	2.01	0.42
1:D:26:PHE:HE1	4:G:4:HIS:H	1.67	0.42
12:B:724:TYR:CZ	12:B:728:MET:HE3	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:C:67:ARG:NH2	13:C:149:LEU:O	2.38	0.42
12:B:718:GLN:HB2	12:B:721:ARG:HG3	2.01	0.42
11:A:783:GLN:HG2	11:A:788:VAL:HA	2.01	0.42
12:B:952:GLU:HB2	13:C:36:ARG:HB2	2.00	0.42
14:N:102:TYR:HE1	14:N:104:LEU:HD12	1.85	0.42
2:E:142:HIS:HD2	2:E:144:LEU:HB2	1.85	0.42
12:B:588:ARG:HB3	12:B:592:ARG:NH1	2.35	0.42
4:G:14:HIS:HD2	4:G:16:ARG:HG3	1.85	0.41
4:G:91:GLN:NE2	4:G:93:ASN:OD1	2.50	0.41
11:A:1245:CYS:HB3	11:A:1257:LEU:HD11	2.02	0.41
12:B:51:ILE:HG23	12:B:93:LEU:HD13	2.02	0.41
13:C:74:ILE:HD12	13:C:128:ILE:HG13	2.02	0.41
2:E:103:LEU:HD12	2:E:103:LEU:HA	1.88	0.41
11:A:1142:PHE:O	11:A:1353:ASP:N	2.50	0.41
12:B:48:ASP:OD1	12:B:158:SER:OG	2.37	0.41
7:J:51:ALA:O	12:B:755:GLN:HB2	2.19	0.41
11:A:1005:HIS:ND1	11:A:1007:ILE:HG12	2.35	0.41
2:E:133:GLN:HA	2:E:136:LEU:HD12	2.01	0.41
12:B:848:LEU:HD23	12:B:852:GLY:HA2	2.02	0.41
12:B:941:GLN:NE2	12:B:975:ARG:HD2	2.34	0.41
11:A:1304:ILE:HA	11:A:1340:GLY:HA3	2.03	0.41
12:B:235:ILE:HG22	12:B:261:PRO:HD3	2.02	0.41
5:H:103:GLU:OE2	11:A:999:ARG:NH2	2.49	0.41
7:J:8:PHE:HB2	7:J:47:ARG:NH2	2.36	0.41
12:B:972:ILE:HA	12:B:976:MET:O	2.21	0.41
6:I:99:SER:HB2	6:I:111:TYR:HE2	1.84	0.41
12:B:733:MET:HG2	12:B:1050:ARG:HB3	2.02	0.41
2:E:45:GLY:HA3	2:E:53:PRO:HB3	2.03	0.41
2:E:193:ILE:HD12	2:E:207:ARG:HG3	2.03	0.41
5:H:13:LYS:NZ	5:H:31:GLU:O	2.53	0.41
7:J:23:GLY:HA3	10:M:34:LEU:HD11	2.03	0.41
11:A:473:ARG:NH1	11:A:516:GLN:HE22	2.19	0.41
11:A:1164:THR:HA	11:A:1168:LYS:HD2	2.02	0.41
12:B:59:VAL:HG21	12:B:91:ILE:HG21	2.03	0.41
13:C:88:CYS:SG	13:C:97:CYS:HB3	2.60	0.41
13:C:101:PHE:HD2	13:C:120:LEU:HG	1.86	0.41
12:B:92:TYR:HB2	12:B:125:TYR:HB2	2.02	0.41
4:G:86:ASP:OD1	4:G:86:ASP:N	2.53	0.40
5:H:92:MET:HB2	5:H:143:LEU:HB3	2.02	0.40
6:I:78:LEU:HD22	6:I:97:PHE:HB3	2.03	0.40
8:K:94:LEU:HB3	13:C:256:LEU:HD13	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:809:HIS:HE1	12:B:697:GLU:HG3	1.87	0.40
12:B:829:PHE:HE1	12:B:869:LYS:HG3	1.86	0.40
11:A:1016:LEU:HD23	11:A:1045:LEU:HD21	2.03	0.40
12:B:926:VAL:HG21	13:C:62:GLU:HG3	2.03	0.40
12:B:348:LEU:HB3	12:B:351:VAL:HG22	2.02	0.40
2:E:197:SER:N	2:E:201:GLY:O	2.52	0.40
11:A:375:ILE:HA	11:A:485:ASN:HB3	2.03	0.40
12:B:205:VAL:O	12:B:371:ARG:NH2	2.55	0.40
12:B:323:SER:HA	12:B:335:ARG:HD2	2.04	0.40
11:A:379:GLY:HA3	11:A:477:LEU:HD12	2.03	0.40
11:A:578:ALA:H	11:A:590:GLN:HE22	1.69	0.40
12:B:144:HIS:CE1	12:B:431:LEU:HD12	2.56	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	D	127/142 (89%)	123 (97%)	4 (3%)	0	100	100
2	E	207/210 (99%)	199 (96%)	8 (4%)	0	100	100
3	F	77/127 (61%)	72 (94%)	5 (6%)	0	100	100
4	G	169/172 (98%)	161 (95%)	8 (5%)	0	100	100
5	H	146/150 (97%)	142 (97%)	4 (3%)	0	100	100
6	I	112/125 (90%)	106 (95%)	6 (5%)	0	100	100
7	J	63/67 (94%)	60 (95%)	3 (5%)	0	100	100
8	K	113/117 (97%)	108 (96%)	5 (4%)	0	100	100
9	L	42/58 (72%)	37 (88%)	5 (12%)	0	100	100
10	M	126/368 (34%)	118 (94%)	8 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	A	1015/1970 (52%)	975 (96%)	40 (4%)	0	100	100
12	B	1007/1174 (86%)	952 (94%)	55 (6%)	0	100	100
13	C	261/275 (95%)	255 (98%)	6 (2%)	0	100	100
14	N	151/612 (25%)	137 (91%)	14 (9%)	0	100	100
All	All	3616/5567 (65%)	3445 (95%)	171 (5%)	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	D	119/126 (94%)	119 (100%)	0	100	100
2	E	191/192 (100%)	191 (100%)	0	100	100
3	F	69/111 (62%)	69 (100%)	0	100	100
4	G	152/153 (99%)	152 (100%)	0	100	100
5	H	129/131 (98%)	129 (100%)	0	100	100
6	I	103/112 (92%)	103 (100%)	0	100	100
7	J	54/56 (96%)	54 (100%)	0	100	100
8	K	104/106 (98%)	104 (100%)	0	100	100
9	L	41/55 (74%)	41 (100%)	0	100	100
10	M	118/332 (36%)	118 (100%)	0	100	100
11	A	915/1748 (52%)	915 (100%)	0	100	100
12	B	894/1028 (87%)	894 (100%)	0	100	100
13	C	242/252 (96%)	242 (100%)	0	100	100
14	N	141/561 (25%)	141 (100%)	0	100	100
All	All	3272/4963 (66%)	3272 (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 (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	89	GLN
1	D	135	GLN
2	E	35	GLN
2	E	107	GLN
2	E	132	GLN
2	E	174	GLN
3	F	72	GLN
4	G	139	GLN
5	H	76	ASN
6	I	41	ASN
6	I	100	HIS
8	K	2	ASN
8	K	113	GLN
10	M	319	ASN
11	A	377	GLN
11	A	410	ASN
11	A	516	GLN
11	A	562	ASN
11	A	590	GLN
11	A	620	HIS
11	A	673	GLN
11	A	735	GLN
11	A	791	GLN
11	A	792	ASN
11	A	825	ASN
11	A	904	GLN
11	A	1032	GLN
11	A	1146	GLN
11	A	1163	HIS
11	A	1190	GLN
11	A	1299	GLN
12	B	90	GLN
12	B	227	ASN
12	B	254	GLN
12	B	287	HIS
12	B	312	GLN
12	B	460	HIS
12	B	503	ASN
12	B	518	HIS
12	B	593	GLN
12	B	699	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	B	777	ASN
12	B	906	GLN
12	B	930	GLN
12	B	948	GLN
12	B	986	GLN
12	B	1040	GLN
13	C	32	ASN
13	C	51	GLN
13	C	66	HIS
13	C	114	HIS
13	C	260	GLN
13	C	262	GLN
14	N	106	GLN
14	N	174	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 6 ligands modelled in this entry, 6 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.

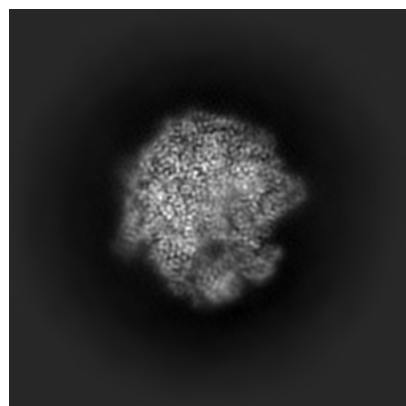
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-56542. These allow visual inspection of the internal detail of the map and identification of artifacts.

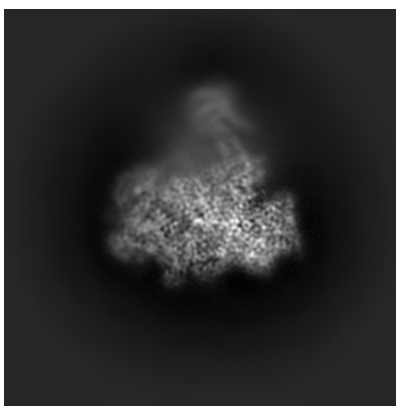
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

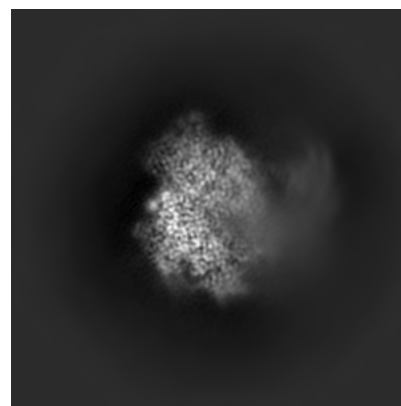
6.1.1 Primary map



X

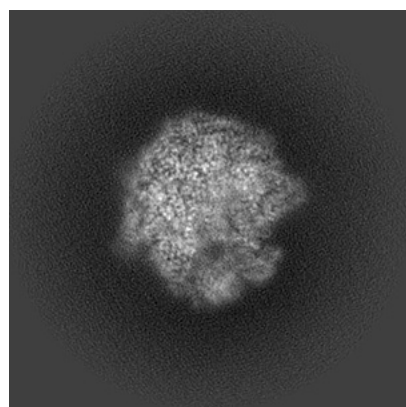


Y

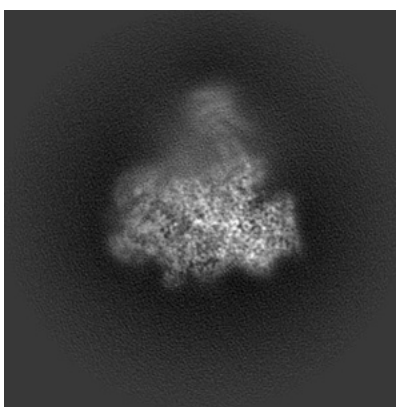


Z

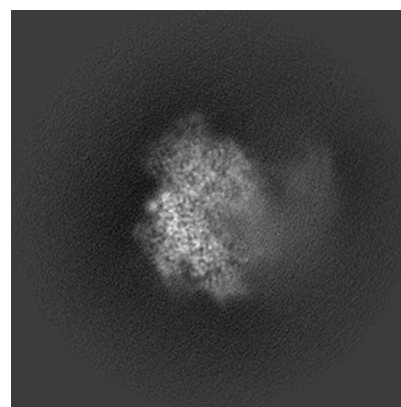
6.1.2 Raw map



X



Y

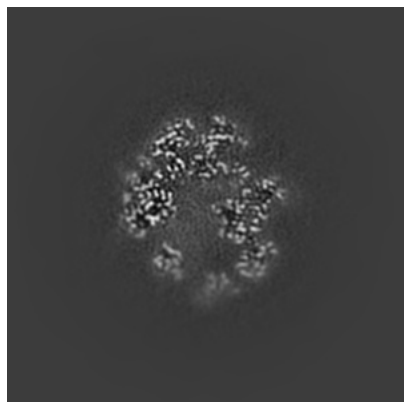


Z

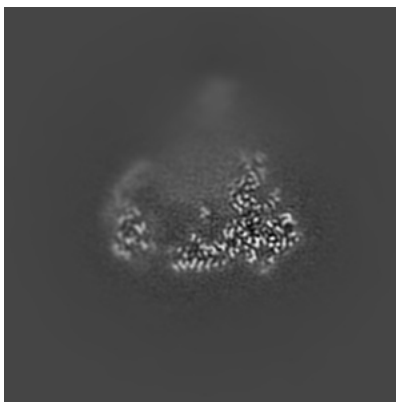
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

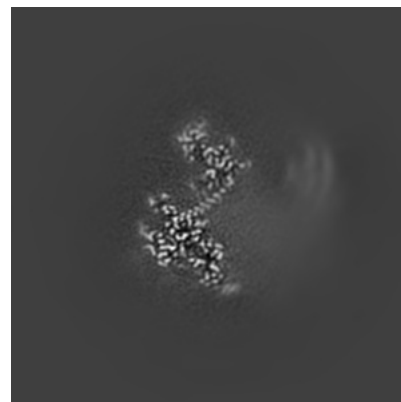
6.2.1 Primary map



X Index: 140

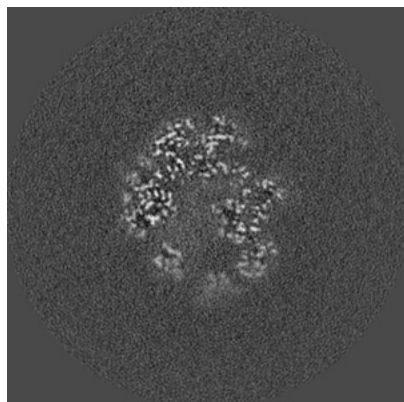


Y Index: 140

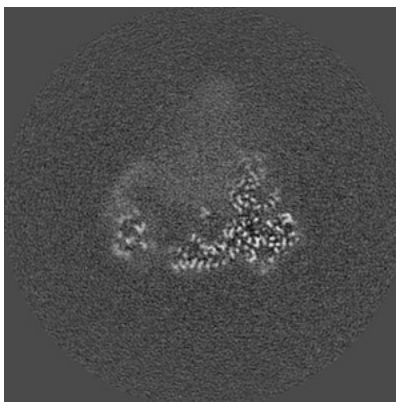


Z Index: 140

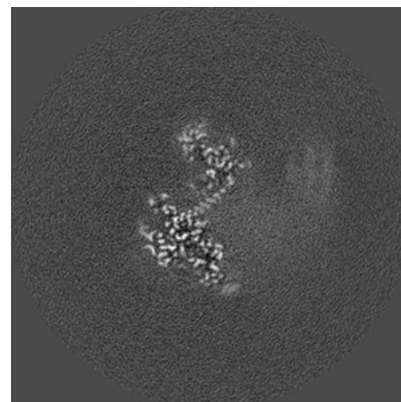
6.2.2 Raw map



X Index: 140



Y Index: 140

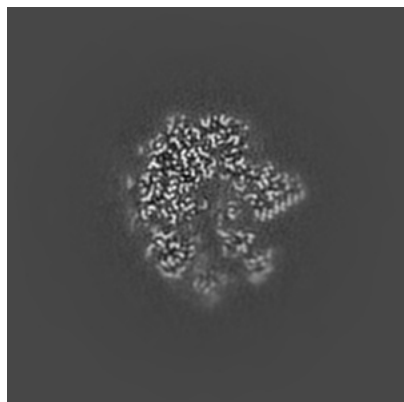


Z Index: 140

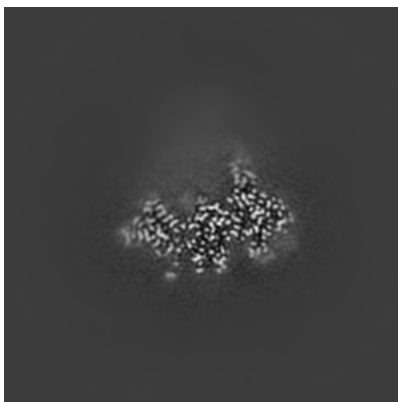
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

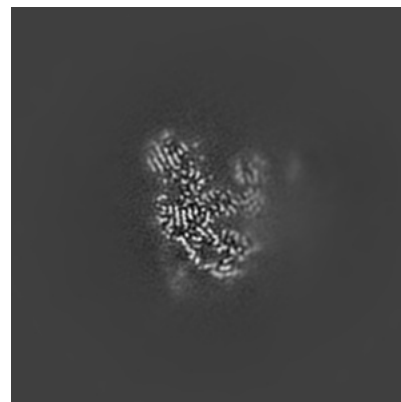
6.3.1 Primary map



X Index: 130

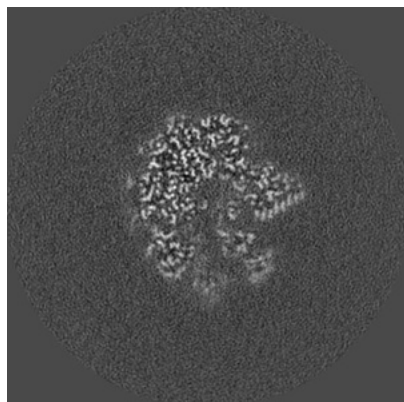


Y Index: 114

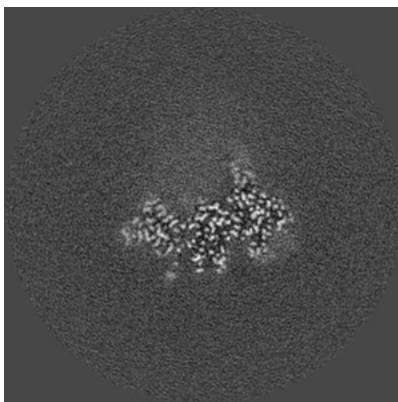


Z Index: 170

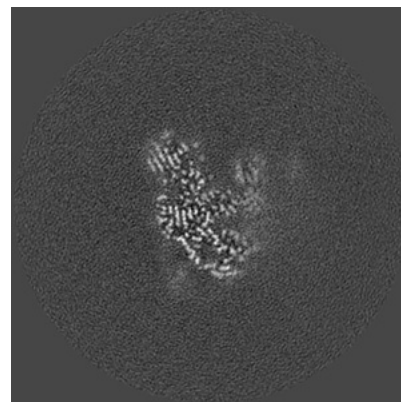
6.3.2 Raw map



X Index: 130



Y Index: 114

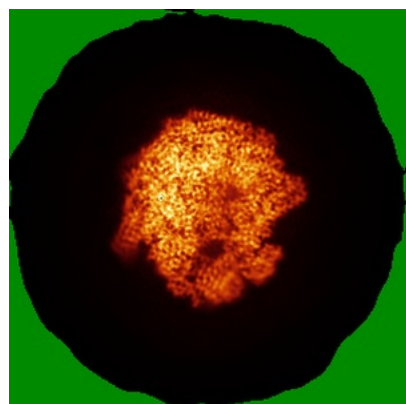


Z Index: 170

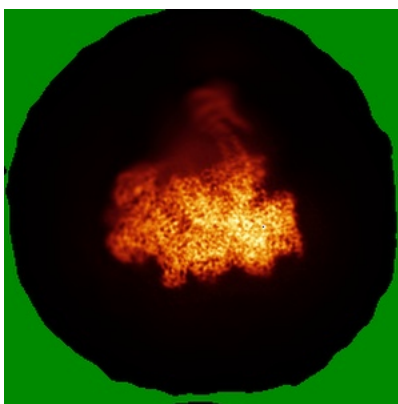
The images above show the largest variance slices of the map in three orthogonal directions.

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

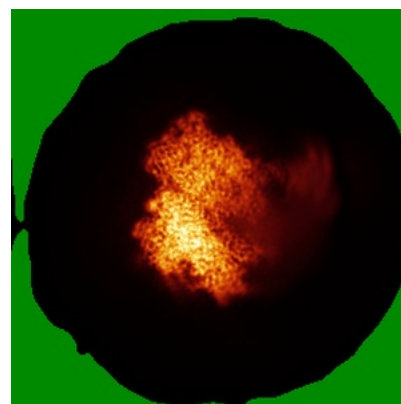
6.4.1 Primary map



X

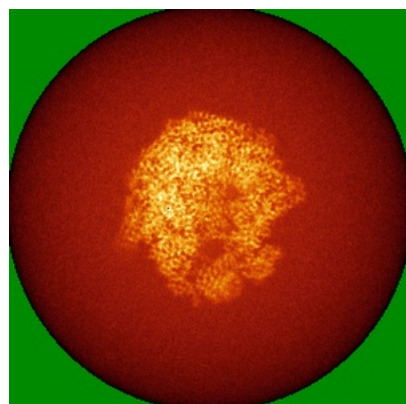


Y

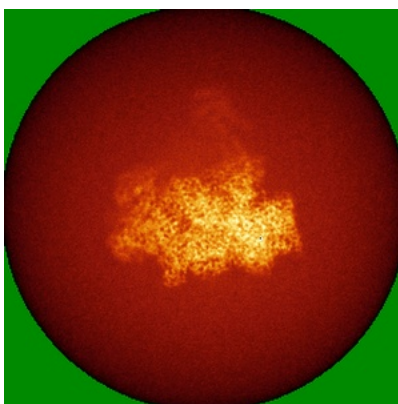


Z

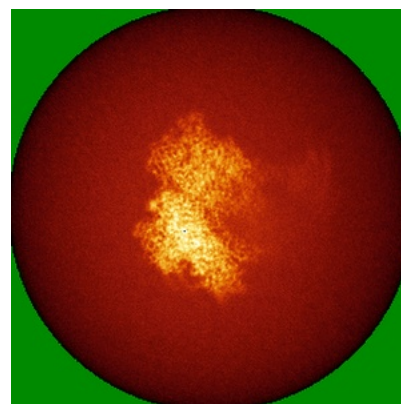
6.4.2 Raw map



X



Y

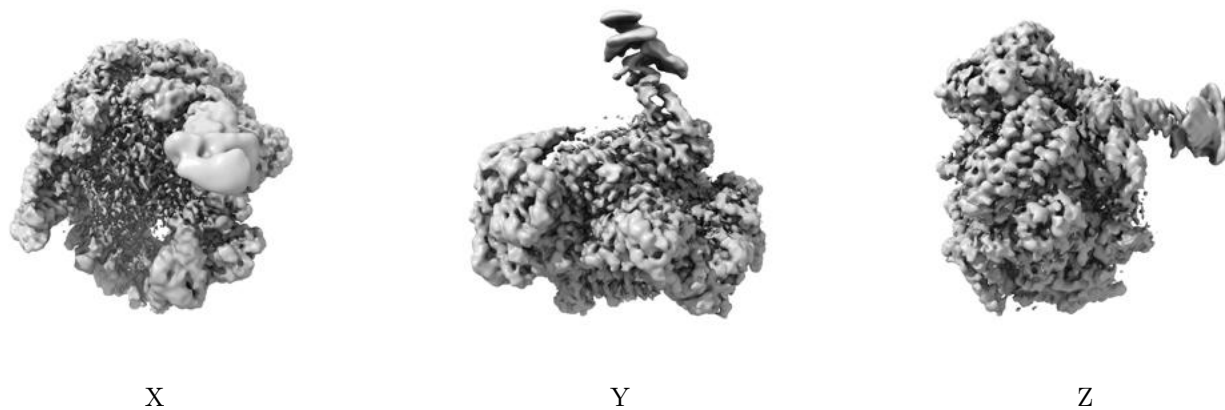


Z

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.

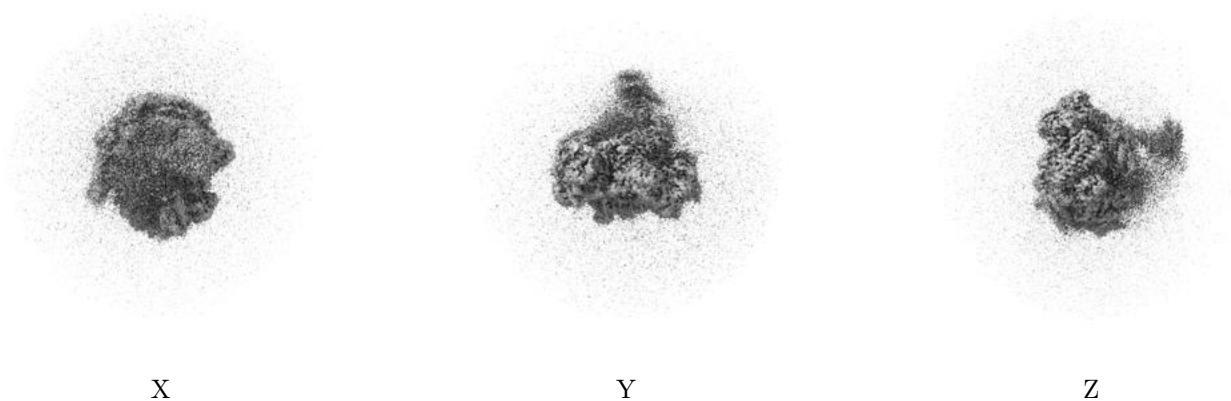
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00511. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

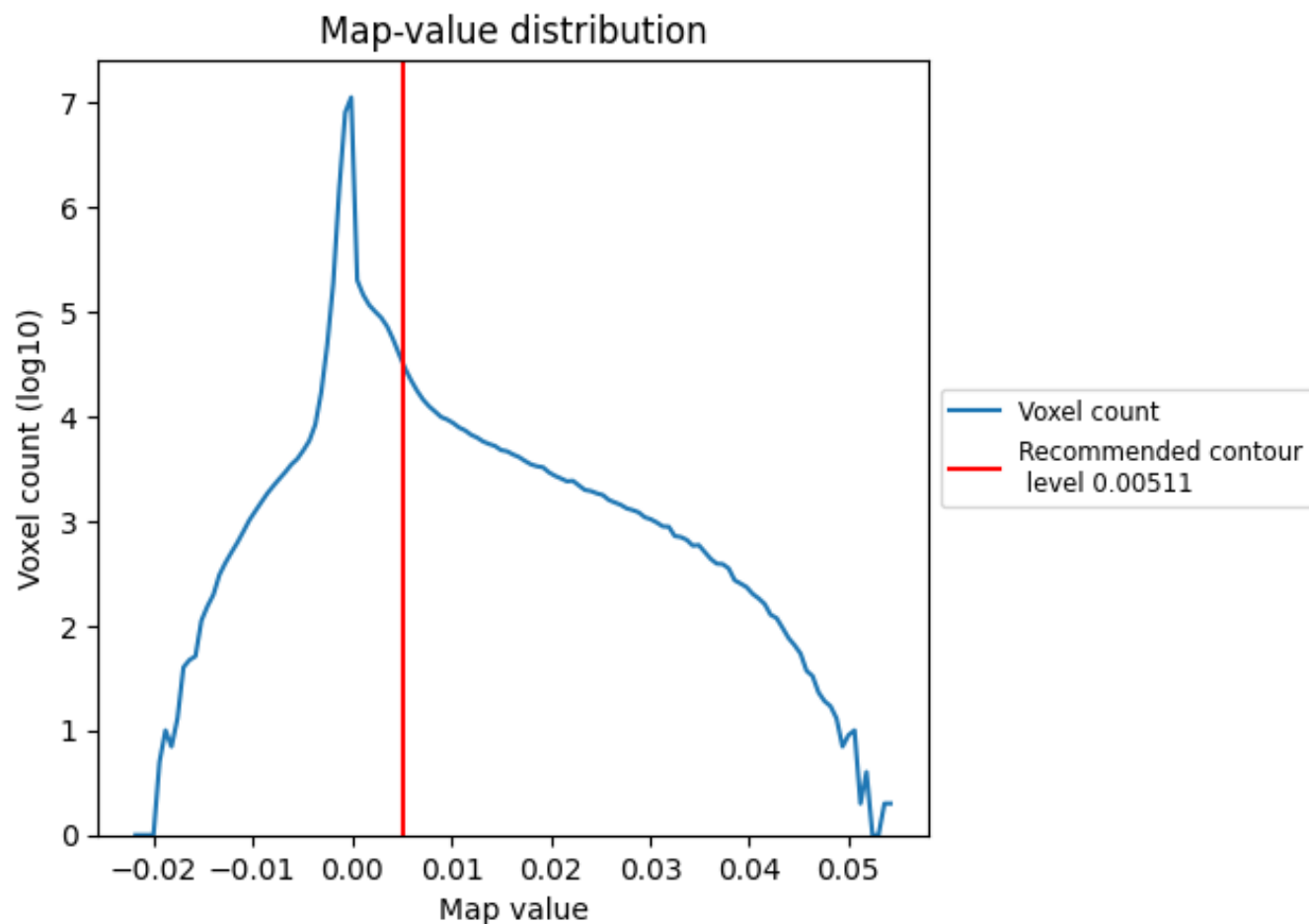
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

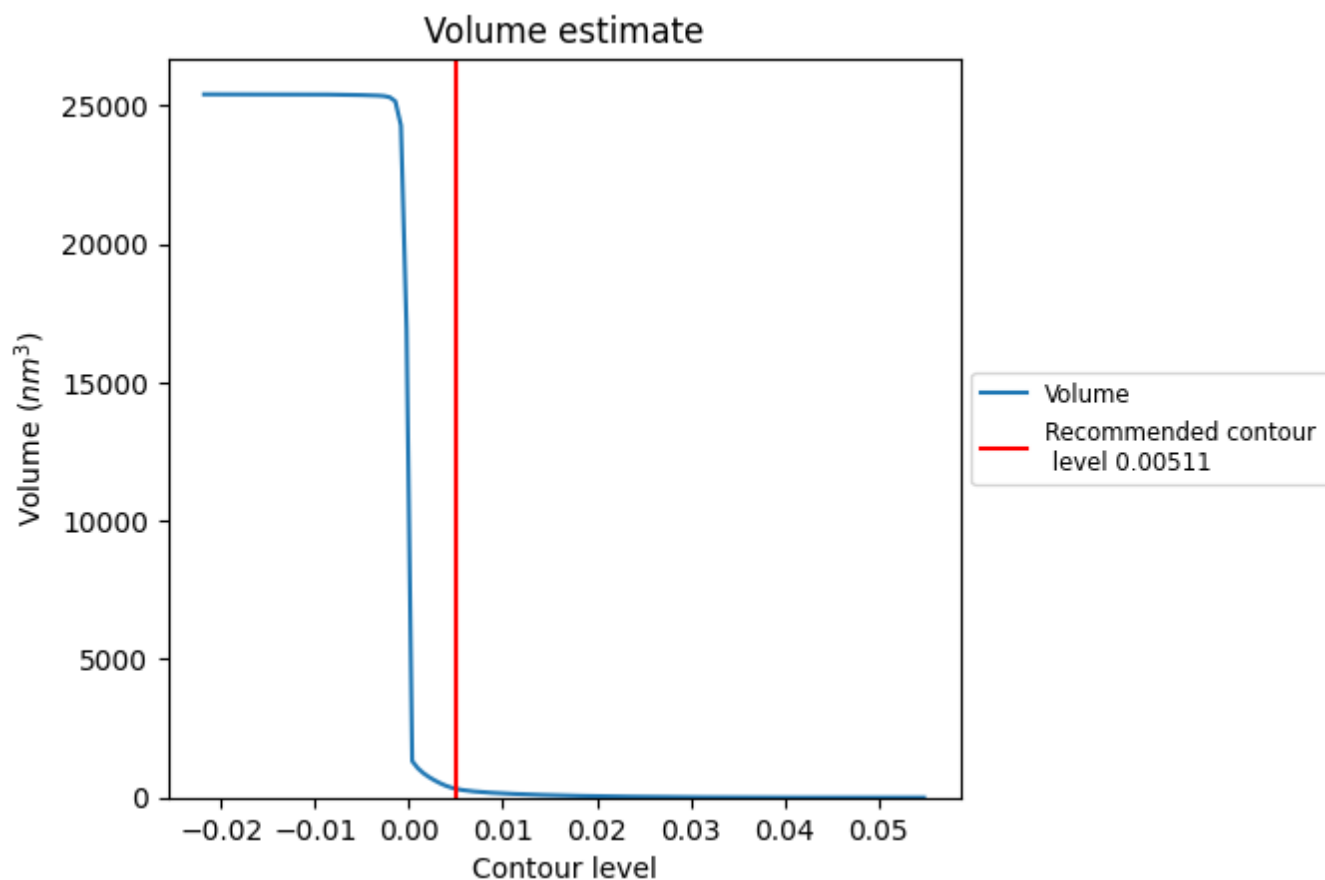
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

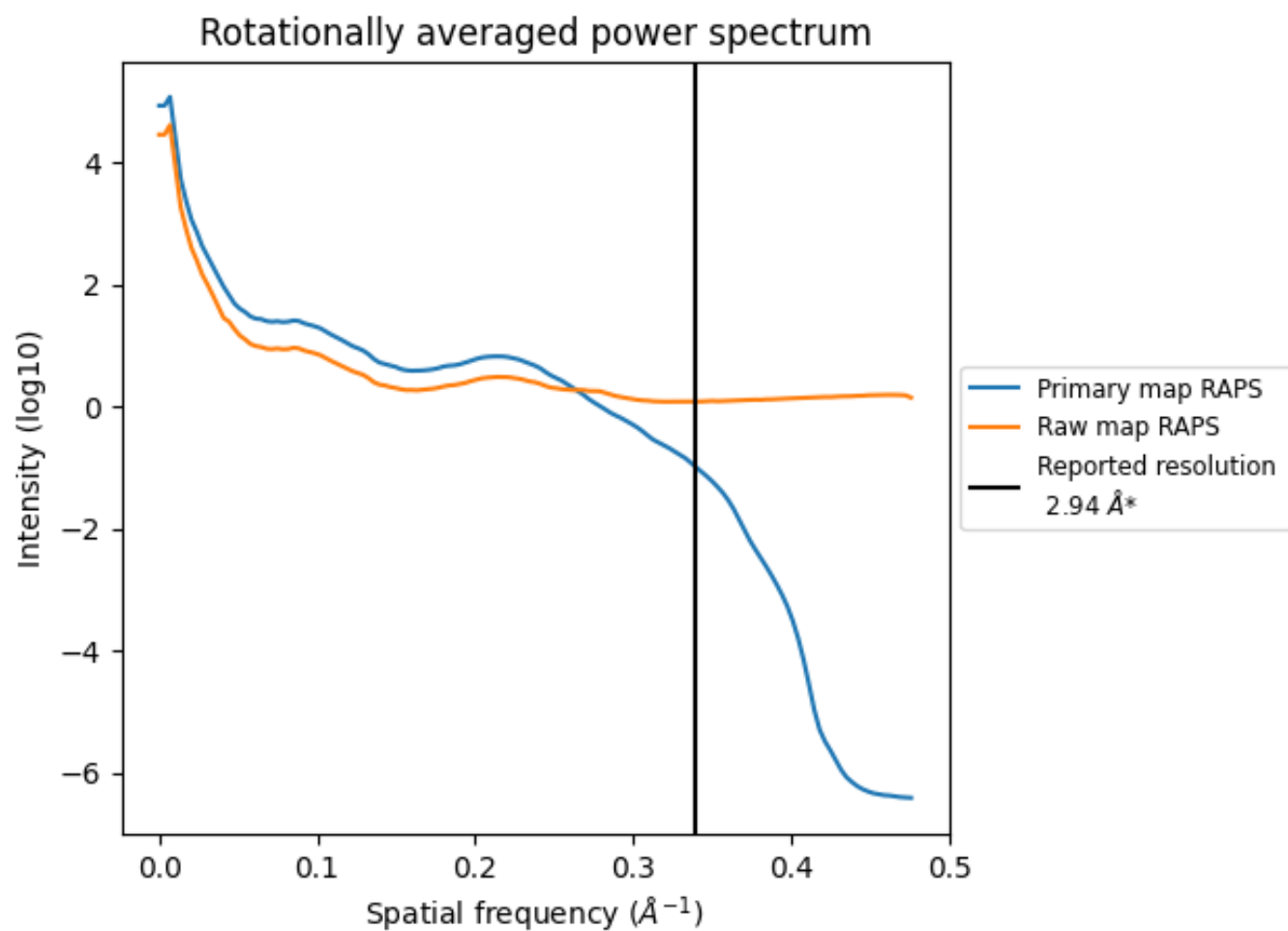
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 309 nm^3 ; this corresponds to an approximate mass of 280 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 ⓘ

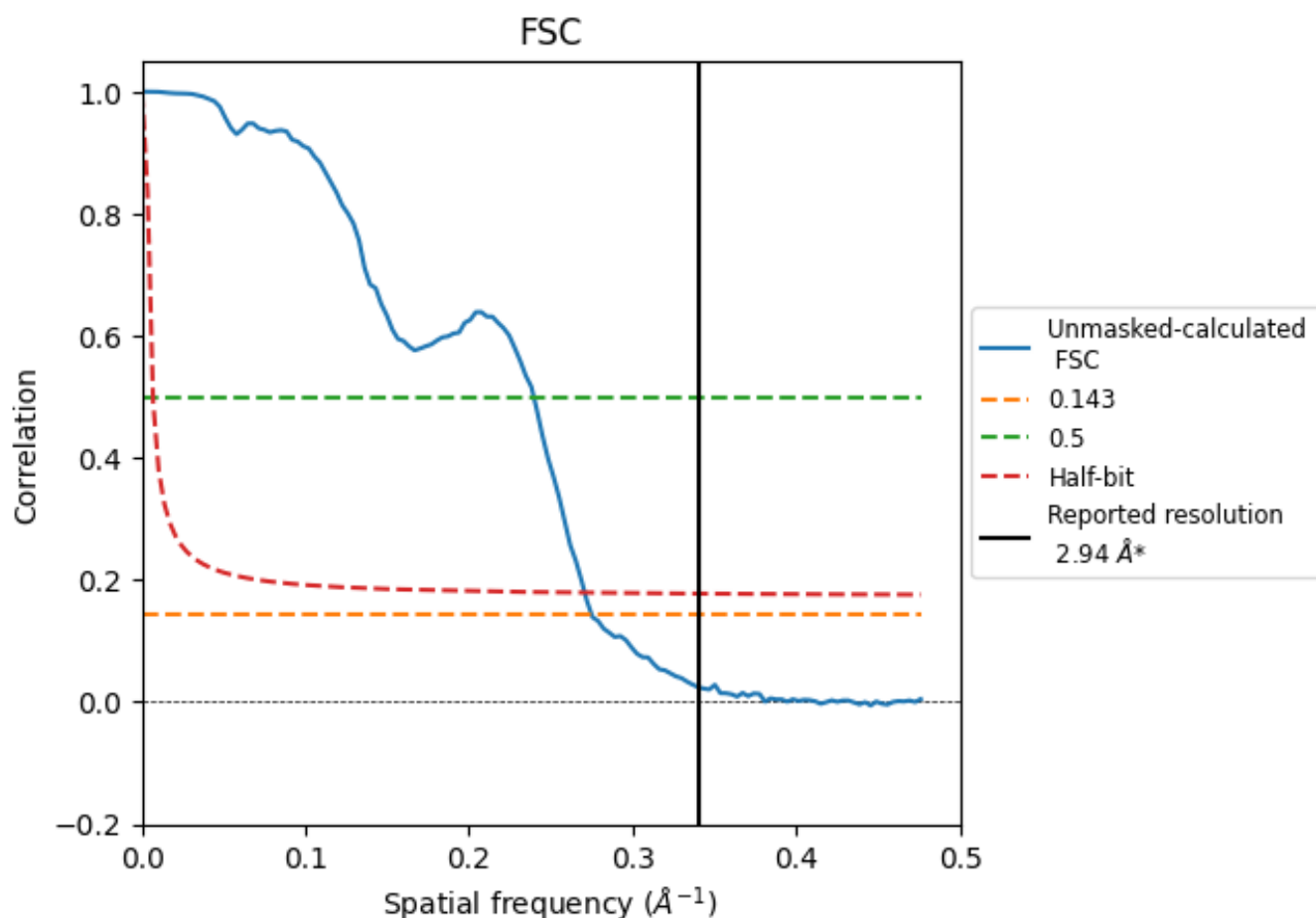


*Reported resolution corresponds to spatial frequency of 0.340 $\text{\AA}^{-1}$

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 0.340 Å⁻¹

8.2 Resolution estimates [i](#)

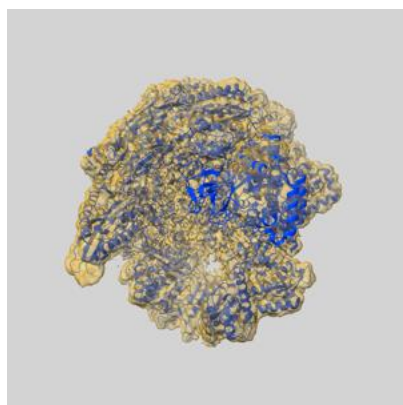
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.94	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.64	4.18	3.69

*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 3.64 differs from the reported value 2.94 by more than 10 %

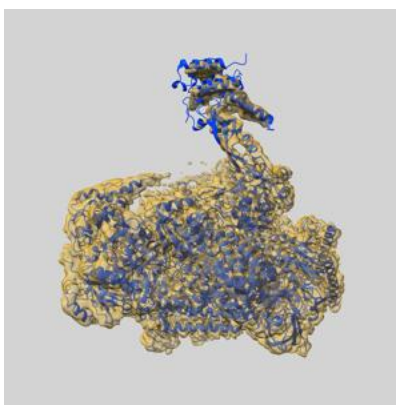
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-56542 and PDB model 28JC. Per-residue inclusion information can be found in section [3](#) on page [7](#).

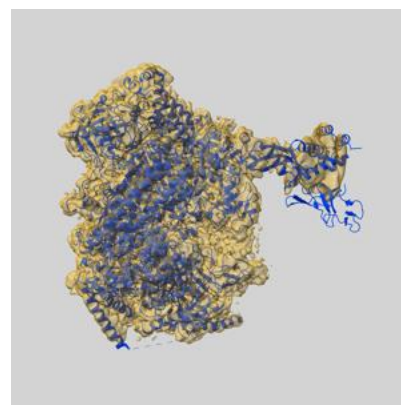
9.1 Map-model overlay [i](#)



X



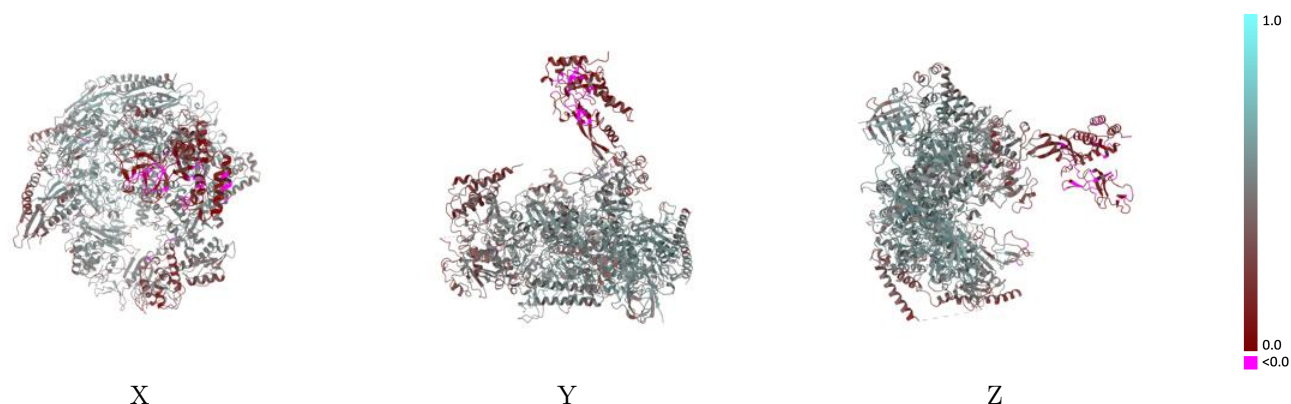
Y



Z

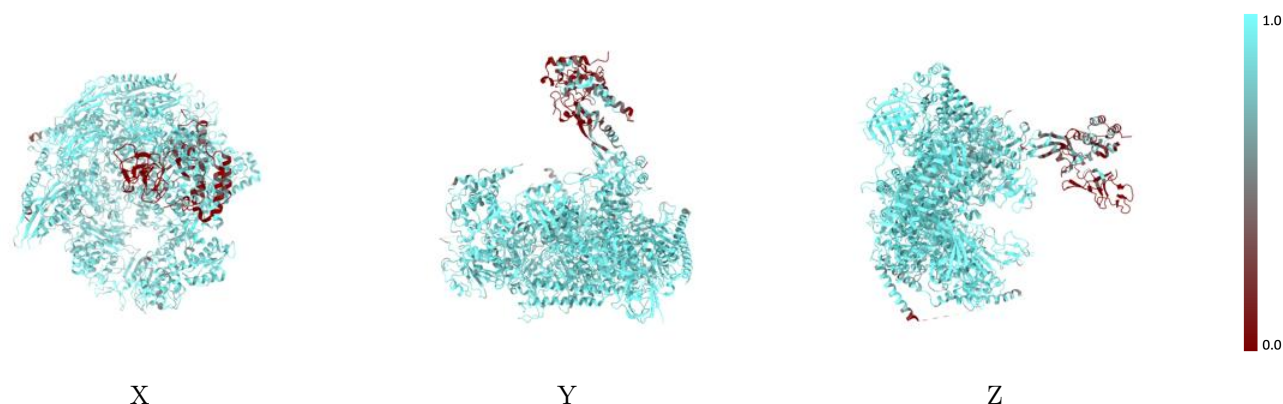
The images above show the 3D surface view of the map at the recommended contour level 0.00511 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



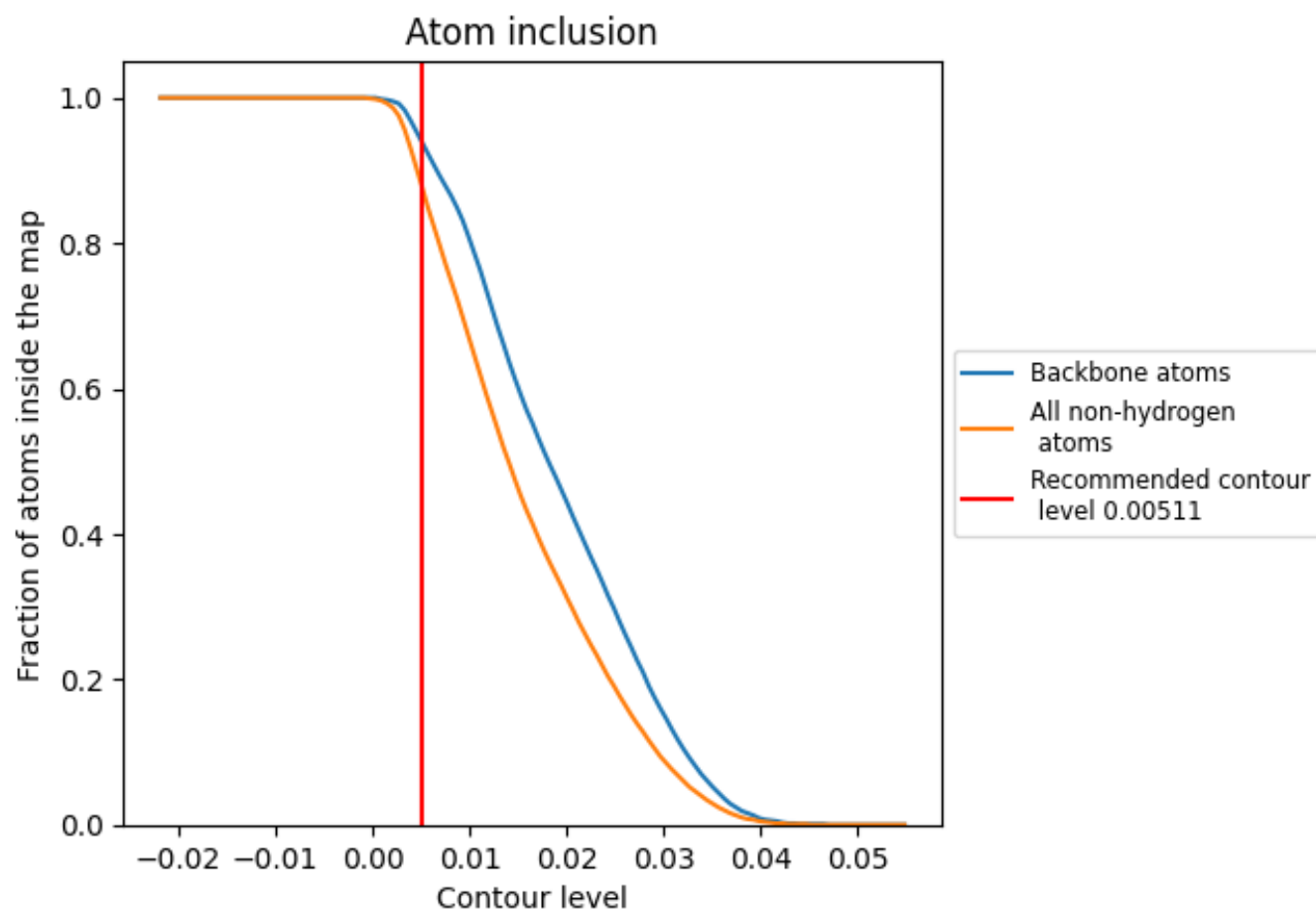
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00511).

9.4 Atom inclusion ⓘ



At the recommended contour level, 94% of all backbone atoms, 88% 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 (0.00511) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8790	 0.4530
A	 0.9310	 0.4850
B	 0.9500	 0.5170
C	 0.9570	 0.5350
D	 0.3320	 0.1260
E	 0.9320	 0.4480
F	 0.8720	 0.4210
G	 0.3080	 0.1250
H	 0.9530	 0.5030
I	 0.9440	 0.4630
J	 0.9660	 0.5500
K	 0.9610	 0.5310
L	 0.9550	 0.4650
M	 0.7430	 0.3250
N	 0.8450	 0.3050

