wwPDB EM Validation Summary Report

Jul 14, 2026 – 12:16 PM JST

PDB ID	:	9XAE / pdb_00009xae
EMDB ID	:	EMD-66684
Title	:	Cryo-EM structure of the pre-40S ribosome (Enp1-Rrp12 WT) from Chaetomium thermophilum, state Rio2-C
Authors	:	Lau, B.; Li, Y.; Zhu, J.; Fischer, P.; Hong, X.; Yuan, R.; Beckmann, R.; Hurt, E.; Cheng, J.
Deposited on	:	2025-10-22
Resolution	:	3.00 Å(reported)
Based on initial model	:	6G18

This is a wwPDB EM Validation Summary 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:

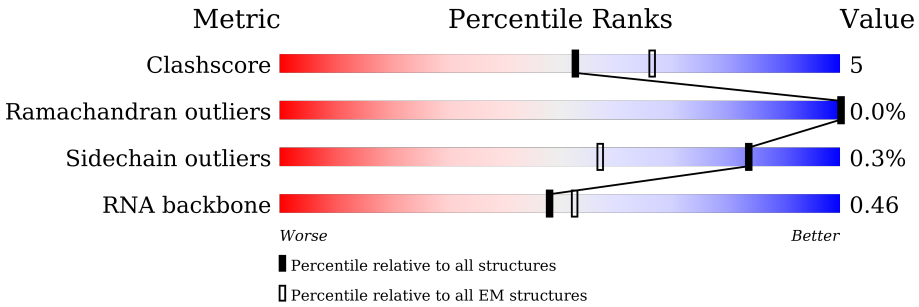
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh &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

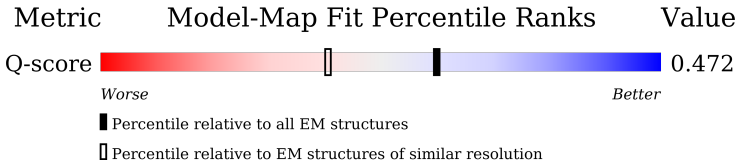
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14081 (2.50 - 3.50)

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 <=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	285	58% 15% 27%
2	E	255	68% 15% 16%
3	F	263	69% 8% 22%

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Mol	Chain	Length	Quality of chain
4	H	264	86% 13%
5	I	212	71% 23% 6%
6	J	239	82% 15%
7	K	203	83% 13%
8	L	202	88% 12%
9	M	190	83% 11% 6%
10	O	161	87% 6% 7%
11	P	144	62% 20% 18%
12	Q	151	93% 7%
13	R	150	67% 23% 10%
14	S	153	58% 22% 20%
15	T	143	65% 19% 16%
16	U	143	14% 65% 11% 24%
17	V	156	69% 9% 22%
18	W	153	67% 25% 7%
19	Y	98	82% 6% 12%
20	Z	130	91% 8%
21	a	145	83% 15%
22	b	136	86% 11%
23	c	99	6% 48% 21% 30%
24	e	82	87% 12%
25	f	68	84% 6% 10%
26	h	62	27% 6% 66%
27	i	154	36% 6% 58%
28	A	1796	58% 33% 5%

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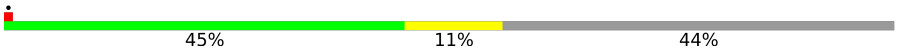
Mol	Chain	Length	Quality of chain
29	2	830	
30	3	259	
31	4	480	
32	5	445	

2 Entry composition (i)

There are 35 unique types of molecules in this entry. The entry contains 76910 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 Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	D	208	1641	1051	289	295	6	0	0

- Molecule 2 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	213	1723	1096	319	303	5	0	0

- Molecule 3 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	F	204	1573	1017	269	284	3	0	0

- Molecule 4 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	H	261	2072	1314	389	362	7	0	0

- Molecule 5 is a protein called 40S ribosomal protein s5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	I	199	1557	971	294	285	7	0	0

- Molecule 6 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	J	232	1875	1171	376	323	5	0	0

- Molecule 7 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	K	195	Total	C	N	O	0	0
			1562	983	300	279		

- Molecule 8 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	201	Total	C	N	O	S	0	0
			1621	1009	330	281	1		

- Molecule 9 is a protein called 40S ribosomal protein s9-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	179	Total	C	N	O	S	0	0
			1466	933	290	241	2		

- Molecule 10 is a protein called 40S ribosomal protein S11-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	O	150	Total	C	N	O	S	0	0
			1222	780	236	201	5		

- Molecule 11 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	118	Total	C	N	O	S	0	0
			923	577	167	171	8		

- Molecule 12 is a protein called 40S ribosomal protein S13-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Q	150	Total	C	N	O	S	0	0
			1182	756	220	205	1		

- Molecule 13 is a protein called 40S ribosomal protein S14-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	135	Total	C	N	O	S	0	0
			993	610	196	182	5		

- Molecule 14 is a protein called 40S ribosomal protein s15-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S	123	Total	C	N	O	S	0	0
			986	628	184	171	3		

- Molecule 15 is a protein called 40S ribosomal protein S16-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	120	Total	C	N	O	S	0	0
			935	603	168	163	1		

- Molecule 16 is a protein called 40S ribosomal protein S17-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	109	Total	C	N	O	S	0	0
			876	552	161	160	3		

- Molecule 17 is a protein called Putative ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	V	122	Total	C	N	O	S	0	0
			995	628	191	175	1		

- Molecule 18 is a protein called 40S ribosomal protein S19-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	142	Total	C	N	O	S	0	0
			1117	694	221	201	1		

- Molecule 19 is a protein called 40S ribosomal protein S21-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Y	86	Total	C	N	O	S	0	0
			664	408	124	128	4		

- Molecule 20 is a protein called 40S ribosomal protein S22-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Z	129	Total	C	N	O	S	0	0
			1037	659	195	178	5		

- Molecule 21 is a protein called 40S ribosomal protein s23-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	a	142	Total	C	N	O	S	0	0
			1099	694	215	188	2		

- Molecule 22 is a protein called Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	b	132	Total	C	N	O	S	0	0
			1061	668	209	182	2		

- Molecule 23 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	c	69	Total	C	N	O	S	0	0
			546	345	101	98	2		

- Molecule 24 is a protein called Ribosomal protein s27-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	e	81	Total	C	N	O	S	0	0
			611	386	111	107	7		

- Molecule 25 is a protein called 40S ribosomal protein S28-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	f	61	Total	C	N	O	S	0	0
			472	292	91	88	1		

- Molecule 26 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	h	21	Total	C	N	O	0	0
			173	112	37	24		

- Molecule 27 is a protein called 40S ribosomal protein S27a-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	i	65	Total	C	N	O	S	0	0
			528	332	97	93	6		

- Molecule 28 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	A	1720	Total	C	N	O	P	0	0
			36686	16390	6537	12039	1720		

- Molecule 29 is a protein called Bms1-type G domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	2	683	Total	C	N	O	S	0	0
			5458	3445	991	1004	18		

- Molecule 30 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	3	184	Total	C	N	O	S	0	0
			1435	912	260	256	7		

- Molecule 31 is a protein called Bystin-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4	270	Total	C	N	O	S	0	0
			2154	1401	377	366	10		

- Molecule 32 is a protein called Putative low-temperature viability protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	5	81	Total	C	N	O	S	0	0
			660	416	113	130	1		

- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
33	a	1	Total	Mg	0
			1	1	
33	A	1	Total	Mg	0
			1	1	

- Molecule 34 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
34	e	1	Total	Zn	0
			1	1	

- Molecule 35 is water.

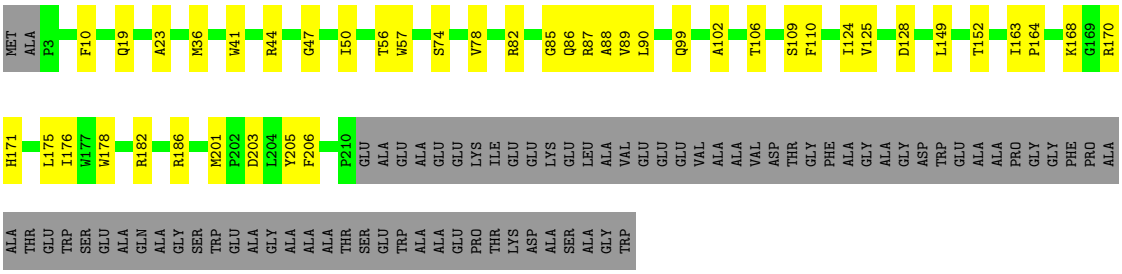
Mol	Chain	Residues	Atoms	AltConf
35	Q	1	Total O 1 1	0
35	A	3	Total O 3 3	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

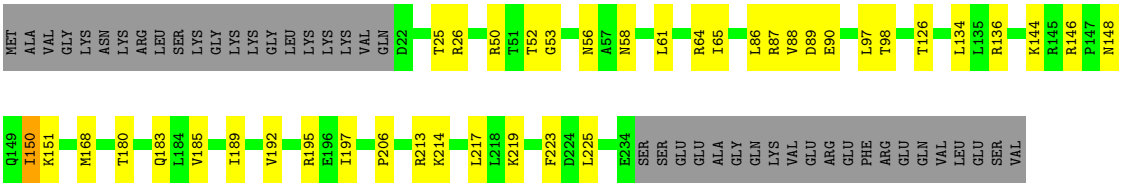
• Molecule 1: Small ribosomal subunit protein uS2

Chain D:



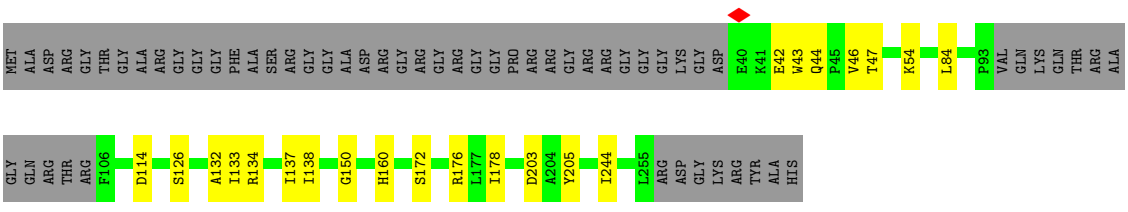
• Molecule 2: Small ribosomal subunit protein eS1

Chain E:



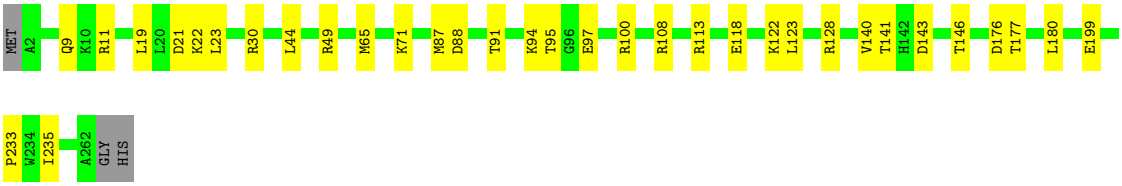
• Molecule 3: Small ribosomal subunit protein uS5

Chain F:



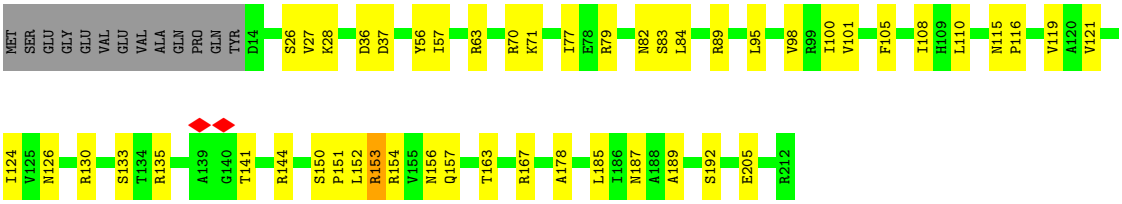
• Molecule 4: 40S ribosomal protein S4

Chain H:



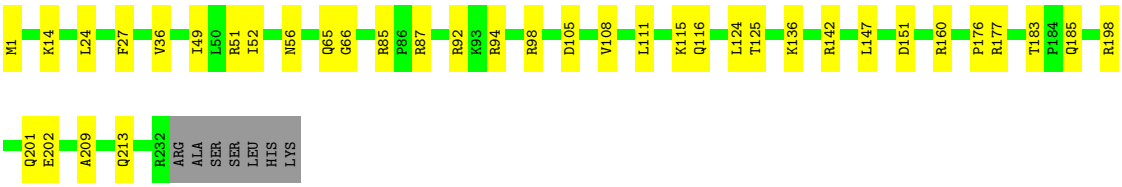
• Molecule 5: 40S ribosomal protein s5-like protein

Chain I:



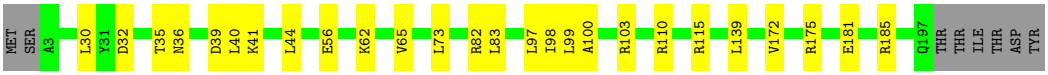
• Molecule 6: 40S ribosomal protein S6

Chain J:



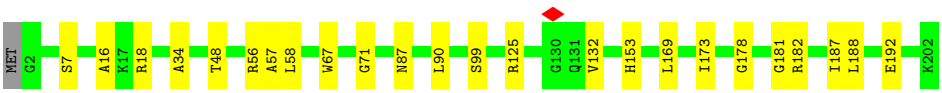
• Molecule 7: 40S ribosomal protein S7

Chain K:



• Molecule 8: 40S ribosomal protein S8

Chain L:

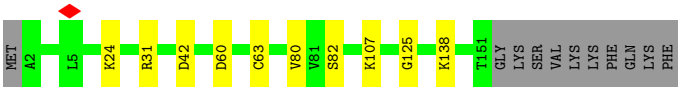


• Molecule 9: 40S ribosomal protein s9-like protein

Chain M:

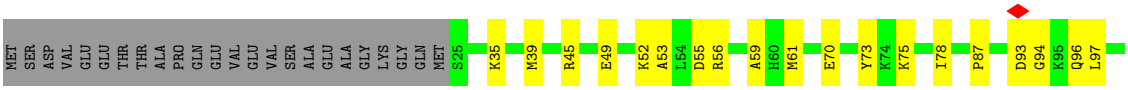
• Molecule 10: 40S ribosomal protein S11-like protein

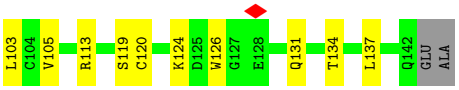
Chain O:



• Molecule 11: 40S ribosomal protein S12

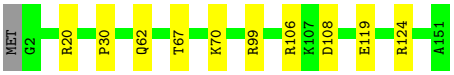
Chain P:





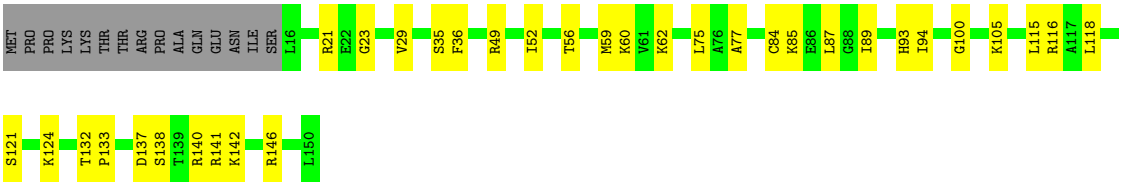
• Molecule 12: 40S ribosomal protein S13-like protein

Chain Q:



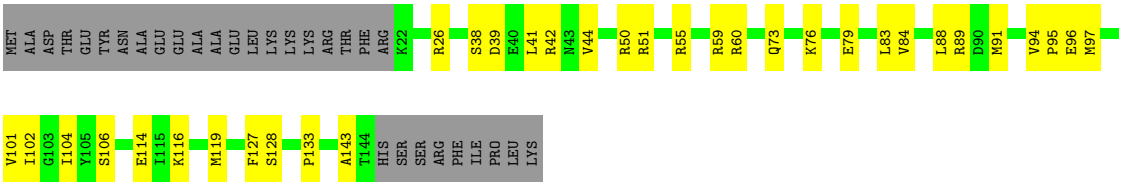
• Molecule 13: 40S ribosomal protein S14-like protein

Chain R:



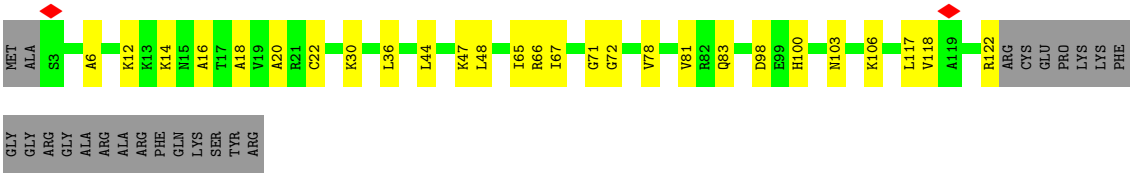
• Molecule 14: 40S ribosomal protein s15-like protein

Chain S:



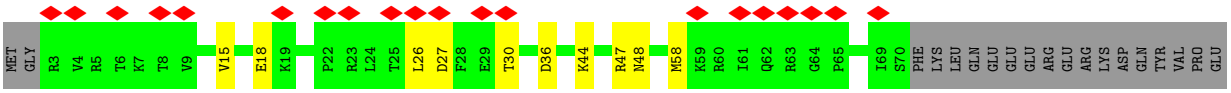
• Molecule 15: 40S ribosomal protein S16-like protein

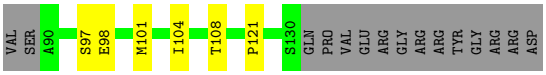
Chain T:



• Molecule 16: 40S ribosomal protein S17-like protein

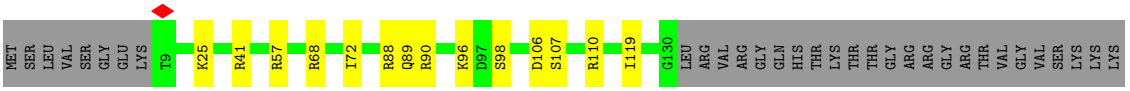
Chain U:





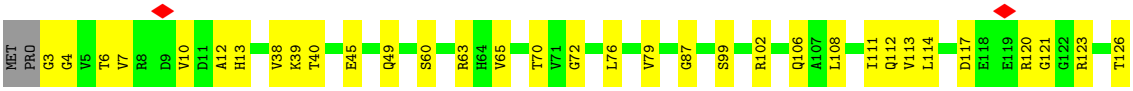
• Molecule 17: Putative ribosomal protein

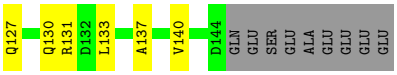
Chain V:



• Molecule 18: 40S ribosomal protein S19-like protein

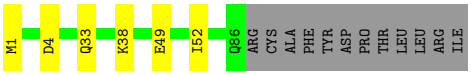
Chain W:





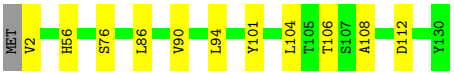
• Molecule 19: 40S ribosomal protein S21-like protein

Chain Y:



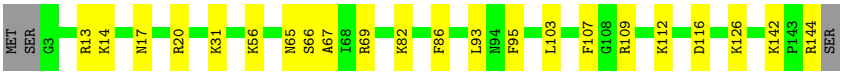
• Molecule 20: 40S ribosomal protein S22-like protein

Chain Z:



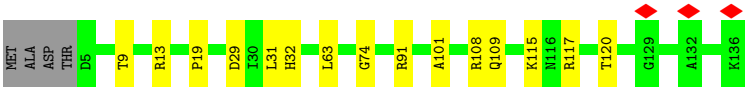
• Molecule 21: 40S ribosomal protein s23-like protein

Chain a:



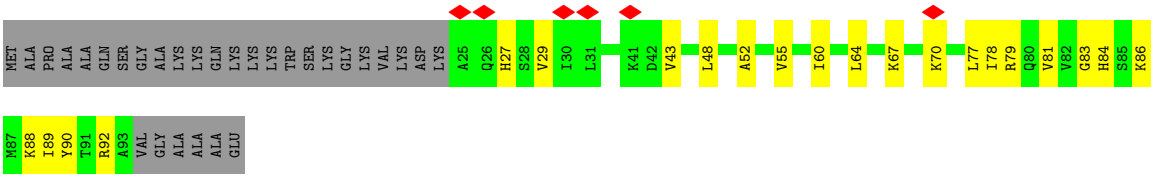
• Molecule 22: Small ribosomal subunit protein eS24

Chain b:



• Molecule 23: 40S ribosomal protein S25

Chain c:

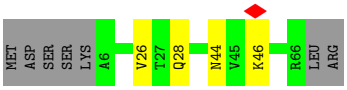


• Molecule 24: Ribosomal protein s27-like protein

Chain e:

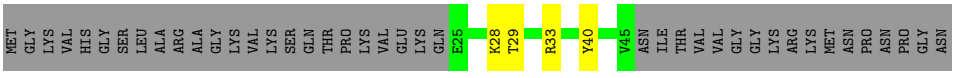
• Molecule 25: 40S ribosomal protein S28-like protein

Chain f:



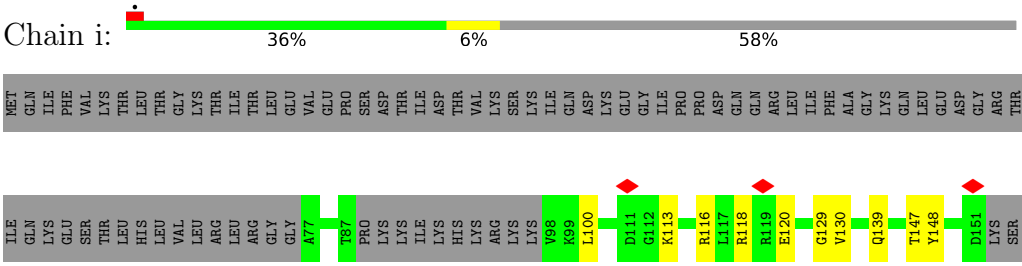
• Molecule 26: 40S ribosomal protein S30

Chain h:



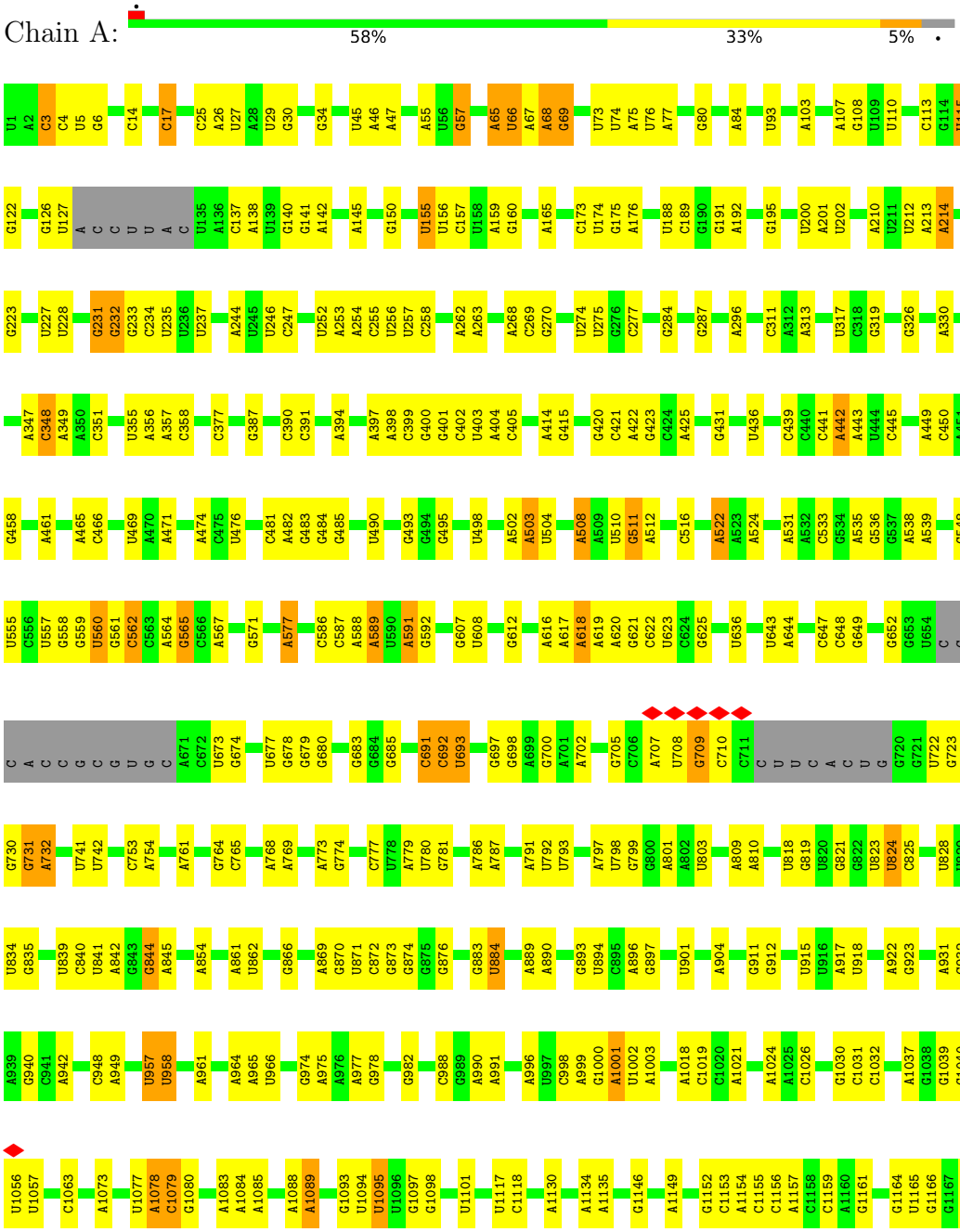
• Molecule 27: 40S ribosomal protein S27a-like protein

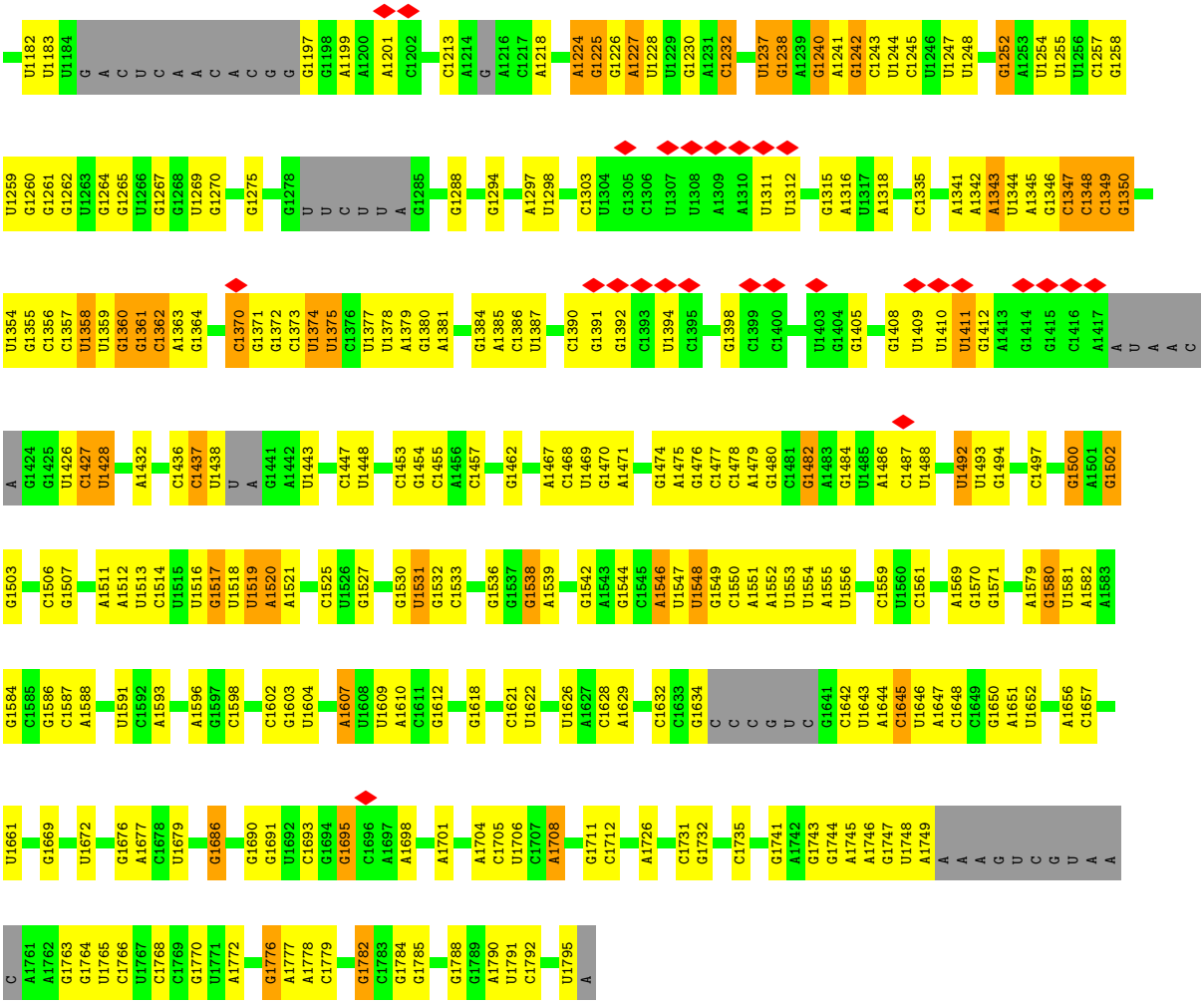
Chain i:



• Molecule 28: 18S rRNA

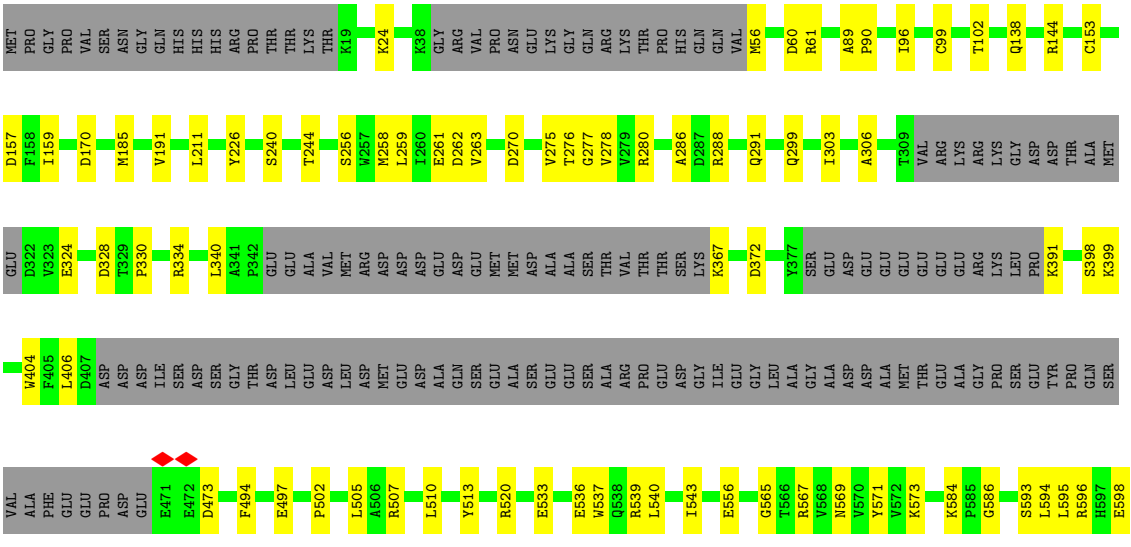
Chain A:

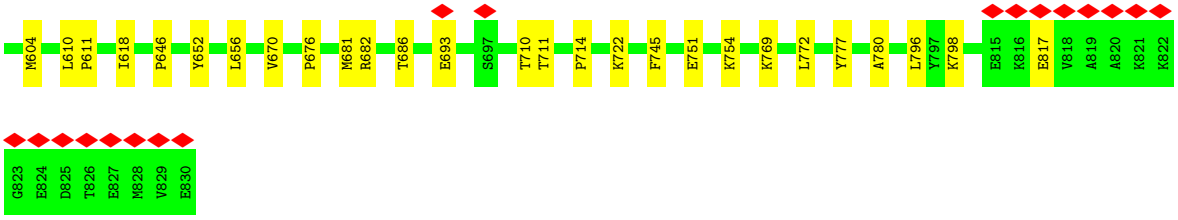




• Molecule 29: Bms1-type G domain-containing protein

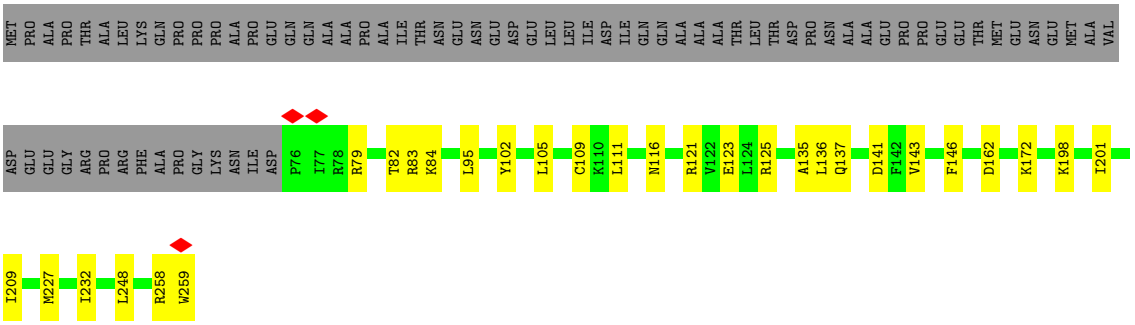
Chain 2:





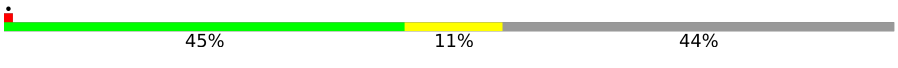
• Molecule 30: Pre-rRNA-processing protein PNO1

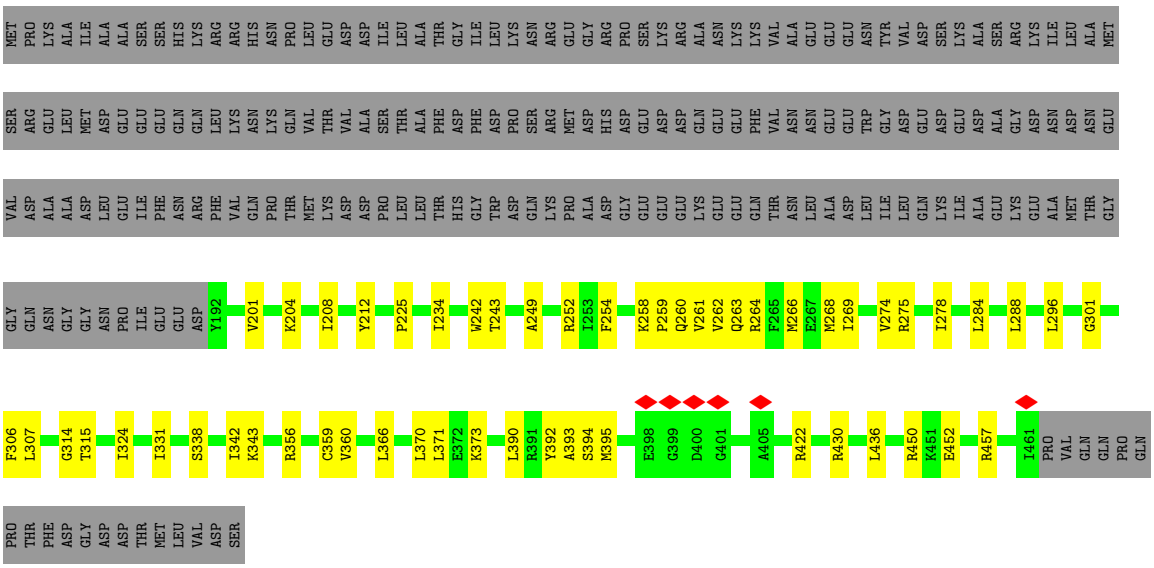
Chain 3:



• Molecule 31: Bystin-like protein

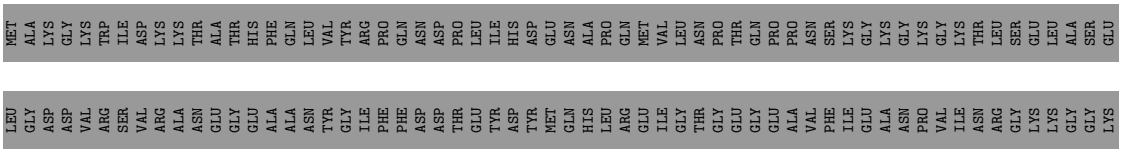
Chain 4:

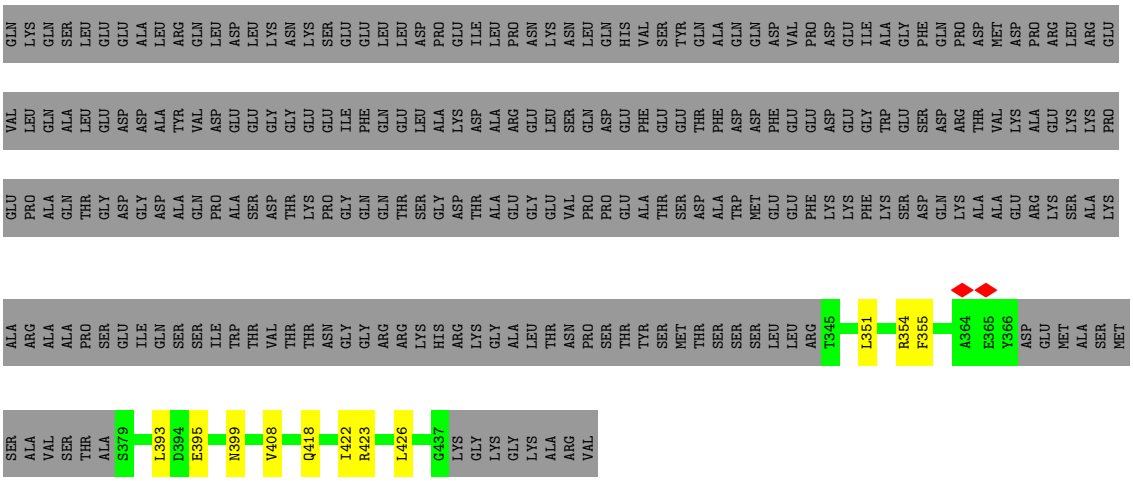




• Molecule 32: Putative low-temperature viability protein

Chain 5:




GLN LYS GLN SER LEU GLU GLU ALA LEU ARG GLN LEU ASP LEU LYS ASN LYS SER GLU GLU LEU LEU ASP PRO GLU ILE LEU PRO ASN LYS ASN LEU GLN HIS VAL SER TYR GLN ALA GLN GLN ASP VAL PRO ASP GLU ILE ALA GLY PHE GLN PRO ASP MET ASP PRO ARG LEU ARG GLU
VAL LEU GLN ALA LEU GLU ASP ASP ALA TYR VAL ASP GLU GLU GLY GLY GLU GLU ILE PHE GLN GLU LEU ALA LYS ASP ALA ARG GLU LEU SER GLN ASP GLU PHE GLU GLU THR PHE ASP ASP PHE GLU GLU ASP GLU GLY TRP GLU SER ASP ARG THR VAL LYS ALA GLU LYS LYS PRO
GLU PRO ALA GLN THR GLY ASP GLY ASP ALA GLN PRO ALA SER ASP THR LYS PRO GLY GLN GLN THR SER GLY ASP THR ALA GLU GLY GLU VAL PRO PRO GLU ALA THR SER ASP ALA TRP MET GLU GLU PHE LYS LYS PHE LYS SER ASP GLN LYS ALA ALA GLU ARG LYS SER ALA LYS
ALA ARG ALA ALA PRO SER GLU ILE GLN SER SER ILE TRP THR VAL THR THR ASN GLY GLY ARG ARG LYS HIS ARG LYS GLY ALA LEU THR ASN PRO SER THR TYR SER MET THR SER SER SER LEU LEU ARG T345 L351 R354 F355 A364 E365 Y366 ASP GLU MET ALA SER MET
SER ALA VAL SER THR ALA S379 L393 D394 E395 N399 V408 Q418 I422 R423 L426 G437 LYS GLY LYS GLY LYS ALA ARG VAL

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	85384	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; Relion	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.752	Depositor
Minimum map value	-0.357	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	412.56, 412.56, 412.56	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.146, 1.146, 1.146	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.18	0/1683	0.47	0/2299
2	E	0.30	0/1752	0.59	1/2361 (0.0%)
3	F	0.18	0/1603	0.46	0/2169
4	H	0.22	0/2112	0.48	0/2842
5	I	0.32	0/1578	0.65	0/2130
6	J	0.27	0/1906	0.57	0/2547
7	K	0.23	0/1587	0.50	0/2140
8	L	0.20	0/1654	0.50	0/2213
9	M	0.19	0/1489	0.42	0/1993
10	O	0.23	0/1249	0.43	0/1678
11	P	0.22	0/934	0.63	0/1255
12	Q	0.17	0/1205	0.33	0/1627
13	R	0.35	0/1005	0.63	1/1350 (0.1%)
14	S	0.18	0/1003	0.53	0/1342
15	T	0.20	0/949	0.52	0/1278
16	U	0.21	0/887	0.45	0/1191
17	V	0.22	0/1009	0.63	0/1356
18	W	0.19	0/1137	0.54	0/1533
19	Y	0.16	0/671	0.36	0/900
20	Z	0.23	0/1055	0.53	0/1416
21	a	0.22	0/1116	0.49	0/1489
22	b	0.19	0/1075	0.43	0/1431
23	c	0.20	0/550	0.63	0/736
24	e	0.21	0/623	0.52	0/843
25	f	0.18	0/475	0.45	0/639
26	h	0.52	0/176	0.68	0/233
27	i	0.14	0/535	0.45	0/710
28	A	0.23	0/41025	0.39	1/63918 (0.0%)
29	2	0.16	0/5573	0.42	0/7533
30	3	0.21	0/1459	0.51	0/1964
31	4	0.24	0/2205	0.64	0/2990
32	5	0.25	0/670	0.75	0/896

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
All	All	0.22	0/81950	0.45	3/119002 (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
5	I	0	1
14	S	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(^{o})	Ideal(^{o})
2	E	150	ILE	N-CA-C	-6.02	107.63	113.53
28	A	1531	U	C2'-C3'-O3'	6.02	118.53	109.50
13	R	138	SER	N-CA-C	5.21	118.14	110.59

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	I	153	ARG	Sidechain
14	S	73	GLN	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	D	1641	0	1650	24	0
2	E	1723	0	1804	22	0
3	F	1573	0	1669	13	0
4	H	2072	0	2155	22	0
5	I	1557	0	1608	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	J	1875	0	1983	23	0
7	K	1562	0	1641	16	0
8	L	1621	0	1645	16	0
9	M	1466	0	1582	18	0
10	O	1222	0	1289	8	0
11	P	923	0	946	19	0
12	Q	1182	0	1264	9	0
13	R	993	0	1021	20	0
14	S	986	0	1045	27	0
15	T	935	0	997	17	0
16	U	876	0	921	9	0
17	V	995	0	1040	14	0
18	W	1117	0	1133	27	0
19	Y	664	0	662	5	0
20	Z	1037	0	1076	8	0
21	a	1099	0	1169	18	0
22	b	1061	0	1150	12	0
23	c	546	0	591	16	0
24	e	611	0	634	6	0
25	f	472	0	491	2	0
26	h	173	0	192	2	0
27	i	528	0	541	7	0
28	A	36686	0	18488	297	0
29	2	5458	0	5501	63	0
30	3	1435	0	1491	18	0
31	4	2154	0	2242	35	0
32	5	660	0	648	10	0
33	A	1	0	0	0	0
33	a	1	0	0	0	0
34	e	1	0	0	0	0
35	A	3	0	0	0	0
35	Q	1	0	0	0	0
All	All	76910	0	60269	702	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.

The worst 5 of 702 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)
28:A:1079:C:H42	28:A:1089:A:N6	1.48	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:A:1079:C:N4	28:A:1089:A:H62	1.50	1.09
28:A:214:A:N6	28:A:840:C:H42	1.55	1.03
28:A:1695:G:H21	28:A:1698:A:N6	1.57	1.03
28:A:214:A:H61	28:A:840:C:N4	1.60	0.99

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	D	206/285 (72%)	197 (96%)	9 (4%)	0	100	100
2	E	211/255 (83%)	199 (94%)	12 (6%)	0	100	100
3	F	200/263 (76%)	194 (97%)	6 (3%)	0	100	100
4	H	259/264 (98%)	250 (96%)	9 (4%)	0	100	100
5	I	197/212 (93%)	182 (92%)	15 (8%)	0	100	100
6	J	230/239 (96%)	222 (96%)	8 (4%)	0	100	100
7	K	193/203 (95%)	184 (95%)	9 (5%)	0	100	100
8	L	199/202 (98%)	188 (94%)	11 (6%)	0	100	100
9	M	177/190 (93%)	173 (98%)	4 (2%)	0	100	100
10	O	148/161 (92%)	143 (97%)	5 (3%)	0	100	100
11	P	116/144 (81%)	103 (89%)	13 (11%)	0	100	100
12	Q	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
13	R	133/150 (89%)	124 (93%)	8 (6%)	1 (1%)	16	50
14	S	121/153 (79%)	118 (98%)	3 (2%)	0	100	100
15	T	118/143 (82%)	111 (94%)	7 (6%)	0	100	100
16	U	105/143 (73%)	102 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	V	120/156 (77%)	112 (93%)	8 (7%)	0	100	100
18	W	140/153 (92%)	131 (94%)	9 (6%)	0	100	100
19	Y	84/98 (86%)	82 (98%)	2 (2%)	0	100	100
20	Z	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
21	a	140/145 (97%)	132 (94%)	8 (6%)	0	100	100
22	b	130/136 (96%)	126 (97%)	4 (3%)	0	100	100
23	c	67/99 (68%)	65 (97%)	2 (3%)	0	100	100
24	e	79/82 (96%)	76 (96%)	3 (4%)	0	100	100
25	f	59/68 (87%)	59 (100%)	0	0	100	100
26	h	19/62 (31%)	19 (100%)	0	0	100	100
27	i	61/154 (40%)	57 (93%)	4 (7%)	0	100	100
29	2	671/830 (81%)	651 (97%)	19 (3%)	1 (0%)	48	80
30	3	182/259 (70%)	178 (98%)	4 (2%)	0	100	100
31	4	268/480 (56%)	255 (95%)	13 (5%)	0	100	100
32	5	77/445 (17%)	75 (97%)	2 (3%)	0	100	100
All	All	4985/6455 (77%)	4775 (96%)	208 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	R	137	ASP
29	2	372	ASP

5.3.2 Protein sidechains (i)

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	178/225 (79%)	178 (100%)	0	100	100
2	E	187/223 (84%)	182 (97%)	5 (3%)	39	71
3	F	171/206 (83%)	171 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	H	219/221 (99%)	219 (100%)	0	100 100
5	I	167/178 (94%)	166 (99%)	1 (1%)	78 88
6	J	198/204 (97%)	195 (98%)	3 (2%)	57 80
7	K	169/177 (96%)	169 (100%)	0	100 100
8	L	163/164 (99%)	163 (100%)	0	100 100
9	M	154/162 (95%)	153 (99%)	1 (1%)	78 88
10	O	133/143 (93%)	133 (100%)	0	100 100
11	P	101/121 (84%)	101 (100%)	0	100 100
12	Q	129/130 (99%)	129 (100%)	0	100 100
13	R	100/117 (86%)	100 (100%)	0	100 100
14	S	106/132 (80%)	106 (100%)	0	100 100
15	T	98/115 (85%)	97 (99%)	1 (1%)	68 84
16	U	100/131 (76%)	100 (100%)	0	100 100
17	V	107/135 (79%)	107 (100%)	0	100 100
18	W	114/124 (92%)	114 (100%)	0	100 100
19	Y	69/80 (86%)	69 (100%)	0	100 100
20	Z	112/113 (99%)	112 (100%)	0	100 100
21	a	113/116 (97%)	113 (100%)	0	100 100
22	b	112/115 (97%)	112 (100%)	0	100 100
23	c	60/80 (75%)	60 (100%)	0	100 100
24	e	70/71 (99%)	70 (100%)	0	100 100
25	f	52/61 (85%)	52 (100%)	0	100 100
26	h	17/52 (33%)	15 (88%)	2 (12%)	5 22
27	i	57/139 (41%)	57 (100%)	0	100 100
29	2	589/714 (82%)	589 (100%)	0	100 100
30	3	152/215 (71%)	152 (100%)	0	100 100
31	4	229/411 (56%)	229 (100%)	0	100 100
32	5	70/373 (19%)	70 (100%)	0	100 100
All	All	4296/5448 (79%)	4283 (100%)	13 (0%)	84 91

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	J	201	GLN
6	J	202	GLU
26	h	29	THR
15	T	83	GLN
26	h	28	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
29	2	63	ASN
32	5	382	GLN
29	2	112	ASN
31	4	290	ASN
6	J	129	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	A	1709/1796 (95%)	413 (24%)	23 (1%)

5 of 413 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
28	A	3	C
28	A	4	C
28	A	14	C
28	A	17	C
28	A	25	C

5 of 23 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
28	A	1264	G
28	A	1468	C
28	A	1378	U
28	A	1469	U
28	A	414	A

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

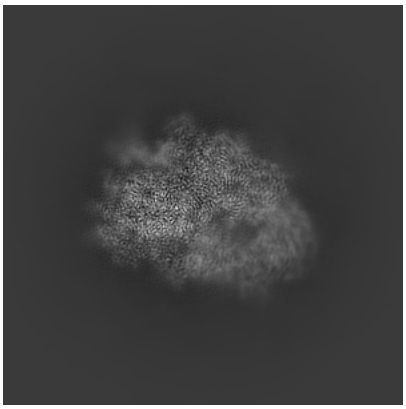
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-66684. These allow visual inspection of the internal detail of the map and identification of artifacts.

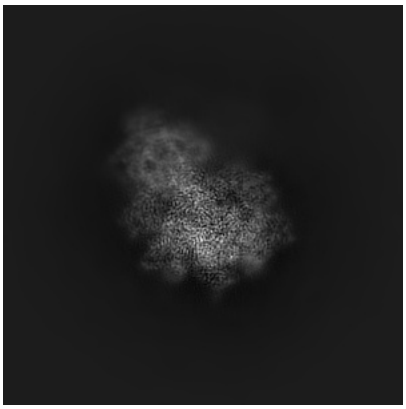
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

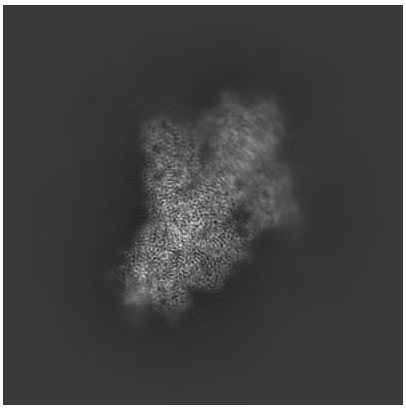
6.1.1 Primary map



X

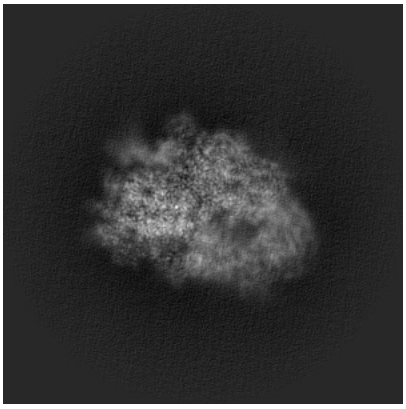


Y

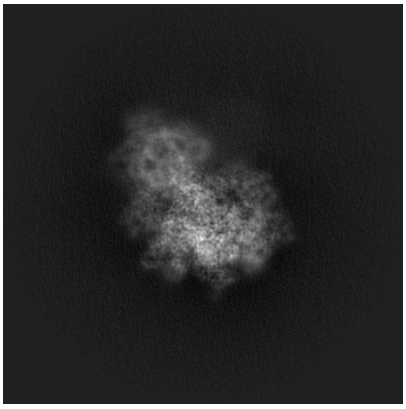


Z

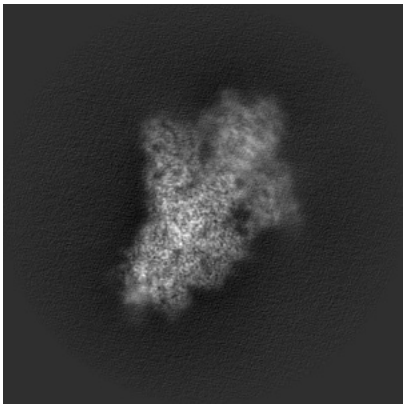
6.1.2 Raw map



X



Y

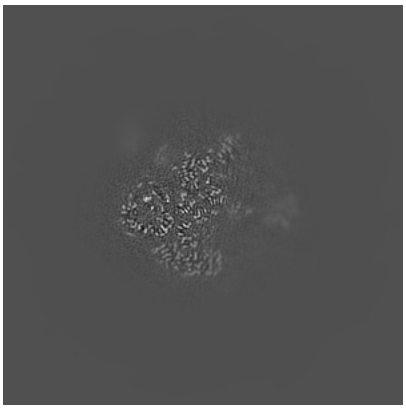


Z

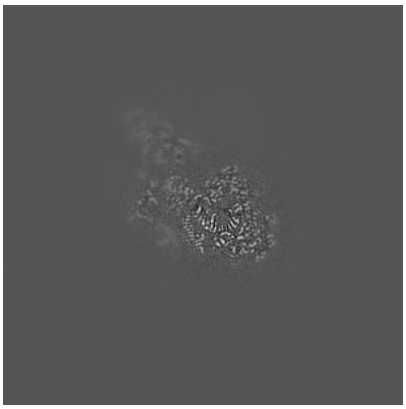
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

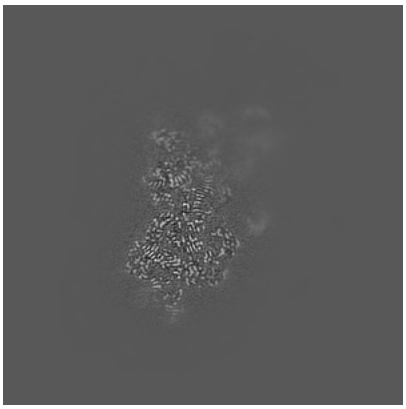
6.2.1 Primary map



X Index: 180

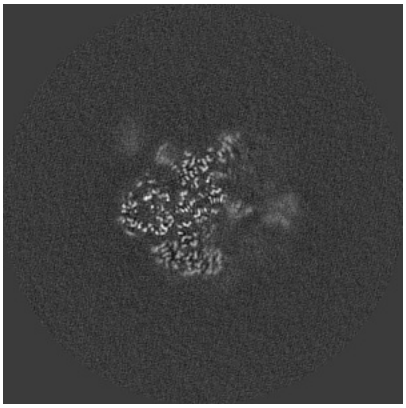


Y Index: 180

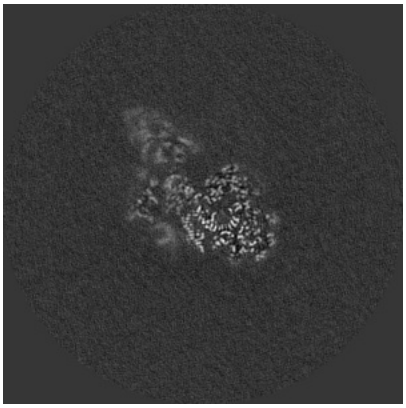


Z Index: 180

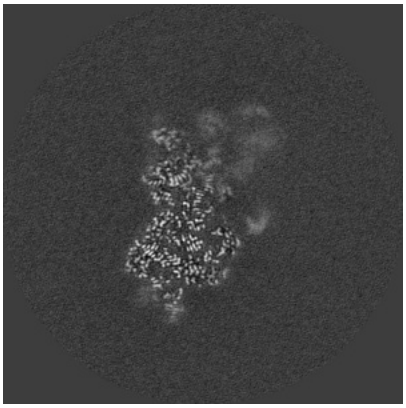
6.2.2 Raw map



X Index: 180



Y Index: 180

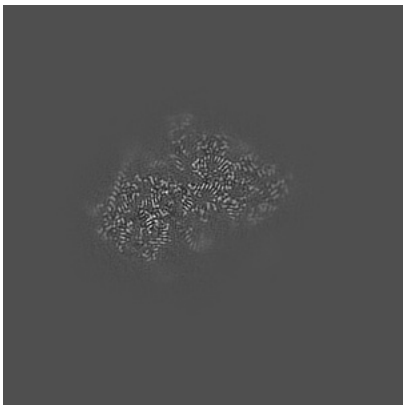


Z Index: 180

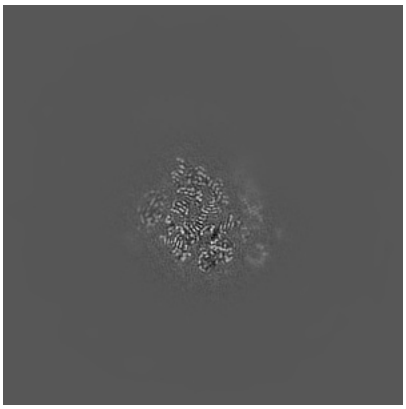
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



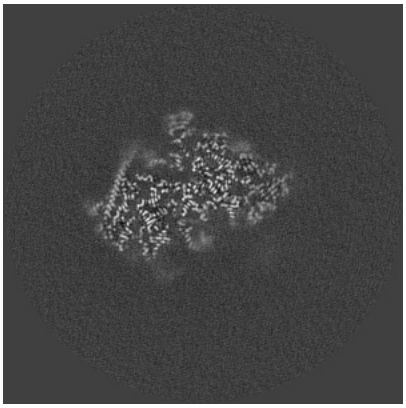
X Index: 147



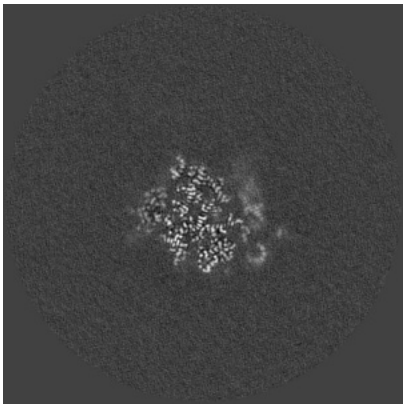
Y Index: 144

Z Index: 178

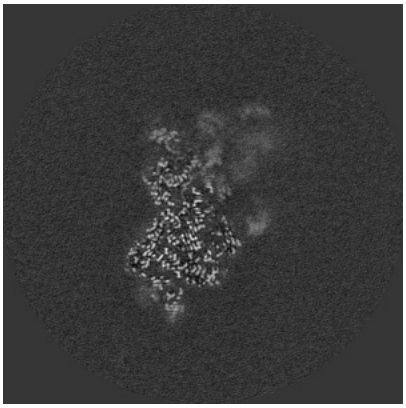
6.3.2 Raw map



X Index: 148



Y Index: 145

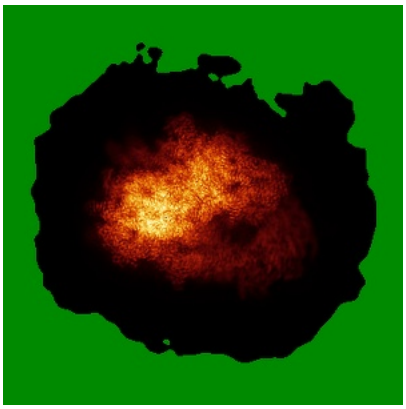


Z Index: 179

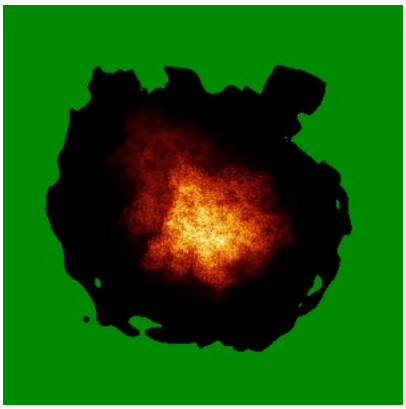
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

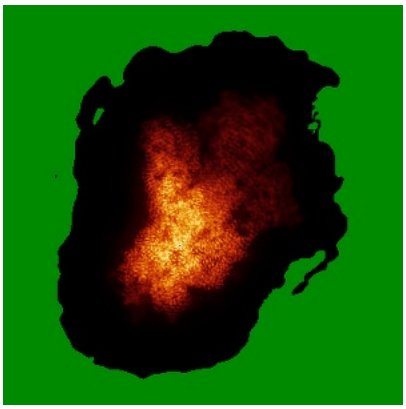
6.4.1 Primary map



X

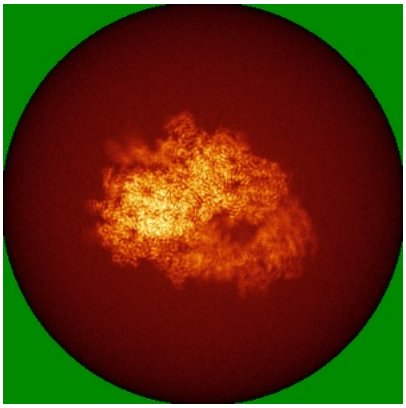


Y

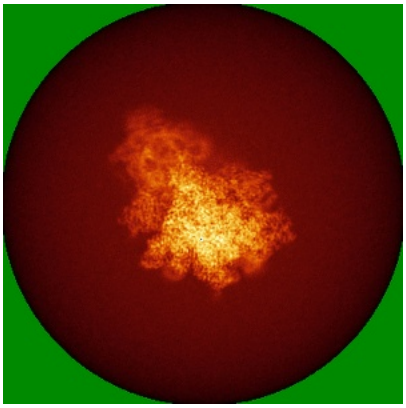


Z

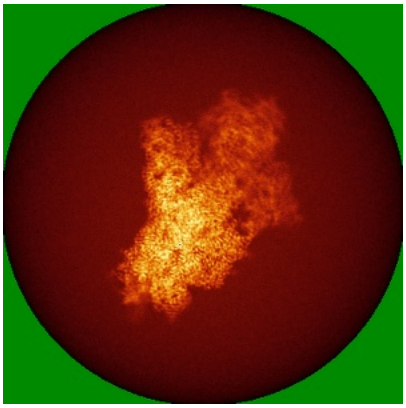
6.4.2 Raw map



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.

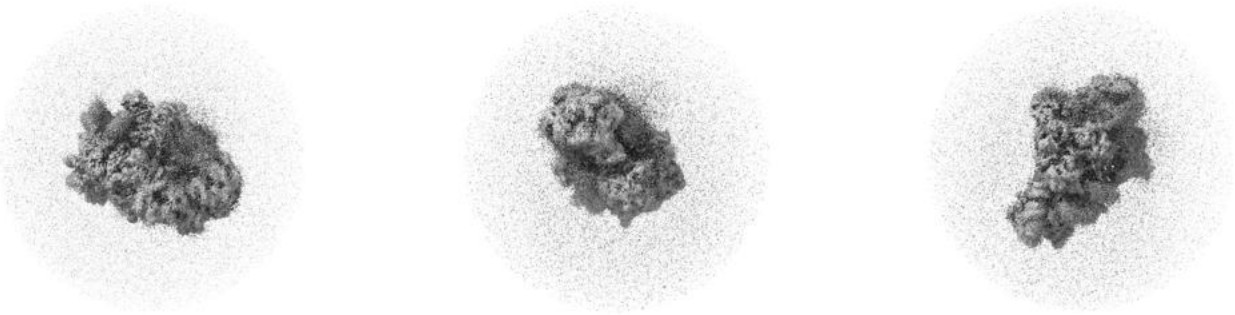
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. 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



X Y Z

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.

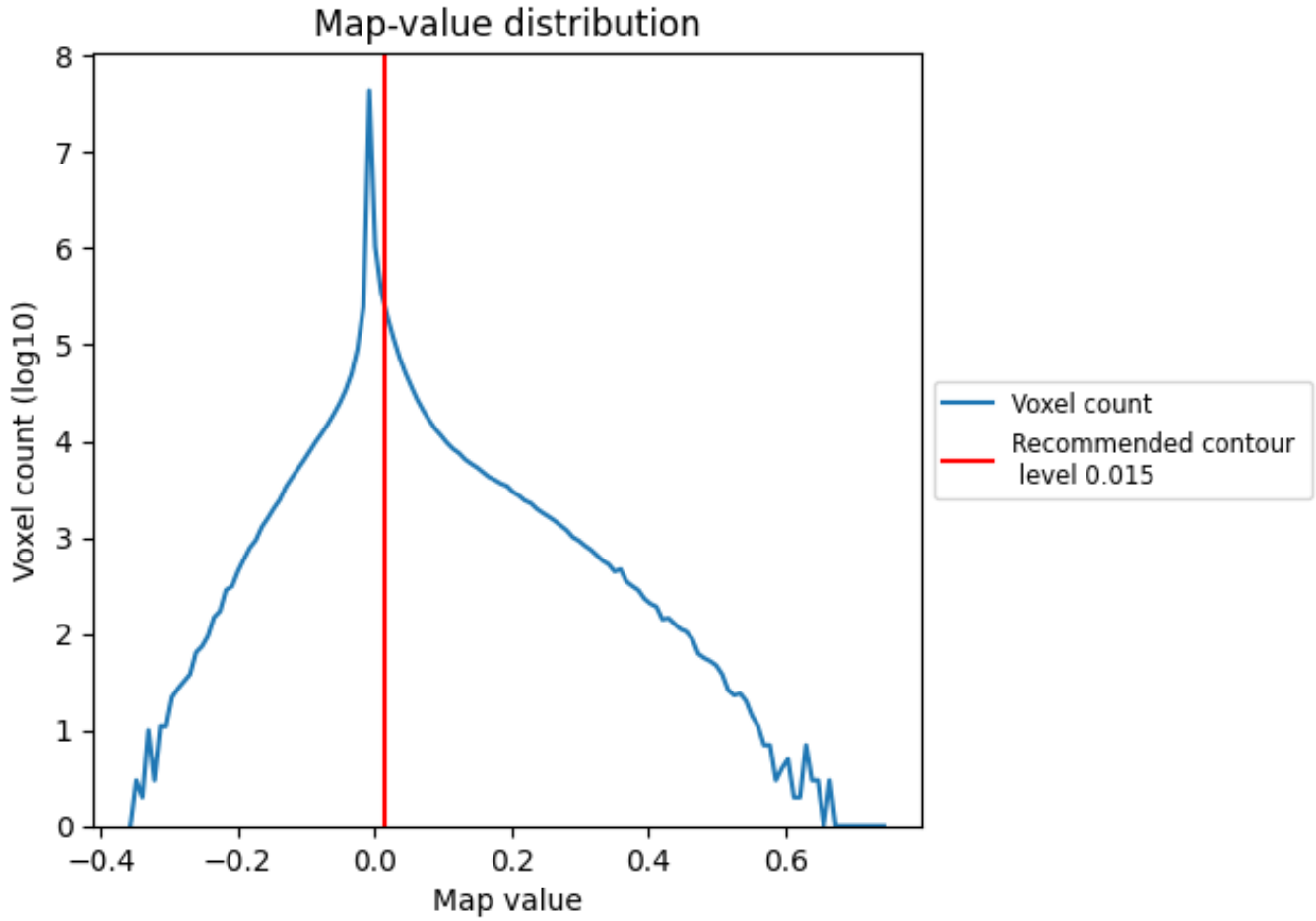
6.6 Mask visualisation (i)

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

7 Map analysis

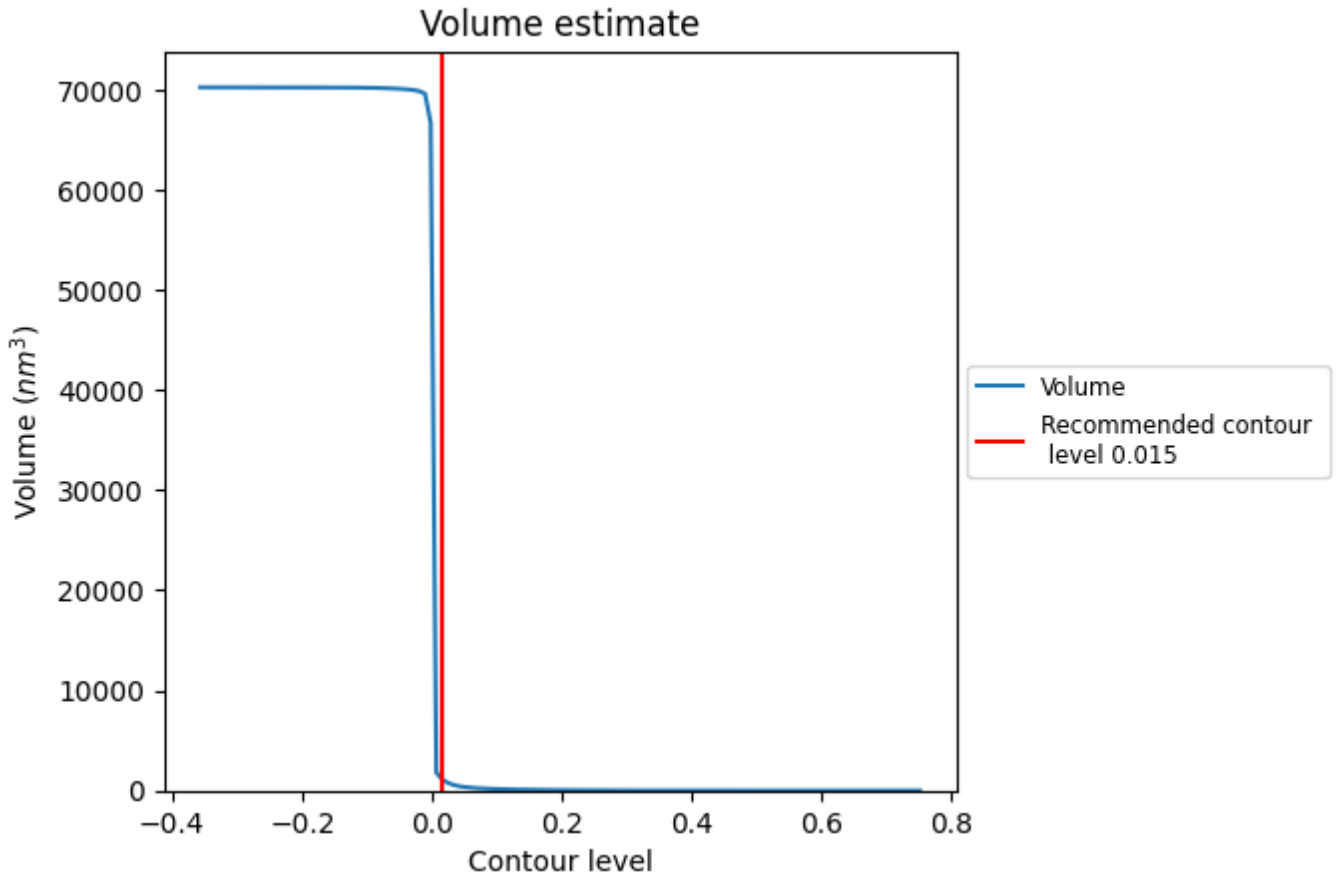
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

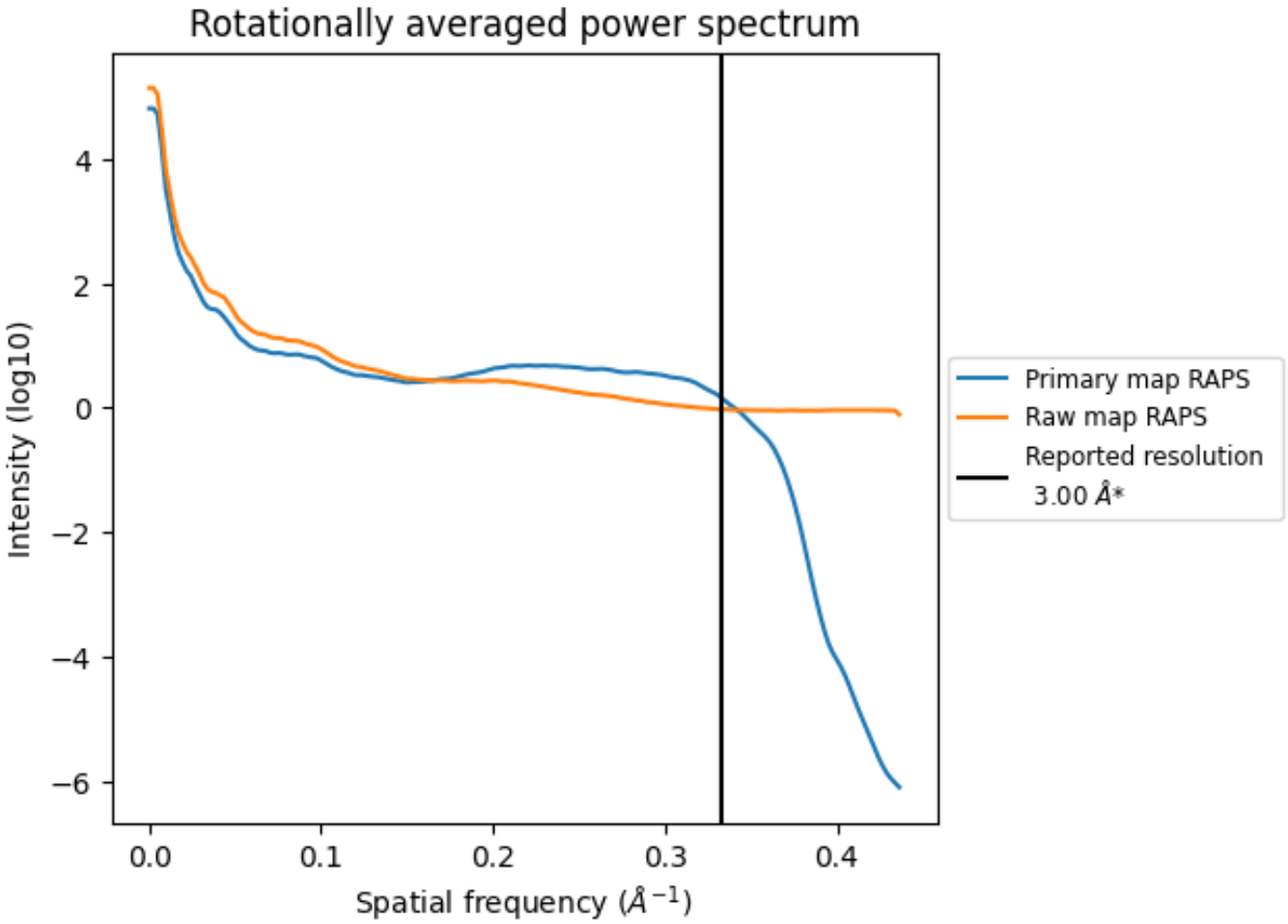
7.2 Volume estimate (i)



The volume at the recommended contour level is 1189 nm^3; this corresponds to an approximate mass of 1074 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 (i)

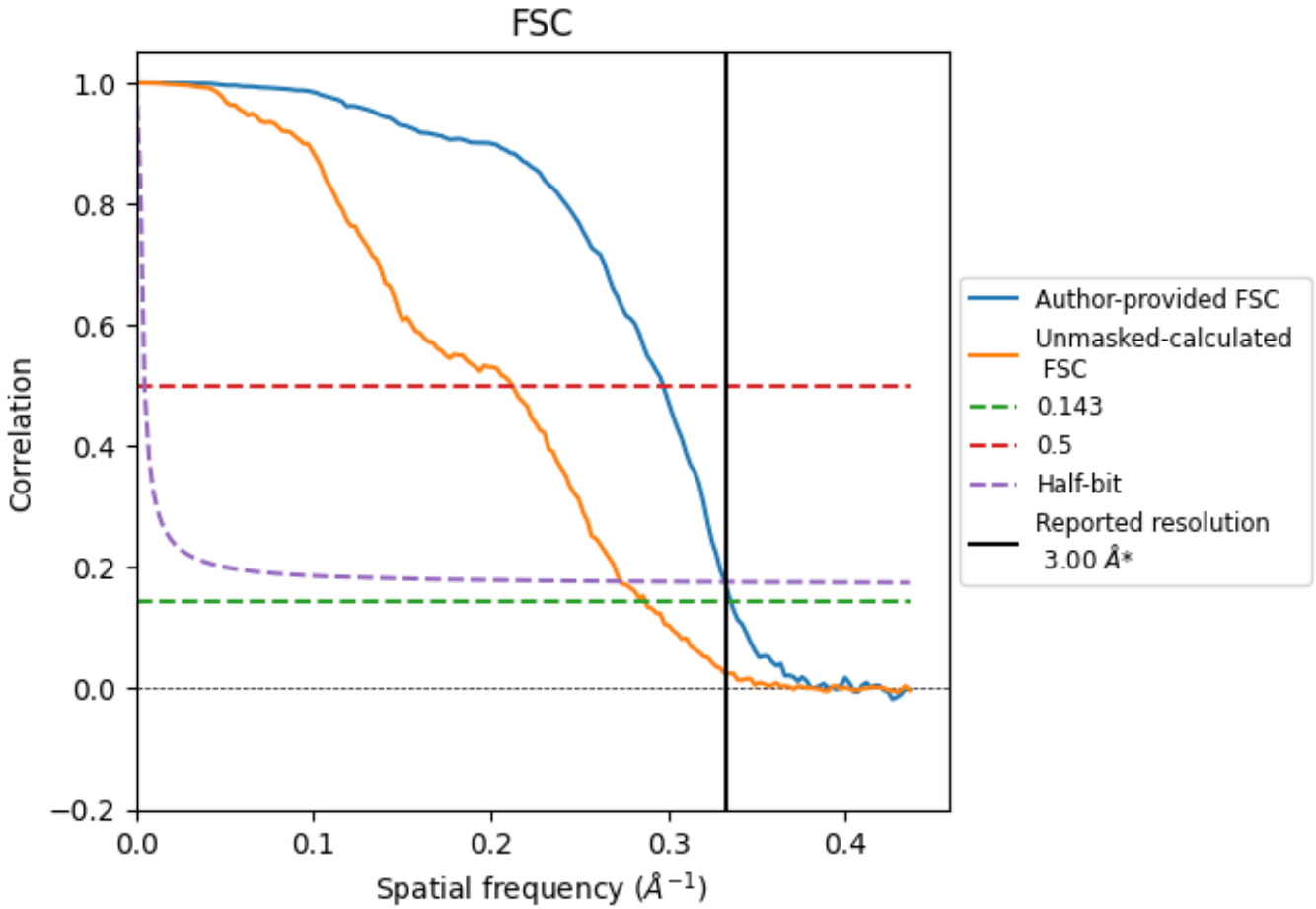


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8.2 Resolution estimates (i)

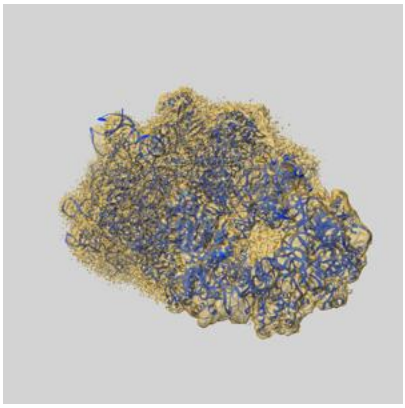
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.98	3.36	3.01
Unmasked-calculated*	3.48	4.72	3.66

*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 3.48 differs from the reported value 3.0 by more than 10 %

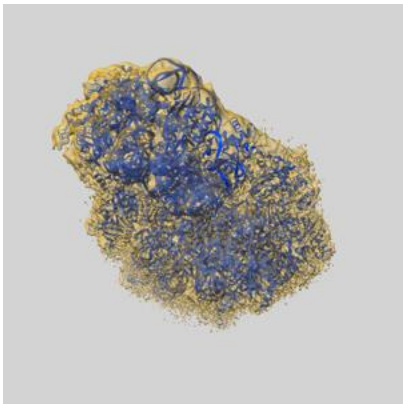
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-66684 and PDB model 9XAE. Per-residue inclusion information can be found in section 3 on page 11.

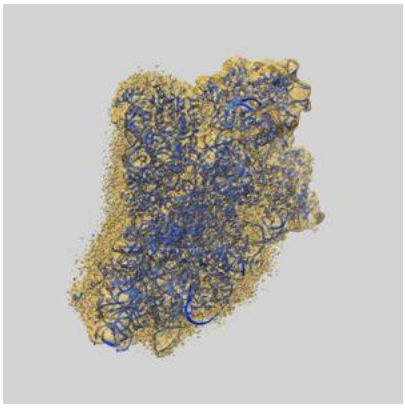
9.1 Map-model overlay



X



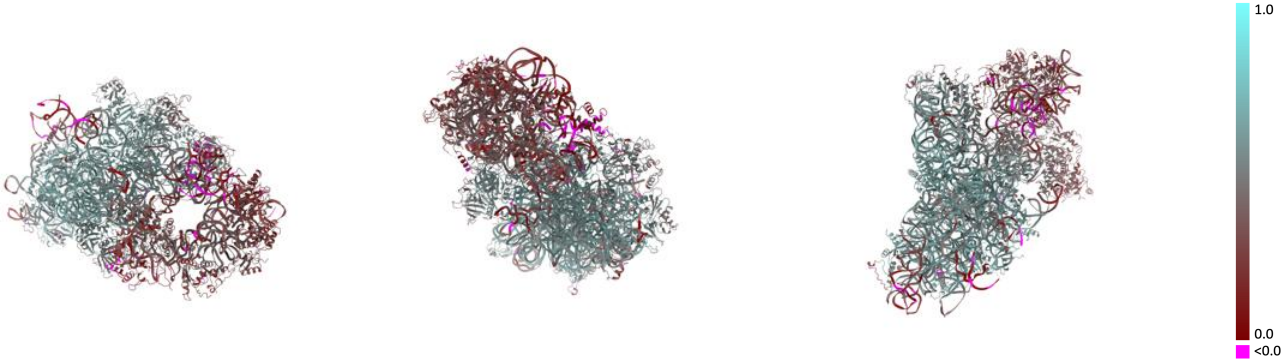
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 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.

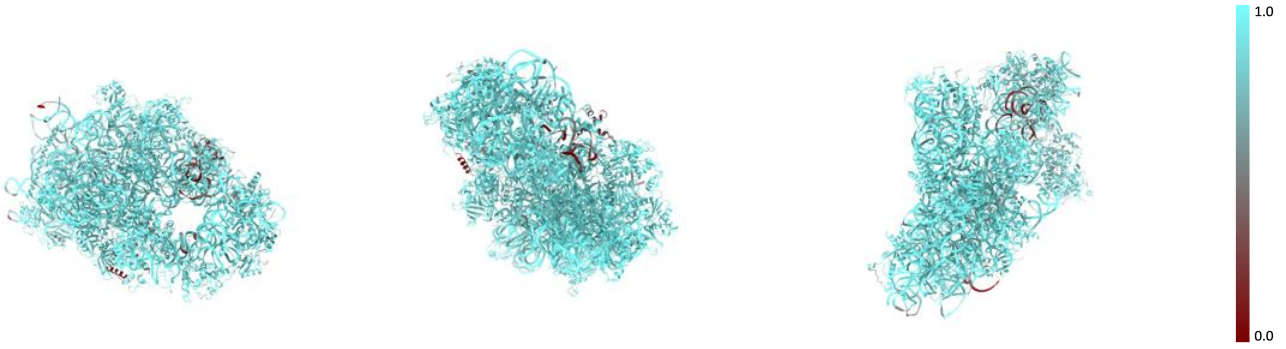
9.2 Q-score mapped to coordinate model



X Y Z

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.

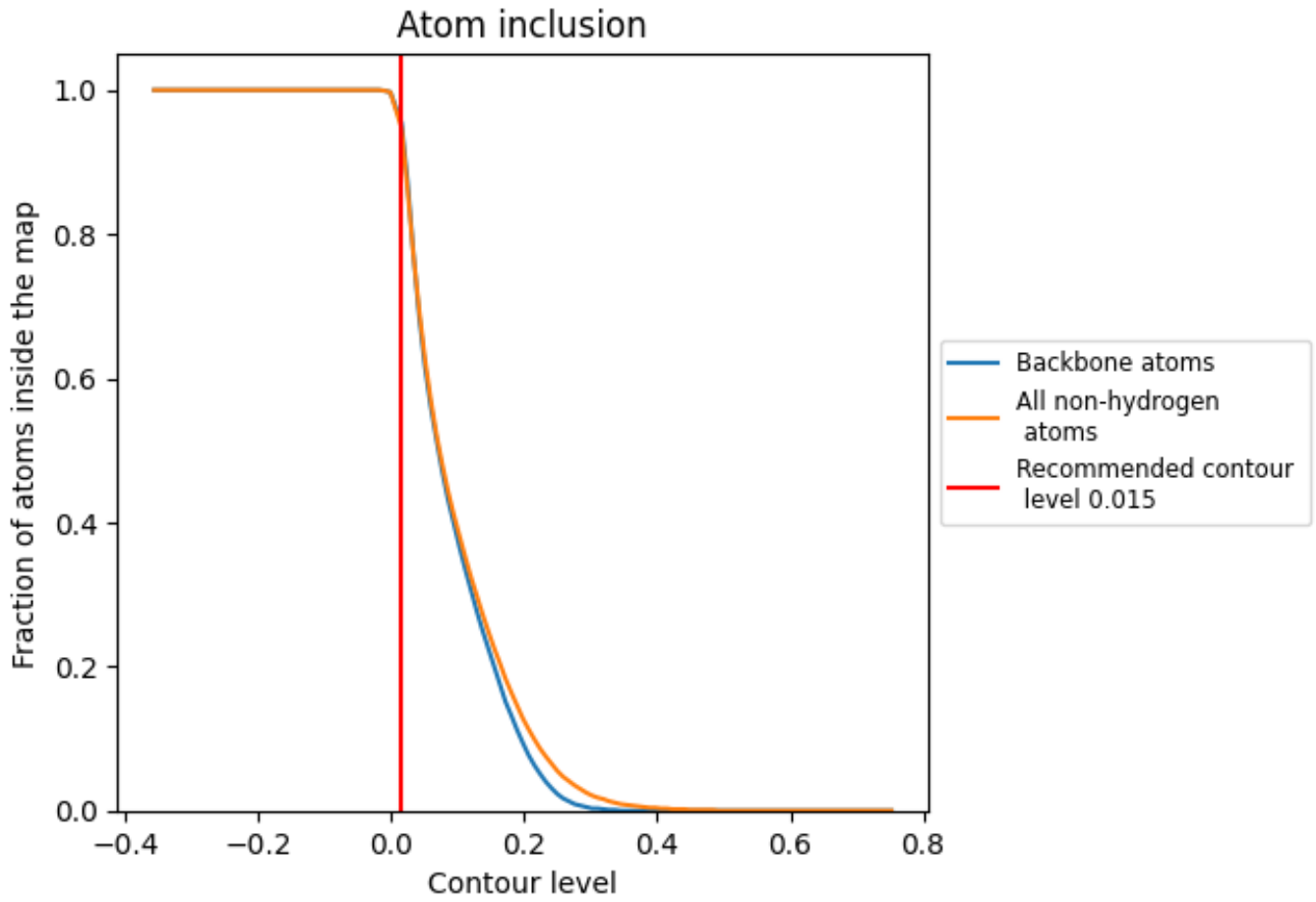
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 95% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9480	0.4720
2	0.9320	0.4850
3	0.9440	0.4860
4	0.9030	0.3490
5	0.8970	0.2540
A	0.9550	0.4750
D	0.9580	0.4800
E	0.9740	0.5270
F	0.9790	0.5730
H	0.9880	0.6210
I	0.8980	0.2610
J	0.9730	0.5500
K	0.9760	0.5240
L	0.9710	0.5750
M	0.9840	0.6080
O	0.9810	0.6170
P	0.9040	0.2200
Q	0.9820	0.6010
R	0.9600	0.5060
S	0.9330	0.3410
T	0.8780	0.2420
U	0.7490	0.1890
V	0.9000	0.3160
W	0.9200	0.2900
Y	0.9860	0.5760
Z	0.9940	0.6390
a	0.9760	0.5950
b	0.9610	0.5760
c	0.7950	0.2000
e	0.9880	0.5800
f	0.9060	0.2240
h	0.9820	0.5780
i	0.9060	0.2140