Full wwPDB EM Validation Report

Dec 18, 2022 – 10:48 am GMT

PDB ID	:	6YBD
EMDB ID	:	EMD-10769
Title	:	Structure of a human 48S translational initiation complex - eIF3
Authors	:	Brito Querido, J.; Sokabe, M.; Kraatz, S.; Gordiyenko, Y.; Skehel, M.; Fraser, C.; Ramakrishnan, V.
Deposited on	:	2020-03-16
Resolution	:	3.30 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:

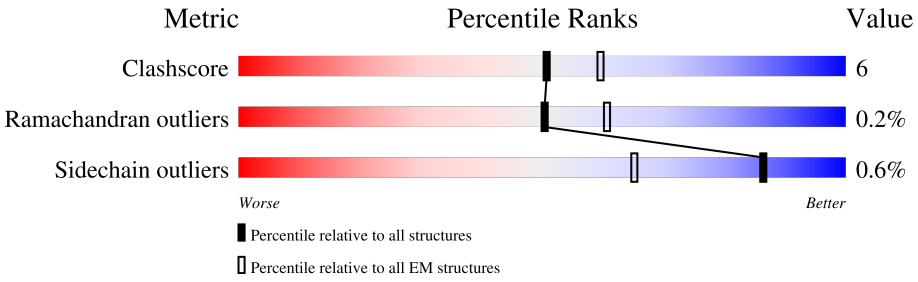
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	6	374	88% 6% 6%
2	4	357	69% 28%
3	u	1382	41% 59%
4	v	445	85% 14%
5	y	913	58% 41%
6	8	352	7% 88% 10%
7	G	194	77% 14% 9%
8	H	84	87% 10%

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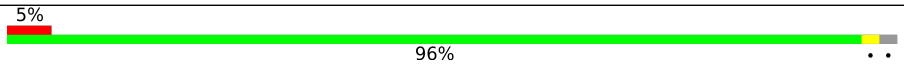
Mol	Chain	Length	Quality of chain
9	K	83	
10	M	135	
11	L	293	
12	O	264	
13	N	295	
14	Q	115	
15	P	151	
16	I	151	
17	x	548	
18	3	218	
19	5	564	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 30742 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 Eukaryotic translation initiation factor 3 subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	6	350	1917	1159	376	380	2	0	0

- Molecule 2 is a protein called Eukaryotic translation initiation factor 3 subunit F.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	4	257	1272	757	257	258	0	0

- Molecule 3 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	u	572	4708	2975	847	863	23	1	0

- Molecule 4 is a protein called Eukaryotic translation initiation factor 3 subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	v	384	2635	1657	477	489	12	0	0

- Molecule 5 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	y	535	4325	2723	768	801	33	0	0

- Molecule 6 is a protein called Eukaryotic translation initiation factor 3 subunit H.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	8	317	1571	936	317	318	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	177	Total	C	N	O	S	0	0
			1430	917	260	252	1		

- Molecule 8 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	81	Total	C	N	O	S	0	0
			631	397	116	111	7		

- Molecule 9 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	81	Total	C	N	O	S	0	0
			617	380	114	118	5		

- Molecule 10 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	54	Total	C	N	O	S	0	0
			432	270	72	88	2		

- Molecule 11 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	220	Total	C	N	O	S	0	0
			1707	1104	292	301	10		

- Molecule 12 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	211	Total	C	N	O	S	0	0
			1715	1088	307	306	14		

- Molecule 13 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	207	Total	C	N	O	S	0	0
			1633	1040	288	297	8		

- Molecule 14 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	99	Total	C	N	O	S	0	0
			792	492	165	130	5		

- Molecule 15 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	133	Total	C	N	O	S	0	0
			997	610	196	185	6		

- Molecule 16 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 17 is a protein called Eukaryotic translation initiation factor 3 subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	x	61	Total	C	N	O	S	0	0
			514	325	86	102	1		

- Molecule 18 is a protein called Eukaryotic translation initiation factor 3 subunit K.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	3	213	Total	C	N	O	0	0
			1057	631	213	213		

- Molecule 19 is a protein called Eukaryotic translation initiation factor 3 subunit L.

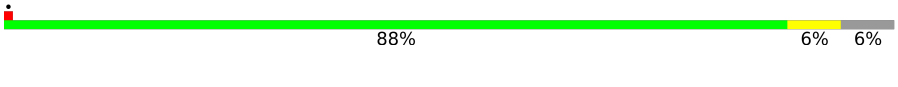
Mol	Chain	Residues	Atoms				AltConf	Trace
19	5	319	Total	C	N	O	0	0
			1581	943	319	319		

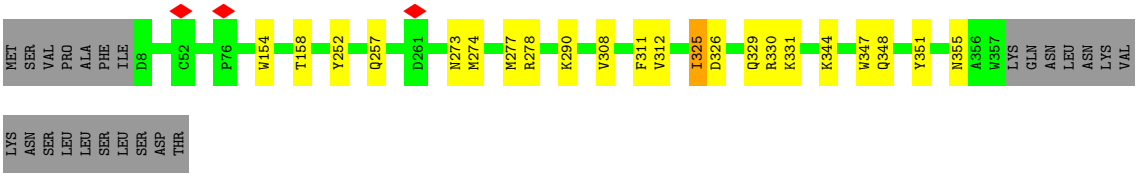
3 Residue-property plots (i)

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: Eukaryotic translation initiation factor 3 subunit M

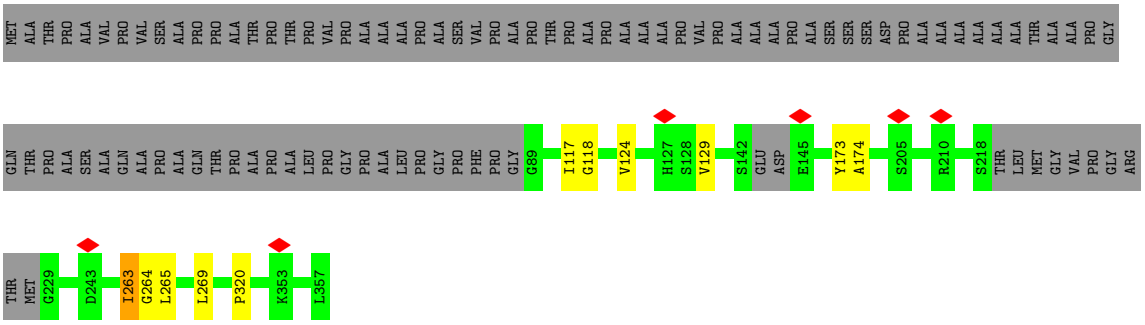
Chain 6:





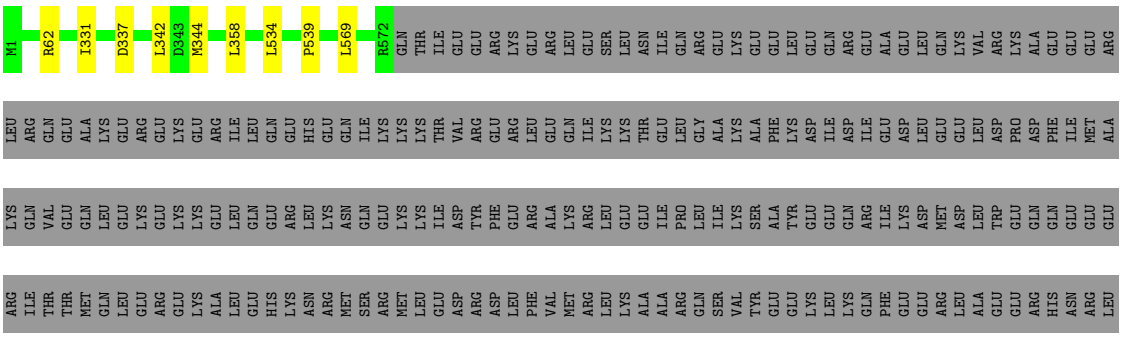
• Molecule 2: Eukaryotic translation initiation factor 3 subunit F

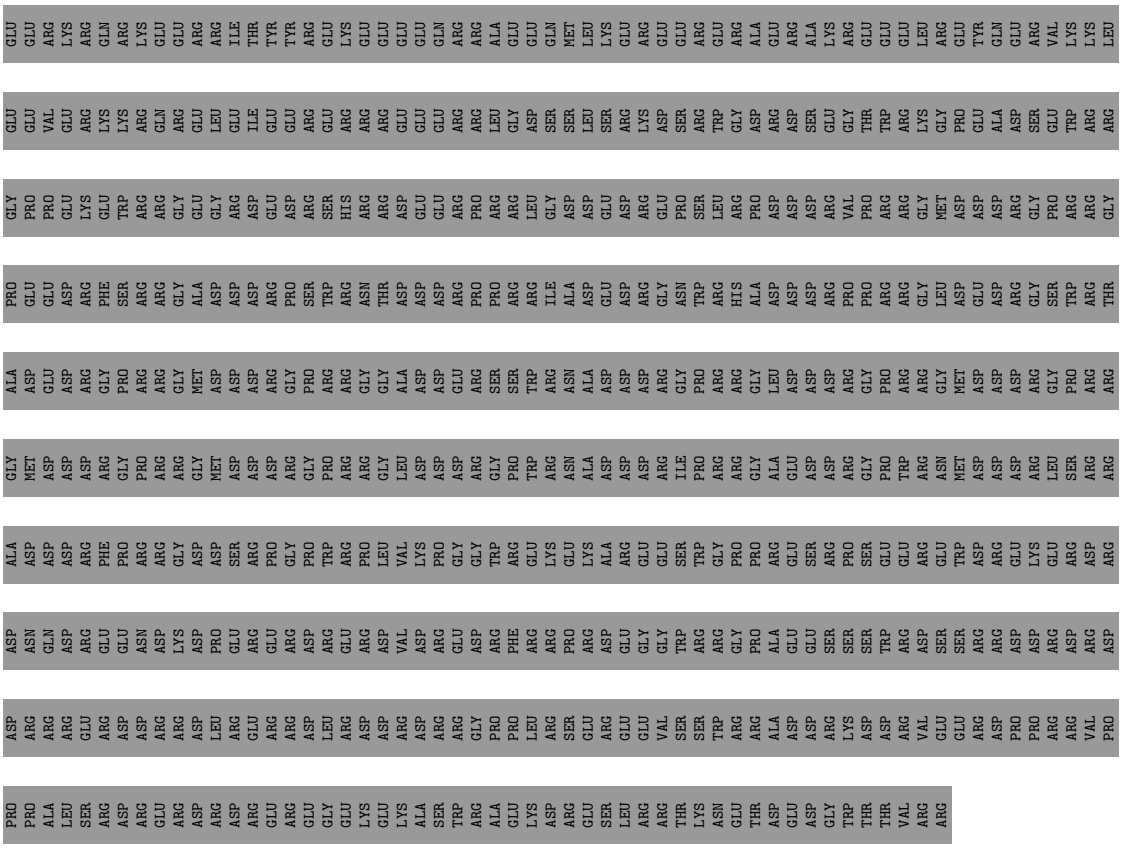
Chain 4:



• Molecule 3: Eukaryotic translation initiation factor 3 subunit A

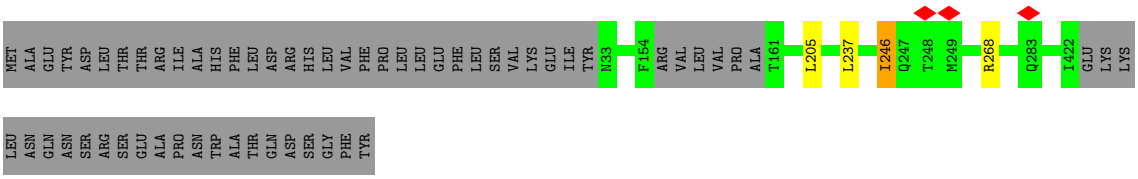
Chain u:





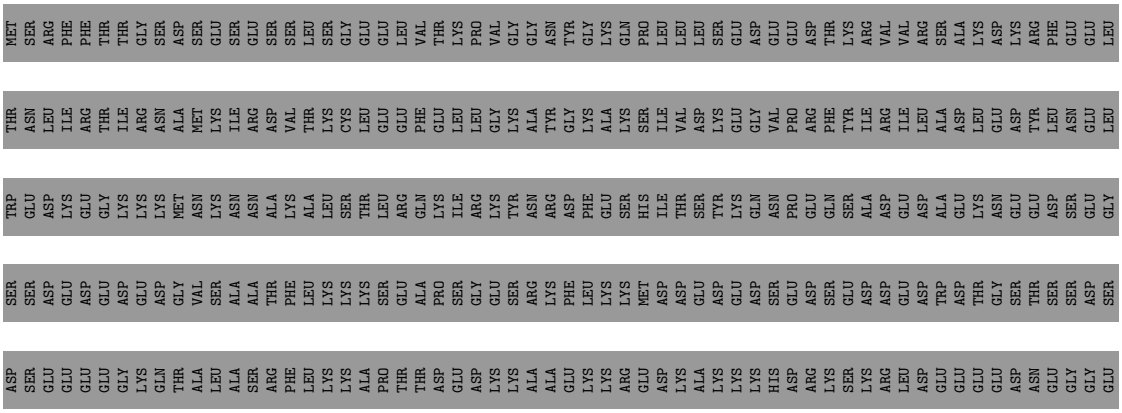
• Molecule 4: Eukaryotic translation initiation factor 3 subunit E

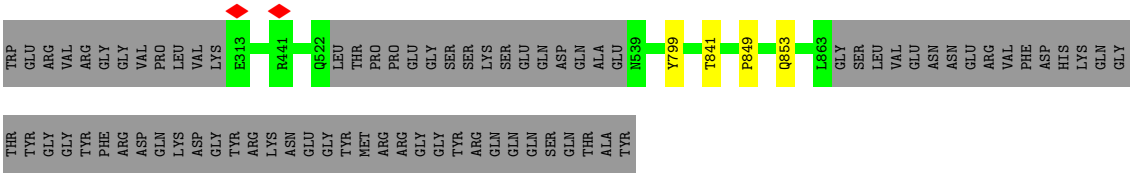
Chain v:



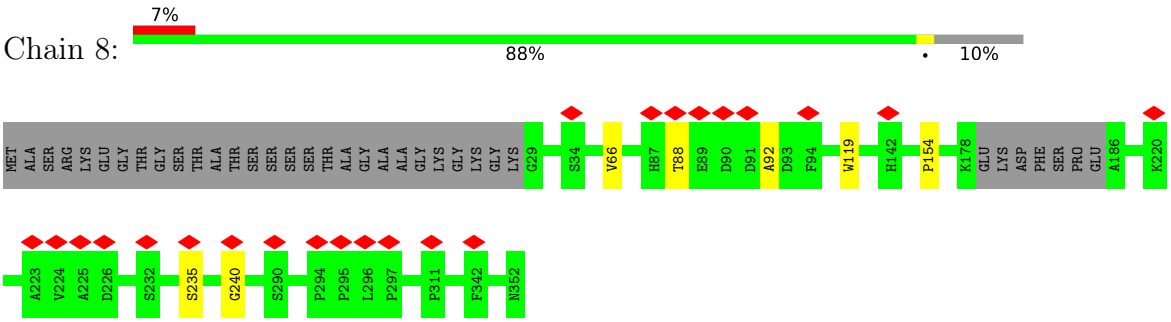
• Molecule 5: Eukaryotic translation initiation factor 3 subunit C

Chain y:

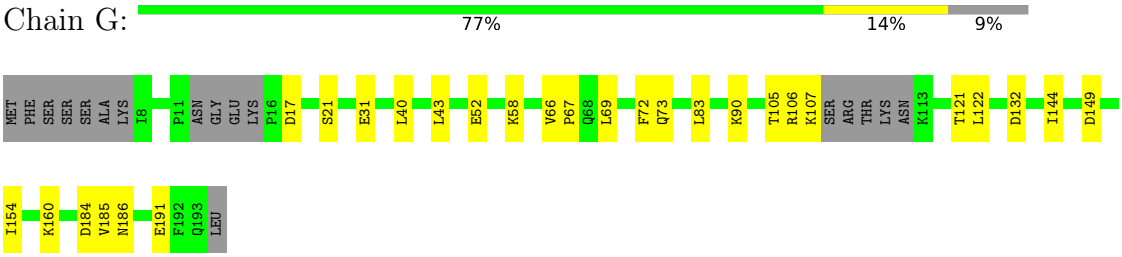




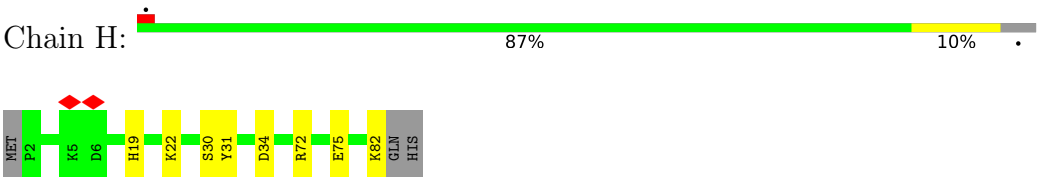
• Molecule 6: Eukaryotic translation initiation factor 3 subunit H



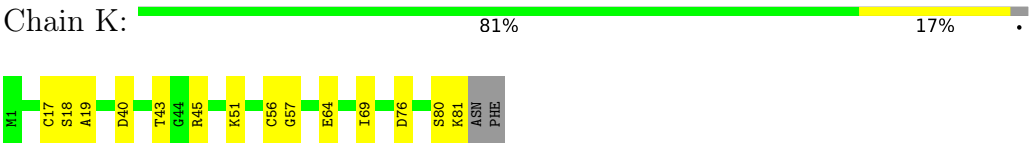
• Molecule 7: 40S ribosomal protein S7



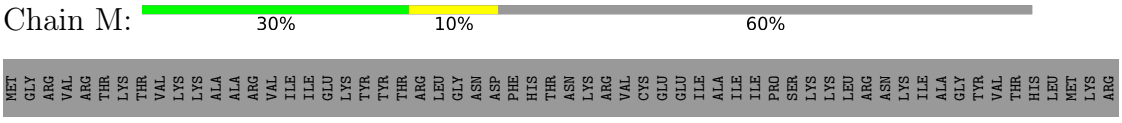
• Molecule 8: 40S ribosomal protein S27

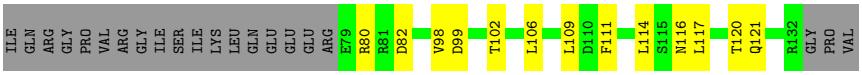


• Molecule 9: 40S ribosomal protein S21



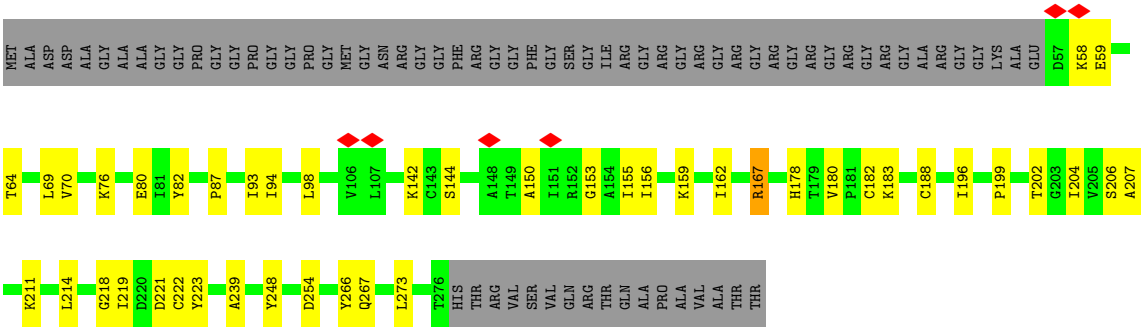
• Molecule 10: 40S ribosomal protein S17





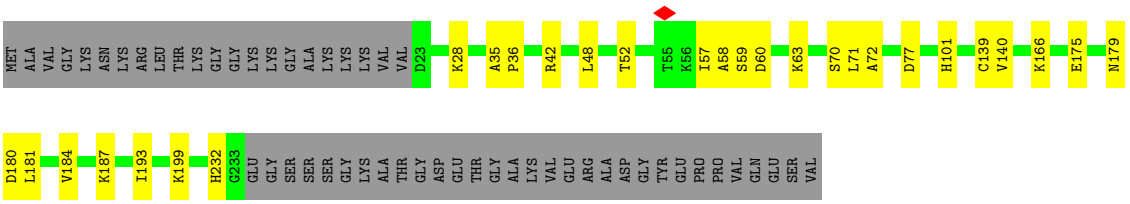
• Molecule 11: 40S ribosomal protein S2

Chain L:



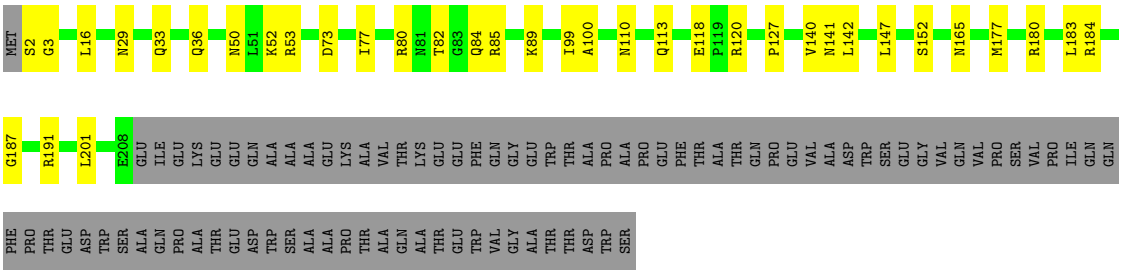
• Molecule 12: 40S ribosomal protein S3a

Chain O:



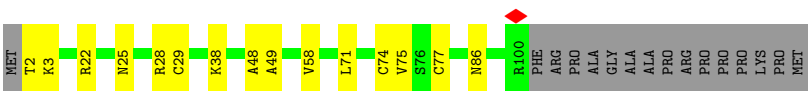
• Molecule 13: 40S ribosomal protein SA

Chain N:



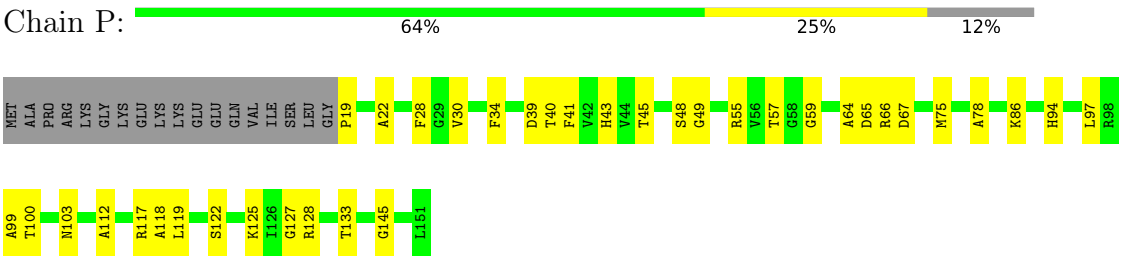
• Molecule 14: 40S ribosomal protein S26

Chain Q:



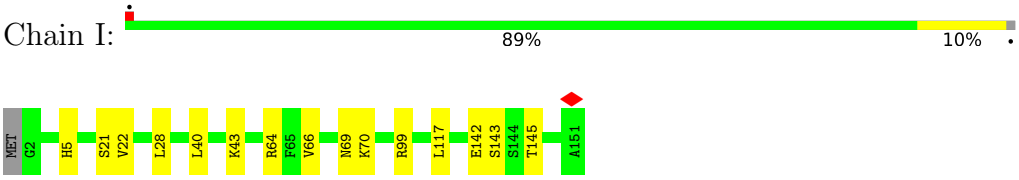
• Molecule 15: 40S ribosomal protein S14

Chain P:



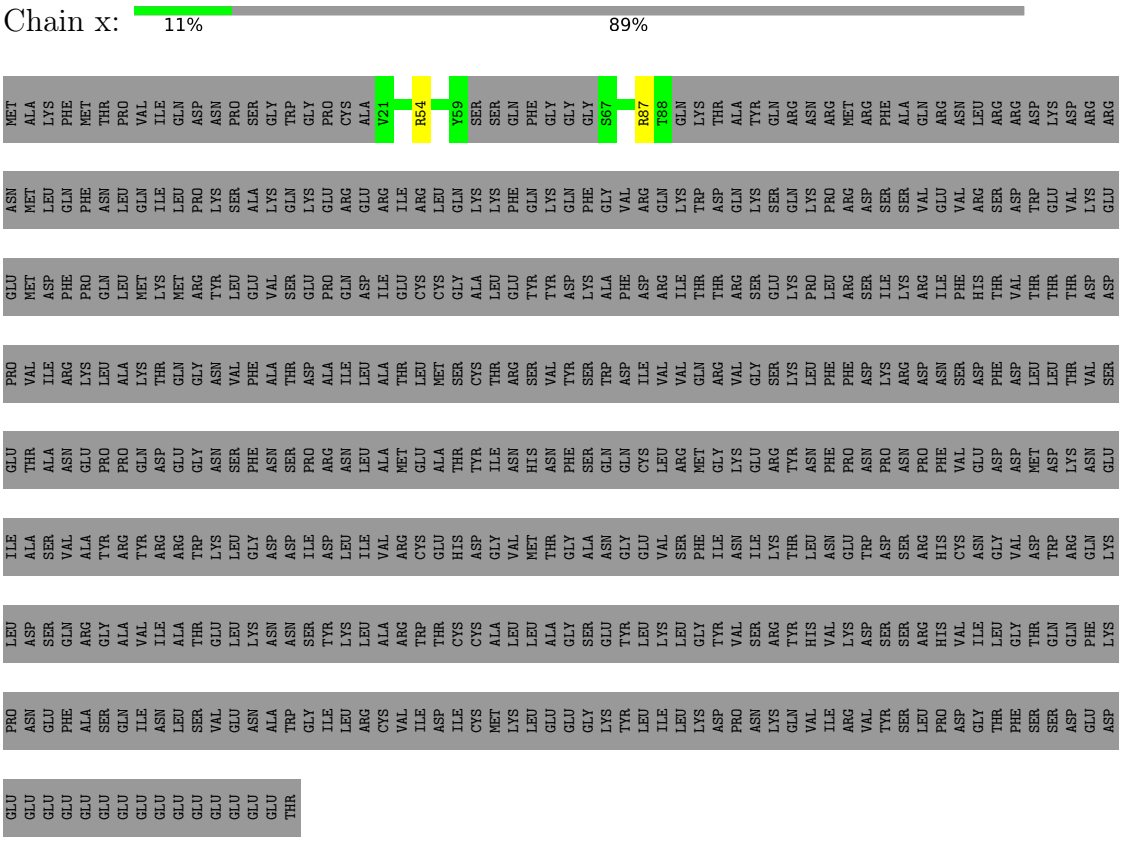
• Molecule 16: 40S ribosomal protein S13

Chain I:



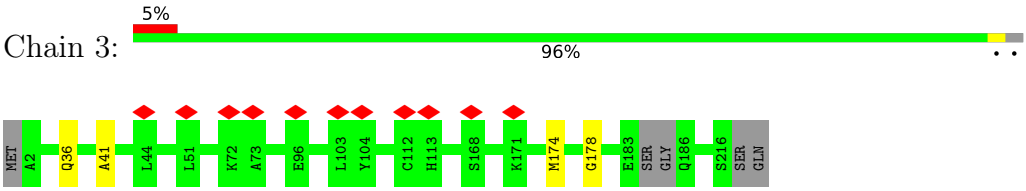
• Molecule 17: Eukaryotic translation initiation factor 3 subunit D

Chain x:



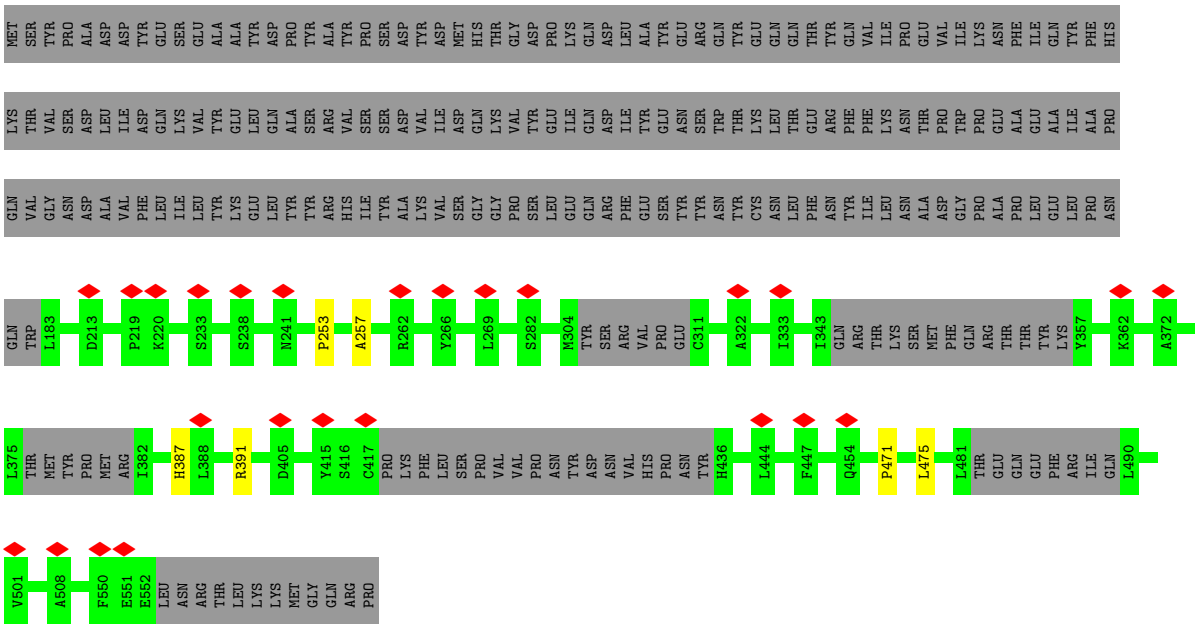
• Molecule 18: Eukaryotic translation initiation factor 3 subunit K

Chain 3:



• Molecule 19: Eukaryotic translation initiation factor 3 subunit L

Chain 5:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	11882	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	107	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.295	Depositor
Minimum map value	-0.181	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	300.72, 300.72, 300.72	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.074, 1.074, 1.074	Depositor

5 Model quality

5.1 Standard geometry

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	6	0.28	0/1926	0.52	1/2669 (0.0%)
2	4	0.28	0/1269	0.61	0/1762
3	u	0.44	0/4800	0.66	5/6488 (0.1%)
4	v	0.36	0/2672	0.62	0/3647
5	y	0.51	0/4400	0.62	0/5939
6	8	0.29	0/1569	0.60	0/2183
7	G	0.42	0/1451	0.61	0/1942
8	H	0.60	0/644	0.66	0/864
9	K	0.49	0/623	0.58	0/833
10	M	0.43	0/438	0.57	0/593
11	L	0.42	0/1743	0.62	0/2354
12	O	0.59	0/1742	0.61	0/2330
13	N	0.51	0/1670	0.60	0/2271
14	Q	0.58	0/805	0.69	0/1079
15	P	0.44	0/1010	0.64	0/1353
16	I	0.53	0/1232	0.60	0/1656
17	x	0.49	0/528	0.73	0/712
18	3	0.25	0/1055	0.48	0/1469
19	5	0.26	0/1575	0.44	0/2187
All	All	0.44	0/31152	0.61	6/42331 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	325	ILE	CG1-CB-CG2	-6.07	98.06	111.40
3	u	342	LEU	CA-CB-CG	5.98	129.05	115.30
3	u	358	LEU	CA-CB-CG	5.51	127.98	115.30
3	u	569	LEU	CA-CB-CG	5.42	127.77	115.30
3	u	534	LEU	CA-CB-CG	5.41	127.75	115.30
3	u	344	MET	CA-CB-CG	5.12	122.01	113.30

There are no chirality outliers.

There are no planarity outliers.

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	6	1917	0	1096	12	0
2	4	1272	0	564	5	0
3	u	4708	0	4785	0	0
4	v	2635	0	2207	0	0
5	y	4325	0	4328	0	0
6	8	1571	0	683	3	0
7	G	1430	0	1520	18	0
8	H	631	0	657	4	0
9	K	617	0	622	9	0
10	M	432	0	429	11	0
11	L	1707	0	1794	27	0
12	O	1715	0	1785	20	0
13	N	1633	0	1640	25	0
14	Q	792	0	845	11	0
15	P	997	0	1021	24	0
16	I	1208	0	1294	11	0
17	x	514	0	466	0	0
18	3	1057	0	475	2	0
19	5	1581	0	689	4	0
All	All	30742	0	26900	170	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 (170) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:325:ILE:HD13	1:6:329:GLN:HB3	1.76	0.68
11:L:182:CYS:SG	11:L:183:LYS:N	2.67	0.68
9:K:17:CYS:SG	9:K:18:SER:N	2.68	0.67
9:K:56:CYS:SG	9:K:57:GLY:N	2.69	0.66
12:O:72:ALA:HB3	15:P:128:ARG:HH12	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:154:ILE:HB	7:G:185:VAL:HG12	1.82	0.62
14:Q:2:THR:OG1	14:Q:3:LYS:N	2.33	0.62
14:Q:74:CYS:SG	14:Q:75:VAL:N	2.73	0.61
8:H:30:SER:OG	8:H:31:TYR:N	2.33	0.61
14:Q:38:LYS:HB3	14:Q:71:LEU:HB2	1.82	0.61
1:6:351:TYR:O	1:6:355:ASN:ND2	2.34	0.61
13:N:147:LEU:O	13:N:165:ASN:ND2	2.33	0.61
7:G:105:THR:HG23	7:G:107:LYS:H	1.66	0.60
12:O:139:CYS:SG	12:O:140:VAL:N	2.74	0.60
1:6:308:VAL:HA	1:6:311:PHE:HB3	1.84	0.59
13:N:84:GLN:HG2	13:N:100:ALA:HB1	1.84	0.59
18:3:36:GLN:HA	18:3:41:ALA:HB3	1.83	0.59
15:P:99:ALA:H	15:P:133:THR:HG22	1.67	0.59
2:4:263:ILE:O	2:4:265:LEU:N	2.36	0.59
16:I:99:ARG:HH12	16:I:143:SER:HB2	1.68	0.58
12:O:175:GLU:O	12:O:179:ASN:ND2	2.37	0.58
14:Q:49:ALA:HB2	15:P:117:ARG:HD2	1.84	0.58
15:P:64:ALA:HB3	15:P:67:ASP:HB2	1.84	0.58
12:O:28:LYS:HD3	12:O:48:LEU:HD13	1.86	0.57
15:P:48:SER:OG	15:P:49:GLY:N	2.37	0.57
13:N:80:ARG:NH2	13:N:82:THR:OG1	2.38	0.57
7:G:121:THR:OG1	7:G:122:LEU:N	2.37	0.56
15:P:57:THR:HG22	15:P:59:GLY:H	1.70	0.56
11:L:266:TYR:O	13:N:120:ARG:NH1	2.38	0.56
14:Q:28:ARG:NH1	14:Q:29:CYS:O	2.39	0.56
1:6:344:LYS:HA	1:6:347:TRP:HB2	1.86	0.56
16:I:5:HIS:HD2	16:I:117:LEU:HD22	1.71	0.56
7:G:184:ASP:OD1	7:G:184:ASP:N	2.39	0.55
11:L:76:LYS:NZ	11:L:80:GLU:OE1	2.40	0.54
13:N:140:VAL:HG13	13:N:142:LEU:HG	1.88	0.54
15:P:86:LYS:NZ	15:P:122:SER:O	2.39	0.54
7:G:149:ASP:OD1	7:G:149:ASP:N	2.41	0.54
16:I:5:HIS:HB3	16:I:117:LEU:HD13	1.88	0.54
8:H:34:ASP:OD2	8:H:82:LYS:NZ	2.34	0.53
12:O:52:THR:HG22	12:O:58:ALA:H	1.74	0.53
12:O:175:GLU:OE1	12:O:187:LYS:NZ	2.40	0.53
12:O:70:SER:OG	12:O:71:LEU:N	2.42	0.53
9:K:80:SER:OG	9:K:81:LYS:N	2.40	0.53
13:N:184:ARG:HH11	13:N:191:ARG:HD3	1.74	0.53
16:I:22:VAL:HG12	16:I:66:VAL:HG12	1.91	0.52
10:M:106:LEU:HB3	10:M:111:PHE:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:85:ARG:NH2	13:N:201:LEU:O	2.42	0.52
7:G:66:VAL:HG23	7:G:67:PRO:HD3	1.91	0.52
12:O:101:HIS:O	12:O:101:HIS:ND1	2.43	0.52
13:N:127:PRO:HG2	13:N:152:SER:HB3	1.92	0.52
11:L:267:GLN:HG3	13:N:120:ARG:HH22	1.75	0.51
11:L:155:ILE:HG12	11:L:159:LYS:HE3	1.93	0.51
13:N:177:MET:SD	13:N:180:ARG:NH1	2.83	0.51
11:L:180:VAL:HG22	11:L:219:ILE:HD13	1.92	0.51
18:3:174:MET:O	18:3:178:GLY:N	2.42	0.51
11:L:206:SER:OG	11:L:207:ALA:N	2.42	0.51
12:O:180:ASP:N	12:O:180:ASP:OD1	2.44	0.51
1:6:290:LYS:HA	1:6:331:LYS:H	1.75	0.51
15:P:30:VAL:N	15:P:45:THR:O	2.44	0.51
11:L:70:VAL:HG11	11:L:93:ILE:HG23	1.93	0.50
10:M:120:THR:OG1	10:M:121:GLN:N	2.45	0.50
15:P:65:ASP:OD2	15:P:66:ARG:NH1	2.44	0.50
1:6:252:TYR:O	1:6:257:GLN:N	2.44	0.50
14:Q:48:ALA:O	15:P:117:ARG:NH2	2.44	0.50
14:Q:25:ASN:ND2	14:Q:77:CYS:SG	2.84	0.49
9:K:64:GLU:HG3	13:N:33:GLN:HE21	1.78	0.49
15:P:34:PHE:O	15:P:41:PHE:N	2.46	0.49
2:4:118:GLY:N	2:4:173:TYR:O	2.45	0.49
11:L:254:ASP:N	11:L:254:ASP:OD1	2.43	0.49
10:M:109:LEU:HD11	13:N:52:LYS:HB2	1.95	0.49
19:5:471:PRO:O	19:5:475:LEU:N	2.44	0.49
15:P:78:ALA:HB1	15:P:119:LEU:HG	1.93	0.49
2:4:265:LEU:O	2:4:269:LEU:N	2.40	0.48
12:O:57:ILE:HG23	12:O:59:SER:H	1.77	0.48
15:P:19:PRO:HD2	15:P:22:ALA:HB2	1.95	0.48
9:K:51:LYS:NZ	9:K:76:ASP:OD2	2.47	0.48
14:Q:22:ARG:NH2	15:P:145:GLY:O	2.47	0.48
19:5:253:PRO:O	19:5:257:ALA:CB	2.63	0.47
7:G:52:GLU:HA	7:G:58:LYS:HG3	1.97	0.47
10:M:116:ASN:OD1	10:M:116:ASN:N	2.41	0.47
1:6:274:MET:O	1:6:278:ARG:N	2.47	0.46
7:G:17:ASP:O	7:G:21:SER:N	2.44	0.46
13:N:2:SER:OG	13:N:3:GLY:N	2.47	0.46
9:K:43:THR:OG1	9:K:45:ARG:NH2	2.46	0.46
7:G:43:LEU:HD22	7:G:72:PHE:HD1	1.81	0.46
9:K:40:ASP:OD1	9:K:40:ASP:N	2.45	0.46
11:L:82:TYR:OH	11:L:162:ILE:O	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:183:LEU:O	13:N:187:GLY:N	2.47	0.46
11:L:87:PRO:HD3	13:N:141:ASN:HD22	1.81	0.46
14:Q:58:VAL:HG13	15:P:125:LYS:HB3	1.98	0.46
7:G:132:ASP:OD1	7:G:132:ASP:N	2.46	0.46
11:L:142:LYS:HD3	11:L:153:GLY:HA3	1.98	0.46
11:L:222:CYS:SG	11:L:223:TYR:N	2.89	0.46
15:P:97:LEU:HD11	15:P:112:ALA:HB1	1.97	0.46
1:6:326:ASP:OD1	1:6:326:ASP:N	2.47	0.45
19:5:387:HIS:O	19:5:391:ARG:N	2.37	0.45
11:L:199:PRO:HG2	11:L:202:THR:HG21	1.99	0.45
13:N:73:ASP:O	13:N:120:ARG:N	2.47	0.45
8:H:72:ARG:NH1	8:H:75:GLU:OE1	2.42	0.45
12:O:166:LYS:HB3	12:O:166:LYS:HE3	1.78	0.45
7:G:160:LYS:NZ	7:G:191:GLU:O	2.47	0.45
11:L:64:THR:OG1	13:N:118:GLU:OE2	2.35	0.45
7:G:105:THR:OG1	7:G:106:ARG:N	2.50	0.45
10:M:82:ASP:O	13:N:85:ARG:NH2	2.50	0.44
6:8:66:VAL:HA	6:8:119:TRP:HA	1.99	0.44
15:P:103:ASN:OD1	15:P:103:ASN:N	2.49	0.44
13:N:50:ASN:HD22	13:N:53:ARG:HB2	1.83	0.44
10:M:99:ASP:HB2	10:M:102:THR:HG22	2.00	0.44
12:O:59:SER:OG	12:O:63:LYS:NZ	2.43	0.44
15:P:43:HIS:CD2	15:P:55:ARG:HB3	2.53	0.44
13:N:77:ILE:HG12	13:N:99:ILE:HB	1.98	0.44
7:G:83:LEU:HD23	7:G:83:LEU:HA	1.78	0.44
9:K:17:CYS:SG	9:K:19:ALA:N	2.82	0.44
2:4:124:VAL:HA	2:4:129:VAL:HA	1.98	0.44
16:I:21:SER:OG	16:I:22:VAL:O	2.33	0.43
10:M:116:ASN:HD21	13:N:16:LEU:HD13	1.83	0.43
11:L:69:LEU:HG	11:L:273:LEU:HD21	2.01	0.43
16:I:69:ASN:N	16:I:69:ASN:OD1	2.49	0.43
10:M:114:LEU:HD13	10:M:117:LEU:HD11	2.00	0.43
10:M:114:LEU:HD23	10:M:114:LEU:HA	1.82	0.43
10:M:82:ASP:OD2	13:N:89:LYS:NZ	2.38	0.43
6:8:235:SER:O	6:8:240:GLY:N	2.42	0.43
15:P:94:HIS:HD2	15:P:127:GLY:HA3	1.84	0.43
19:5:253:PRO:O	19:5:257:ALA:HB2	2.19	0.43
13:N:110:ASN:HB3	13:N:113:GLN:HG3	1.99	0.42
14:Q:86:ASN:OD1	14:Q:86:ASN:N	2.50	0.42
16:I:64:ARG:HD3	16:I:70:LYS:HG2	2.01	0.42
1:6:273:ASN:O	1:6:277:MET:CB	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:M:98:VAL:HG13	10:M:102:THR:HG23	2.01	0.42
11:L:144:SER:HB3	11:L:150:ALA:HB2	2.01	0.42
7:G:144:ILE:HG23	7:G:154:ILE:HG12	2.00	0.42
11:L:196:ILE:HB	11:L:223:TYR:HB2	2.01	0.42
11:L:204:ILE:O	11:L:211:LYS:NZ	2.39	0.42
12:O:35:ALA:O	12:O:42:ARG:NE	2.50	0.42
16:I:43:LYS:HB3	16:I:43:LYS:HE2	1.79	0.42
14:Q:58:VAL:HG21	15:P:28:PHE:HZ	1.84	0.42
9:K:69:ILE:HD13	9:K:69:ILE:HA	1.90	0.42
11:L:153:GLY:HA2	11:L:156:ILE:HG12	2.02	0.42
12:O:72:ALA:HB3	15:P:128:ARG:NH1	2.33	0.42
16:I:40:LEU:HD23	16:I:40:LEU:HA	1.88	0.42
6:8:88:THR:HA	6:8:92:ALA:HB2	2.01	0.42
7:G:58:LYS:HB2	7:G:90:LYS:HE2	2.01	0.42
8:H:19:HIS:HB3	8:H:22:LYS:HB2	2.02	0.42
1:6:154:TRP:O	1:6:158:THR:N	2.43	0.42
2:4:117:ILE:HA	2:4:174:ALA:HA	2.02	0.42
11:L:94:ILE:HG21	11:L:162:ILE:HD12	2.00	0.42
16:I:28:LEU:HD23	16:I:28:LEU:HA	1.94	0.42
7:G:31:GLU:HA	7:G:40:LEU:HD23	2.02	0.41
7:G:185:VAL:O	7:G:186:ASN:ND2	2.53	0.41
11:L:188:CYS:HB3	11:L:239:ALA:HB2	2.03	0.41
12:O:60:ASP:OD1	12:O:60:ASP:N	2.51	0.41
15:P:39:ASP:OD1	15:P:40:THR:N	2.53	0.41
11:L:94:ILE:O	11:L:98:LEU:N	2.44	0.41
15:P:34:PHE:HE1	15:P:100:THR:HA	1.84	0.41
11:L:204:ILE:HD13	11:L:214:LEU:HB3	2.02	0.41
12:O:36:PRO:HA	12:O:232:HIS:CD2	2.55	0.41
11:L:167:ARG:NH2	11:L:218:GLY:O	2.49	0.41
11:L:58:LYS:NZ	11:L:59:GLU:O	2.51	0.41
12:O:175:GLU:HG3	12:O:193:ILE:HG12	2.02	0.41
12:O:181:LEU:HA	12:O:184:VAL:HG12	2.03	0.41
1:6:312:VAL:HG12	1:6:330:ARG:HH11	1.87	0.40
12:O:71:LEU:HA	12:O:71:LEU:HD12	1.85	0.40
13:N:29:ASN:HD22	13:N:29:ASN:HA	1.69	0.40
13:N:36:GLN:H	13:N:36:GLN:HG2	1.51	0.40
16:I:142:GLU:HB3	16:I:145:THR:HG22	2.01	0.40
7:G:69:LEU:O	7:G:73:GLN:HG3	2.22	0.40
12:O:199:LYS:HA	12:O:199:LYS:HD3	1.61	0.40
15:P:75:MET:HG3	15:P:118:ALA:HB2	2.03	0.40
1:6:344:LYS:NZ	1:6:348:GLN:HE22	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:178:HIS:ND1	11:L:221:ASP:OD1	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	6	348/374 (93%)	300 (86%)	48 (14%)	0	100	100
2	4	251/357 (70%)	216 (86%)	32 (13%)	3 (1%)	13	42
3	u	571/1382 (41%)	524 (92%)	46 (8%)	1 (0%)	47	77
4	v	380/445 (85%)	328 (86%)	51 (13%)	1 (0%)	41	71
5	y	531/913 (58%)	490 (92%)	40 (8%)	1 (0%)	47	77
6	8	313/352 (89%)	264 (84%)	48 (15%)	1 (0%)	41	71
7	G	171/194 (88%)	159 (93%)	12 (7%)	0	100	100
8	H	79/84 (94%)	72 (91%)	7 (9%)	0	100	100
9	K	79/83 (95%)	73 (92%)	6 (8%)	0	100	100
10	M	52/135 (38%)	45 (86%)	7 (14%)	0	100	100
11	L	218/293 (74%)	205 (94%)	13 (6%)	0	100	100
12	O	209/264 (79%)	190 (91%)	19 (9%)	0	100	100
13	N	205/295 (70%)	189 (92%)	16 (8%)	0	100	100
14	Q	97/115 (84%)	88 (91%)	9 (9%)	0	100	100
15	P	131/151 (87%)	119 (91%)	12 (9%)	0	100	100
16	I	148/151 (98%)	139 (94%)	9 (6%)	0	100	100
17	x	57/548 (10%)	41 (72%)	16 (28%)	0	100	100
18	3	209/218 (96%)	204 (98%)	5 (2%)	0	100	100
19	5	307/564 (54%)	300 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	4356/6918 (63%)	3946 (91%)	403 (9%)	7 (0%)	50 77

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	4	264	GLY
4	v	246	ILE
6	8	154	PRO
2	4	263	ILE
3	u	539	PRO
5	y	849	PRO
2	4	320	PRO

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	6	49/335 (15%)	49 (100%)	0	100 100
3	u	526/1259 (42%)	523 (99%)	3 (1%)	86 91
4	v	206/406 (51%)	202 (98%)	4 (2%)	57 77
5	y	473/811 (58%)	470 (99%)	3 (1%)	86 91
7	G	159/174 (91%)	159 (100%)	0	100 100
8	H	73/76 (96%)	73 (100%)	0	100 100
9	K	65/67 (97%)	65 (100%)	0	100 100
10	M	51/122 (42%)	50 (98%)	1 (2%)	55 76
11	L	186/225 (83%)	184 (99%)	2 (1%)	73 85
12	O	192/231 (83%)	191 (100%)	1 (0%)	88 93
13	N	173/243 (71%)	173 (100%)	0	100 100
14	Q	86/98 (88%)	86 (100%)	0	100 100
15	P	104/119 (87%)	104 (100%)	0	100 100
16	I	130/131 (99%)	130 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	x	54/494 (11%)	52 (96%)	2 (4%)	34 63
All	All	2527/4791 (53%)	2511 (99%)	16 (1%)	86 91

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

Mol	Chain	Res	Type
3	u	62	ARG
3	u	331	ILE
3	u	337	ASP
4	v	205	LEU
4	v	237	LEU
4	v	246	ILE
4	v	268	ARG
5	y	799	TYR
5	y	841	THR
5	y	853	GLN
10	M	80	ARG
11	L	167	ARG
11	L	248	TYR
12	O	77	ASP
17	x	54	ARG
17	x	87	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	6	348	GLN
3	u	109	GLN
3	u	110	GLN
3	u	222	ASN
3	u	229	HIS
3	u	392	ASN
3	u	466	GLN
3	u	522	GLN
4	v	231	ASN
4	v	244	ASN
4	v	252	HIS
4	v	373	ASN
4	v	377	ASN
5	y	364	ASN
5	y	432	HIS

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Mol	Chain	Res	Type
5	y	460	GLN
5	y	784	GLN
5	y	840	GLN
5	y	852	GLN
5	y	853	GLN
7	G	186	ASN
10	M	93	GLN
12	O	186	ASN
12	O	202	GLN
12	O	208	HIS
13	N	29	ASN
13	N	50	ASN
13	N	132	GLN
15	P	94	HIS
16	I	5	HIS
16	I	36	GLN
16	I	101	HIS
16	I	105	ASN
16	I	123	HIS
17	x	31	GLN
17	x	57	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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.

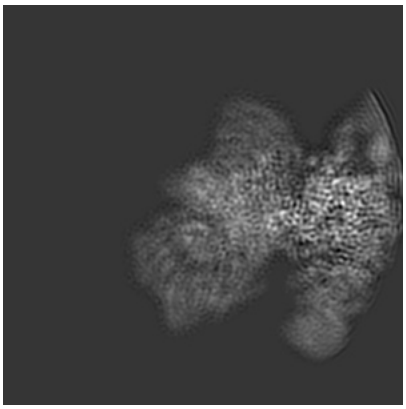
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10769. These allow visual inspection of the internal detail of the map and identification of artifacts.

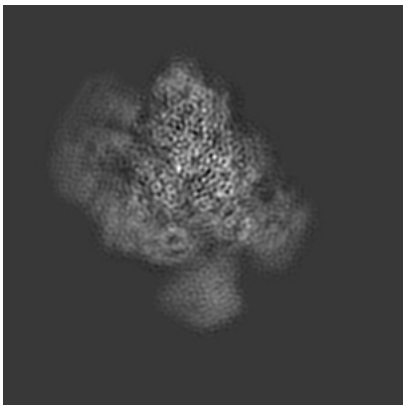
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

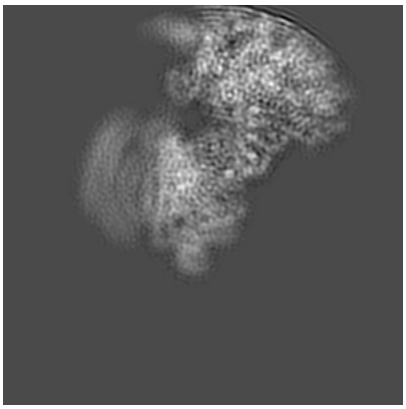
6.1.1 Primary map



X

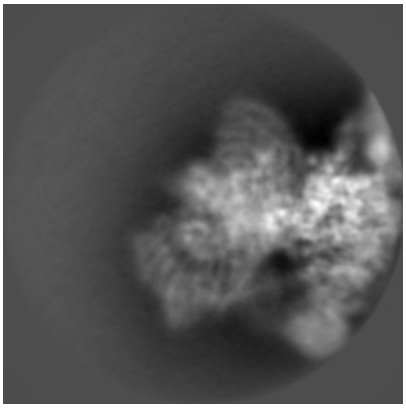


Y

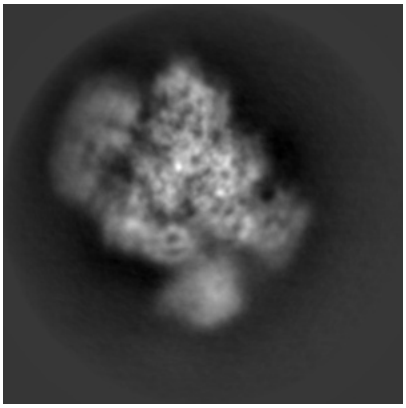


Z

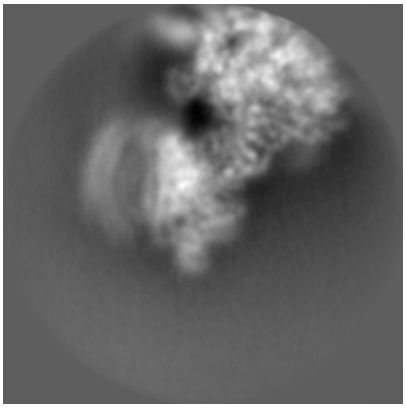
6.1.2 Raw map



X



Y

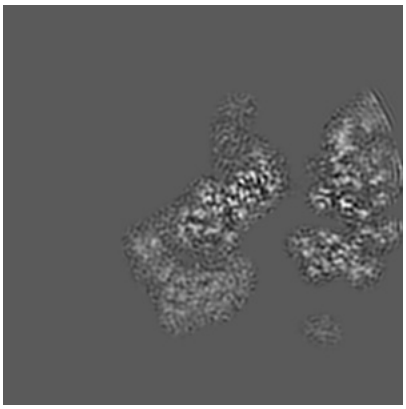


Z

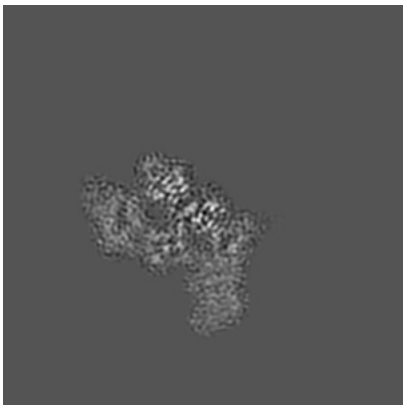
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

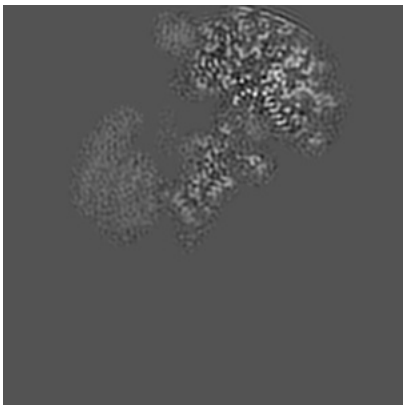
6.2.1 Primary map



X Index: 140

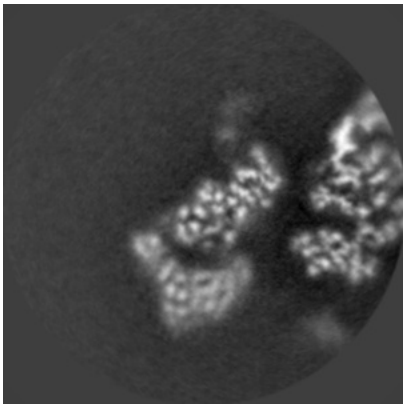


Y Index: 140

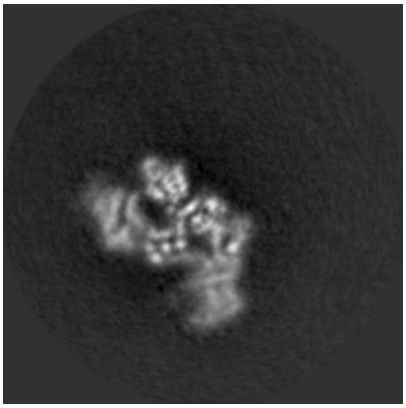


Z Index: 140

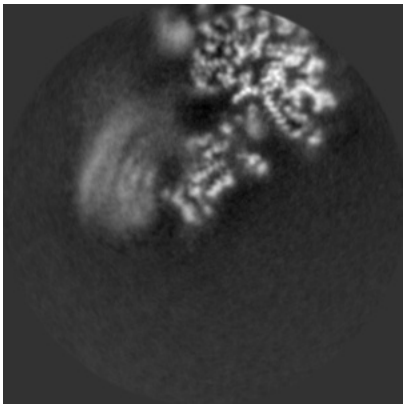
6.2.2 Raw map



X Index: 140



Y Index: 140

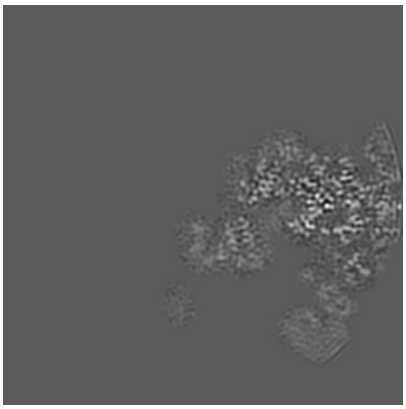


Z Index: 140

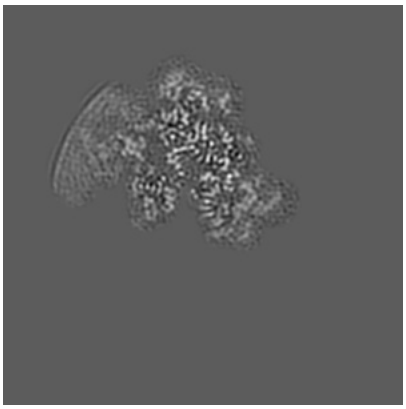
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

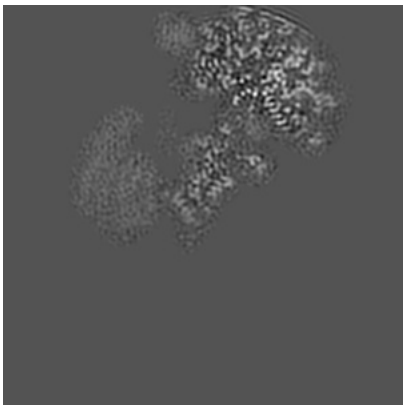
6.3.1 Primary map



X Index: 166

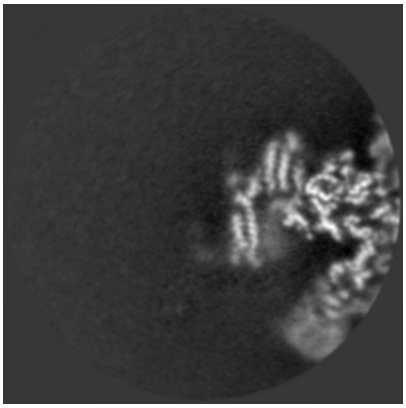


Y Index: 233

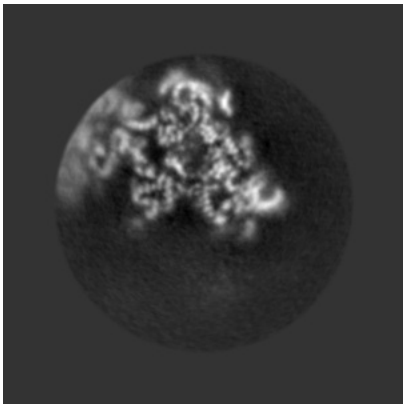


Z Index: 140

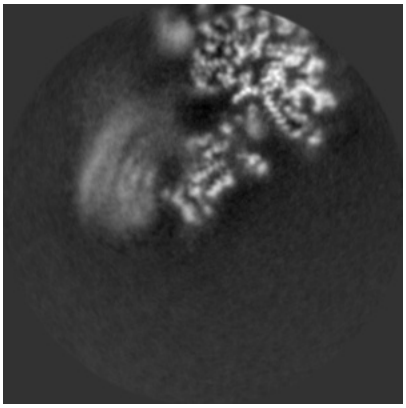
6.3.2 Raw map



X Index: 173



Y Index: 236



Z Index: 140

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

6.4 Orthogonal surface views (i)

6.4.1 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.

6.4.2 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.

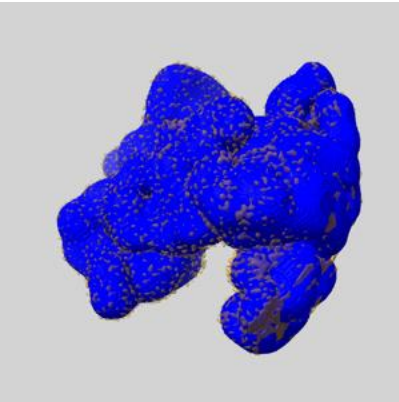
6.5 Mask visualisation (i)

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

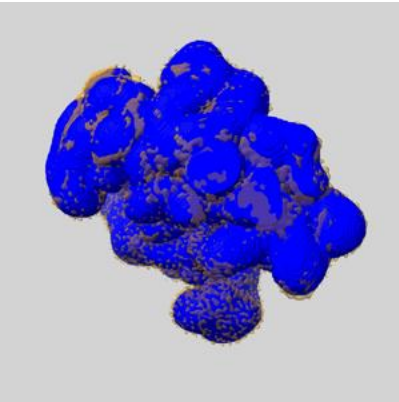
A mask typically either:

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

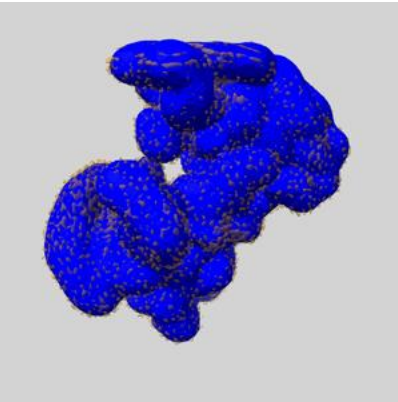
6.5.1 emd_10769_msk_1.map (i)



X



Y

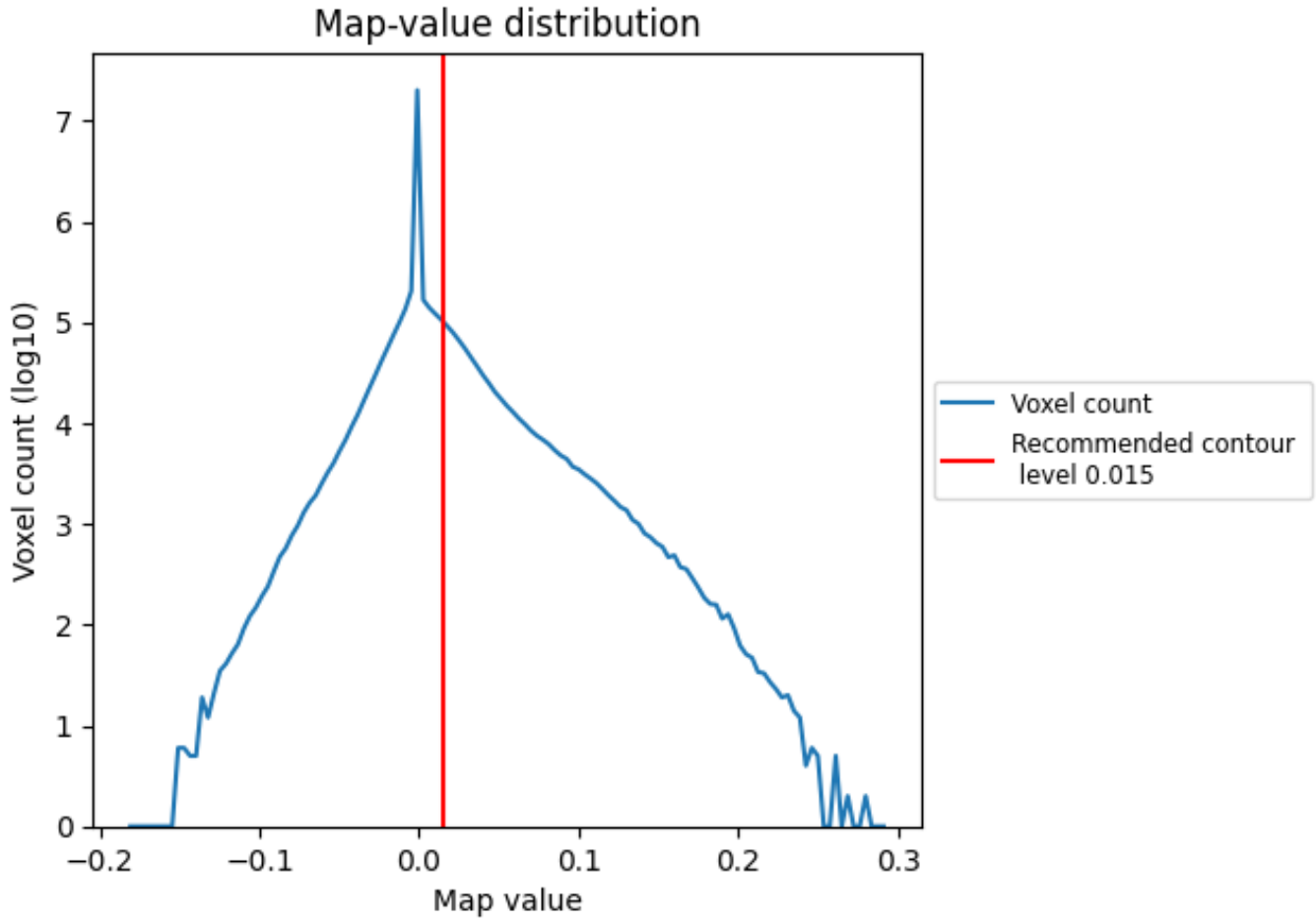


Z

7 Map analysis

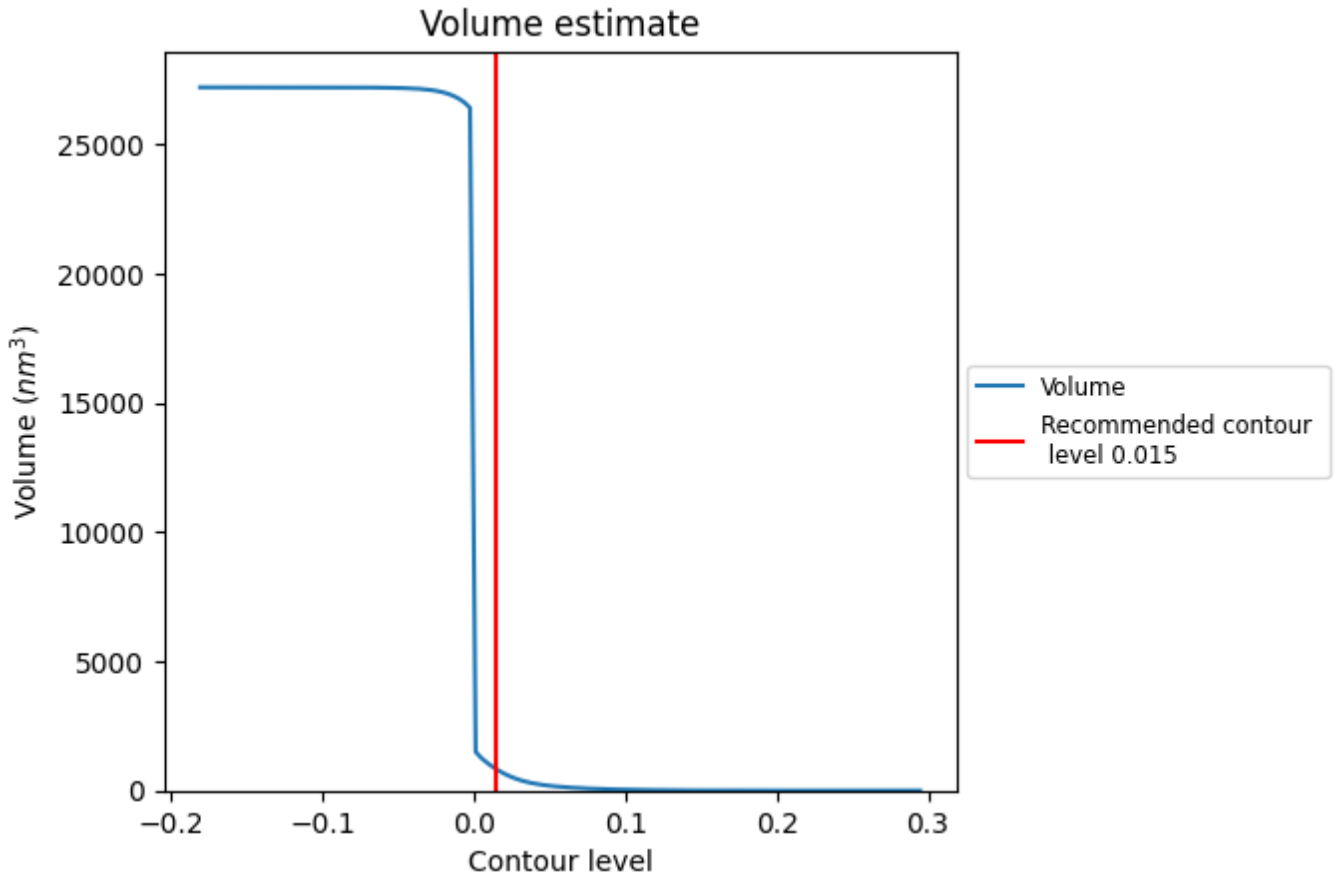
This section contains the results of statistical analysis of the map.

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.

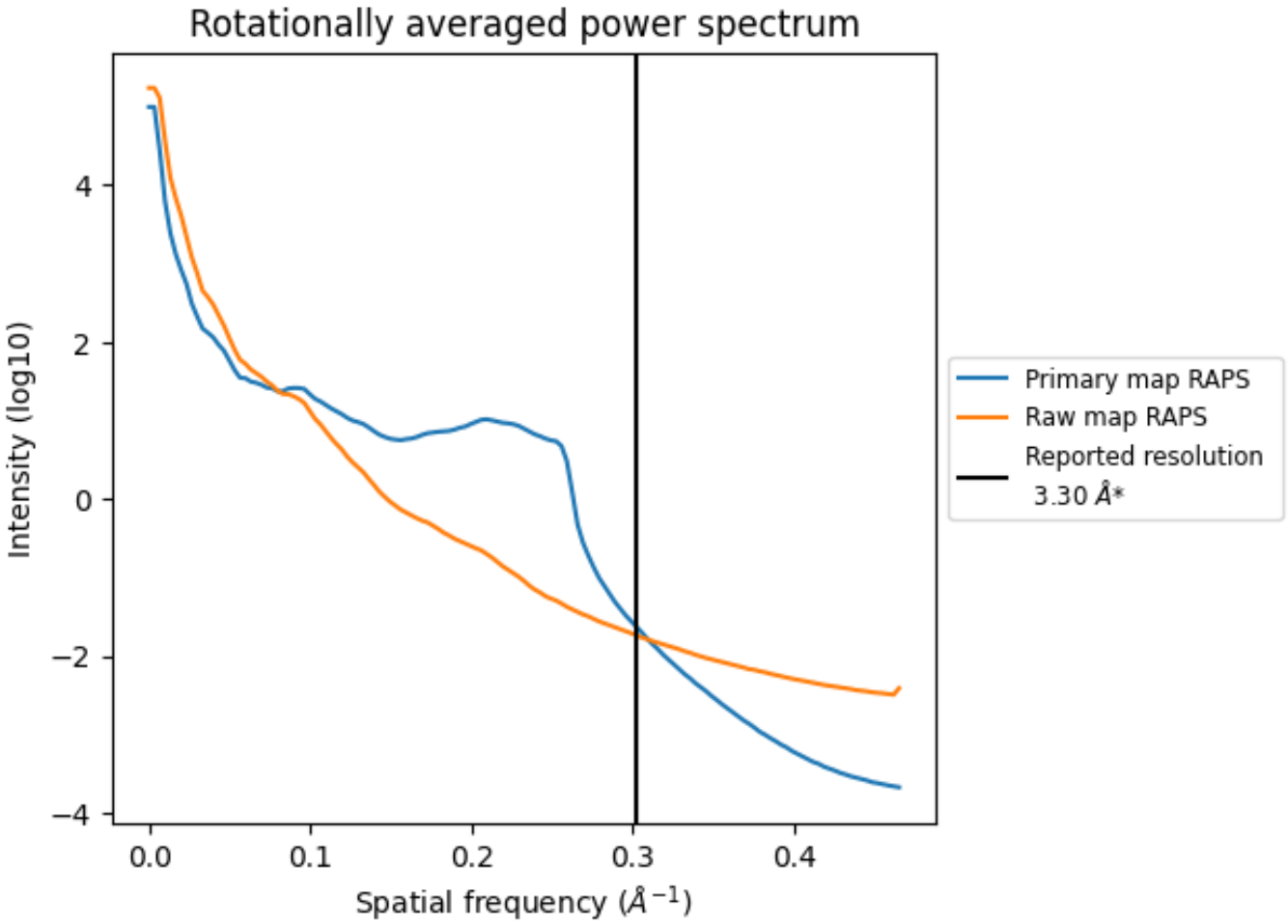
7.2 Volume estimate



The volume at the recommended contour level is 822 nm^3; this corresponds to an approximate mass of 742 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)

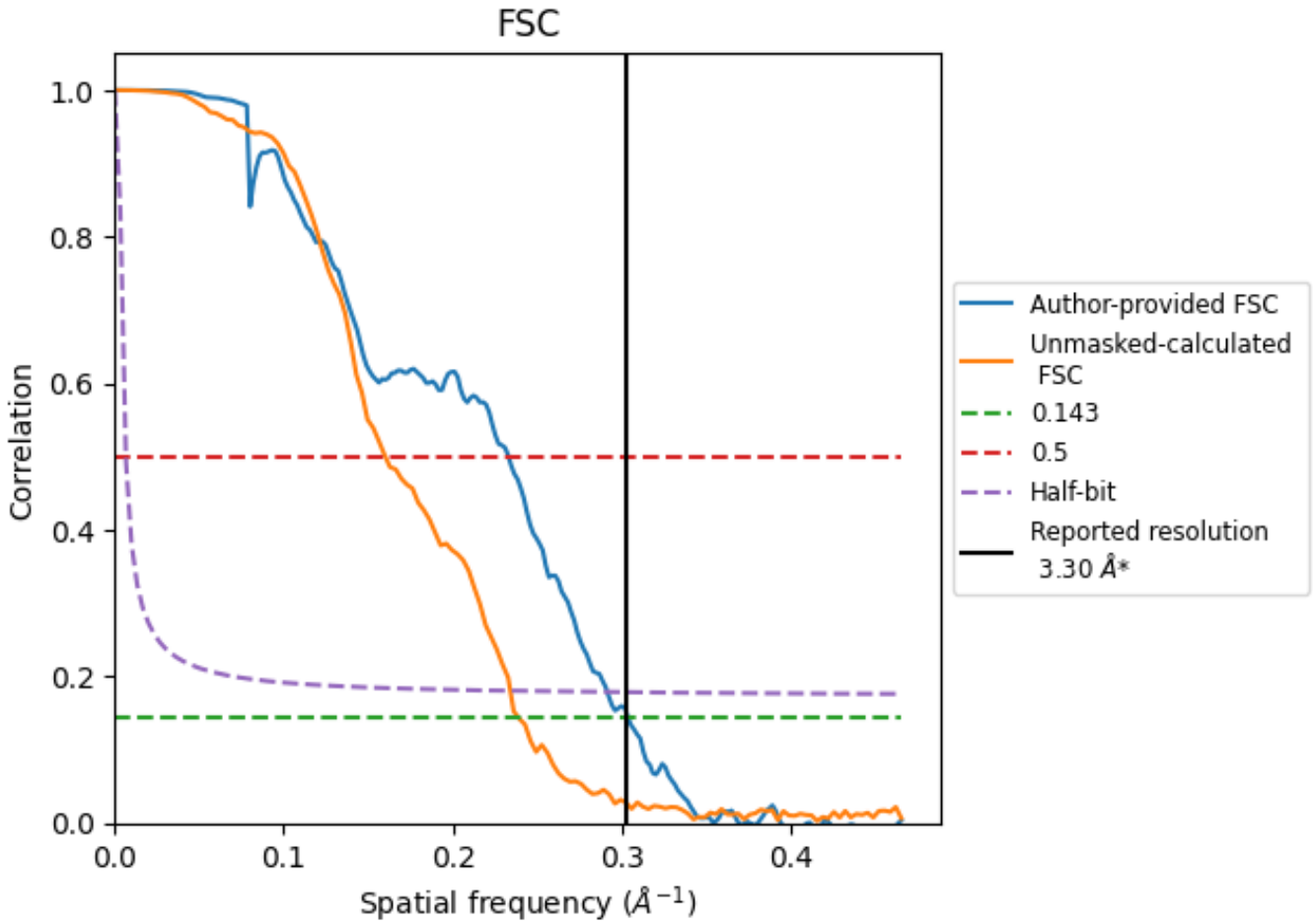


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

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 0.303 Å^{-1}

8.2 Resolution estimates (i)

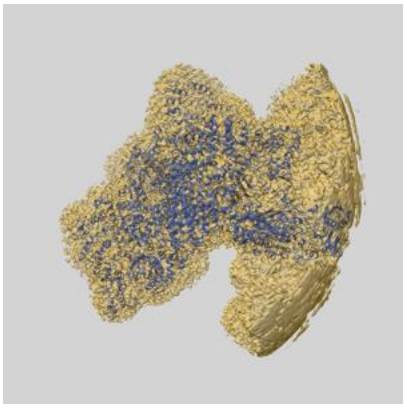
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.29	4.29	3.43
Unmasked-calculated*	4.18	6.25	4.27

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

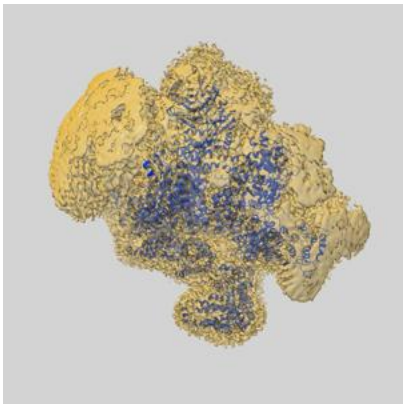
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10769 and PDB model 6YBD. Per-residue inclusion information can be found in section 3 on page 7.

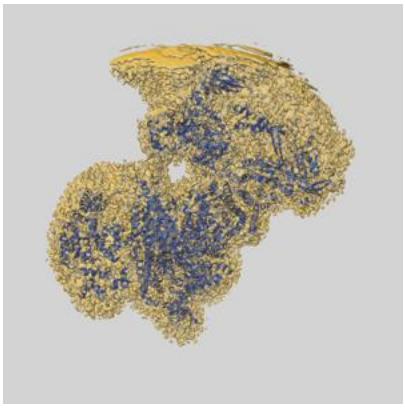
9.1 Map-model overlay



X



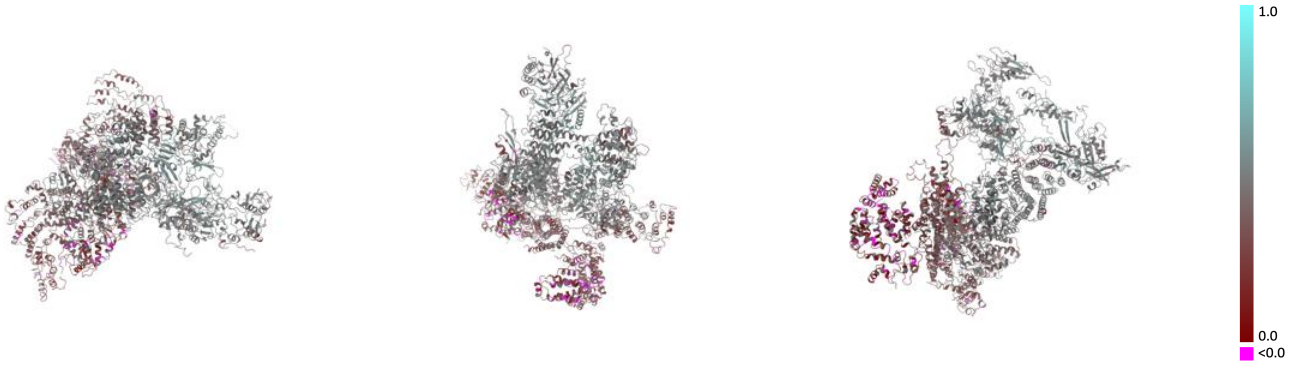
Y



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 (i)



X Y Z

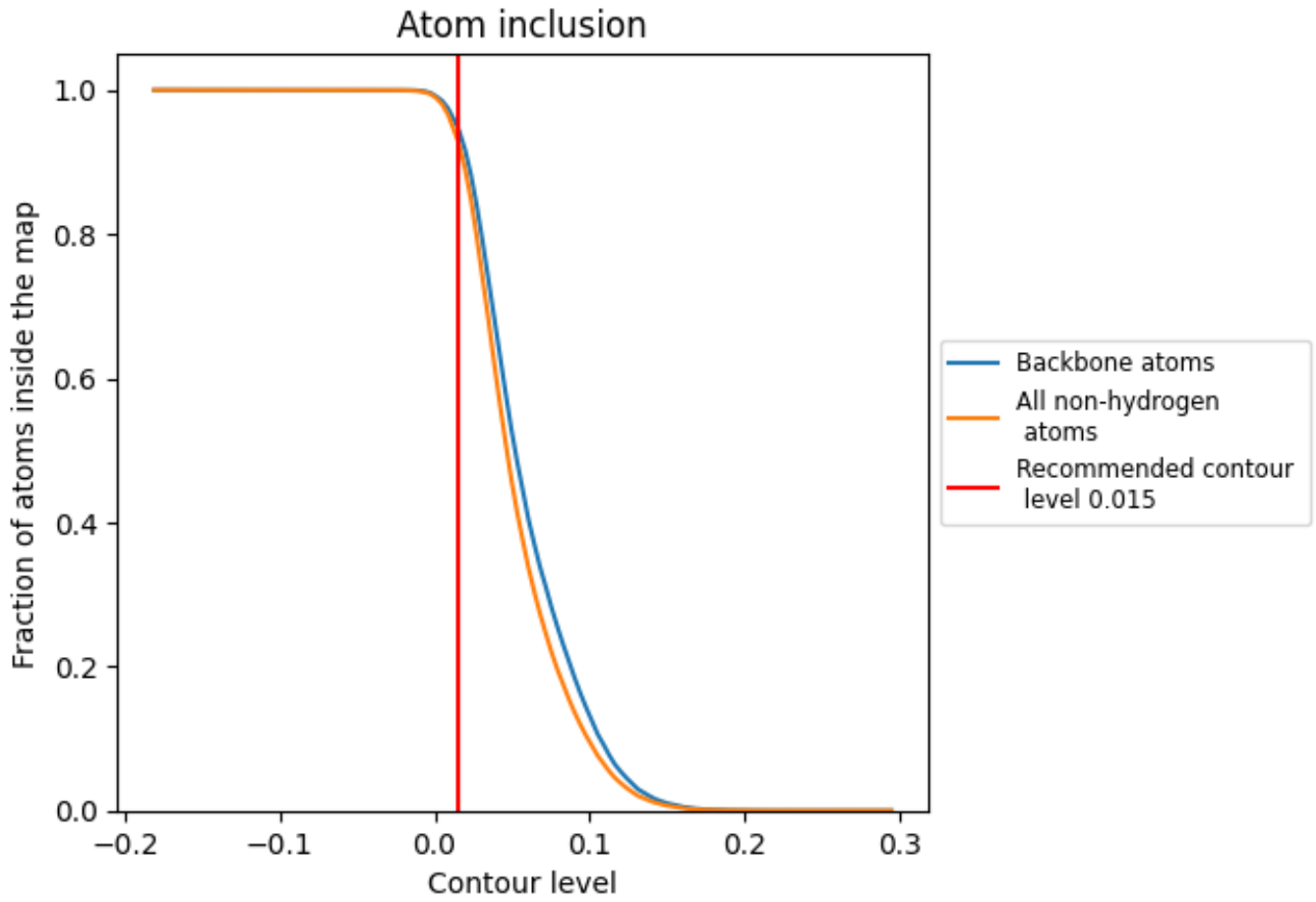
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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, 95% of all backbone atoms, 93% 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	0.9297	0.4160
3	0.8780	0.2450
4	0.9198	0.2880
5	0.8223	0.2280
6	0.9481	0.3320
8	0.8689	0.2880
G	0.9615	0.4690
H	0.9257	0.5170
I	0.9693	0.5060
K	0.9519	0.4880
L	0.8782	0.4470
M	0.9506	0.4810
N	0.9384	0.4820
O	0.9596	0.5070
P	0.9411	0.4810
Q	0.9448	0.5120
u	0.9469	0.4410
v	0.9354	0.3740
x	0.9539	0.4680
y	0.9487	0.4610