wwPDB EM Validation Summary Report (i)

Jul 7, 2021 – 11:16 am BST

PDB ID	:	7OE1
EMDB ID	:	EMD-12857
Title	:	30S ribosomal subunit from E. coli
Authors	:	Maksimova, E.; Korepanov, A.; Baymukhametov, T.; Kravchenko, O.; Stolboushkina, E.
Deposited on	:	2021-04-30
Resolution	:	3.05 Å(reported)
Based on initial model	:	4V4Q

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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

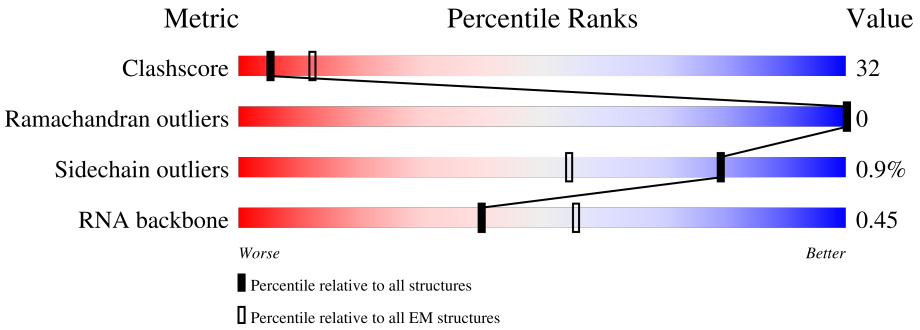
EMDB validation analysis	:	0.0.0.dev84
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.22

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 3.05 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
RNA backbone	4643	859

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	A	1542	24% 52% 22%
2	D	205	18% 52% 48%
3	E	166	5% 49% 41% 10%
4	F	135	24% 33% 41% 26%
5	H	129	54% 46%
6	K	128	41% 40% 51% 9%
7	L	123	46% 52%

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Mol	Chain	Length	Quality of chain
8	O	89	6% 57% 42%
9	P	82	7% 73% 27%
10	Q	83	7% 53% 43%
11	R	74	11% 39% 34% 26%
12	T	86	8% 64% 35%
13	B	240	25% 34% 57% 9%
14	U	71	18% 8% 17% 75%
15	C	232	55% 33% 55% 11%
16	G	178	74% 39% 45% 16%
17	I	129	73% 30% 67%
18	J	103	81% 42% 50% 5%
19	M	117	81% 36% 62%
20	N	100	60% 36% 58%
21	S	91	54% 31% 53% 13%

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 51092 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 RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	1530	32831	14642	6024	10635	1530	0	0

- Molecule 2 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	205	1643	1026	315	298	4	0	0

- Molecule 3 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	150	1105	687	211	201	6	0	0

- Molecule 4 is a protein called 30S ribosomal protein S6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	F	100	817	515	148	148	6	0	0

- Molecule 5 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	H	129	979	616	173	184	6	0	0

- Molecule 6 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	K	117	877	540	174	160	3	0	0

- Molecule 7 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 8 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	88	Total	C	N	O	S	0	0
			716	440	146	129	1		

- Molecule 9 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	P	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 10 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 11 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	R	55	Total	C	N	O	0	0
			455	288	86	81		

- Molecule 12 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 13 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	B	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 14 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	U	18	Total	C	N	O	0	0
			148	94	28	26		

- Molecule 15 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	C	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 16 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	G	150	Total	C	N	O	S	0	0
			1174	730	226	214	4		

- Molecule 17 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 18 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 19 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 20 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	96	Total	C	N	O	S	0	0
			774	483	160	128	3		

- Molecule 21 is a protein called 30S ribosomal protein S19.

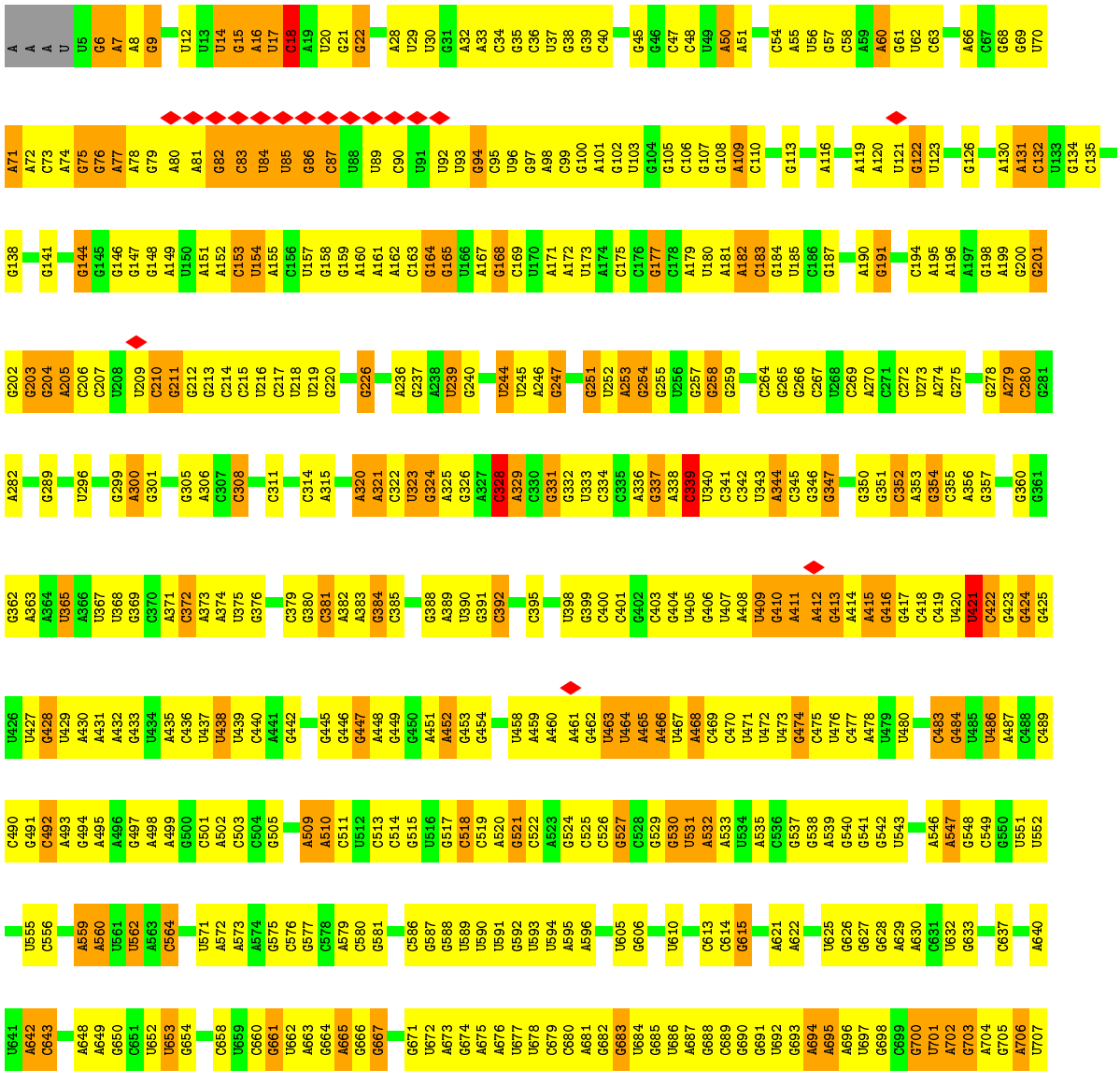
Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

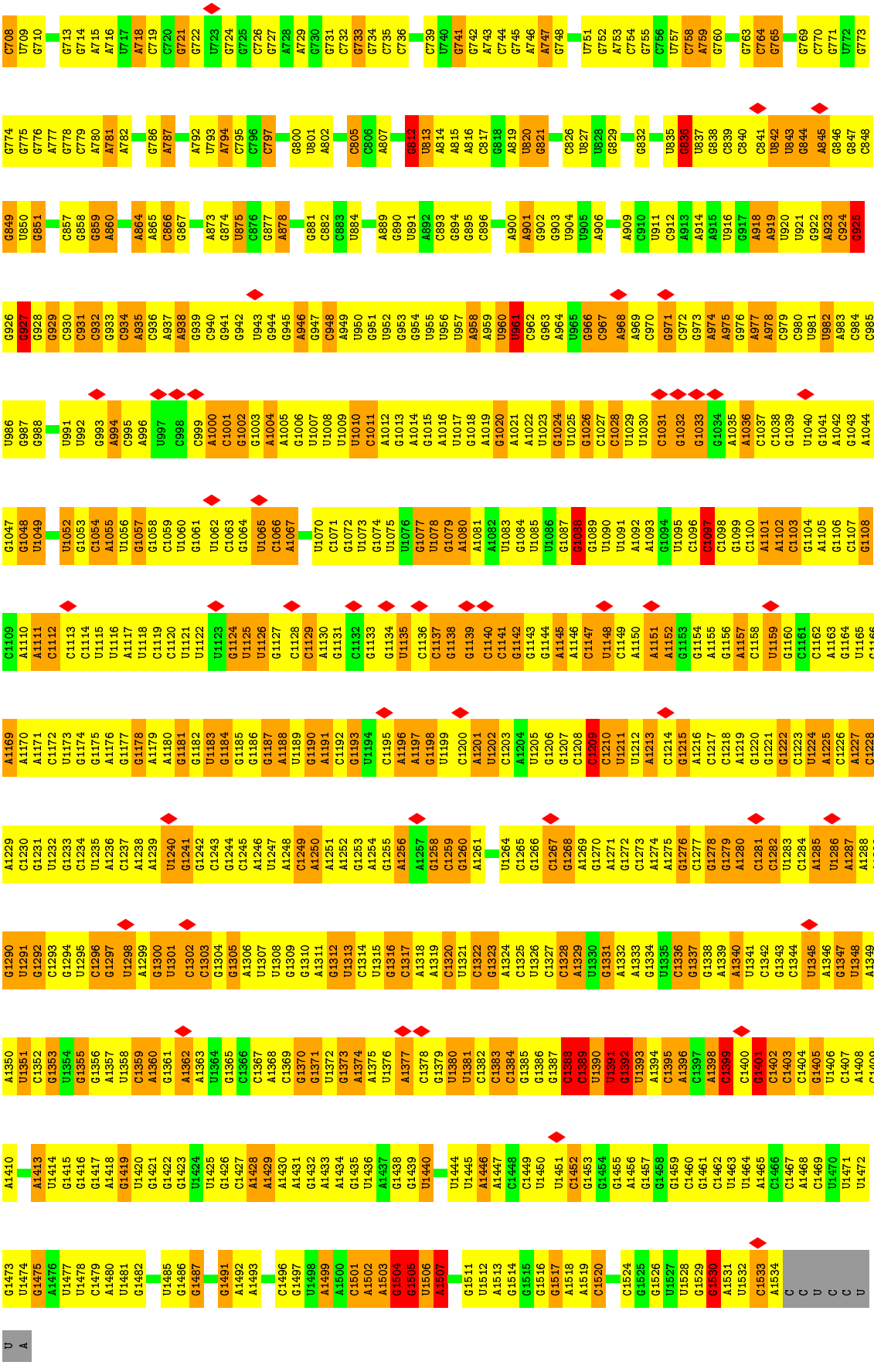
3 Residue-property plots (i)

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: 16S rRNA

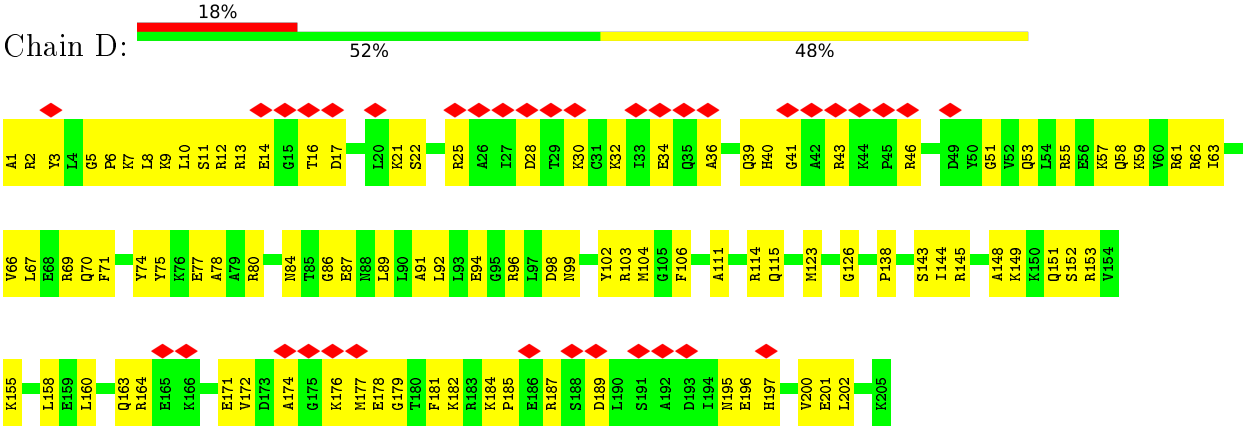
Chain A:





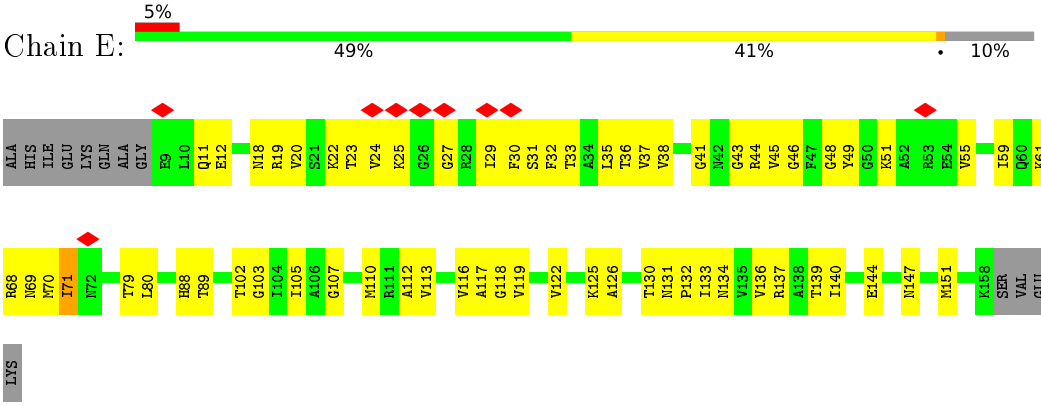
- Molecule 2: 30S ribosomal protein S4

Chain D:



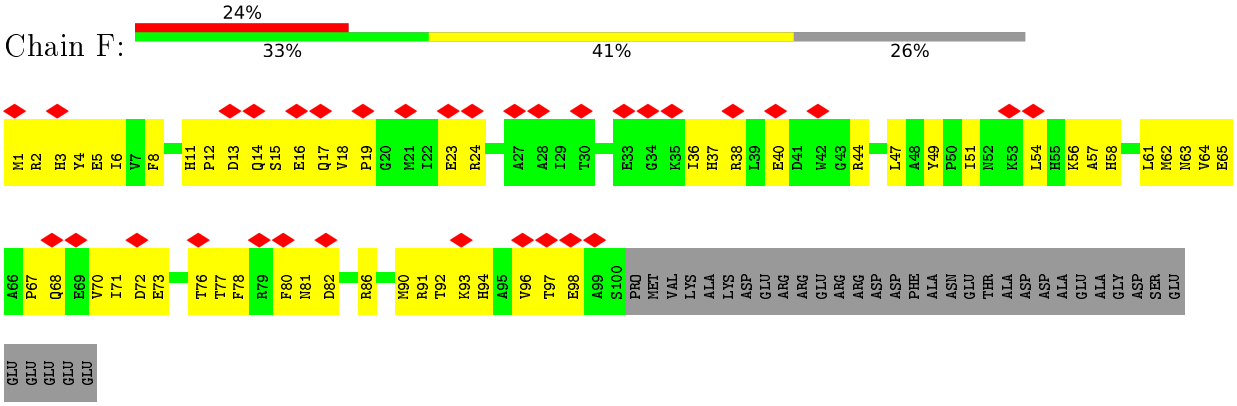
- Molecule 3: 30S ribosomal protein S5

Chain E:



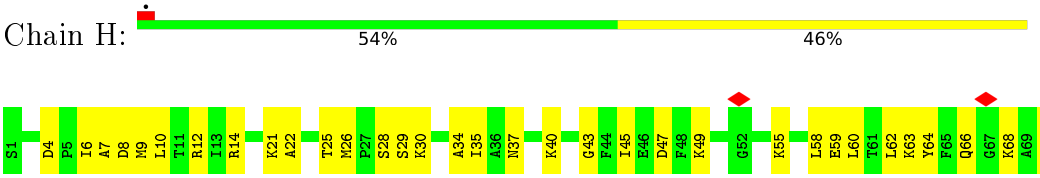
- Molecule 4: 30S ribosomal protein S6, fully modified isoform

Chain F:

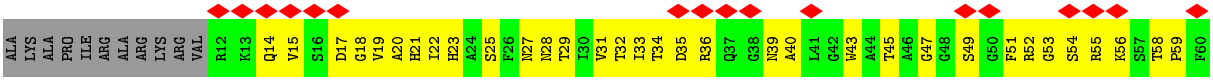


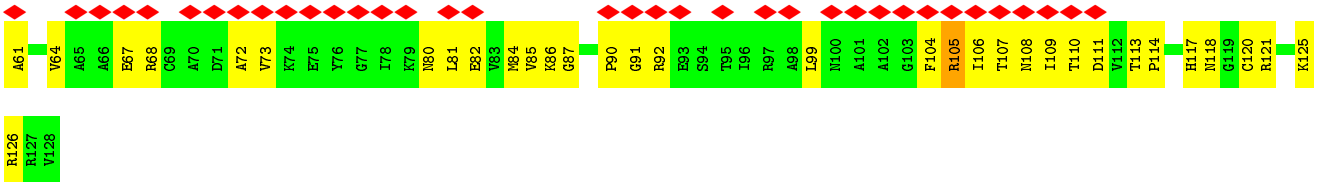
- Molecule 5: 30S ribosomal protein S8

Chain H:

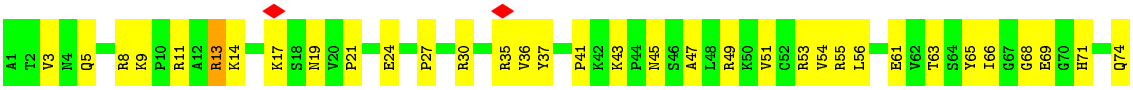


• Molecule 6: 30S ribosomal protein S11

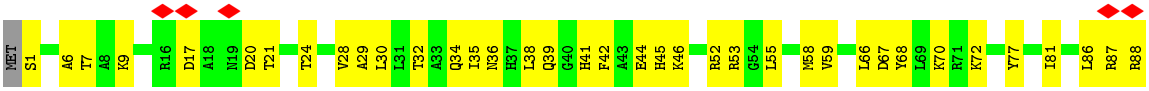




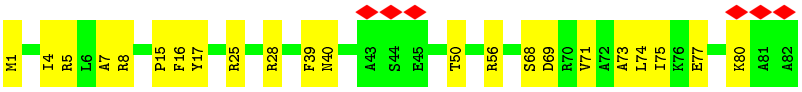
• Molecule 7: 30S ribosomal protein S12



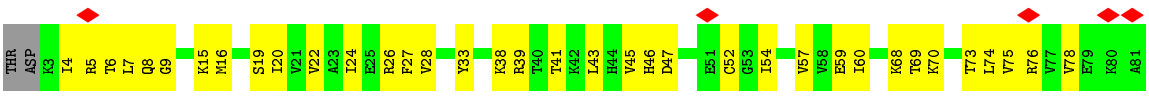
• Molecule 8: 30S ribosomal protein S15



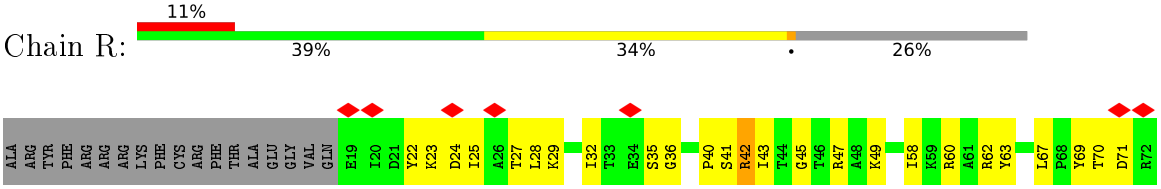
• Molecule 9: 30S ribosomal protein S16



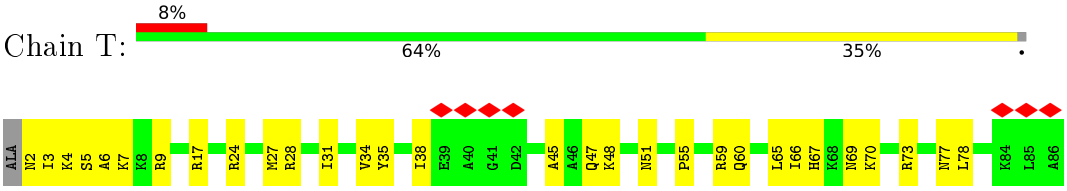
• Molecule 10: 30S ribosomal protein S17



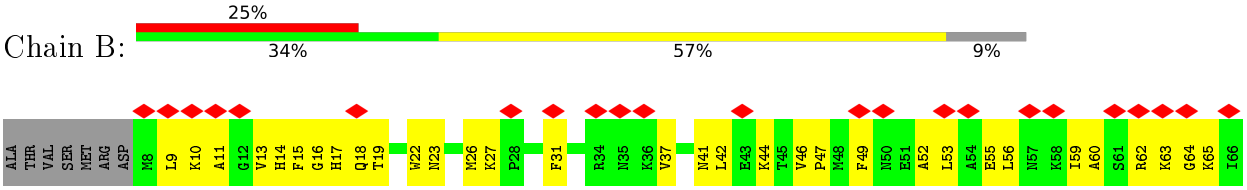
• Molecule 11: 30S ribosomal protein S18

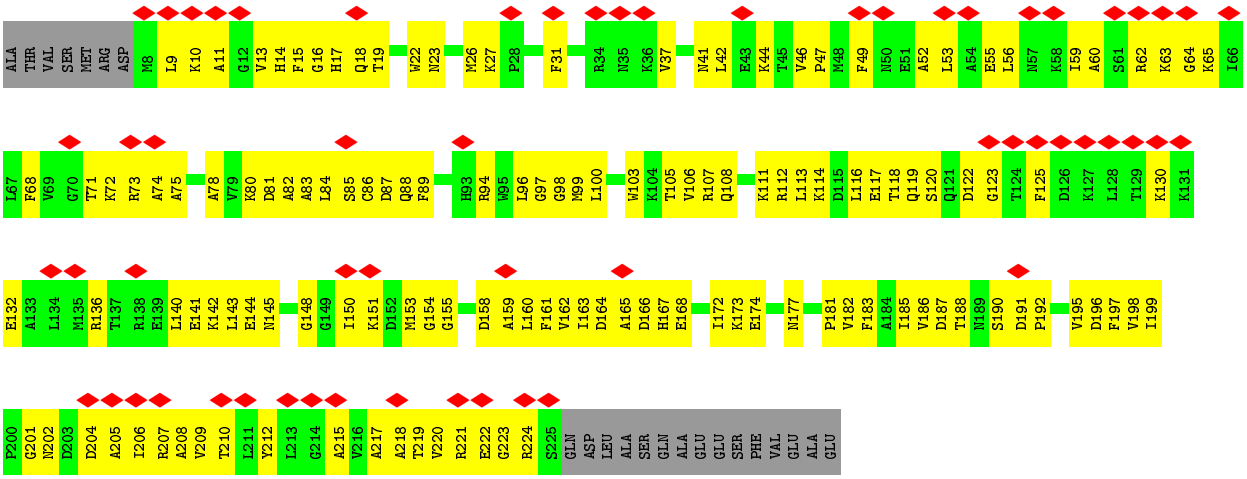


• Molecule 12: 30S ribosomal protein S20

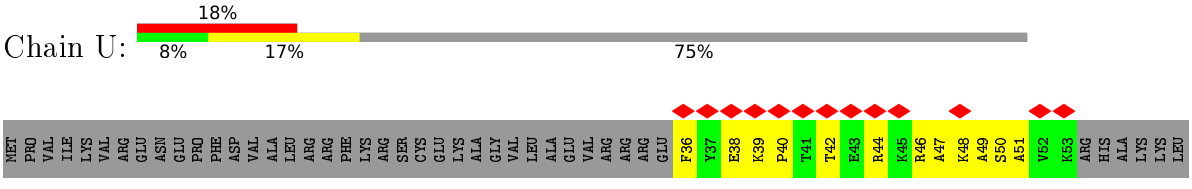


• Molecule 13: 30S ribosomal protein S2



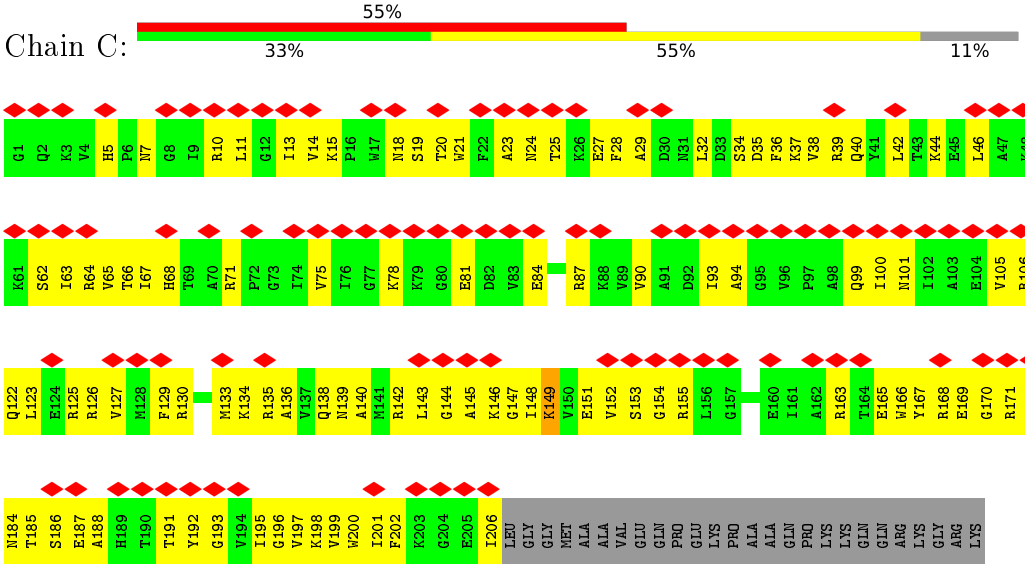


• Molecule 14: 30S ribosomal protein S21



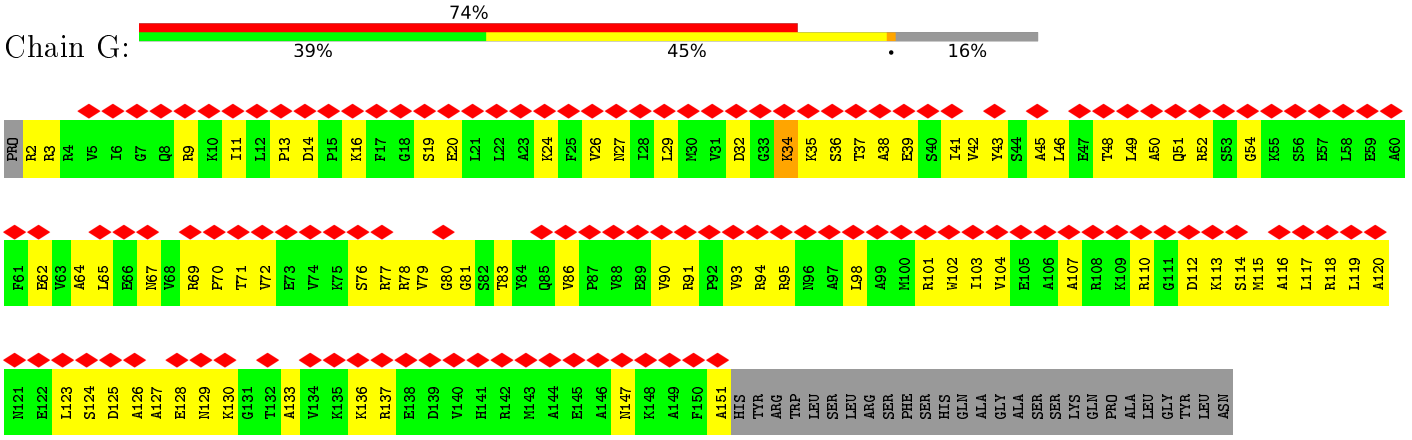
- Molecule 15: 30S ribosomal protein S3

Chain C:



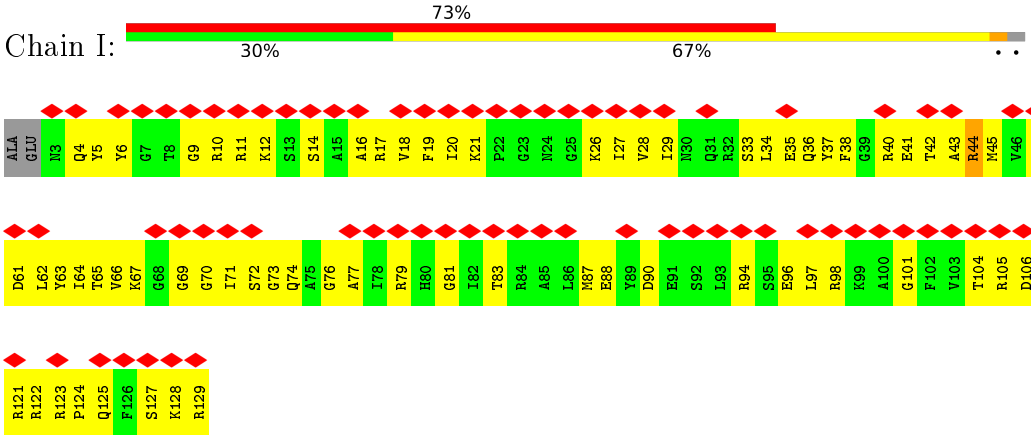
- Molecule 16: 30S ribosomal protein S7

Chain G:



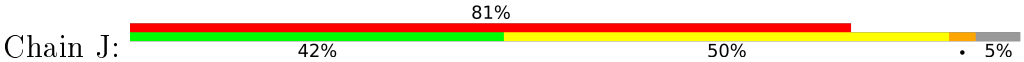
- Molecule 17: 30S ribosomal protein S9

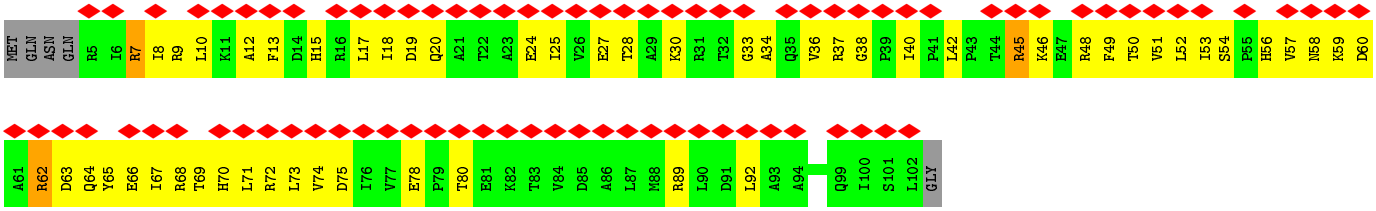
Chain I:



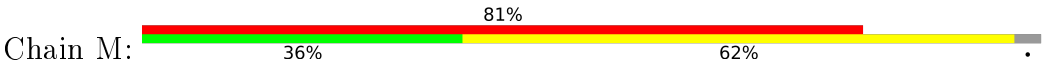
- Molecule 18: 30S ribosomal protein S10

Chain J:

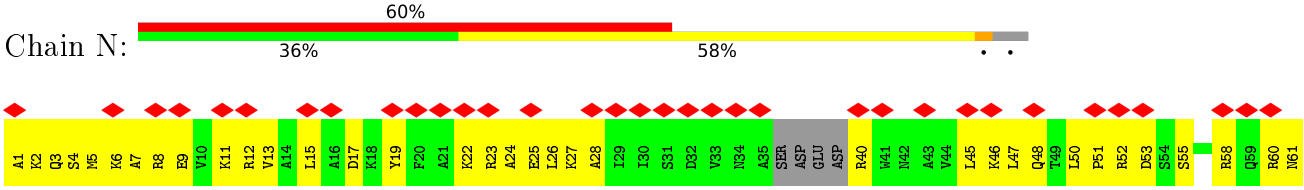




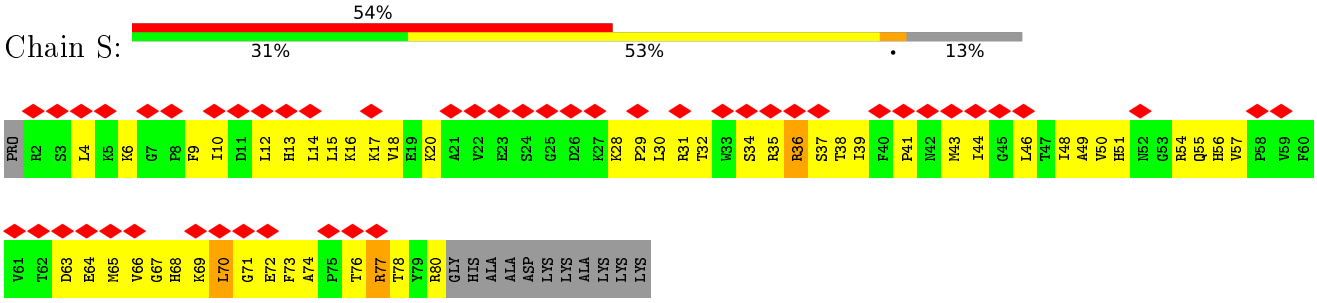
- Molecule 19: 30S ribosomal protein S13



- Molecule 20: 30S ribosomal protein S14



- Molecule 21: 30S ribosomal protein S19



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	169371	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	8.320	Depositor
Minimum map value	-4.514	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.094	Depositor
Recommended contour level	0.428	Depositor
Map size (Å)	344.0, 344.0, 344.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	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	A	1.03	47/36762 (0.1%)	1.07	136/57350 (0.2%)
2	D	0.46	0/1665	0.63	0/2227
3	E	0.59	0/1118	0.71	1/1504 (0.1%)
4	F	0.41	0/835	0.57	0/1128
5	H	0.56	0/989	0.65	0/1326
6	K	0.34	0/893	0.60	0/1205
7	L	0.52	0/969	0.74	1/1300 (0.1%)
8	O	0.49	0/724	0.65	0/966
9	P	0.59	0/659	0.71	0/884
10	Q	0.53	0/657	0.58	0/881
11	R	0.46	0/462	0.70	0/621
12	T	0.38	0/671	0.59	0/888
13	B	0.38	0/1735	0.60	0/2338
14	U	0.34	0/150	0.57	0/198
15	C	0.28	0/1651	0.52	0/2225
16	G	0.27	0/1187	0.50	0/1591
17	I	0.30	0/1034	0.54	0/1375
18	J	0.26	0/796	0.54	0/1077
19	M	0.26	0/892	0.55	0/1193
20	N	0.29	0/785	0.56	0/1043
21	S	0.30	0/652	0.58	1/877 (0.1%)
All	All	0.88	47/55286 (0.1%)	0.95	139/82197 (0.2%)

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	918	A	C6-N1	-14.72	1.25	1.35
1	A	17	U	C2-N3	-11.04	1.30	1.37
1	A	18	C	N1-C6	-10.28	1.30	1.37
1	A	1401	G	N7-C5	-9.99	1.33	1.39
1	A	17	U	C4-O4	-8.87	1.16	1.23

The worst 5 of 139 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	860	A	O5'-P-OP1	-16.03	91.27	105.70
1	A	859	G	N3-C4-C5	-14.60	121.30	128.60
1	A	17	U	N3-C4-C5	12.56	122.14	114.60
1	A	1401	G	C6-C5-N7	-12.11	123.13	130.40
1	A	17	U	C2-N3-C4	-11.84	119.89	127.00

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	A	32831	0	16519	1541	0
2	D	1643	0	1710	126	0
3	E	1105	0	1148	66	0
4	F	817	0	808	64	0
5	H	979	0	1034	51	0
6	K	877	0	887	86	0
7	L	955	0	1019	74	0
8	O	716	0	742	35	0
9	P	649	0	666	19	0
10	Q	648	0	691	38	0
11	R	455	0	478	43	0
12	T	665	0	714	25	0
13	B	1704	0	1732	133	0
14	U	148	0	157	13	0
15	C	1624	0	1699	145	0
16	G	1174	0	1230	106	0
17	I	1022	0	1070	106	0
18	J	786	0	828	88	0
19	M	883	0	944	95	0
20	N	774	0	827	88	0
21	S	637	0	665	97	0
All	All	51092	0	35568	2694	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 32.

The worst 5 of 2694 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1117:A:C2	1:A:1156:G:N1	2.10	1.19
1:A:945:G:H1	1:A:1236:A:N6	1.37	1.19
1:A:1156:G:N2	1:A:1179:A:C2	2.11	1.18
21:S:39:ILE:HG23	21:S:43:MET:HE3	1.30	1.13
2:D:104:MET:HG2	2:D:106:PHE:CE2	1.91	1.06

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	
2	D	203/205 (99%)	174 (86%)	29 (14%)	0	100	100
3	E	148/166 (89%)	119 (80%)	29 (20%)	0	100	100
4	F	98/135 (73%)	80 (82%)	18 (18%)	0	100	100
5	H	127/129 (98%)	113 (89%)	14 (11%)	0	100	100
6	K	115/128 (90%)	94 (82%)	21 (18%)	0	100	100
7	L	121/123 (98%)	96 (79%)	25 (21%)	0	100	100
8	O	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
9	P	80/82 (98%)	69 (86%)	11 (14%)	0	100	100
10	Q	78/83 (94%)	66 (85%)	12 (15%)	0	100	100
11	R	53/74 (72%)	45 (85%)	8 (15%)	0	100	100
12	T	83/86 (96%)	77 (93%)	6 (7%)	0	100	100
13	B	216/240 (90%)	172 (80%)	44 (20%)	0	100	100
14	U	16/71 (22%)	10 (62%)	6 (38%)	0	100	100
15	C	204/232 (88%)	176 (86%)	28 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	G	148/178 (83%)	129 (87%)	19 (13%)	0	100	100
17	I	125/129 (97%)	107 (86%)	18 (14%)	0	100	100
18	J	96/103 (93%)	78 (81%)	18 (19%)	0	100	100
19	M	112/117 (96%)	98 (88%)	14 (12%)	0	100	100
20	N	92/100 (92%)	86 (94%)	6 (6%)	0	100	100
21	S	77/91 (85%)	64 (83%)	13 (17%)	0	100	100
All	All	2278/2561 (89%)	1935 (85%)	343 (15%)	0	100	100

There are no Ramachandran outliers to report.

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	
2	D	172/172 (100%)	172 (100%)	0	100	100
3	E	113/125 (90%)	113 (100%)	0	100	100
4	F	87/116 (75%)	87 (100%)	0	100	100
5	H	104/104 (100%)	104 (100%)	0	100	100
6	K	90/98 (92%)	88 (98%)	2 (2%)	52	76
7	L	103/103 (100%)	102 (99%)	1 (1%)	76	89
8	O	76/77 (99%)	76 (100%)	0	100	100
9	P	65/65 (100%)	65 (100%)	0	100	100
10	Q	74/77 (96%)	74 (100%)	0	100	100
11	R	48/64 (75%)	47 (98%)	1 (2%)	53	77
12	T	65/65 (100%)	65 (100%)	0	100	100
13	B	180/198 (91%)	180 (100%)	0	100	100
14	U	15/61 (25%)	14 (93%)	1 (7%)	16	43
15	C	170/189 (90%)	169 (99%)	1 (1%)	86	93
16	G	123/146 (84%)	122 (99%)	1 (1%)	81	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	I	105/106 (99%)	103 (98%)	2 (2%)	57 79
18	J	86/90 (96%)	83 (96%)	3 (4%)	36 66
19	M	92/95 (97%)	91 (99%)	1 (1%)	73 88
20	N	79/83 (95%)	77 (98%)	2 (2%)	47 74
21	S	70/78 (90%)	68 (97%)	2 (3%)	42 70
All	All	1917/2112 (91%)	1900 (99%)	17 (1%)	79 90

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	N	80	ARG
21	S	77	ARG
17	I	44	ARG
17	I	112	ARG
18	J	7	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
13	B	108	GLN
15	C	138	GLN
15	C	101	ASN
6	K	118	ASN
12	T	77	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1529/1542 (99%)	468 (30%)	15 (0%)

5 of 468 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	A
1	A	9	G
1	A	18	C
1	A	20	U

5 of 15 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	923	A
1	A	1388	C
1	A	931	C
1	A	1390	U
1	A	1210	C

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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.

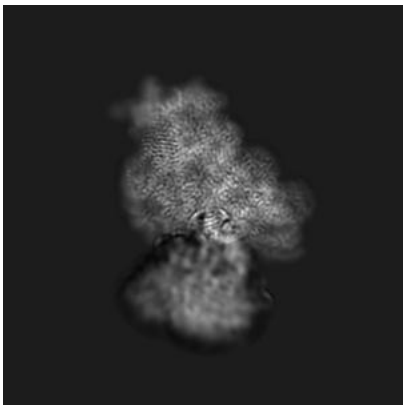
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12857. These allow visual inspection of the internal detail of the map and identification of artifacts.

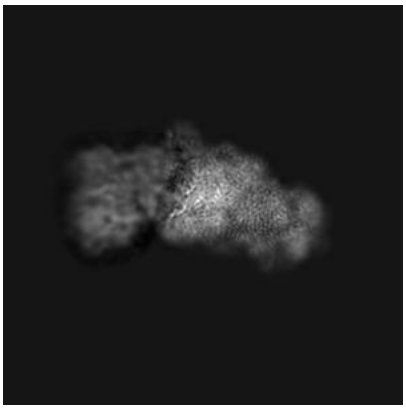
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

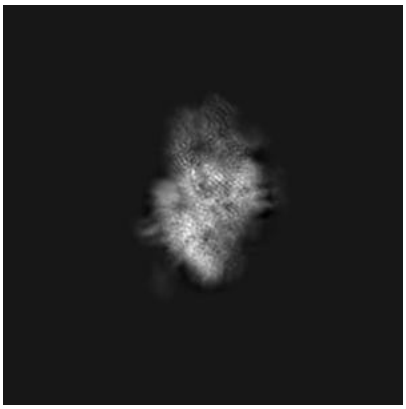
6.1.1 Primary map



X

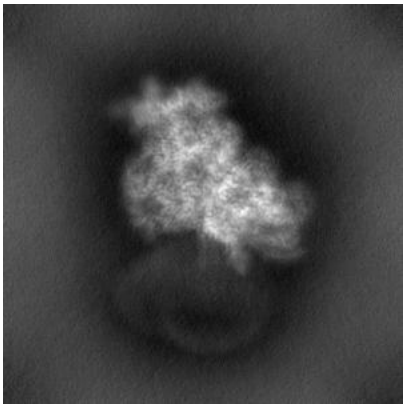


Y

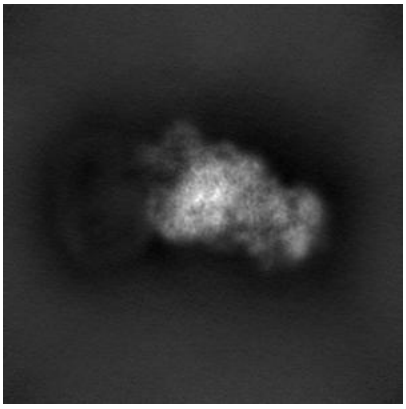


Z

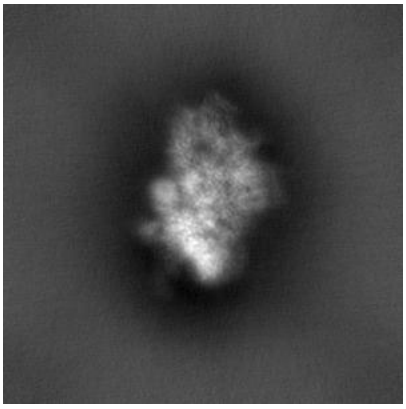
6.1.2 Raw map



X



Y

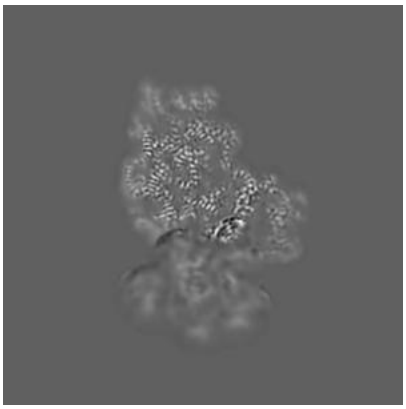


Z

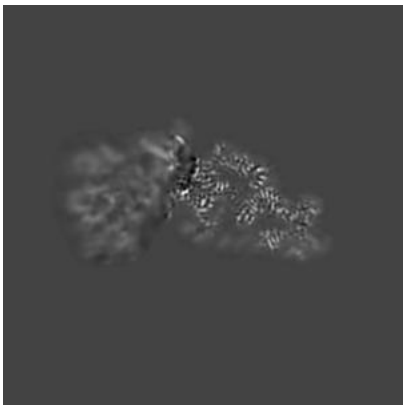
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

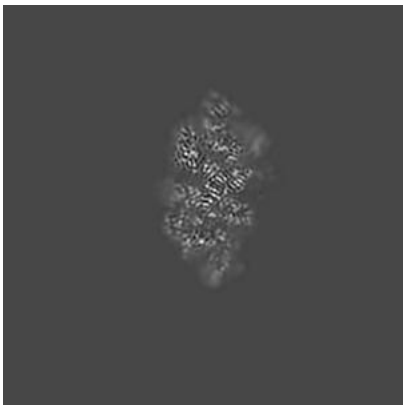
6.2.1 Primary map



X Index: 200

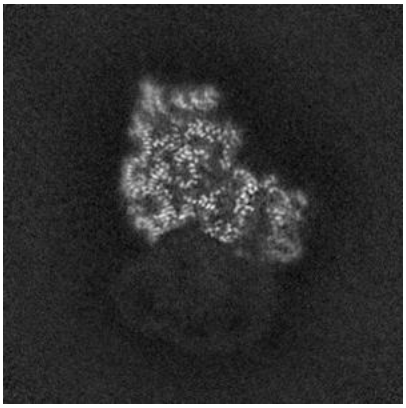


Y Index: 200

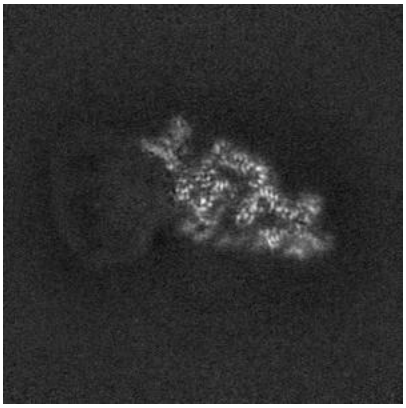


Z Index: 200

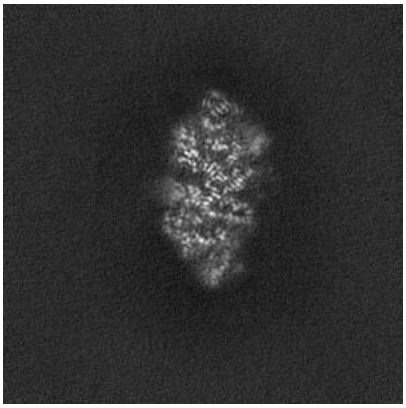
6.2.2 Raw map



X Index: 200



Y Index: 200

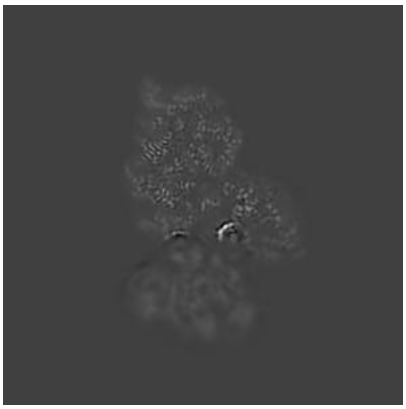


Z Index: 200

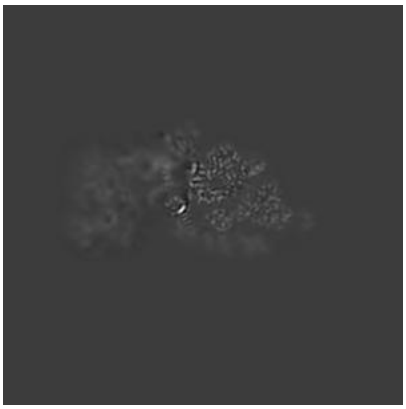
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

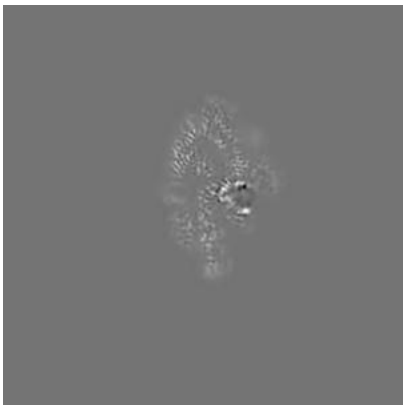
6.3.1 Primary map



X Index: 194

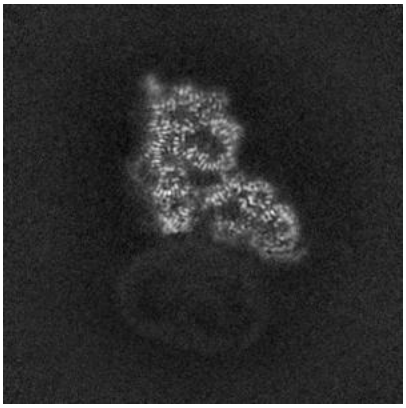


Y Index: 222

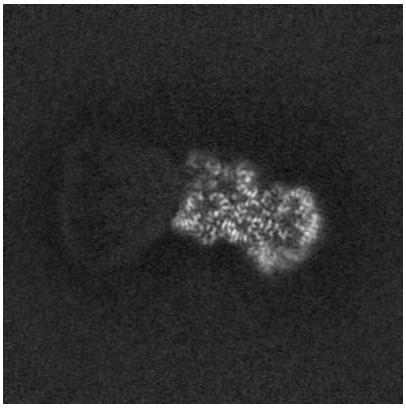


Z Index: 191

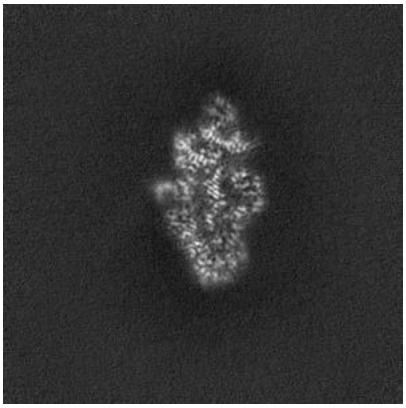
6.3.2 Raw map



X Index: 187



Y Index: 177



Z Index: 214

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 0.428. 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.

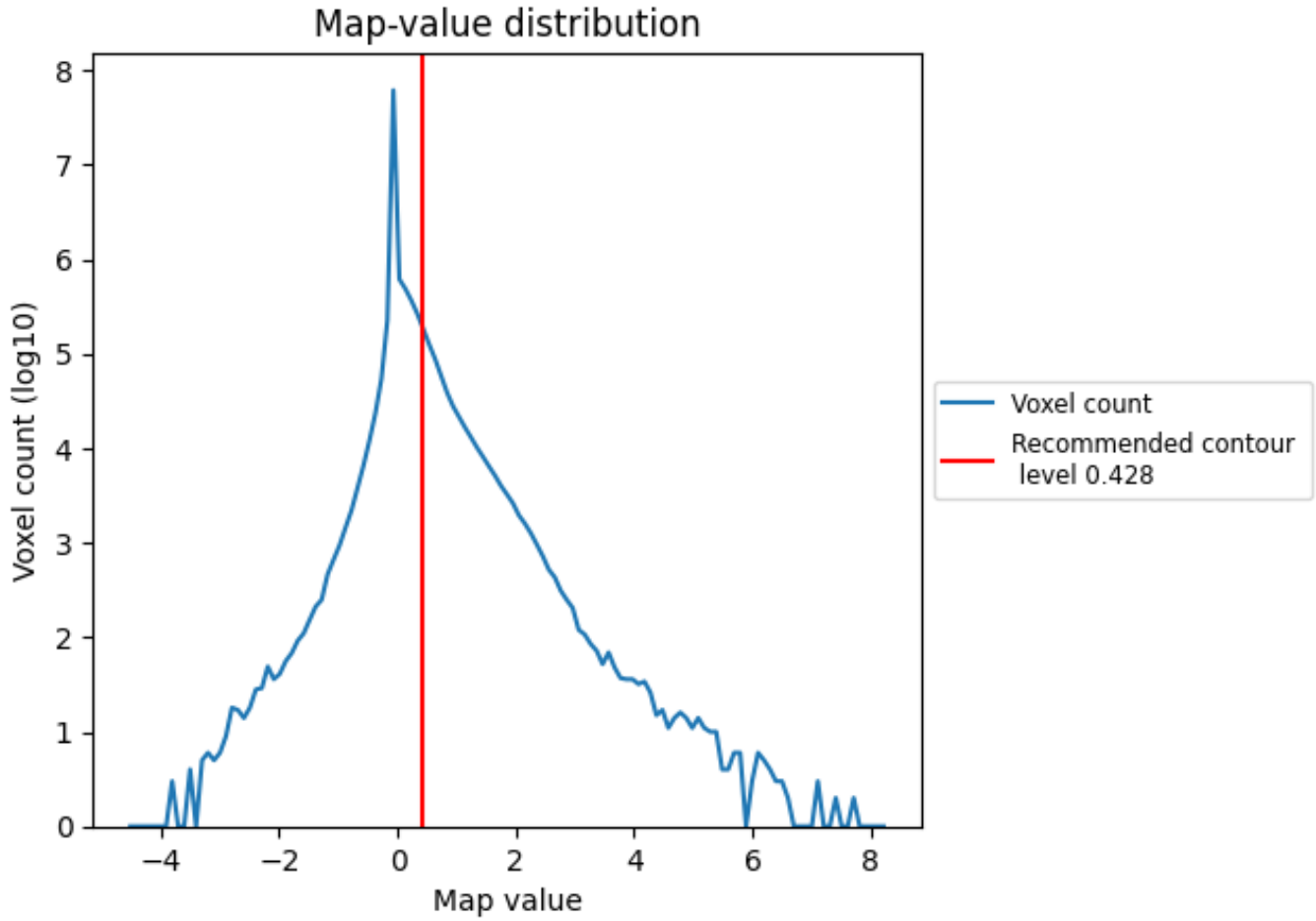
6.5 Mask visualisation (i)

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

7 Map analysis

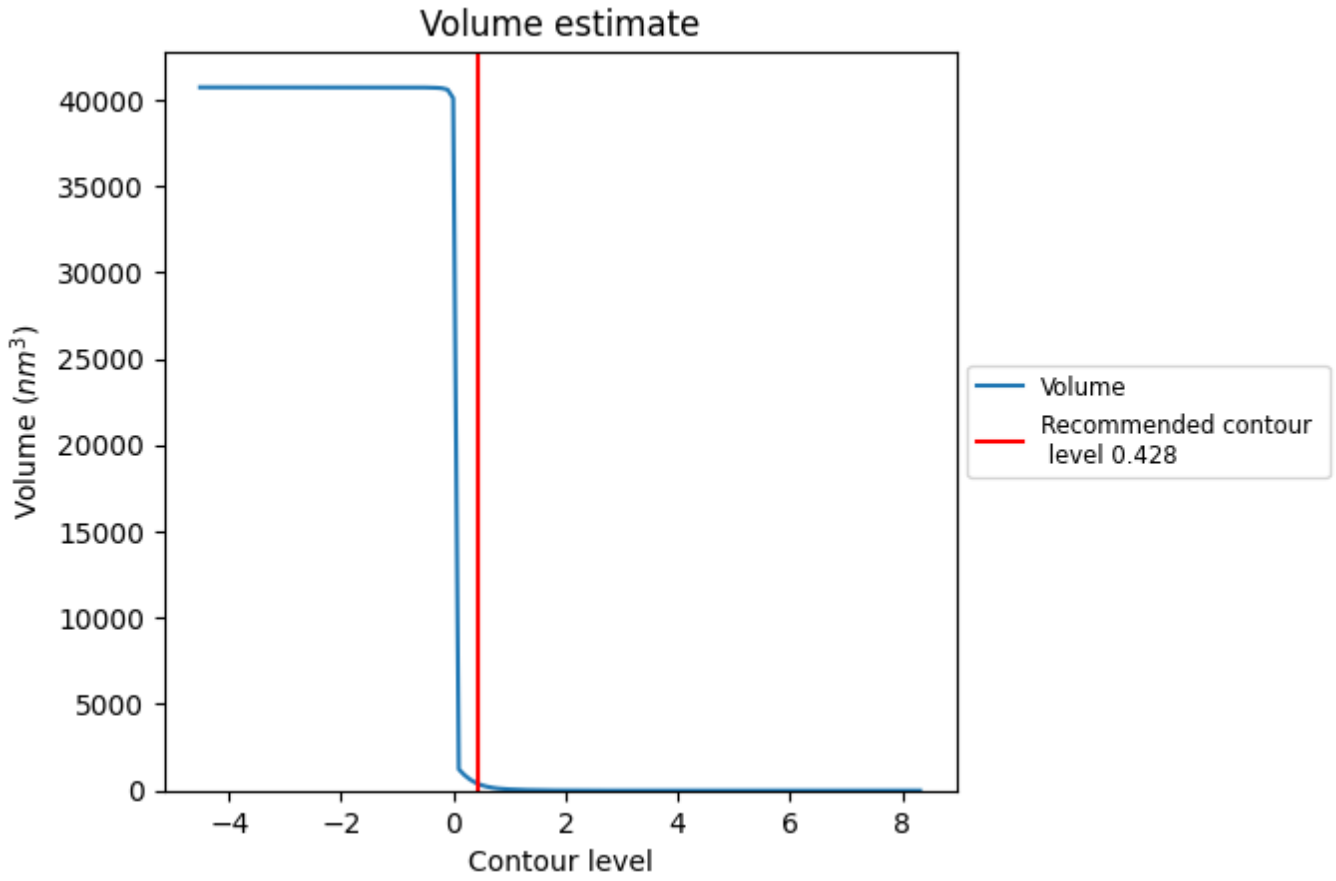
This section contains the results of statistical analysis of the map.

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.

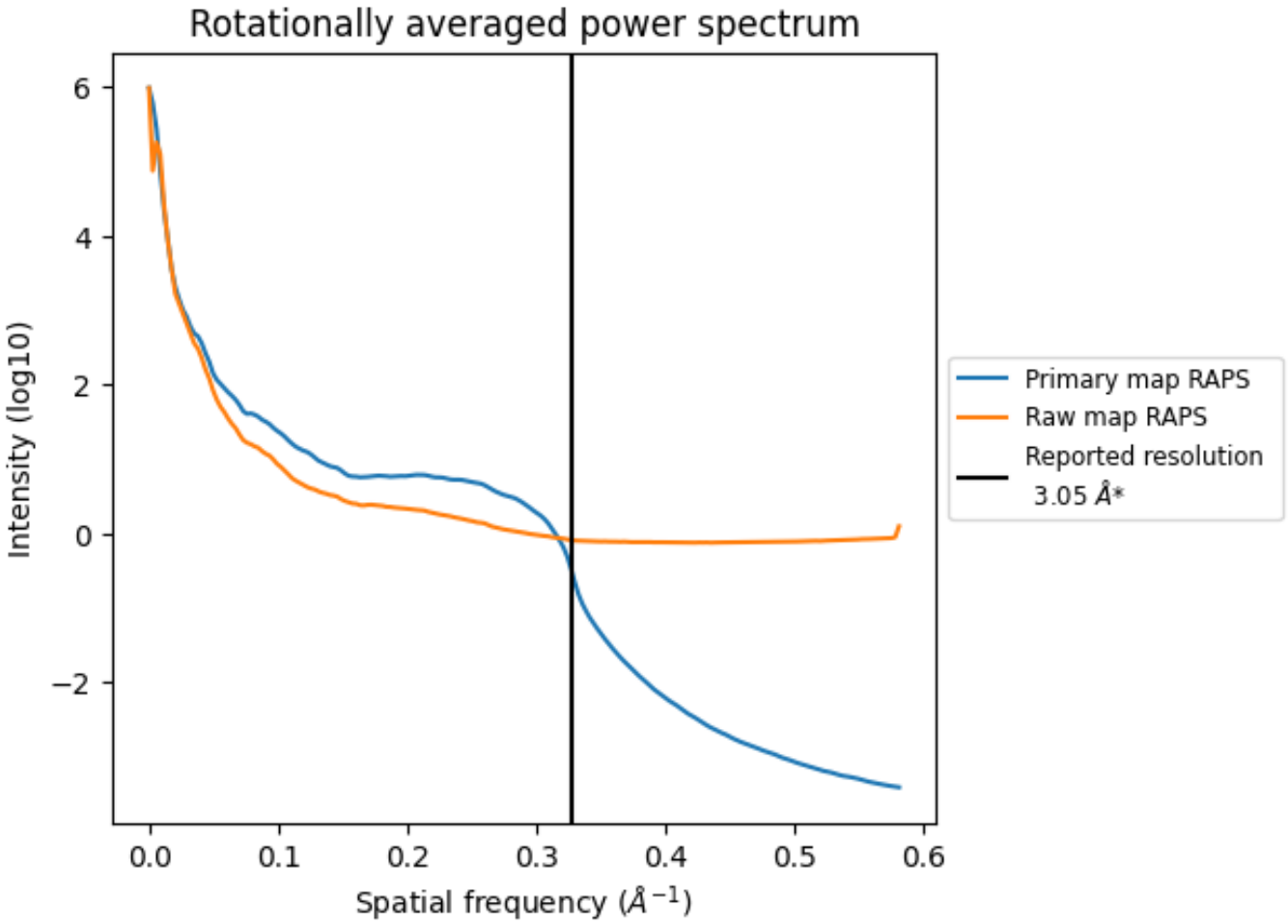
7.2 Volume estimate



The volume at the recommended contour level is 412 nm^3; this corresponds to an approximate mass of 373 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)

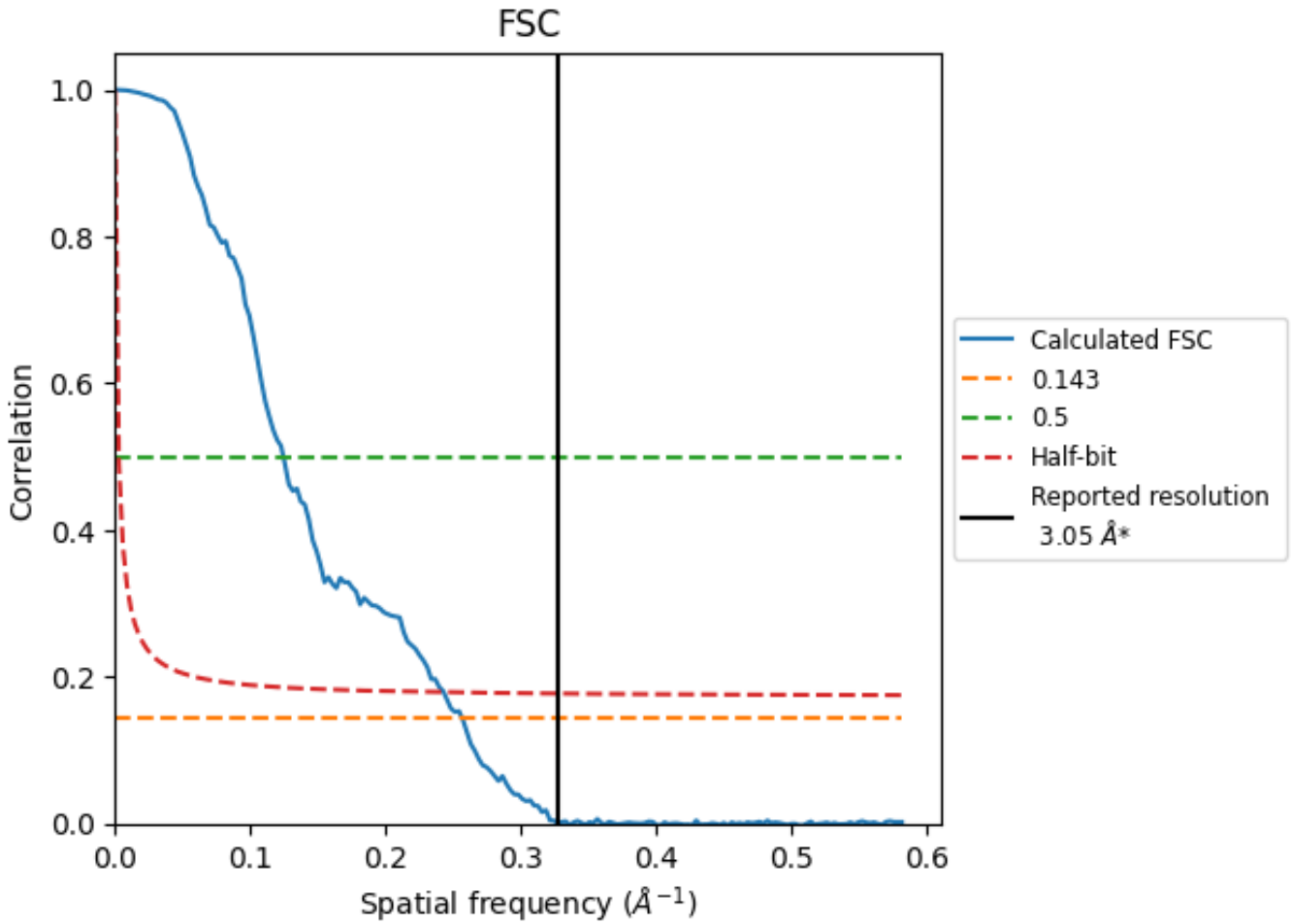


*Reported resolution corresponds to spatial frequency of 0.328 $Å^{-1}$

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 0.328 Å^{-1}

8.2 Resolution estimates (i)

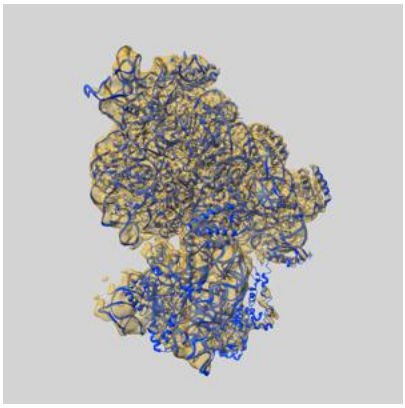
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.05	-	-
Author-provided FSC curve	-	-	-
Calculated*	3.90	8.04	4.12

*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 3.90 differs from the reported value 3.05 by more than 10 %

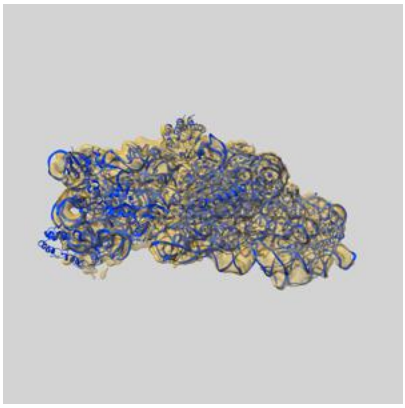
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12857 and PDB model 7OE1. Per-residue inclusion information can be found in section 3 on page 8.

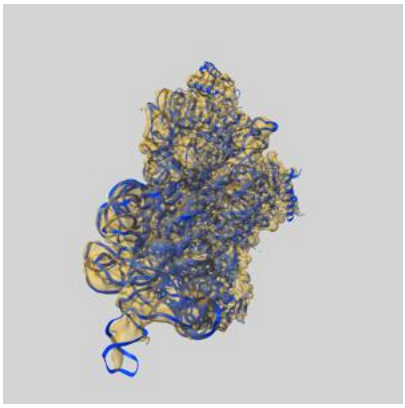
9.1 Map-model overlay



X



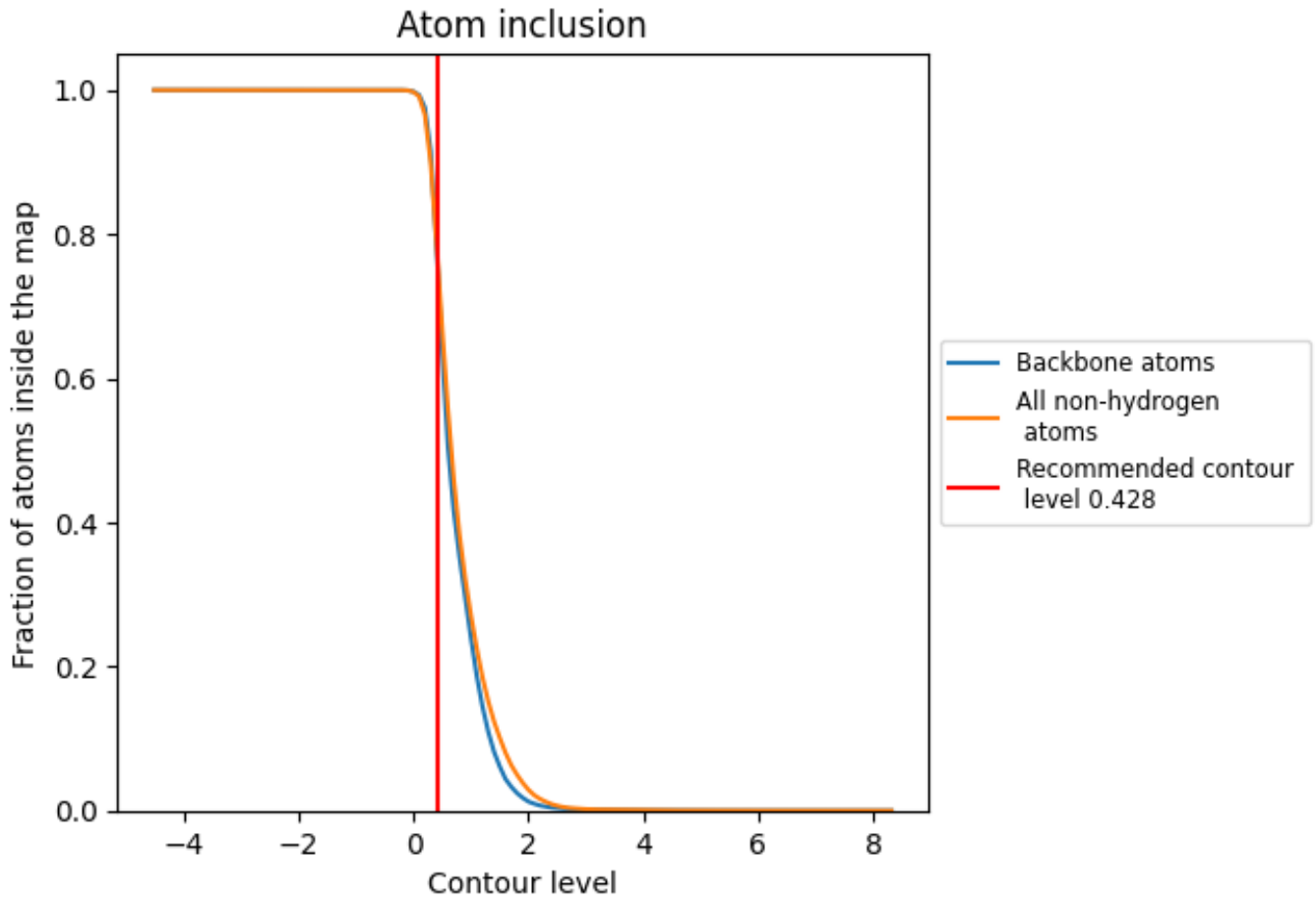
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.428 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 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.