



wwPDB EM Validation Summary Report ⓘ

Dec 10, 2022 – 08:36 am GMT

PDB ID : 5AN9
EMDB ID : EMD-3145
Title : Mechanism of eIF6 release from the nascent 60S ribosomal subunit
Authors : Weis, F.; Giudice, E.; Churcher, M.; Jin, L.; Hilcenko, C.; Wong, C.C.;
Traynor, D.; Kay, R.R.; Warren, A.J.
Deposited on : 2015-09-06
Resolution : 3.30 Å(reported)

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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:

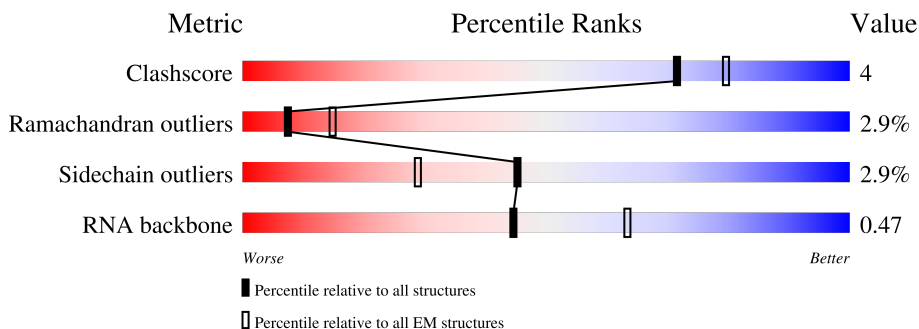
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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.



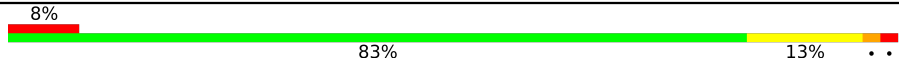
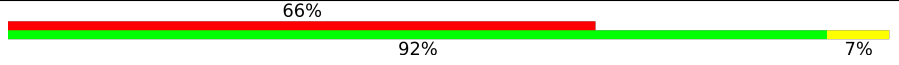
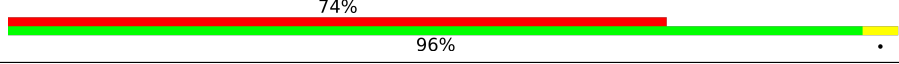

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	398	
2	B	188	
3	C	205	
4	D	166	
5	E	136	
6	F	217	
7	G	69	

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Mol	Chain	Length	Quality of chain
8	H	52	
9	I	224	
10	J	250	
11	N	3741	

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 39693 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 60S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	398	3176	2018	599	547	12	0	0

- Molecule 2 is a protein called 60S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	188	1491	944	264	277	6	0	0

- Molecule 3 is a protein called 60S ACIDIC RIBOSOMAL PROTEIN P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	205	1571	998	271	294	8	0	0

- Molecule 4 is a protein called 60S RIBOSOMAL PROTEIN L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	166	1245	790	220	228	7	0	0

- Molecule 5 is a protein called 60S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	136	1017	640	188	181	8	0	0

- Molecule 6 is a protein called 60S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	217	1721	1079	332	297	13	0	0

- Molecule 7 is a protein called 60S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	69	586	378	105	99	4	0	0

- Molecule 8 is a protein called UBIQUITIN-60S RIBOSOMAL PROTEIN L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	52	427	269	88	64	6	0	0

- Molecule 9 is a protein called EUKARYOTIC TRANSLATION INITIATION FACTOR 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	224	1686	1048	290	338	10	0	0

- Molecule 10 is a protein called RIBOSOME MATURATION PROTEIN SBDS.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	250	2015	1272	352	380	11	0	0

- Molecule 11 is a RNA chain called 26S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
11	N	1162	24758	11082	4431	8087	1158	0	0

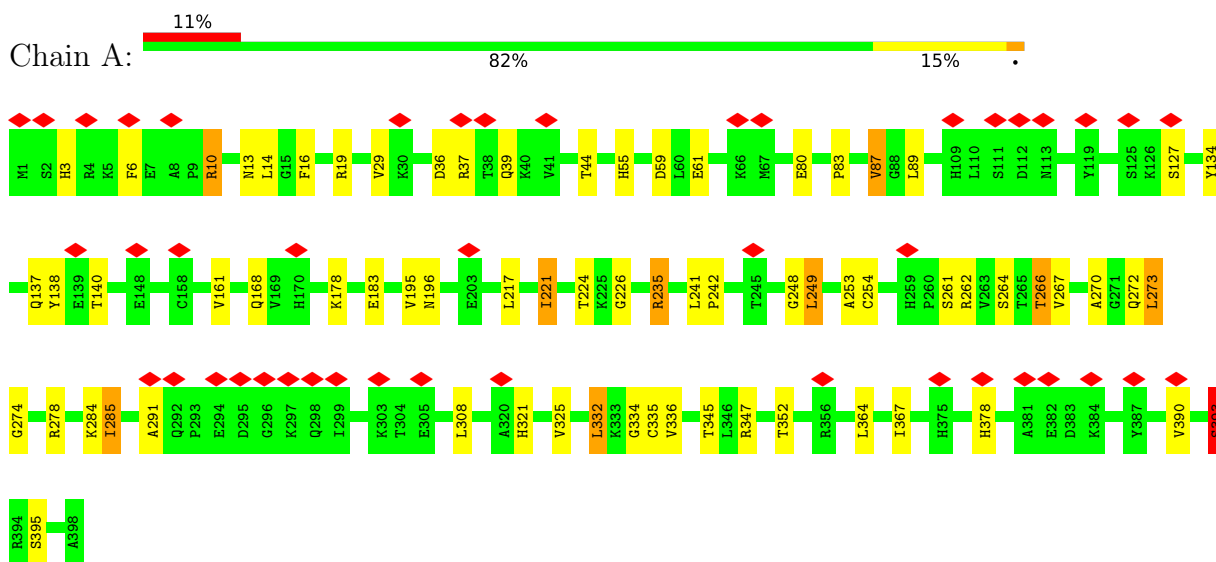
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	3119	C	G	conflict	GB FR733594.

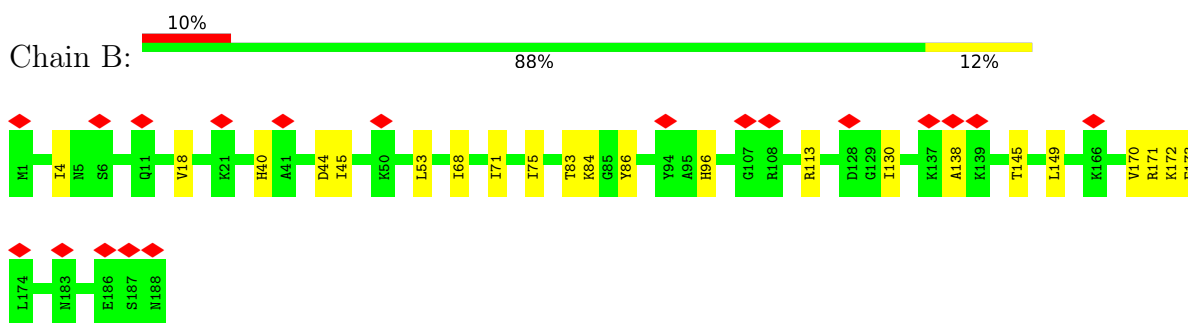
3 Residue-property plots [i](#)

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.

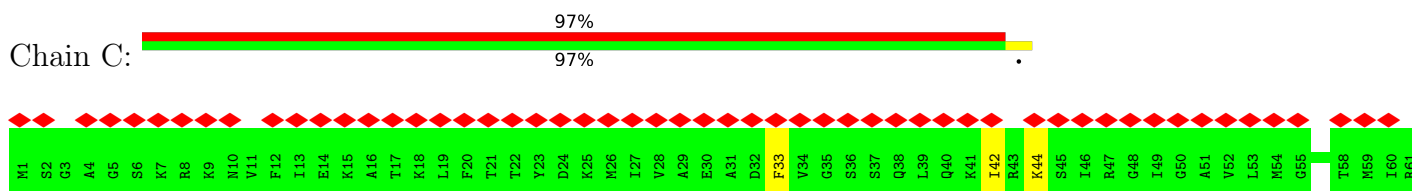
- Molecule 1: 60S RIBOSOMAL PROTEIN L3

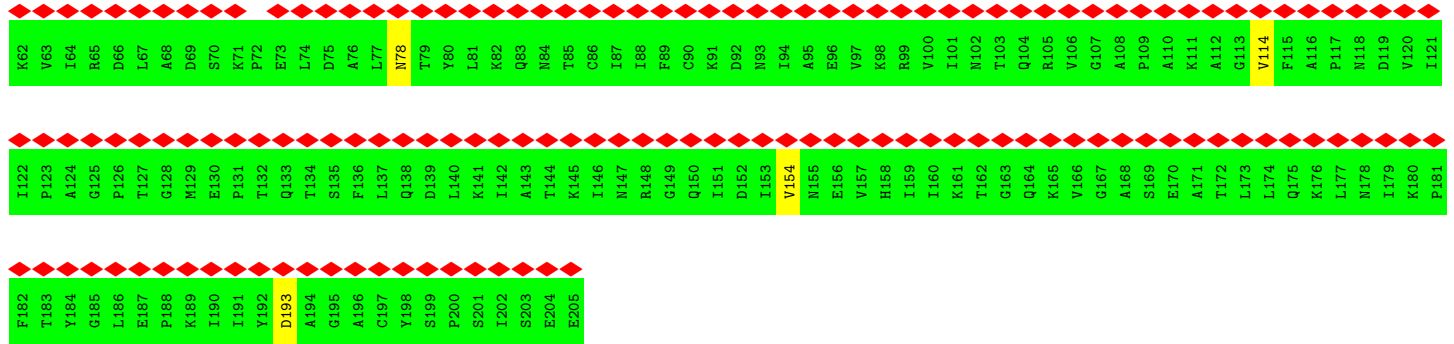


- Molecule 2: 60S RIBOSOMAL PROTEIN L9

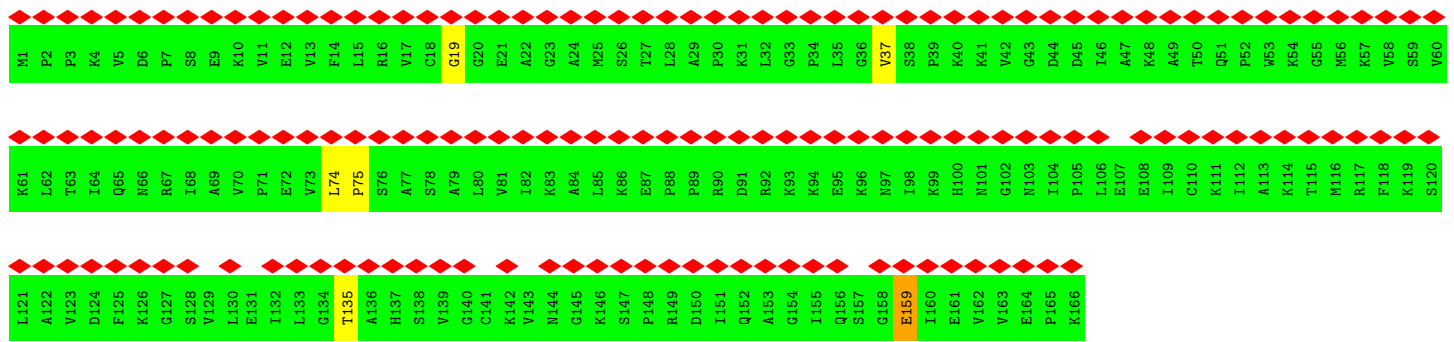


- Molecule 3: 60S ACIDIC RIBOSOMAL PROTEIN P0

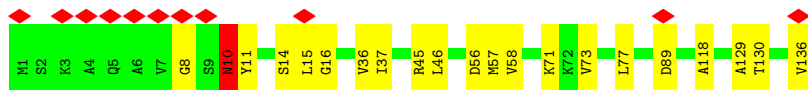
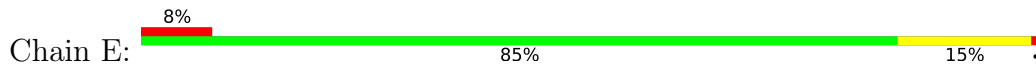




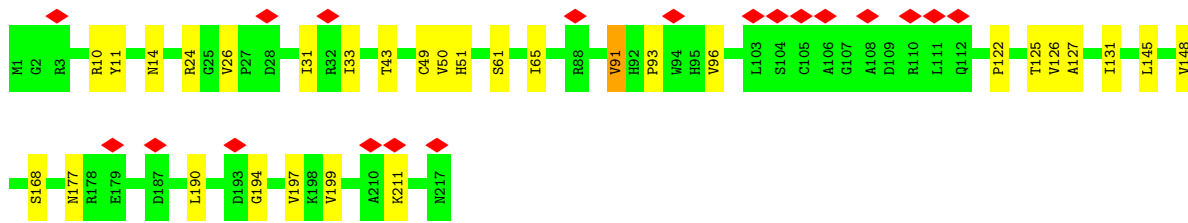
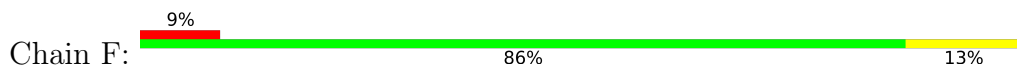
• Molecule 4: 60S RIBOSOMAL PROTEIN L12



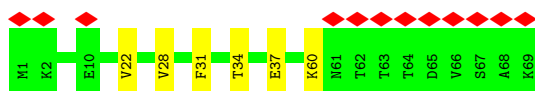
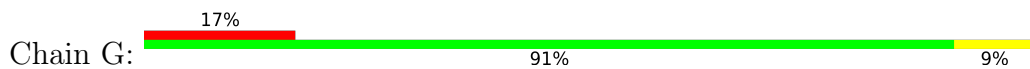
• Molecule 5: 60S RIBOSOMAL PROTEIN L23



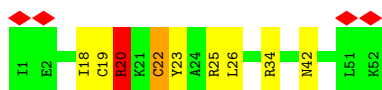
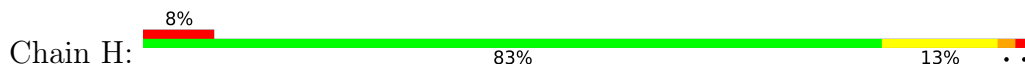
• Molecule 6: 60S RIBOSOMAL PROTEIN L10



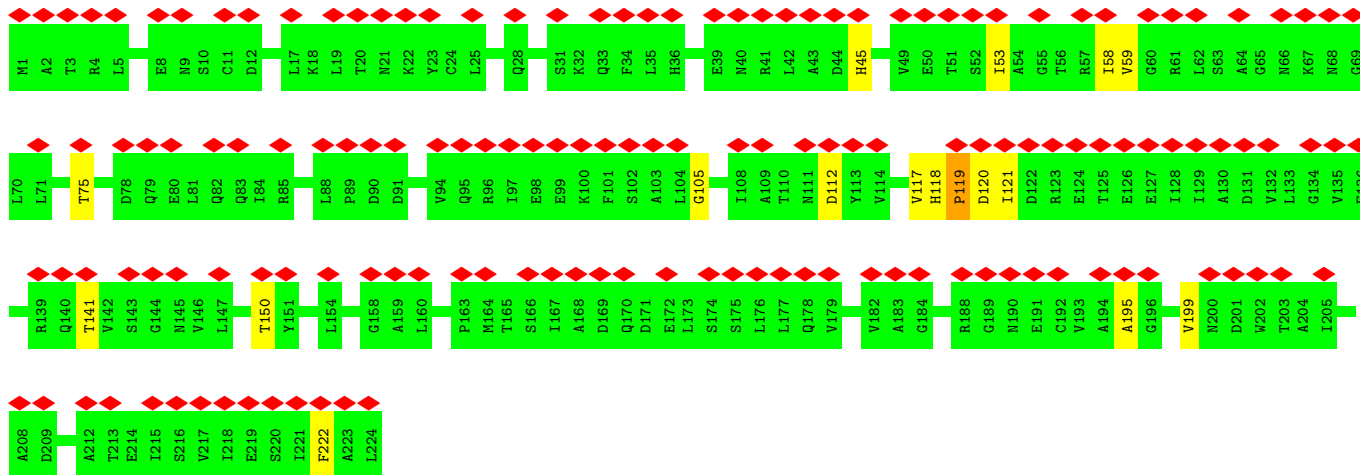
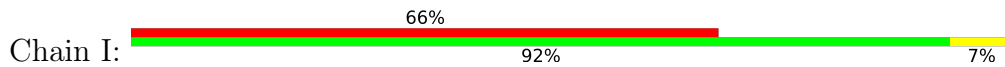
• Molecule 7: 60S RIBOSOMAL PROTEIN L24



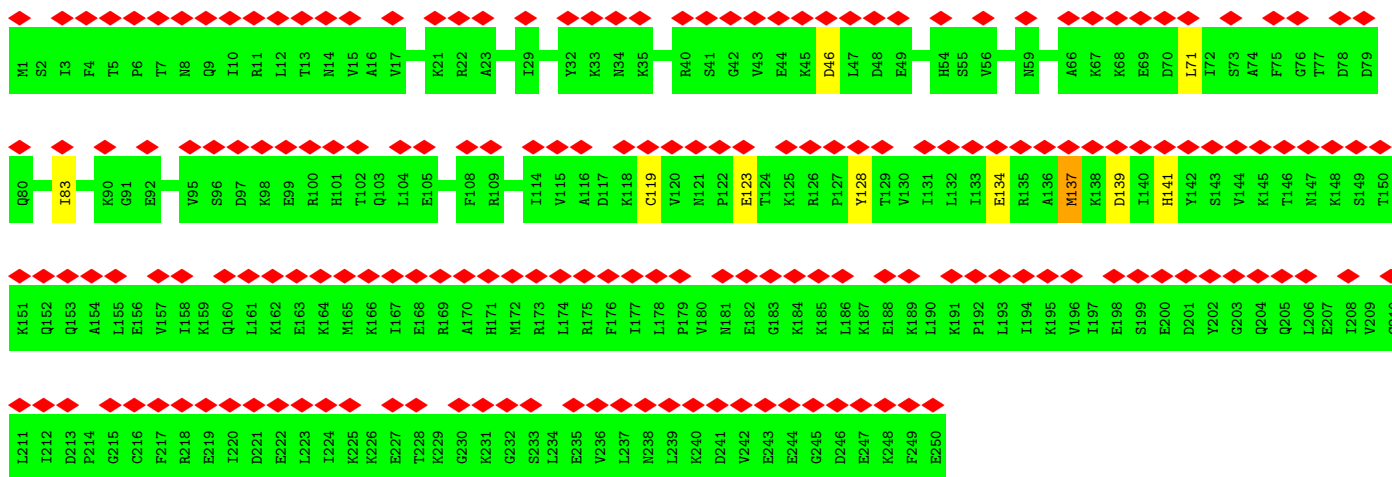
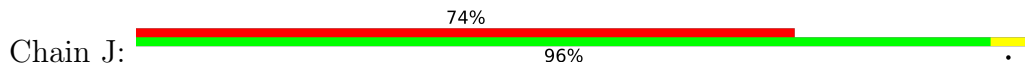
• Molecule 8: UBIQUITIN-60S RIBOSOMAL PROTEIN L40



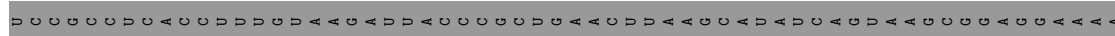
• Molecule 9: EUKARYOTIC TRANSLATION INITIATION FACTOR 6

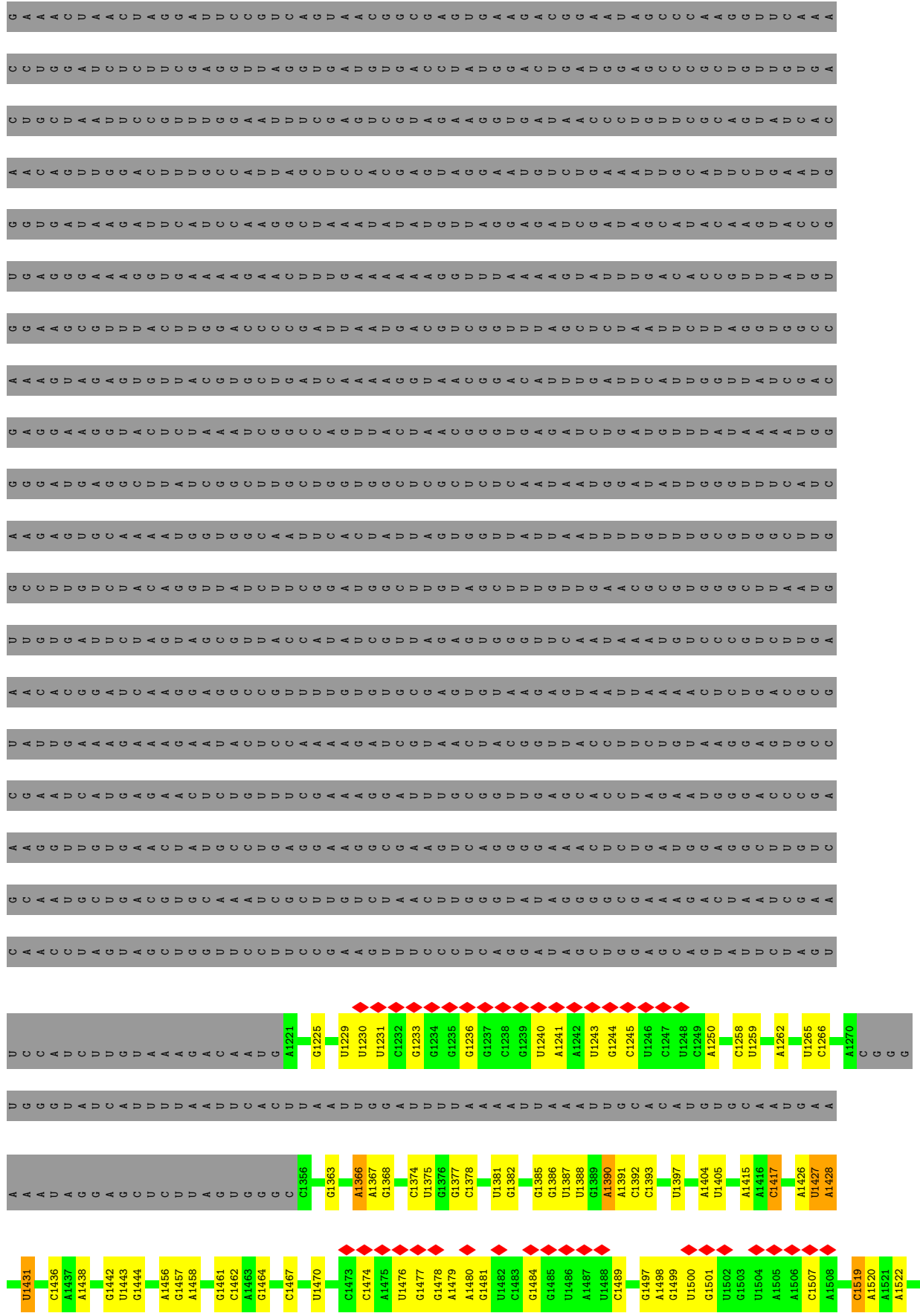


• Molecule 10: RIBOSOME MATURATION PROTEIN SBDS



• Molecule 11: 26S RIBOSOMAL RNA





A3000	G3127	A3220	C3378	A	C	C	U	A
A3007	U3128	G3228	C3379	U	A	A	U	A
G3010	G3129	A3229	C3384	G	U	U	G	U
U3014	A3132	A3230	U3392	C	U	A	A	U
G3015	G3133	G3231	A3395	U	A	A	U	U
U3016	A3134	C3232	G3396	A	C	A	U	U
A3022	A3135	G3245	G3397	A	C	U	G	U
G3023	U3016	U3246	A3401	A	U	U	U	U
A3024	G3143	G3251	U3402	G	U	A	A	C
G3025	A3150	C3261	U3402	C	A	A	A	C
U3026	U3151	C3262	G3414	U	U	U	U	U
A3027	A3155	A3268	U3415	A	A	U	U	U
A3029	G3156	A3269	G3416	U	A	A	U	U
G3032	G3157	A3270	A3417	A	A	U	U	U
A3036	C3158	G3271	C3418	A	A	U	U	U
A3037	U3159	G3272	C3419	C	U	C	U	U
A3038	G3164	C3275	C3422	U	C	U	C	U
G3039	C3165	G3275	C3425	U	C	U	C	U
C3040	A3166	G3278	U3426	C	U	C	U	C
G3043	G3167	A3279	A3427	G	U	A	U	A
C3044	C3168	G3280	C3428	U	A	G	U	U
U3045	C3169	C3281	A3430	A	C	A	C	A
U3046	G3172	U3282	G3283	A	C	A	C	A
G3047	C3173	G3284	A3442	C	C	A	C	A
C3059	U3176	G3285	U3443	U	C	C	U	U
A3060	G3177	U3286	G3444	U	C	A	U	U
G3061	A3178	U3287	C3445	A	C	A	U	U
U3062	G3181	U3288	C3446	C	A	C	U	U
G3070	C3182	A3304	C3453	G	U	A	U	U
A3084	G3186	G3305	C3456	U	C	U	C	U
G3085	C3187	C3316	U3457	U	C	U	C	U
G3086	U3188	C3317	A3458	A	U	C	U	U
C3089	G3189	C3318	C3462	C	C	A	A	A
A3095	C3190	U3319	A3466	G	U	A	U	U
G3104	U3193	G3323	U3467	G	U	U	U	U
U3105	G3204	C3328	A3477	G	G	U	U	U
G3106	A3205	A3329	C3480	A	C	A	A	A
C3107	U3208	A3330	G	U	U	U	U	U
A3110	G3209	U3331	C	A	C	A	A	A
A3111	U3210	U3332	A	U	U	U	U	U
U3116	G3211	G3339	A	C	A	G	G	G
C3120	C3212	A3347	C	U	U	C	C	C
	U3213	G3348	A	U	U	U	U	U
	G3214	C3349	C	A	U	U	U	U
	U3215	G3364	A	C	A	U	U	U
	U3216		A	C	A	U	U	U
	U3219		A	C	A	U	U	U

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	43063	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	2200	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	105263	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	1.554	Depositor
Minimum map value	-1.083	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.14	Depositor
Map size (\AA)	399.0, 399.0, 399.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.33, 1.33, 1.33	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.45	0/3241	0.78	1/4339 (0.0%)
2	B	0.37	0/1510	0.68	0/2030
3	C	0.38	0/1592	0.57	0/2142
4	D	0.37	0/1265	0.58	0/1702
5	E	0.36	0/1032	0.69	0/1386
6	F	0.38	0/1752	0.70	0/2345
7	G	0.44	0/600	0.67	0/801
8	H	0.39	0/433	0.77	0/571
9	I	0.37	0/1706	0.62	0/2325
10	J	0.38	0/2038	0.64	0/2727
11	N	0.35	0/27702	0.74	7/43160 (0.0%)
All	All	0.36	0/42871	0.72	8/63528 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
5	E	0	1
9	I	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	N	2995	G	C2'-C3'-O3'	8.84	128.96	109.50
11	N	1582	A	C2'-C3'-O3'	7.68	126.41	109.50
11	N	1565	G	C4'-C3'-O3'	6.44	125.88	113.00
11	N	1519	C	C2'-C3'-O3'	6.32	123.81	113.70
11	N	2515	G	C2'-C3'-O3'	6.02	123.33	113.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	16	PHE	Peptide
1	A	393	SER	Peptide
5	E	10	ASN	Peptide
9	I	118	HIS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3176	0	3319	26	0
2	B	1491	0	1555	8	0
3	C	1571	0	1657	1	0
4	D	1245	0	1338	1	0
5	E	1017	0	1076	11	0
6	F	1721	0	1778	14	0
7	G	586	0	601	2	0
8	H	427	0	483	5	0
9	I	1686	0	1685	7	0
10	J	2015	0	2112	2	0
11	N	24758	0	12487	174	0
All	All	39693	0	28091	238	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 4.

The worst 5 of 238 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:285:ILE:CD1	1:A:332:LEU:HD23	2.24	0.68
11:N:1415:A:N3	11:N:1564:C:O2'	2.26	0.67
6:F:96:VAL:HG12	6:F:125:THR:HG22	1.78	0.64
6:F:14:ASN:ND2	11:N:1363:G:OP2	2.29	0.64
5:E:36:VAL:HG13	5:E:58:VAL:HG13	1.79	0.63

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	396/398 (100%)	328 (83%)	50 (13%)	18 (4%)	2	15
2	B	186/188 (99%)	169 (91%)	14 (8%)	3 (2%)	9	36
3	C	203/205 (99%)	185 (91%)	15 (7%)	3 (2%)	10	38
4	D	164/166 (99%)	142 (87%)	17 (10%)	5 (3%)	4	24
5	E	134/136 (98%)	114 (85%)	13 (10%)	7 (5%)	2	13
6	F	215/217 (99%)	188 (87%)	21 (10%)	6 (3%)	5	25
7	G	67/69 (97%)	62 (92%)	4 (6%)	1 (2%)	10	38
8	H	50/52 (96%)	40 (80%)	8 (16%)	2 (4%)	3	18
9	I	222/224 (99%)	199 (90%)	17 (8%)	6 (3%)	5	26
10	J	248/250 (99%)	232 (94%)	13 (5%)	3 (1%)	13	42
All	All	1885/1905 (99%)	1659 (88%)	172 (9%)	54 (3%)	7	24

5 of 54 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	249	LEU
2	B	138	ALA
5	E	46	LEU
9	I	119	PRO
1	A	285	ILE

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	A	337/337 (100%)	317 (94%)	20 (6%)	19	49
2	B	168/168 (100%)	162 (96%)	6 (4%)	35	63
3	C	172/172 (100%)	169 (98%)	3 (2%)	60	78
4	D	139/139 (100%)	138 (99%)	1 (1%)	84	90
5	E	108/108 (100%)	104 (96%)	4 (4%)	34	63
6	F	180/180 (100%)	176 (98%)	4 (2%)	52	74
7	G	65/65 (100%)	64 (98%)	1 (2%)	65	81
8	H	48/48 (100%)	44 (92%)	4 (8%)	11	36
9	I	190/190 (100%)	189 (100%)	1 (0%)	88	93
10	J	228/228 (100%)	224 (98%)	4 (2%)	59	78
All	All	1635/1635 (100%)	1587 (97%)	48 (3%)	45	69

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	193	ASP
6	F	131	ILE
4	D	159	GLU
5	E	45	ARG
6	F	168	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	135	ASN
2	B	147	ASN
6	F	177	ASN
4	D	103	ASN
6	F	133	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	N	1158/3741 (30%)	216 (18%)	36 (3%)

5 of 216 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	N	1225	G
11	N	1229	U
11	N	1230	U
11	N	1231	U
11	N	1233	G

5 of 36 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	N	3231	G
11	N	3477	A
11	N	3283	G
11	N	3391	C
11	N	1582	A

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.

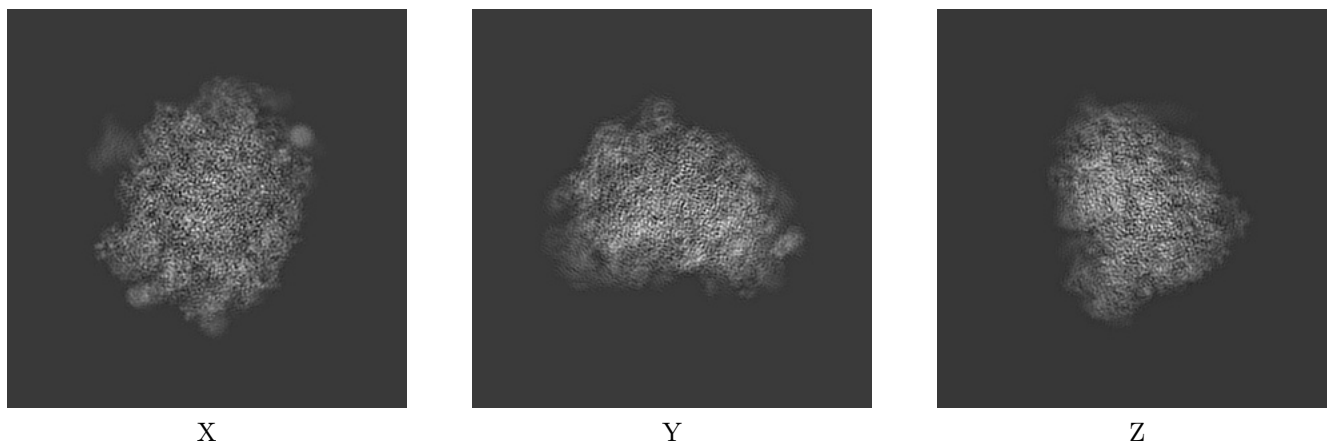
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3145. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

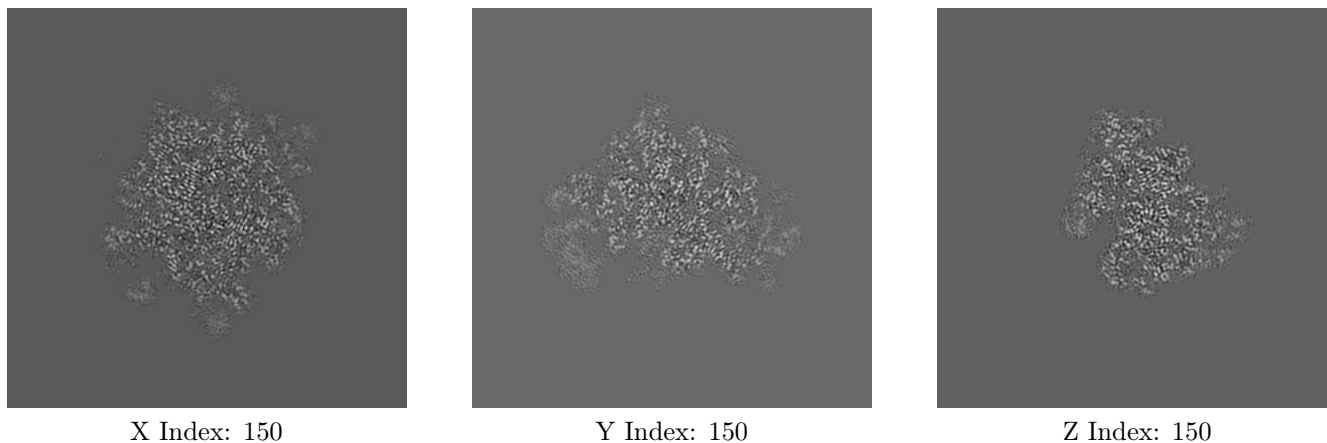
6.1.1 Primary map



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

6.2 Central slices [i](#)

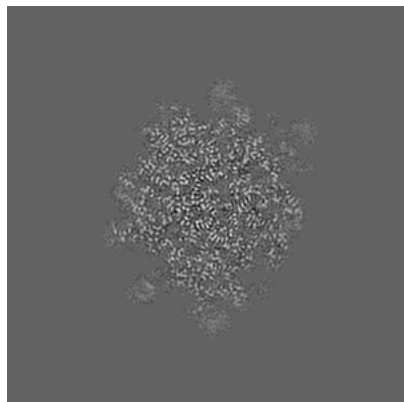
6.2.1 Primary map



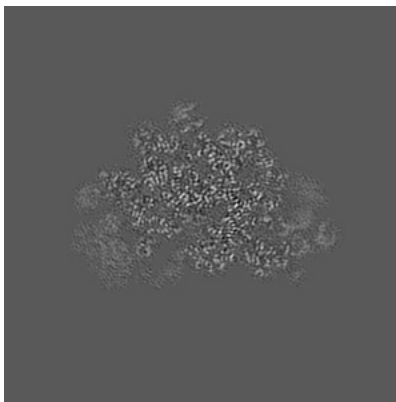
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

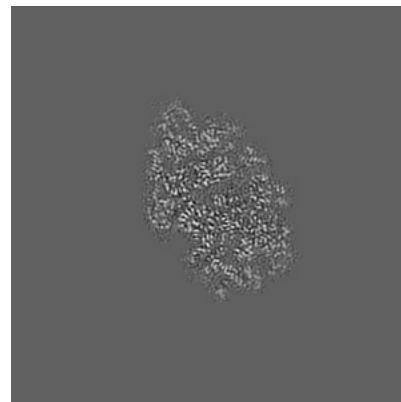
6.3.1 Primary map



X Index: 153



Y Index: 155

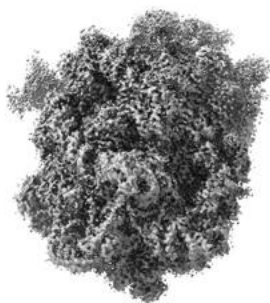


Z Index: 161

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 0.14. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

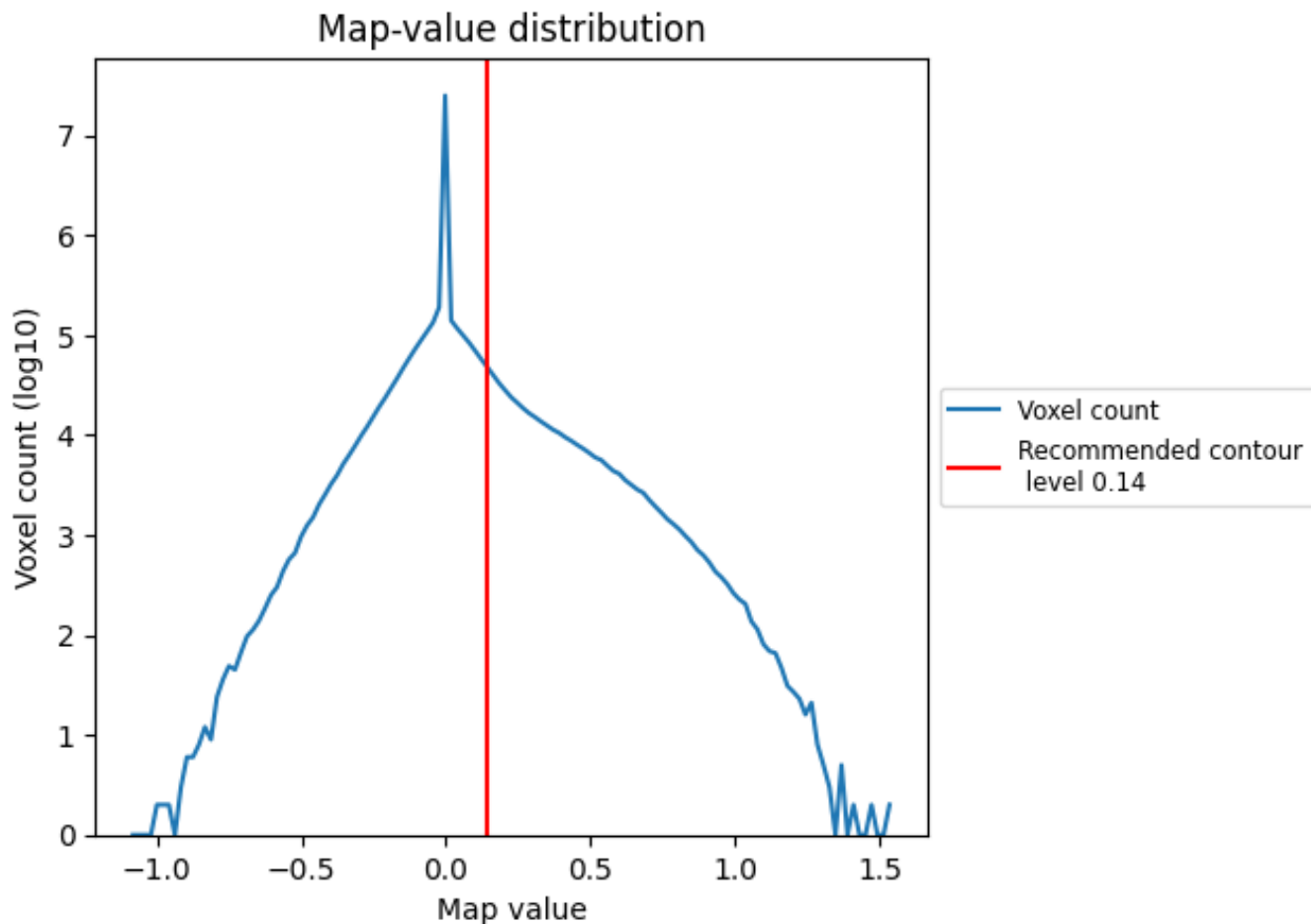
6.5 Mask visualisation

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

7 Map analysis [i](#)

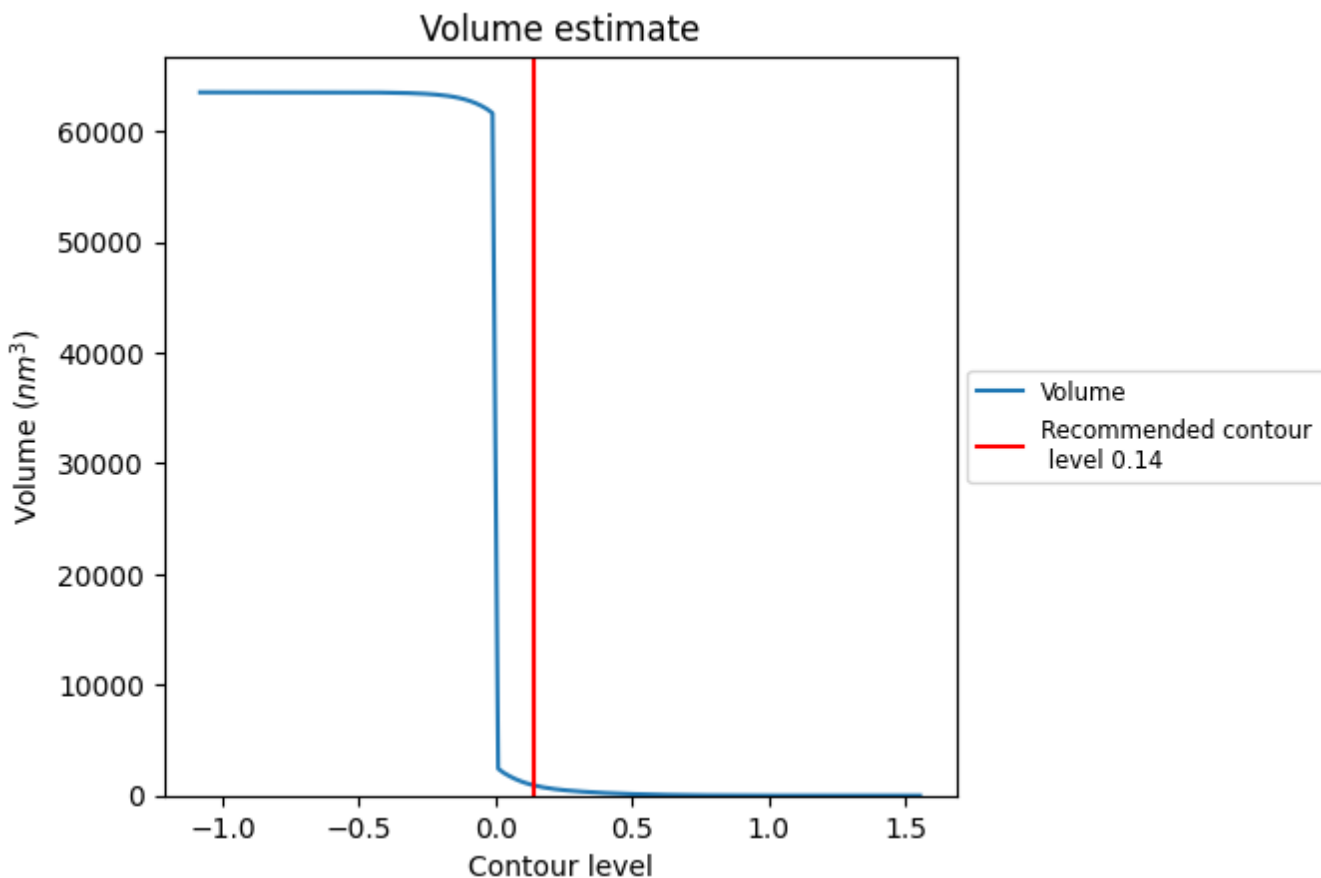
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

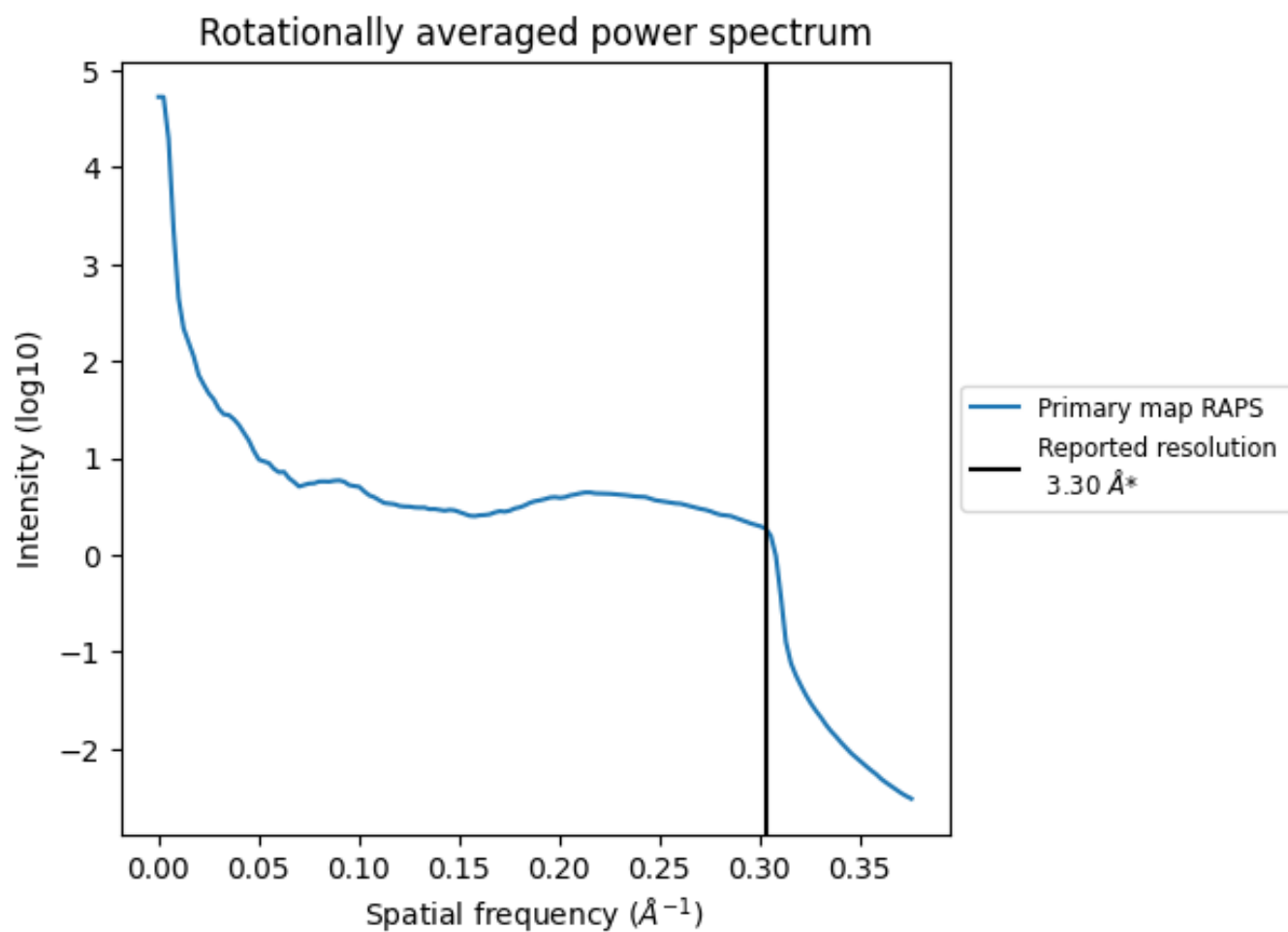
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 926 nm³; this corresponds to an approximate mass of 837 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

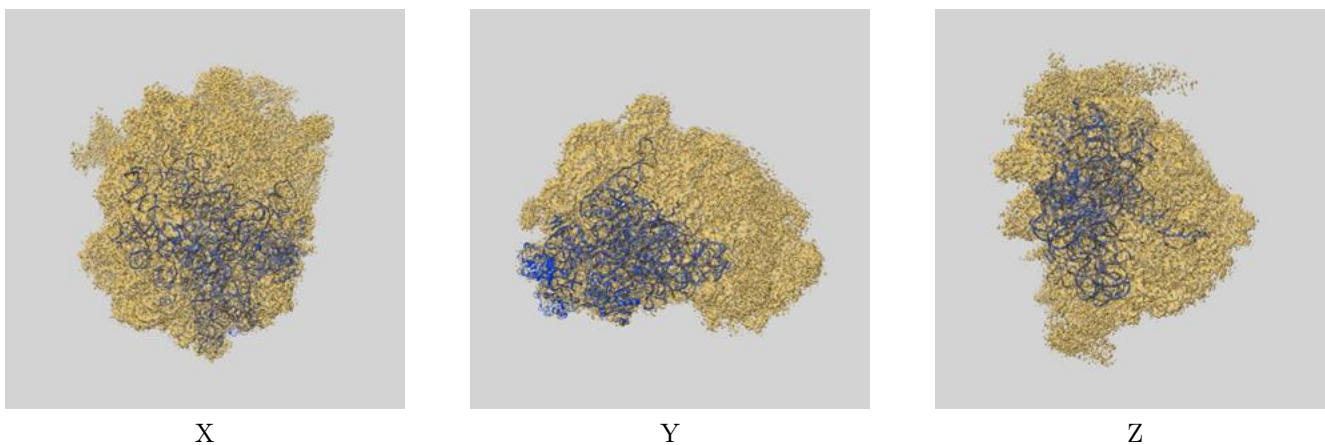
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

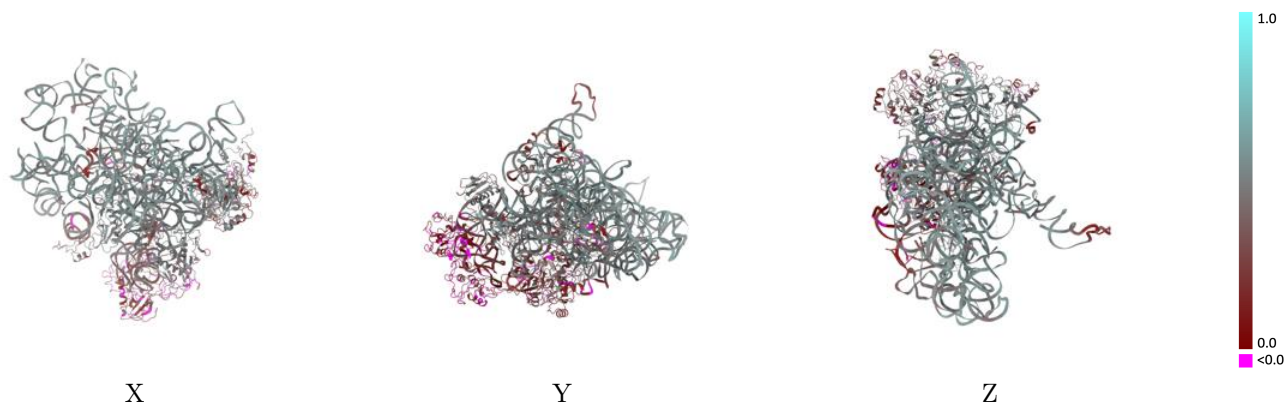
This section contains information regarding the fit between EMDB map EMD-3145 and PDB model 5AN9. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



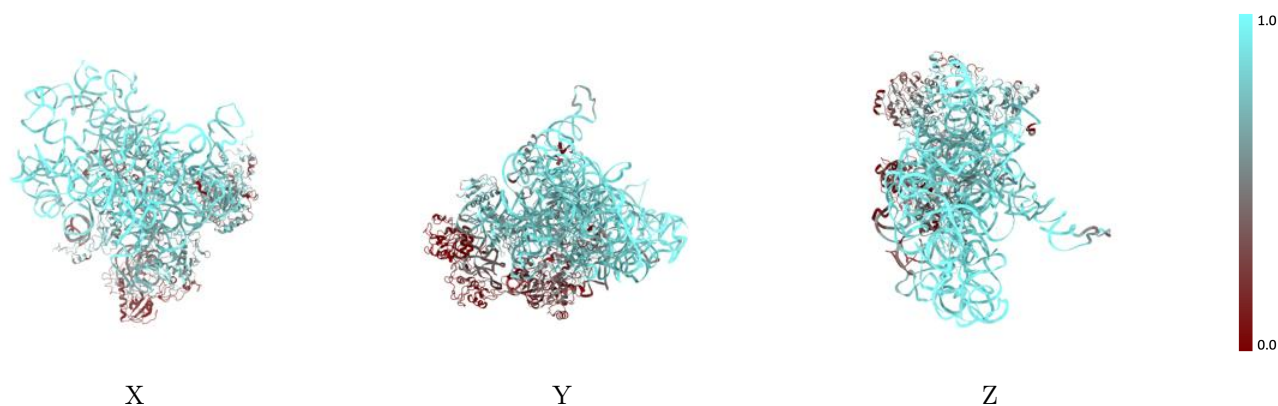
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



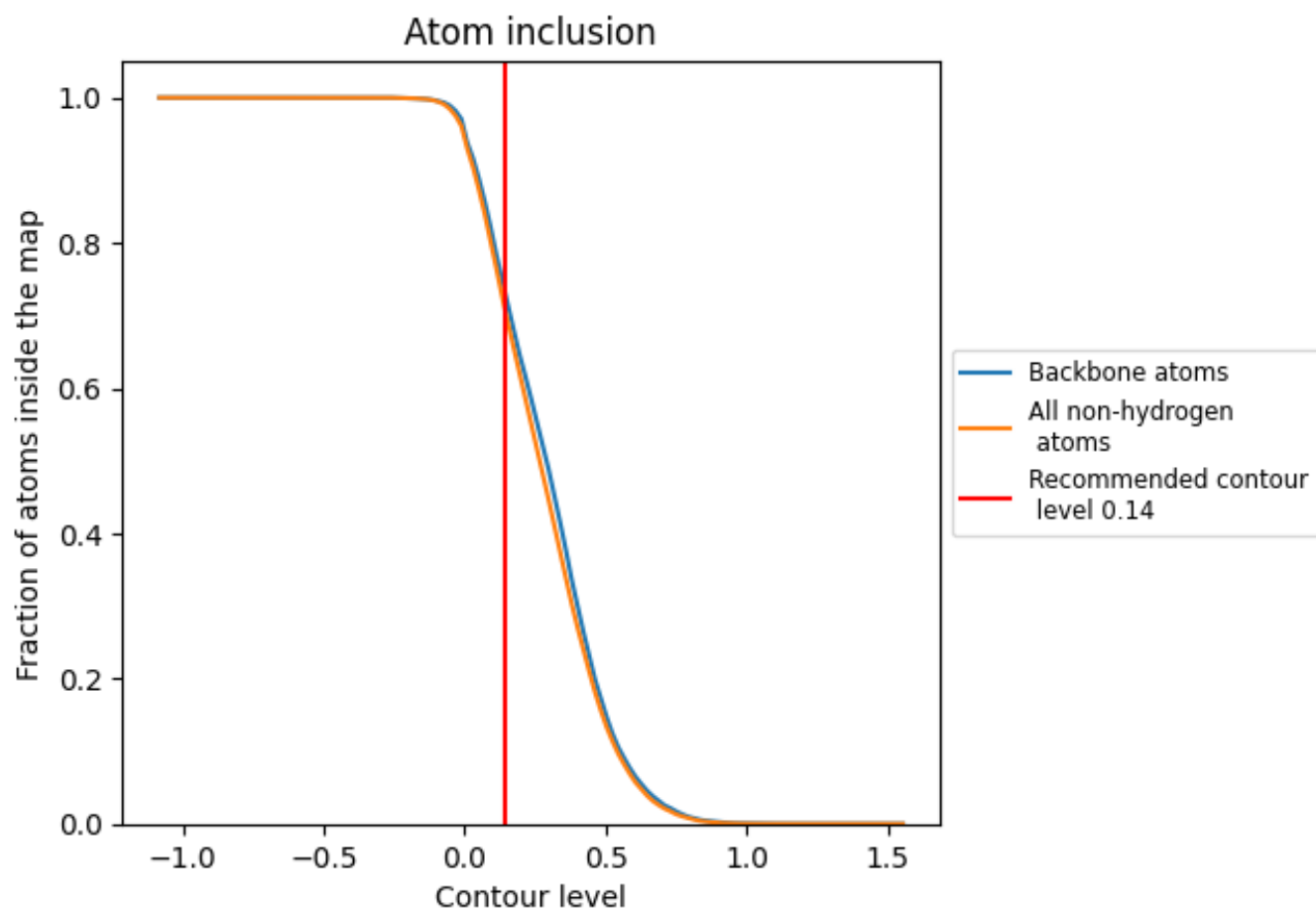
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.14).

























9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7128	 0.4230
A	 0.7032	 0.4140
B	 0.6619	 0.4100
C	 0.0742	 0.1170
D	 0.0909	 0.1010
E	 0.7392	 0.4670
F	 0.6843	 0.4240
G	 0.6261	 0.3910
H	 0.7167	 0.4310
I	 0.3289	 0.2950
J	 0.2843	 0.2180
N	 0.8508	 0.4840

