



wwPDB EM Validation Summary Report ⓘ

Nov 2, 2024 – 04:29 pm GMT

PDB ID : 6HIY
EMDB ID : EMD-0232
Title : Cryo-EM structure of the Trypanosoma brucei mitochondrial ribosome - This entry contains the body of the small mitoribosomal subunit in complex with mt-IF-3
Authors : Ramrath, D.J.F.; Niemann, M.; Leibundgut, M.; Bieri, P.; Prange, C.; Horn, E.K.; Leitner, A.; Boehringer, D.; Schneider, A.; Ban, N.
Deposited on : 2018-08-31
Resolution : 3.27 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

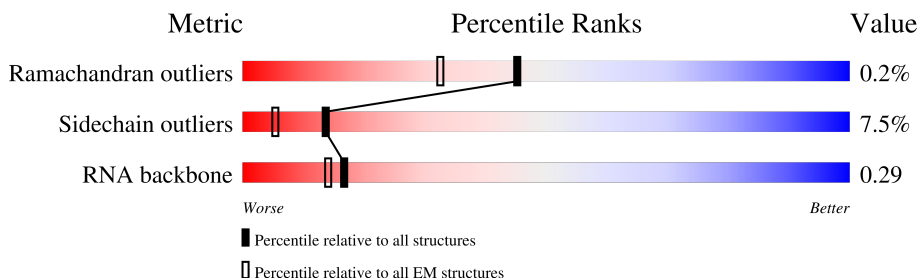
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.27 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.










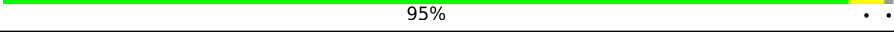



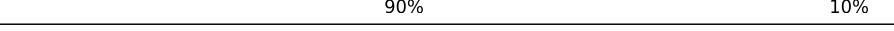







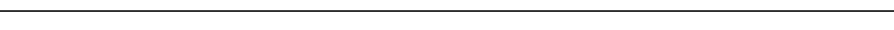

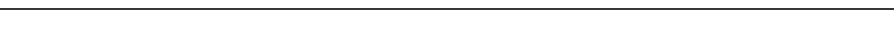
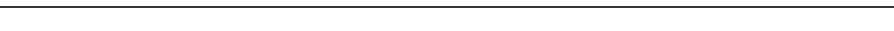


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	DA	1788	
2	DD	812	
3	DI	407	
4	DL	307	
5	DM	294	
6	DN	293	
7	DO	282	
8	DP	274	

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Mol	Chain	Length	Quality of chain
9	DQ	268	 92% . .
10	DR	270	 85% 7% 7%
11	DS	261	 87% 5% 9%
12	DU	228	 86% 8% 7%
13	DZ	94	 84% . 13%
14	Da	64	 80% 6% 14%
15	CE	435	 86% 9% .
16	CF	160	 95% . .
17	CH	282	 88% 9% .
18	CI	443	 43% . 54%
19	CK	326	 68% 6% 26%
20	CL	87	 90% 10%
21	CO	429	 78% 6% 16%
22	CP	188	 89% 7% .
23	CQ	307	 55% 7% 38%
24	CR	320	 92% 6% .
25	CU	193	 90% 5% 5%
26	CZ	360	 39% . 58%
27	Ca	602	 90% 8% .
28	Cb	324	 73% 5% 22%
29	Cd	440	 61% 5% 34%
30	Cj	257	 82% 6% 12%
31	Cm	215	 80% 12% 9%
32	Cn	250	 42% . 56%
33	Cp	187	 87% 6% 6%

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Mol	Chain	Length	Quality of chain
34	Cq	263	 89% 6%
35	Cr	439	 53% 5% 41%
36	Cv	1211	 82% 6% 13%
37	CA	621	 42% 34% 23%
38	UQ	32	 100%
39	UR	8	 100%
40	US	54	 100%
41	UT	44	 100%

2 Entry composition

There are 45 unique types of molecules in this entry. The entry contains 100780 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 mS48.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	DA	1426	Total	C	N	O	S	0	0
			11489	7252	2052	2151	34		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DA	894	HIS	ASN	conflict	UNP Q57UJ2
DA	1181	THR	ILE	conflict	UNP Q57UJ2
DA	1333	ALA	VAL	conflict	UNP Q57UJ2
DA	1700	ARG	HIS	conflict	UNP Q57UJ2
DA	1761	LYS	ARG	conflict	UNP Q57UJ2

- Molecule 2 is a protein called mS51.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	DD	791	Total	C	N	O	S	0	0
			6523	4127	1184	1171	41		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DD	371	PRO	SER	conflict	UNP Q385L8
DD	599	ALA	VAL	conflict	UNP Q385L8

- Molecule 3 is a protein called mS56.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	DI	390	Total	C	N	O	S	0	0
			3182	2020	554	594	14		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DI	92	GLU	GLY	conflict	UNP Q587C2
DI	116	ASP	GLU	conflict	UNP Q587C2

- Molecule 4 is a protein called mS59.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	DL	140	Total	C	N	O	S	0	0
			1134	718	208	199	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DL	274	THR	ALA	conflict	UNP Q38BS2

- Molecule 5 is a protein called mS60.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	DM	294	Total	C	N	O	S	0	0
			2430	1533	459	426	12		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DM	69	PHE	TYR	conflict	UNP Q57XL2
DM	97	ASN	SER	conflict	UNP Q57XL2
DM	138	SER	PRO	conflict	UNP Q57XL2
DM	173	ALA	THR	conflict	UNP Q57XL2
DM	206	ALA	THR	conflict	UNP Q57XL2

- Molecule 6 is a protein called mS61.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	DN	257	Total	C	N	O	S	0	0
			2091	1331	379	371	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DN	51	GLY	SER	conflict	UNP Q38D60

- Molecule 7 is a protein called mS62.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	DO	222	Total	C	N	O	S	0	0
			1804	1127	327	340	10		

- Molecule 8 is a protein called mS63.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	DP	207	Total	C	N	O	S	0	0
			1760	1132	312	307	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DP	3	HIS	ARG	conflict	UNP Q38F25

- Molecule 9 is a protein called mS64.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	DQ	256	Total	C	N	O	S	0	0
			2061	1293	389	370	9		

- Molecule 10 is a protein called mS65.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	DR	251	Total	C	N	O	S	0	0
			2025	1304	369	342	10		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DR	65	GLY	SER	conflict	UNP Q57UA2
DR	94	GLY	GLU	conflict	UNP Q57UA2
DR	128	PRO	SER	conflict	UNP Q57UA2
DR	229	ARG	GLN	conflict	UNP Q57UA2

- Molecule 11 is a protein called mS66.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	DS	238	Total	C	N	O	S	0	0
			1904	1185	356	348	15		

- Molecule 12 is a protein called mS68.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	DU	213	Total	C	N	O	S	0	0
			1754	1103	310	335	6		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DU	119	ILE	LEU	conflict	UNP Q582T9
DU	152	ILE	VAL	conflict	UNP Q582T9

- Molecule 13 is a protein called mS73.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	DZ	82	Total	C	N	O	S	0	0
			697	457	113	123	4		

- Molecule 14 is a protein called mS74.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Da	55	Total	C	N	O	S	0	0
			501	315	109	74	3		

- Molecule 15 is a protein called mS55m.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	CE	417	Total	C	N	O	S	0	0
			3399	2151	632	600	16		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CE	341	ARG	LYS	conflict	UNP Q38AX6

- Molecule 16 is a protein called bS6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	CF	159	Total	C	N	O	S	0	0
			1292	821	228	237	6		

- Molecule 17 is a protein called uS8m.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	CH	273	Total	C	N	O	S	0	0
			2228	1387	432	398	11		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CH	74	ASN	SER	conflict	UNP Q388R7

- Molecule 18 is a protein called uS9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	CI	202	Total	C	N	O	S	0	0
			1632	1035	281	309	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CI	370	ALA	VAL	conflict	UNP Q57W62

- Molecule 19 is a protein called uS11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	CK	241	Total	C	N	O	S	0	0
			1980	1234	368	363	15		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CK	3	ARG	GLN	conflict	UNP Q389T7
CK	138	UNK	ILE	conflict	UNP Q389T7

- Molecule 20 is a protein called uS12m.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	CL	87	Total	C	N	O	S	0	0
			733	503	113	107	10		

- Molecule 21 is a protein called uS15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	CO	361	Total	C	N	O	S	0	0
			3003	1907	560	520	16		

- Molecule 22 is a protein called bS16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	CP	180	Total	C	N	O	S	0	0
			1489	956	274	250	9		

- Molecule 23 is a protein called uS17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	CQ	190	Total	C	N	O	S	0	0
			1584	1015	302	259	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CQ	138	ALA	VAL	conflict	UNP Q38DP8

- Molecule 24 is a protein called bS18m.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	CR	314	Total	C	N	O	S	0	0
			2567	1623	471	465	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CR	8	ILE	VAL	conflict	UNP Q38AS2

- Molecule 25 is a protein called uS21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	CU	184	Total	C	N	O	S	0	0
			1538	965	307	254	12		

- Molecule 26 is a protein called mt-IF-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	CZ	151	Total	C	N	O	S	0	0
			1212	759	231	215	7		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CZ	6	SER	GLY	conflict	UNP Q57WU2
CZ	30	THR	ILE	conflict	UNP Q57WU2
CZ	172	THR	ALA	conflict	UNP Q57WU2

- Molecule 27 is a protein called mS22.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Ca	592	Total	C	N	O	S	0	0
			5004	3201	898	882	23		

- Molecule 28 is a protein called mS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Cb	252	Total	C	N	O	S	0	0
			2056	1300	368	380	8		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Cb	244	SER	ASN	conflict	UNP Q57VB2
Cb	?	-	GLU	deletion	UNP Q57VB2
Cb	312	CYS	-	expression tag	UNP Q57VB2
Cb	313	SER	-	expression tag	UNP Q57VB2
Cb	314	ARG	-	expression tag	UNP Q57VB2
Cb	315	ASP	-	expression tag	UNP Q57VB2
Cb	316	GLY	-	expression tag	UNP Q57VB2
Cb	317	PHE	-	expression tag	UNP Q57VB2
Cb	318	ALA	-	expression tag	UNP Q57VB2
Cb	319	LEU	-	expression tag	UNP Q57VB2
Cb	320	MET	-	expression tag	UNP Q57VB2
Cb	321	LYS	-	expression tag	UNP Q57VB2
Cb	322	ALA	-	expression tag	UNP Q57VB2
Cb	323	ASN	-	expression tag	UNP Q57VB2
Cb	324	LYS	-	expression tag	UNP Q57VB2

- Molecule 29 is a protein called mS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Cd	291	Total	C	N	O	S	0	0
			2389	1491	442	446	10		

- Molecule 30 is a protein called mS34.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Cj	226	Total	C	N	O	S	0	0
			1792	1138	310	340	4		

- Molecule 31 is a protein called mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Cm	196	Total	C	N	O	S	0	0
			1577	975	304	289	9		

- Molecule 32 is a protein called mS38.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Cn	110	Total	C	N	O	S	0	0
			912	585	181	143	3		

- Molecule 33 is a protein called mS41.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Cp	175	Total	C	N	O	S	0	0
			1483	937	268	273	5		

- Molecule 34 is a protein called mS42.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Cq	252	Total	C	N	O	S	0	0
			2005	1285	342	369	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Cq	48	THR	ALA	conflict	UNP Q586A1
Cq	167	MET	VAL	conflict	UNP Q586A1

- Molecule 35 is a protein called mS43.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Cr	257	Total	C	N	O	S	0	0
			1999	1261	368	356	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Cr	351	LYS	GLU	conflict	UNP Q585I1

- Molecule 36 is a protein called mS47.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Cv	1059	Total	C	N	O	S	0	0
			8557	5387	1535	1596	39		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Cv	16	CYS	PRO	conflict	UNP Q383R4
Cv	718	THR	ALA	conflict	UNP Q383R4
Cv	1179	GLU	GLY	conflict	UNP Q383R4

- Molecule 37 is a RNA chain called 9S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	CA	478	Total	C	N	O	P	0	0
			10092	4542	1705	3367	478		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CA	298	U	C	conflict	GB 343546
CA	614	U	-	insertion	GB 343546
CA	615	U	-	insertion	GB 343546
CA	616	U	-	insertion	GB 343546
CA	617	U	-	insertion	GB 343546
CA	618	U	-	insertion	GB 343546
CA	619	U	-	insertion	GB 343546
CA	620	U	-	insertion	GB 343546
CA	621	U	-	insertion	GB 343546

- Molecule 38 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	UQ	32	Total	C	N	O	0	0
			192	128	32	32		

- Molecule 39 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	UR	8	Total	C	N	O	0	0
			48	32	8	8		

- Molecule 40 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	US	54	Total	C	N	O	0	0
			324	216	54	54		

- Molecule 41 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	UT	44	Total	C	N	O	0	0
			264	176	44	44		

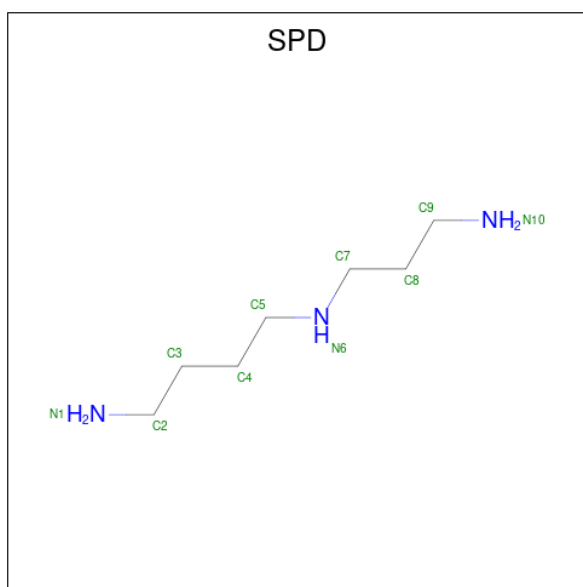
- Molecule 42 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
42	DA	1	Total	Zn	0
			1	1	
42	DS	2	Total	Zn	0
			2	2	
42	Cr	1	Total	Zn	0
			1	1	

- Molecule 43 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

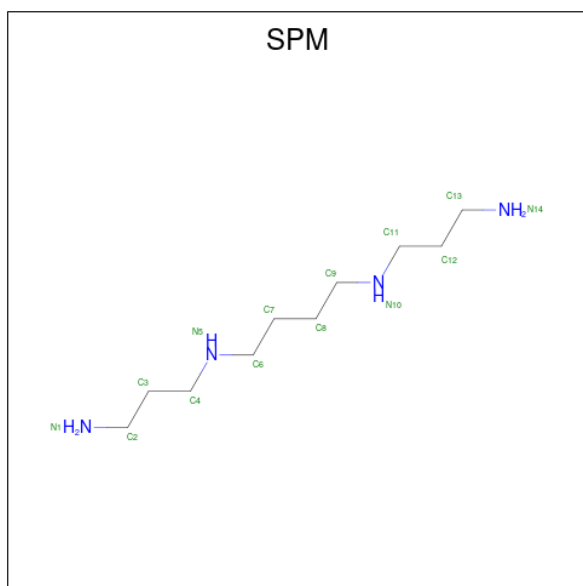
Mol	Chain	Residues	Atoms		AltConf
43	CO	1	Total	Mg	0
			1	1	
43	CQ	1	Total	Mg	0
			1	1	
43	Ca	1	Total	Mg	0
			1	1	
43	Cv	1	Total	Mg	0
			1	1	
43	CA	32	Total	Mg	0
			32	32	

- Molecule 44 is SPERMIDINE (three-letter code: SPD) (formula: C₇H₁₉N₃).

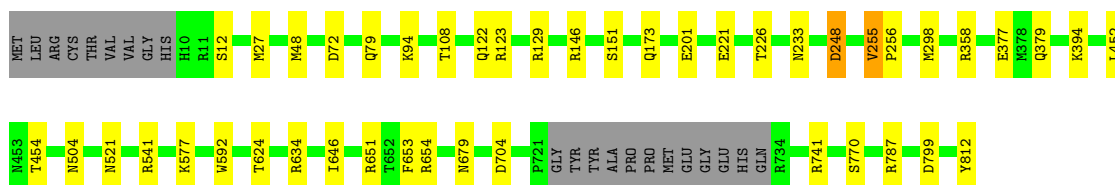


Mol	Chain	Residues	Atoms			AltConf
44	CA	1	Total	C	N	0
			10	7	3	
44	CA	1	Total	C	N	0
			10	7	3	

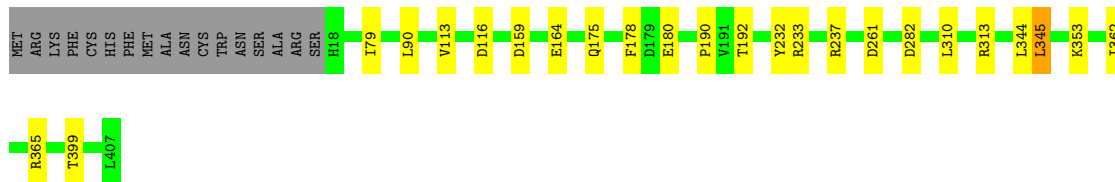
- Molecule 45 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



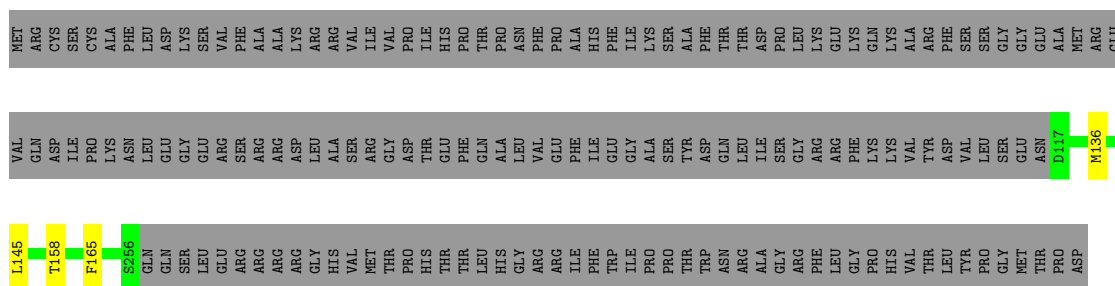
Mol	Chain	Residues	Atoms			AltConf
45	CA	1	Total	C	N	0
			14	10	4	



• Molecule 3: mS56



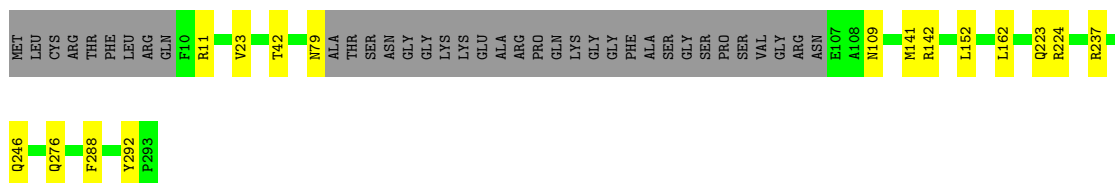
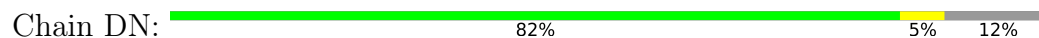
• Molecule 4: mS59



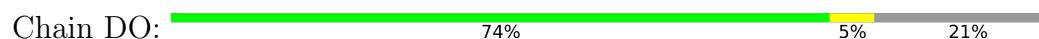
• Molecule 5: mS60

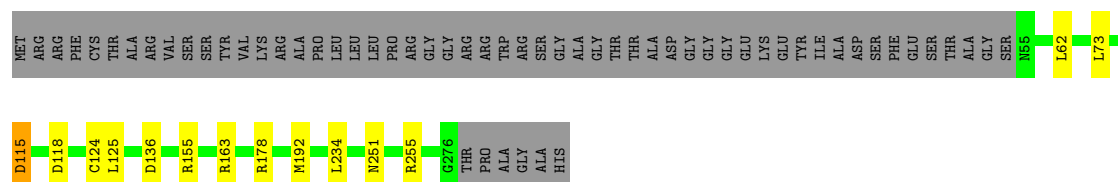


• Molecule 6: mS61

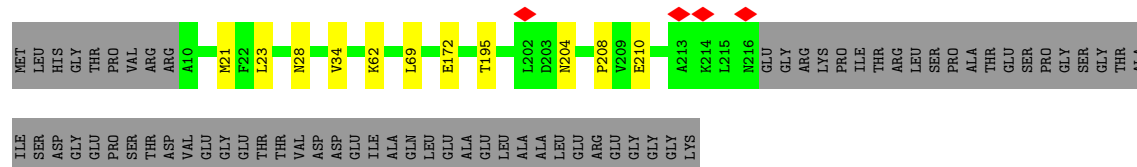
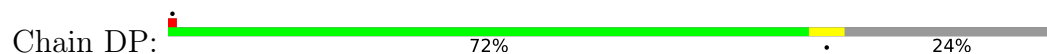


• Molecule 7: mS62





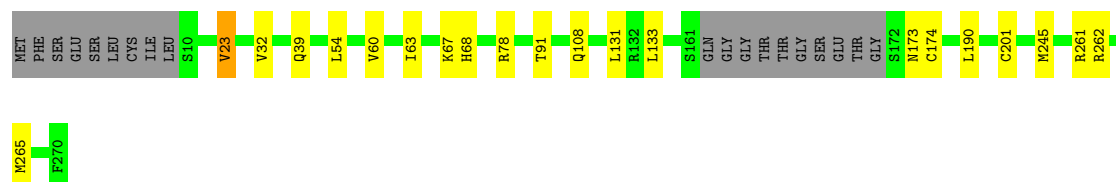
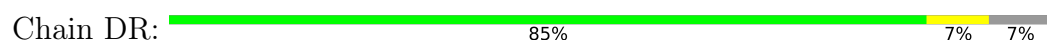
• Molecule 8: mS63



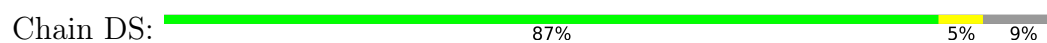
• Molecule 9: mS64



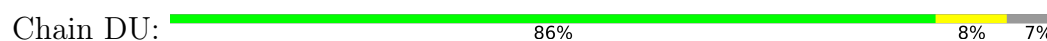
• Molecule 10: mS65



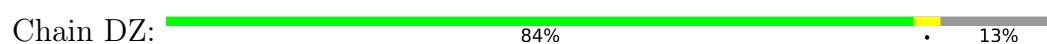
• Molecule 11: mS66



• Molecule 12: mS68

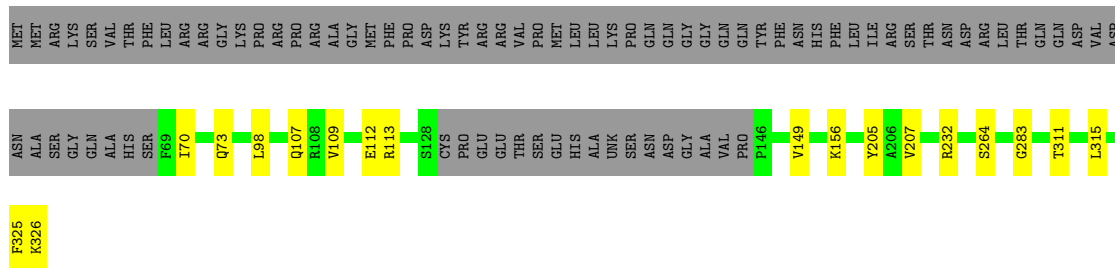


• Molecule 13: mS73



- Molecule 19: uS11m

Chain CK:



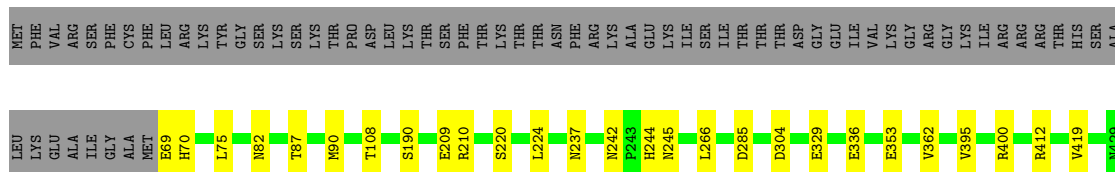
- Molecule 20: uS12m

Chain CL:



- Molecule 21: uS15m

Chain CO:



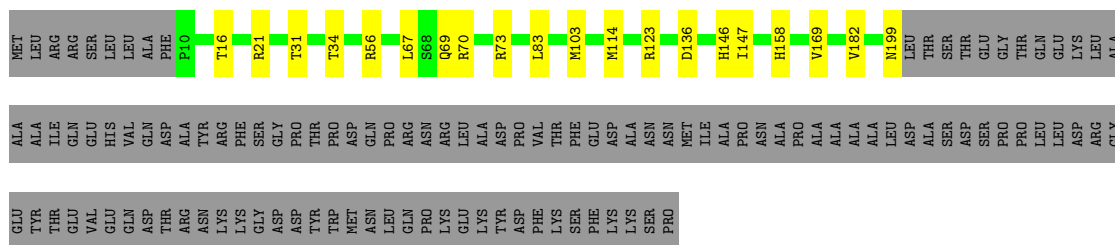
- Molecule 22: bS16m

Chain CP:



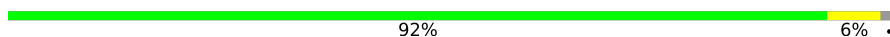
- Molecule 23: uS17m

Chain CQ:

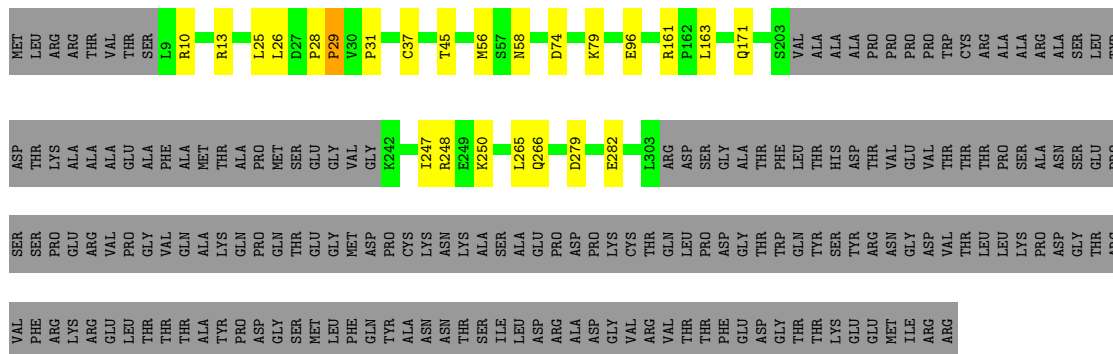


- Molecule 24: bS18m

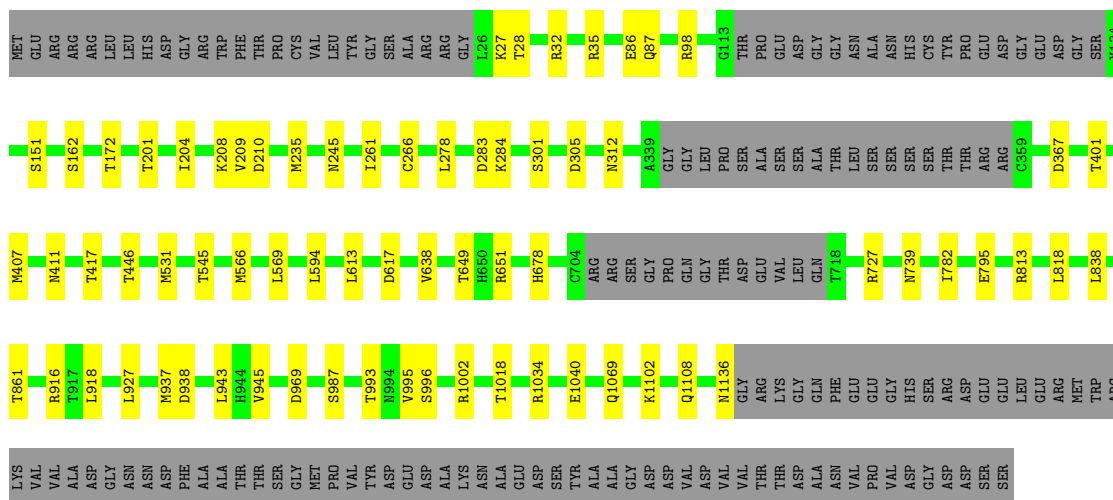
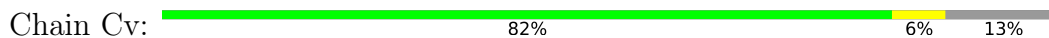
Chain CR:



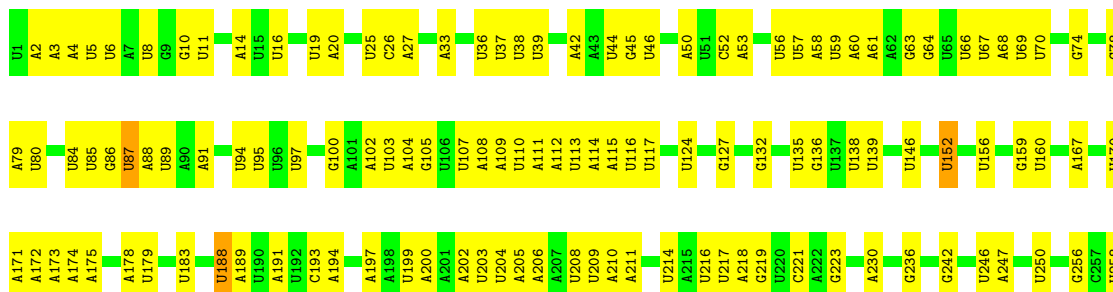
- Molecule 35: mS43

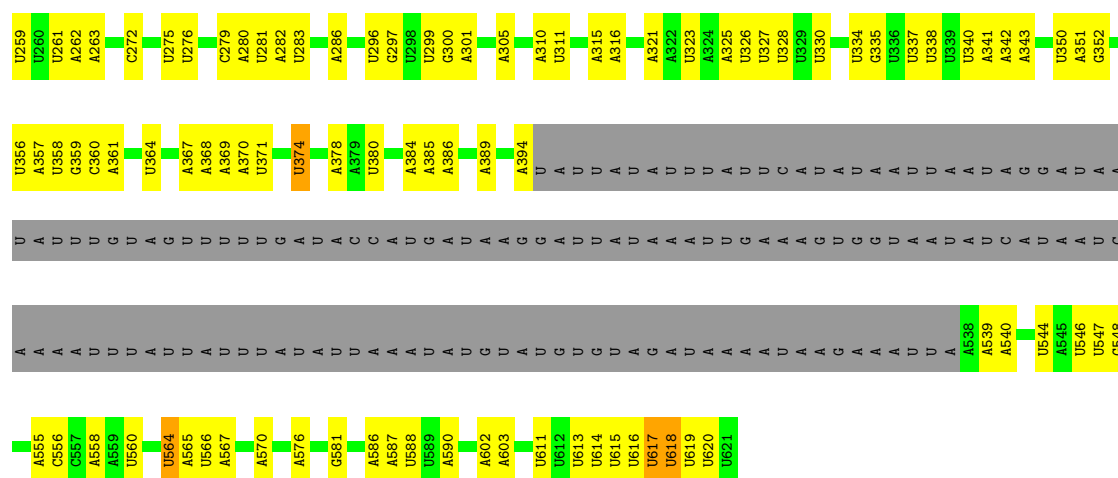


- Molecule 36: mS47



- Molecule 37: 9S rRNA





- Molecule 38: Unknown protein

Chain UQ: 100%

There are no outlier residues recorded for this chain.

- Molecule 39: Unknown protein

Chain UR: 100%

There are no outlier residues recorded for this chain.

- Molecule 40: Unknown protein

Chain US: 100%

There are no outlier residues recorded for this chain.

- Molecule 41: Unknown protein

Chain UT: 100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31911	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 ($e^-/\text{\AA}^2$)	40	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	0.514	Depositor
Minimum map value	-0.265	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.0115	Depositor
Map size (Å)	444.8, 444.8, 444.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	DA	0.38	1/11769 (0.0%)	0.55	2/15925 (0.0%)
2	DD	0.38	0/6710	0.56	1/9087 (0.0%)
3	DI	0.37	0/3248	0.57	2/4401 (0.0%)
4	DL	0.41	0/1160	0.56	0/1560
5	DM	0.39	0/2488	0.55	0/3362
6	DN	0.40	0/2148	0.59	0/2916
7	DO	0.38	0/1840	0.56	0/2482
8	DP	0.52	1/1813 (0.1%)	0.56	0/2457
9	DQ	0.37	0/2111	0.56	0/2863
10	DR	0.36	0/2090	0.56	0/2849
11	DS	0.35	0/1950	0.52	0/2633
12	DU	0.38	0/1799	0.54	0/2438
13	DZ	0.38	0/725	0.55	0/984
14	Da	0.40	0/520	0.54	0/694
15	CE	0.40	0/3484	0.56	0/4708
16	CF	0.38	0/1319	0.53	0/1783
17	CH	0.42	0/2276	0.55	0/3071
18	CI	0.37	0/1670	0.51	0/2260
19	CK	0.37	0/2024	0.56	1/2715 (0.0%)
20	CL	0.42	0/759	0.55	0/1026
21	CO	0.38	0/3085	0.54	0/4165
22	CP	0.42	0/1533	0.57	0/2074
23	CQ	0.46	0/1631	0.59	0/2203
24	CR	0.39	0/2640	0.55	0/3572
25	CU	0.38	0/1576	0.52	0/2115
26	CZ	0.39	0/1237	0.54	1/1659 (0.1%)
27	Ca	0.40	0/5159	0.55	3/6980 (0.0%)
28	Cb	0.39	0/2105	0.54	0/2842
29	Cd	0.40	0/2446	0.51	0/3299
30	Cj	0.35	0/1842	0.55	0/2511
31	Cm	0.42	0/1616	0.60	1/2175 (0.0%)
32	Cn	0.40	0/934	0.57	0/1248

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Cp	0.36	0/1528	0.51	0/2072
34	Cq	0.40	0/2066	0.54	0/2815
35	Cr	0.36	0/2038	0.56	3/2759 (0.1%)
36	Cv	0.37	0/8780	0.55	0/11901
37	CA	0.51	1/11286 (0.0%)	0.96	16/17548 (0.1%)
All	All	0.40	3/103405 (0.0%)	0.62	30/142152 (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	DA	0	1
2	DD	0	2
6	DN	0	2
7	DO	0	2
10	DR	0	1
17	CH	0	1
27	Ca	0	1
30	Cj	0	1
36	Cv	0	2
All	All	0	13

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	DA	323	HIS	CG-CD2	6.72	1.47	1.35
37	CA	310	A	N9-C4	5.63	1.41	1.37
8	DP	210	GLU	CD-OE2	5.46	1.31	1.25

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	CK	283	GLY	N-CA-C	7.77	132.53	113.10
37	CA	188	U	C2-N1-C1'	7.02	126.12	117.70
27	Ca	35	PRO	N-CA-CB	6.53	111.13	103.30
27	Ca	33	PRO	N-CA-CB	6.41	110.99	103.30
27	Ca	32	PRO	N-CA-CB	6.40	110.98	103.30

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	DA	166	TYR	Peptide
2	DD	248	ASP	Peptide
2	DD	255	VAL	Peptide
6	DN	142	ARG	Peptide
6	DN	292	TYR	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	DA	1420/1788 (79%)	1370 (96%)	48 (3%)	2 (0%)	48	77
2	DD	787/812 (97%)	747 (95%)	38 (5%)	2 (0%)	37	67
3	DI	388/407 (95%)	366 (94%)	21 (5%)	1 (0%)	37	67
4	DL	138/307 (45%)	130 (94%)	8 (6%)	0	100	100
5	DM	292/294 (99%)	283 (97%)	9 (3%)	0	100	100
6	DN	253/293 (86%)	242 (96%)	11 (4%)	0	100	100
7	DO	220/282 (78%)	213 (97%)	6 (3%)	1 (0%)	25	56
8	DP	205/274 (75%)	195 (95%)	9 (4%)	1 (0%)	25	56
9	DQ	254/268 (95%)	246 (97%)	6 (2%)	2 (1%)	16	45
10	DR	247/270 (92%)	239 (97%)	8 (3%)	0	100	100
11	DS	234/261 (90%)	227 (97%)	7 (3%)	0	100	100
12	DU	211/228 (92%)	202 (96%)	7 (3%)	2 (1%)	14	44
13	DZ	80/94 (85%)	75 (94%)	5 (6%)	0	100	100
14	Da	53/64 (83%)	52 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	CE	413/435 (95%)	395 (96%)	18 (4%)	0	100	100
16	CF	157/160 (98%)	152 (97%)	5 (3%)	0	100	100
17	CH	271/282 (96%)	265 (98%)	5 (2%)	1 (0%)	30	61
18	CI	200/443 (45%)	196 (98%)	4 (2%)	0	100	100
19	CK	237/326 (73%)	225 (95%)	12 (5%)	0	100	100
20	CL	85/87 (98%)	80 (94%)	5 (6%)	0	100	100
21	CO	359/429 (84%)	343 (96%)	14 (4%)	2 (1%)	22	52
22	CP	178/188 (95%)	171 (96%)	7 (4%)	0	100	100
23	CQ	188/307 (61%)	182 (97%)	6 (3%)	0	100	100
24	CR	312/320 (98%)	297 (95%)	14 (4%)	1 (0%)	37	67
25	CU	182/193 (94%)	177 (97%)	4 (2%)	1 (0%)	25	56
26	CZ	149/360 (41%)	142 (95%)	6 (4%)	1 (1%)	19	49
27	Ca	590/602 (98%)	556 (94%)	29 (5%)	5 (1%)	16	45
28	Cb	248/324 (76%)	242 (98%)	6 (2%)	0	100	100
29	Cd	289/440 (66%)	281 (97%)	6 (2%)	2 (1%)	19	49
30	Cj	224/257 (87%)	216 (96%)	7 (3%)	1 (0%)	30	61
31	Cm	194/215 (90%)	184 (95%)	10 (5%)	0	100	100
32	Cn	108/250 (43%)	103 (95%)	5 (5%)	0	100	100
33	Cp	173/187 (92%)	169 (98%)	4 (2%)	0	100	100
34	Cq	250/263 (95%)	243 (97%)	7 (3%)	0	100	100
35	Cr	253/439 (58%)	243 (96%)	9 (4%)	1 (0%)	30	61
36	Cv	1051/1211 (87%)	1011 (96%)	40 (4%)	0	100	100
All	All	10893/13360 (82%)	10460 (96%)	407 (4%)	26 (0%)	45	72

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	CZ	296	PRO
27	Ca	32	PRO
27	Ca	33	PRO
27	Ca	35	PRO
24	CR	10	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	DA	1211/1514 (80%)	1125 (93%)	86 (7%)	12	36
2	DD	694/711 (98%)	652 (94%)	42 (6%)	15	42
3	DI	350/365 (96%)	328 (94%)	22 (6%)	15	41
4	DL	118/263 (45%)	114 (97%)	4 (3%)	32	58
5	DM	252/252 (100%)	233 (92%)	19 (8%)	11	34
6	DN	229/256 (90%)	215 (94%)	14 (6%)	15	42
7	DO	186/229 (81%)	174 (94%)	12 (6%)	14	40
8	DP	187/239 (78%)	178 (95%)	9 (5%)	21	50
9	DQ	228/239 (95%)	220 (96%)	8 (4%)	31	57
10	DR	220/235 (94%)	199 (90%)	21 (10%)	7	25
11	DS	209/228 (92%)	197 (94%)	12 (6%)	17	44
12	DU	190/201 (94%)	174 (92%)	16 (8%)	9	30
13	DZ	72/84 (86%)	69 (96%)	3 (4%)	25	53
14	Da	50/59 (85%)	46 (92%)	4 (8%)	10	32
15	CE	358/372 (96%)	317 (88%)	41 (12%)	4	19
16	CF	136/144 (94%)	129 (95%)	7 (5%)	20	47
17	CH	237/246 (96%)	215 (91%)	22 (9%)	7	26
18	CI	171/371 (46%)	160 (94%)	11 (6%)	14	40
19	CK	210/283 (74%)	193 (92%)	17 (8%)	9	31
20	CL	79/79 (100%)	70 (89%)	9 (11%)	4	19
21	CO	318/377 (84%)	293 (92%)	25 (8%)	10	32
22	CP	160/168 (95%)	147 (92%)	13 (8%)	9	31
23	CQ	171/270 (63%)	151 (88%)	20 (12%)	4	18
24	CR	275/279 (99%)	258 (94%)	17 (6%)	15	41
25	CU	160/169 (95%)	151 (94%)	9 (6%)	17	44
26	CZ	121/313 (39%)	111 (92%)	10 (8%)	9	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	Ca	516/543 (95%)	473 (92%)	43 (8%)	9	30
28	Cb	219/277 (79%)	203 (93%)	16 (7%)	11	35
29	Cd	240/381 (63%)	219 (91%)	21 (9%)	8	28
30	Cj	193/219 (88%)	179 (93%)	14 (7%)	11	35
31	Cm	165/184 (90%)	141 (86%)	24 (14%)	2	12
32	Cn	95/210 (45%)	89 (94%)	6 (6%)	15	41
33	Cp	163/175 (93%)	151 (93%)	12 (7%)	11	34
34	Cq	210/221 (95%)	193 (92%)	17 (8%)	9	31
35	Cr	211/369 (57%)	190 (90%)	21 (10%)	6	23
36	Cv	912/1034 (88%)	844 (92%)	68 (8%)	11	34
All	All	9516/11559 (82%)	8801 (92%)	715 (8%)	14	34

5 of 715 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	CZ	218	VAL
31	Cm	92	GLN
27	Ca	19	ARG
25	CU	171	VAL
28	Cb	110	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 197 such sidechains are listed below:

Mol	Chain	Res	Type
21	CO	82	ASN
28	Cb	67	GLN
21	CO	359	HIS
25	CU	123	GLN
29	Cd	159	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
37	CA	476/621 (76%)	212 (44%)	2 (0%)

5 of 212 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
37	CA	2	A
37	CA	3	A
37	CA	4	A
37	CA	5	U
37	CA	6	U

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
37	CA	38	U
37	CA	39	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 43 ligands modelled in this entry, 40 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
44	SPD	CA	733	-	9,9,9	0.49	0	8,8,8	0.49	0
45	SPM	CA	735	-	13,13,13	0.34	0	12,12,12	0.85	0
44	SPD	CA	734	-	9,9,9	0.35	0	8,8,8	0.67	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	SPD	CA	733	-	-	5/7/7/7	-
45	SPM	CA	735	-	-	8/11/11/11	-
44	SPD	CA	734	-	-	3/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	CA	735	SPM	N10-C11-C12-C13
45	CA	735	SPM	C2-C3-C4-N5
44	CA	733	SPD	C3-C4-C5-N6
45	CA	735	SPM	C7-C8-C9-N10
45	CA	735	SPM	C6-C7-C8-C9

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

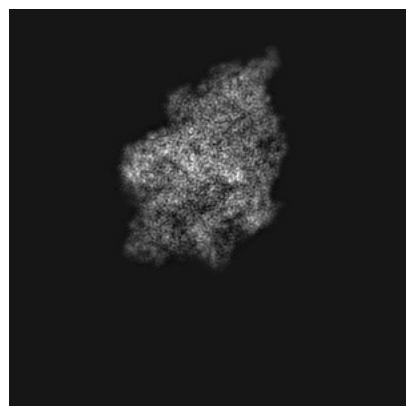
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0232. These allow visual inspection of the internal detail of the map and identification of artifacts.

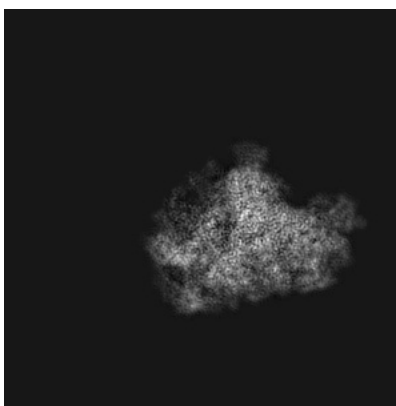
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

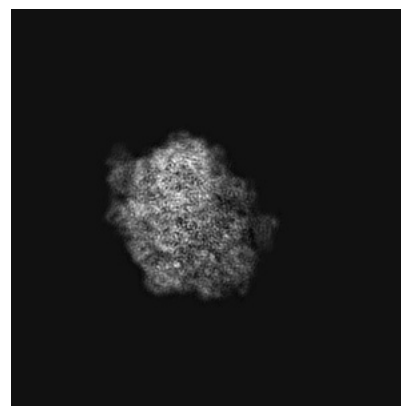
6.1.1 Primary map



X

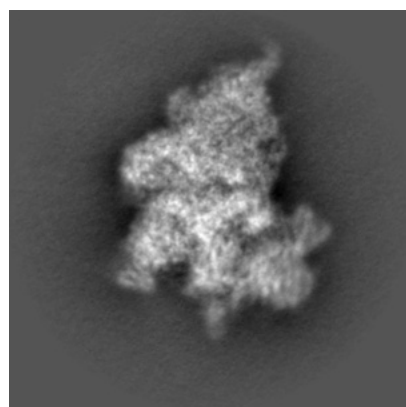


Y

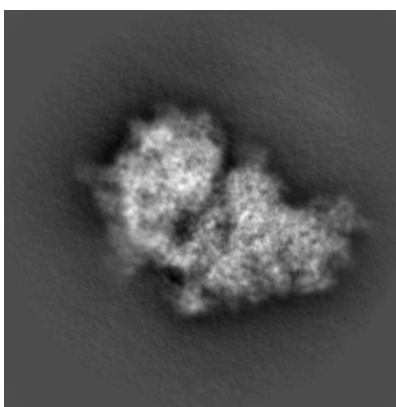


Z

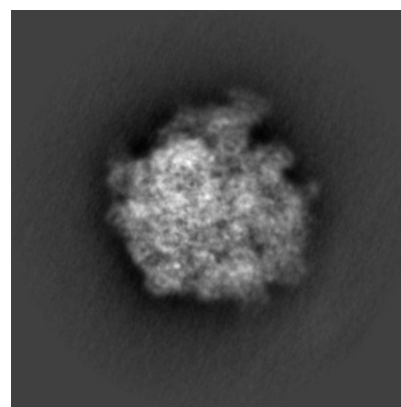
6.1.2 Raw map



X



Y

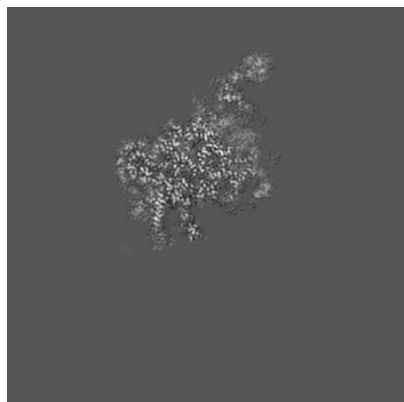


Z

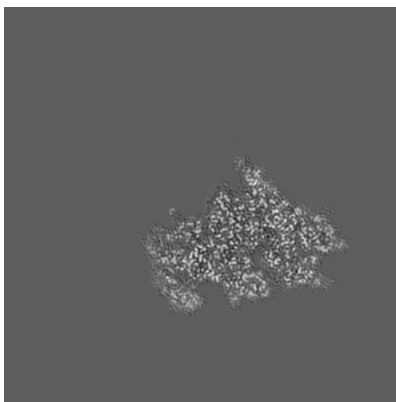
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

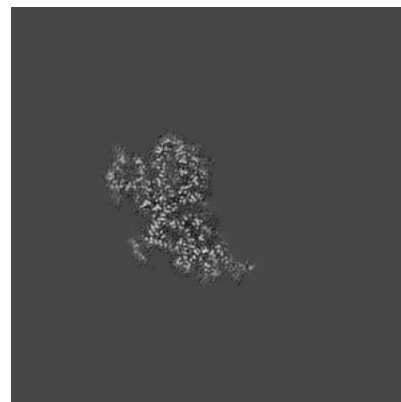
6.2.1 Primary map



X Index: 160

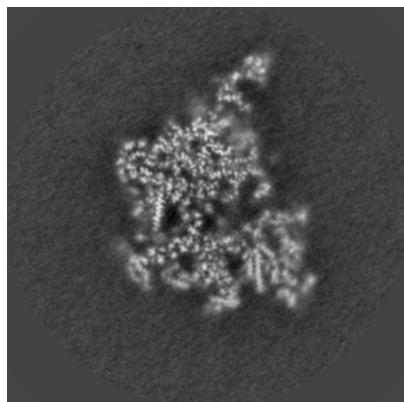


Y Index: 160

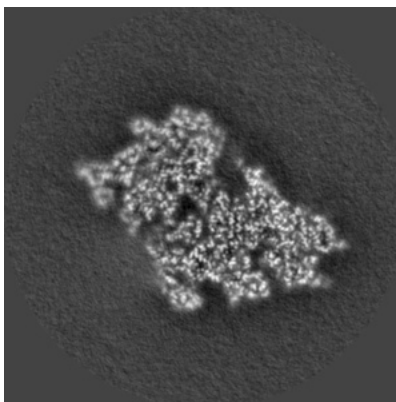


Z Index: 160

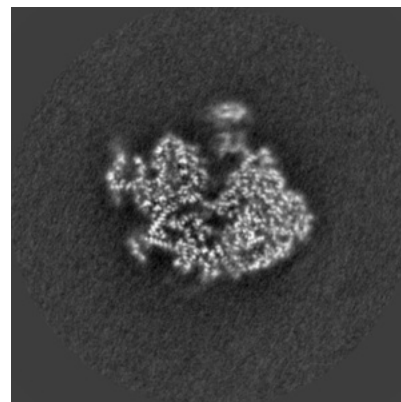
6.2.2 Raw map



X Index: 160



Y Index: 160

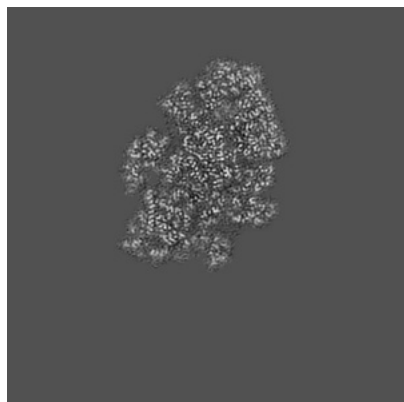


Z Index: 160

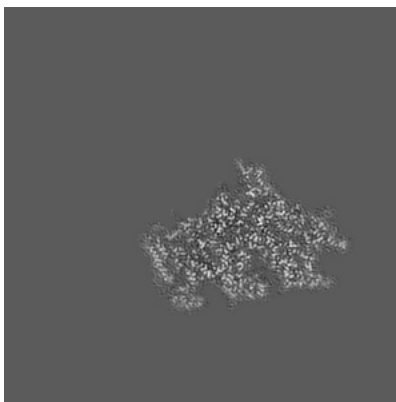
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

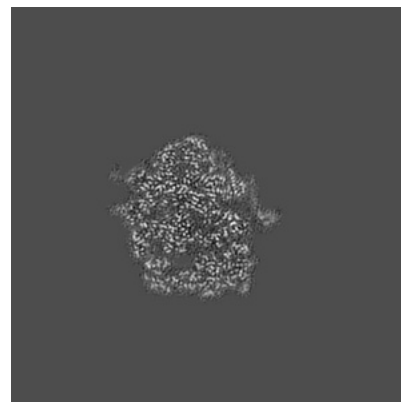
6.3.1 Primary map



X Index: 133

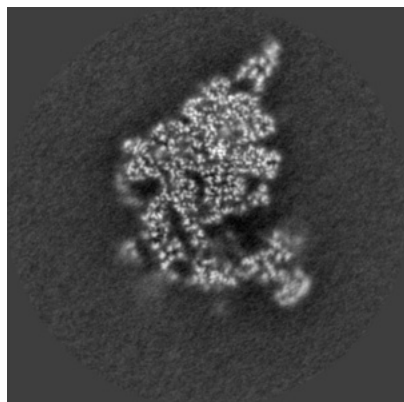


Y Index: 162

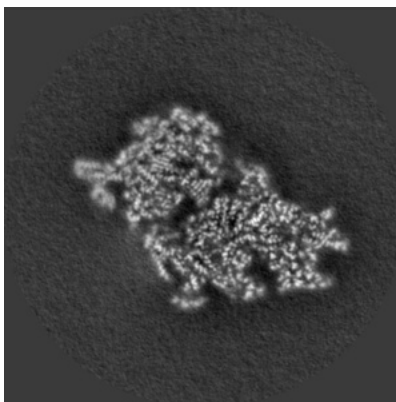


Z Index: 187

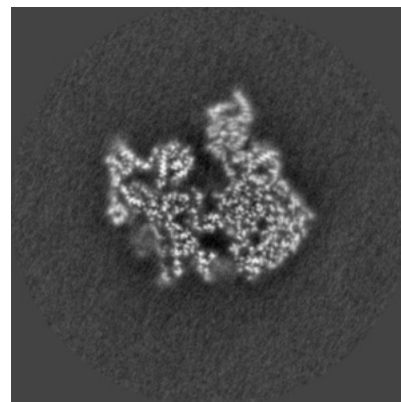
6.3.2 Raw map



X Index: 151



Y Index: 164

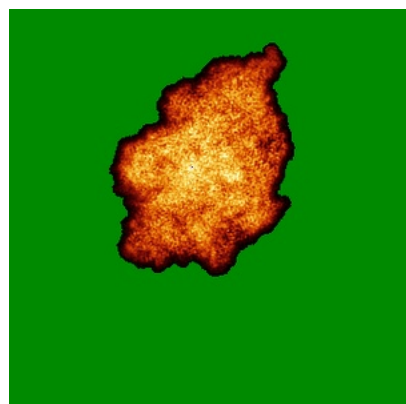


Z Index: 152

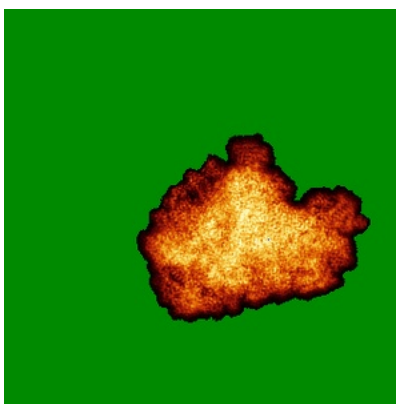
The images above show the largest variance slices of the map in three orthogonal directions.

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

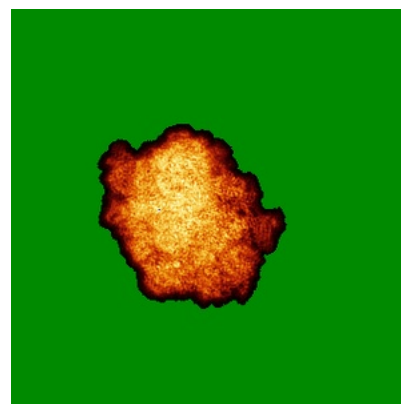
6.4.1 Primary map



X

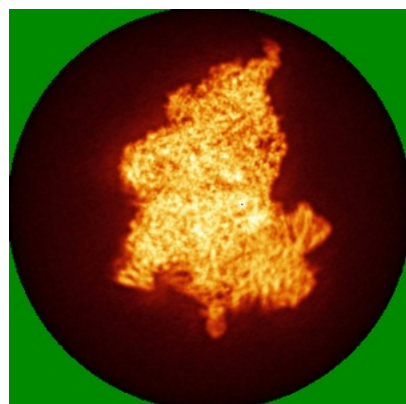


Y

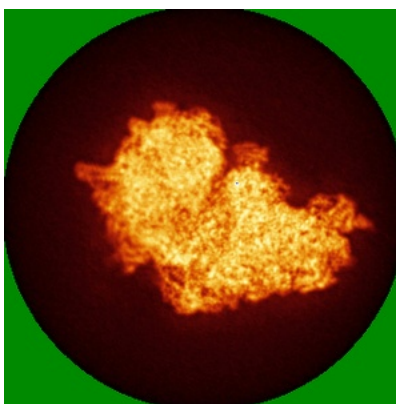


Z

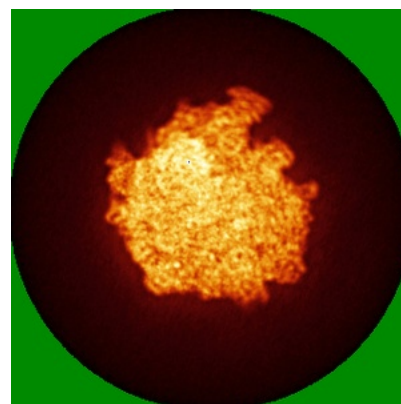
6.4.2 Raw map



X



Y

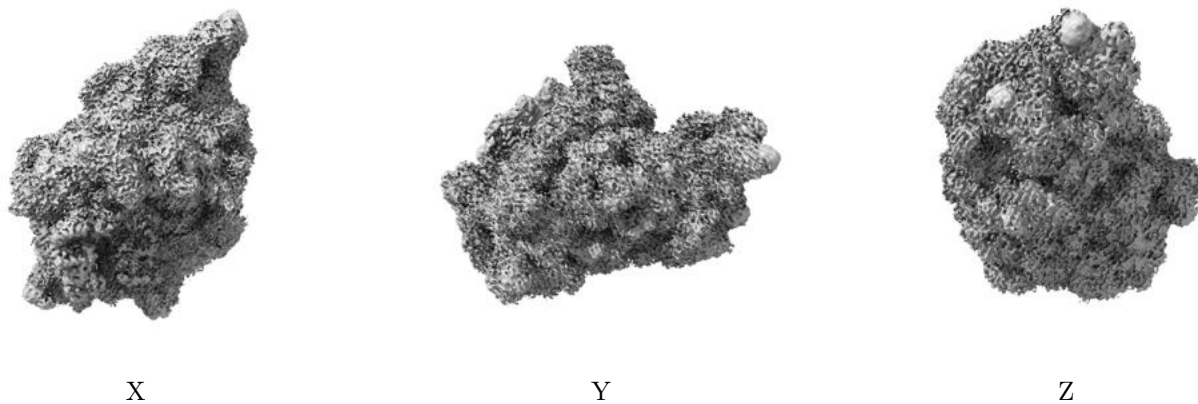


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

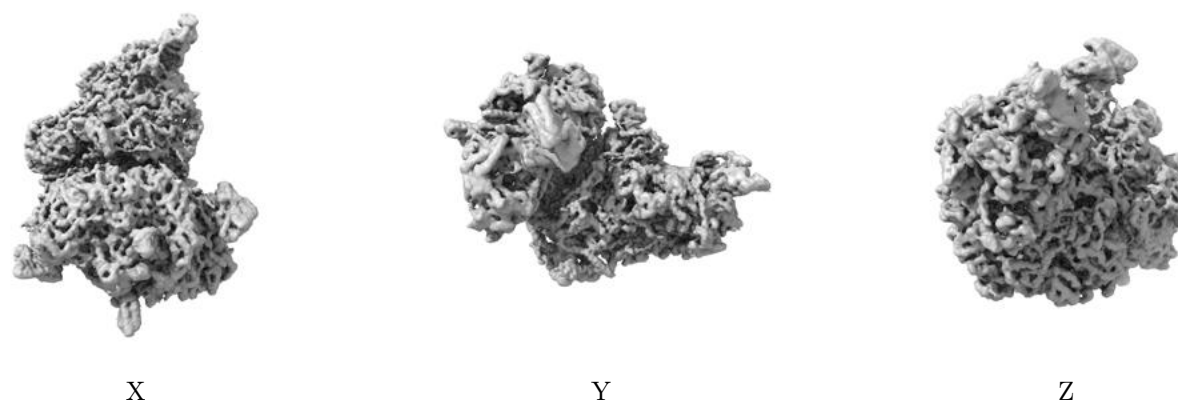
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0115. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

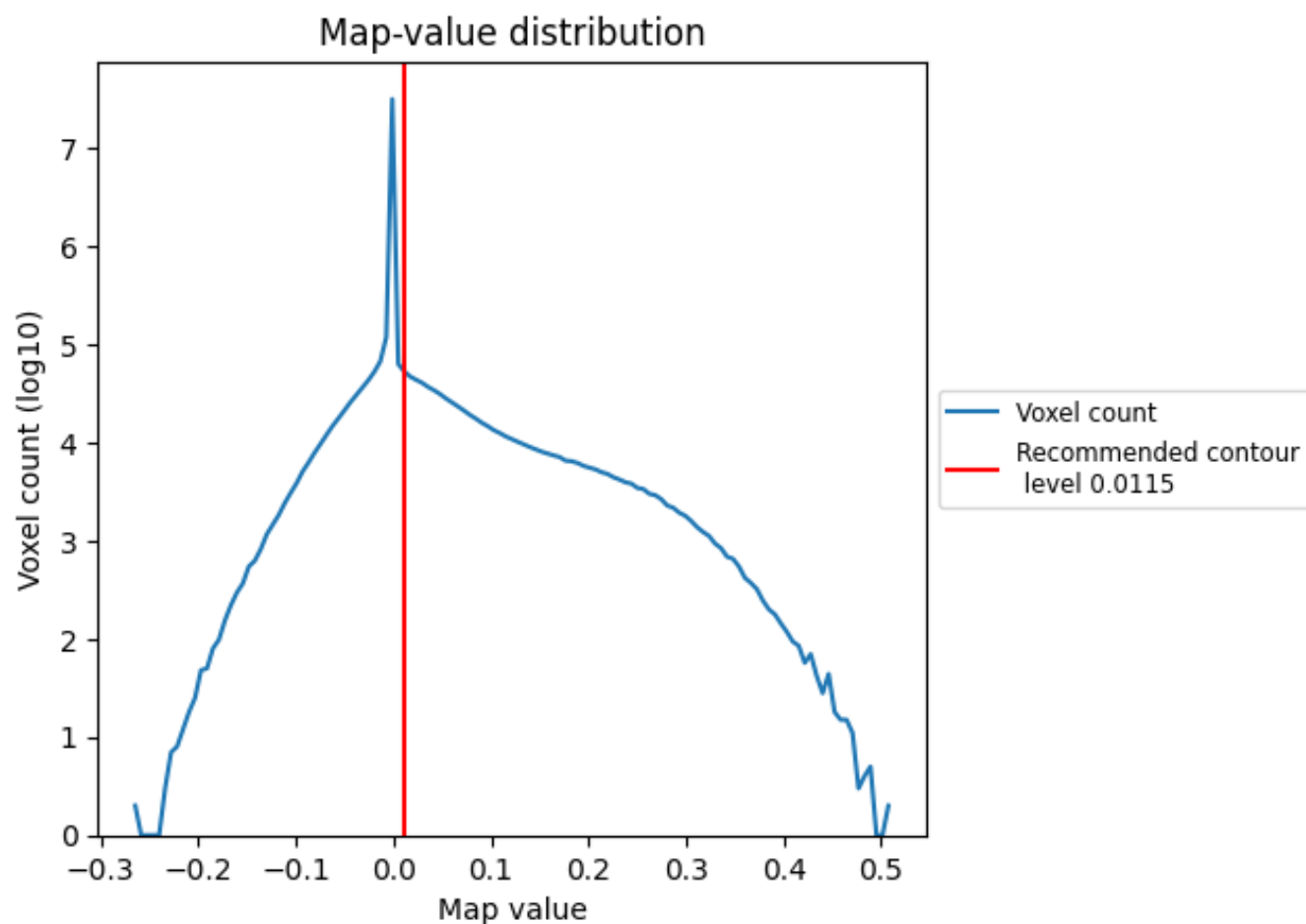
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

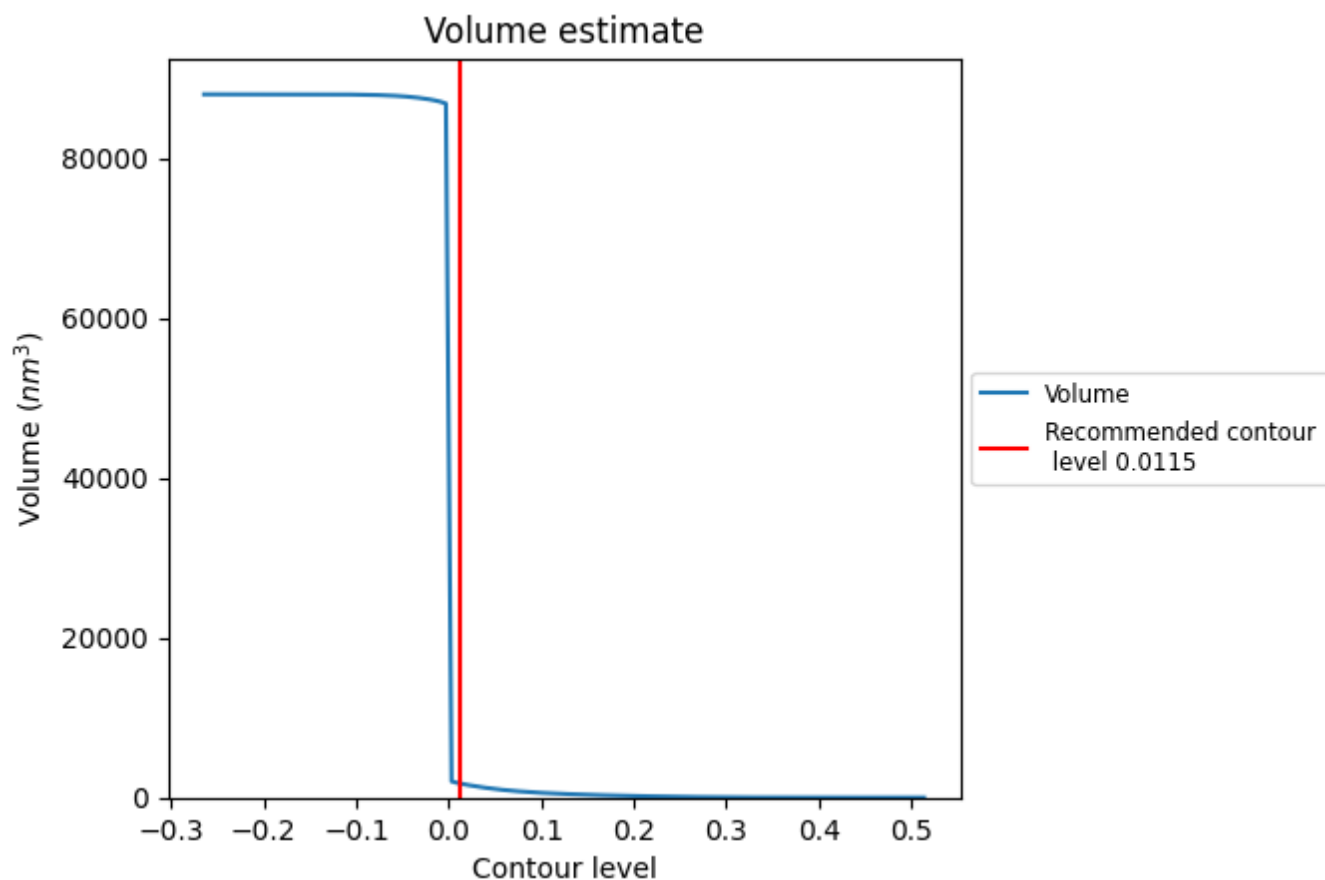
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

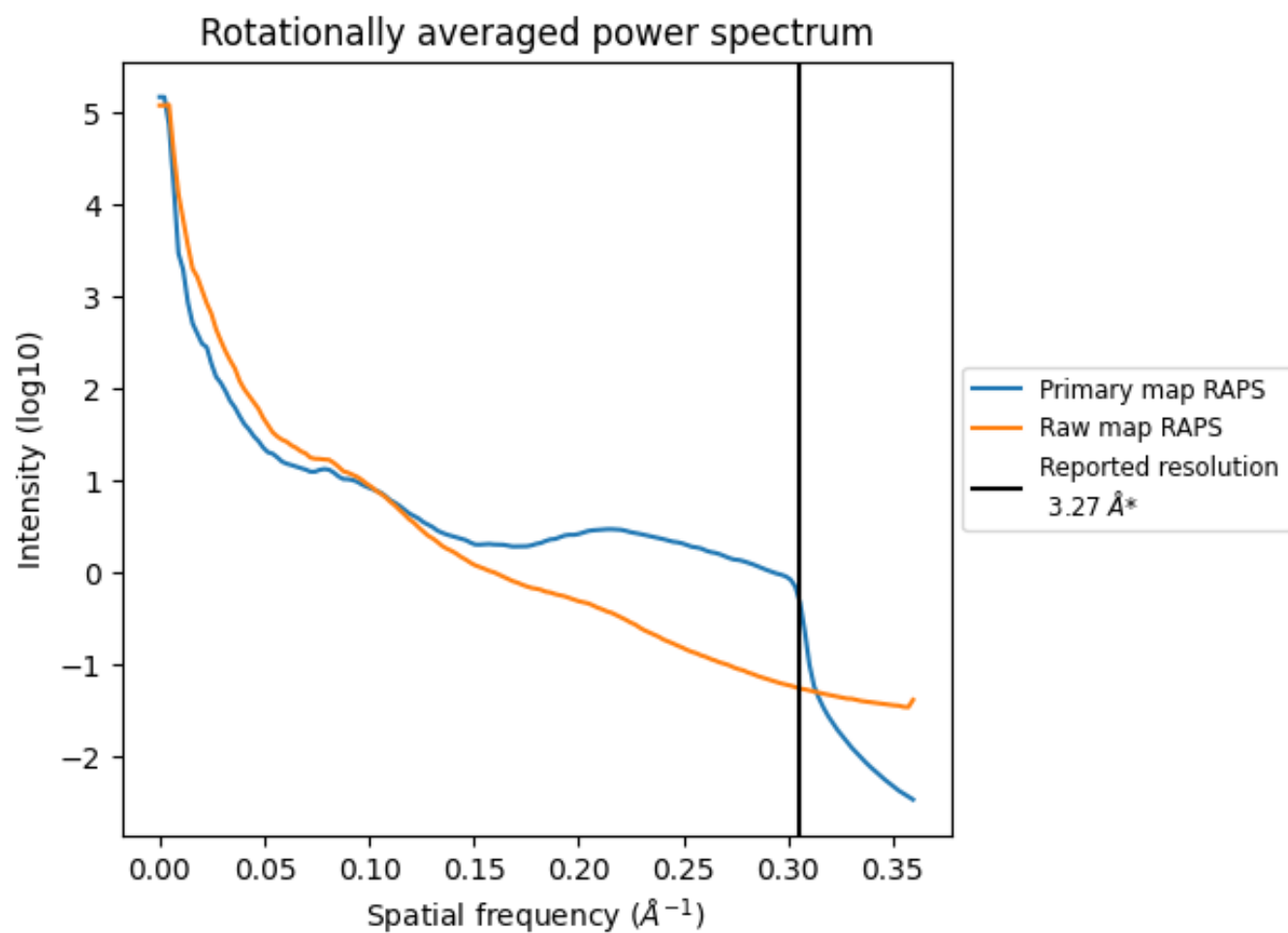
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1779 nm^3 ; this corresponds to an approximate mass of 1607 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

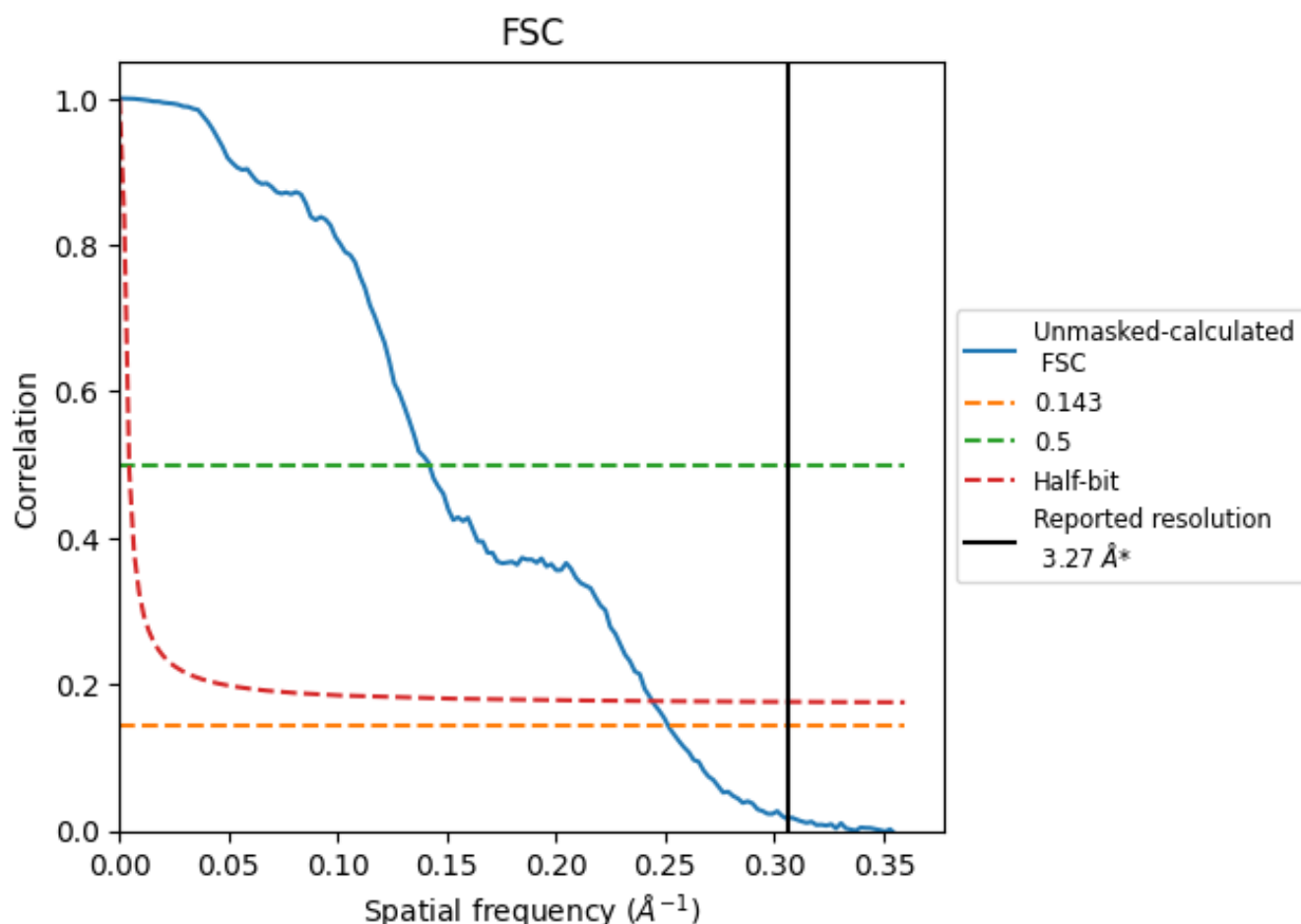


*Reported resolution corresponds to spatial frequency of 0.306 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.306 Å⁻¹

8.2 Resolution estimates [i](#)

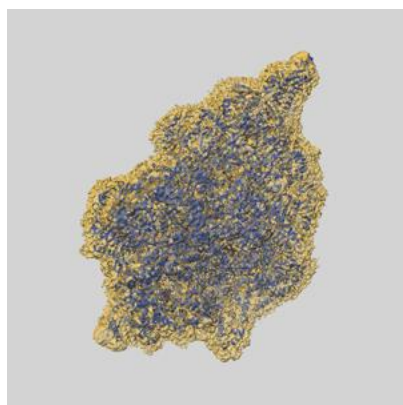
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.27	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.98	7.05	4.10

*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 3.98 differs from the reported value 3.27 by more than 10 %

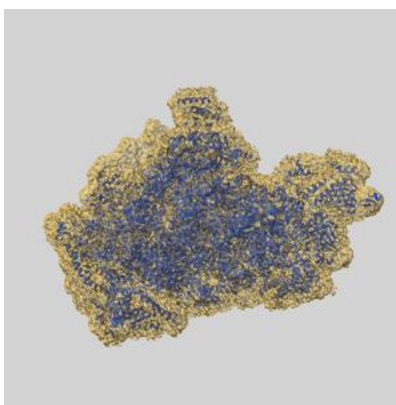
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0232 and PDB model 6HIY. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

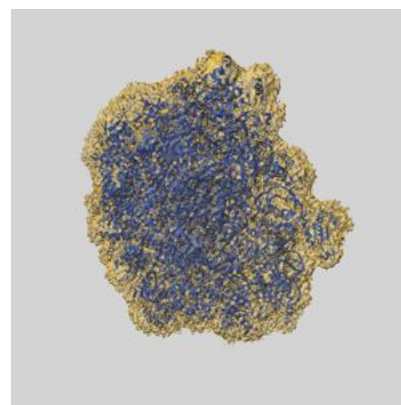
9.1 Map-model overlay [i](#)



X



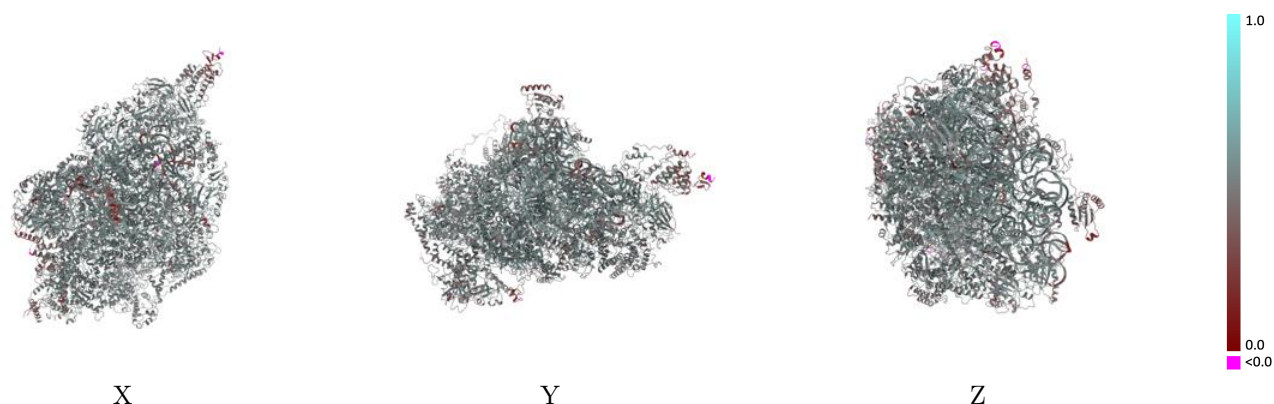
Y



Z

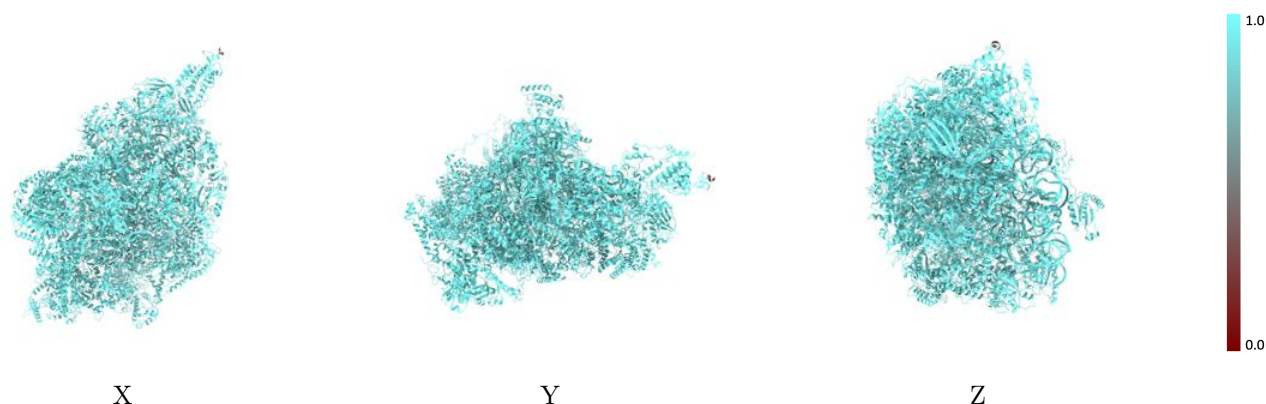
The images above show the 3D surface view of the map at the recommended contour level 0.0115 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



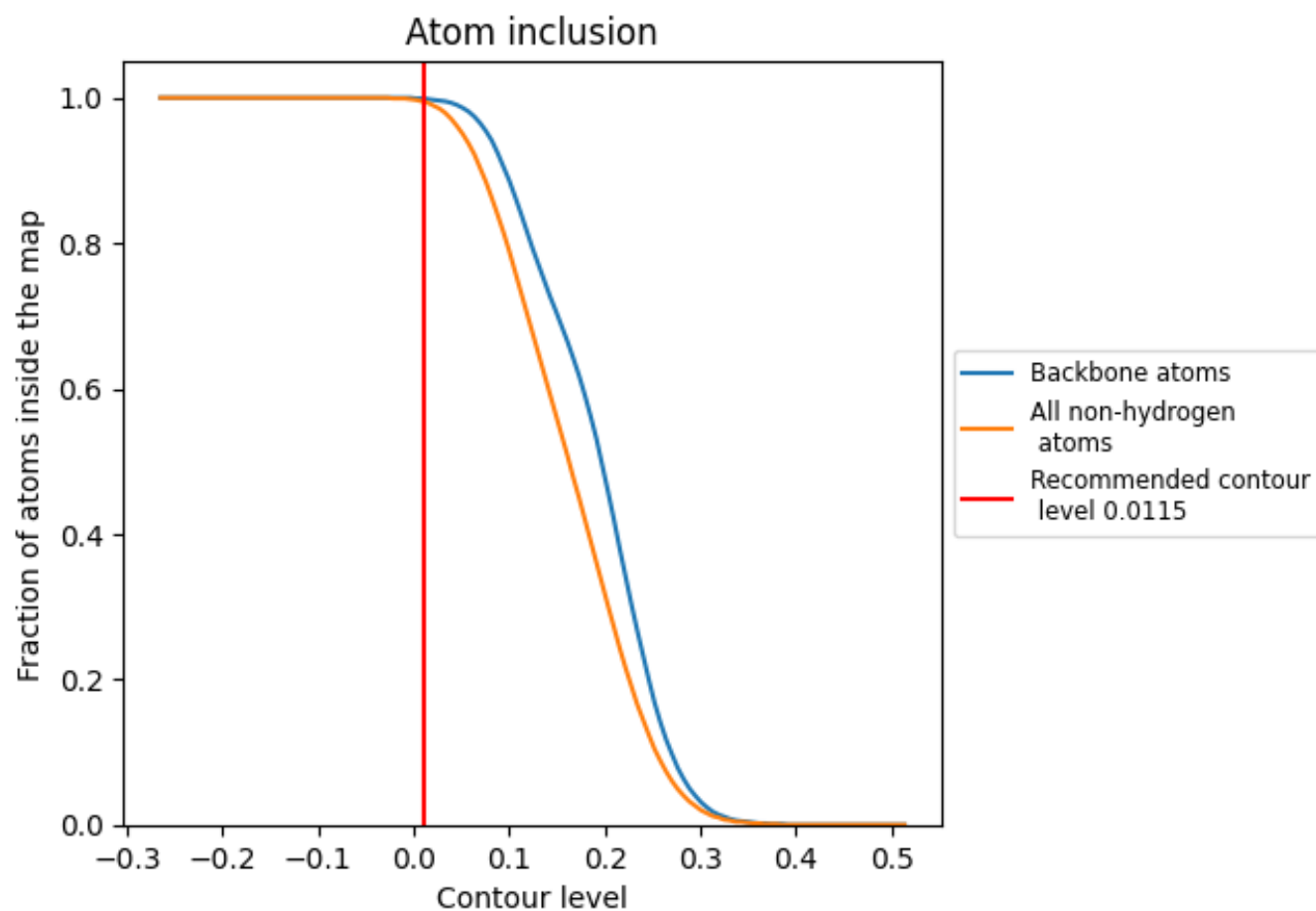
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0115).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 99% 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 (0.0115) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9940	 0.5160
CA	 0.9960	 0.5150
CE	 0.9910	 0.5410
CF	 0.9820	 0.5040
CH	 0.9910	 0.5270
CI	 0.9910	 0.5300
CK	 0.9950	 0.5020
CL	 0.9970	 0.5380
CO	 0.9990	 0.5330
CP	 0.9980	 0.5360
CQ	 0.9980	 0.5640
CR	 0.9880	 0.5220
CU	 0.9970	 0.5270
CZ	 0.9800	 0.4120
Ca	 0.9930	 0.5320
Cb	 0.9930	 0.5060
Cd	 0.9930	 0.5030
Cj	 0.9990	 0.5140
Cm	 0.9840	 0.5160
Cn	 0.9980	 0.5310
Cp	 0.9990	 0.4980
Cq	 0.9910	 0.5240
Cr	 0.9970	 0.4760
Cv	 0.9950	 0.5290
DA	 0.9950	 0.5030
DD	 0.9930	 0.5250
DI	 0.9970	 0.5100
DL	 0.9880	 0.5430
DM	 0.9960	 0.5400
DN	 0.9910	 0.5360
DO	 0.9970	 0.4930
DP	 0.9840	 0.4450
DQ	 0.9970	 0.5010
DR	 1.0000	 0.5020
DS	 0.9970	 0.5160



Continued on next page...

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Chain	Atom inclusion	Q-score
DU	 0.9960	 0.5150
DZ	 0.9930	 0.5400
Da	 0.9980	 0.5600
UQ	 1.0000	 0.4100
UR	 1.0000	 0.4000
US	 0.9880	 0.4230
UT	 0.9660	 0.3910