wwPDB EM Validation Summary Report (i)

Nov 1, 2023 – 10:57 AM EDT

PDB ID	:	8FN2
EMDB ID	:	EMD-29304
Title	:	The structure of a 50S ribosomal subunit in the Lyme disease pathogen Borreliella burgdorferi
Authors	:	Sharma, M.R.; Manjari, S.R.; Agrawal, E.K.; Keshavan, P.; Koripella, R.K.; Majumdar, S.; Marcinkiewicz, A.L.; Lin, Y.P.; Agrawal, R.K.; Banavali, N.K.
Deposited on	:	2022-12-26
Resolution	:	3.40 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 (i) 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 (i)) were used in the production of this report:

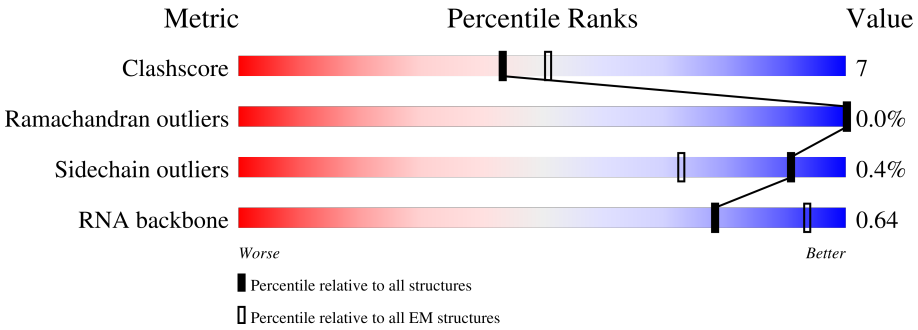
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.40 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	2929	64% 25% 5% 6%
2	B	112	55% 35% 10%
3	D	277	7% 78% 22%
4	E	206	82% 17%
5	F	209	80% 20%
6	G	182	46% 71% 29%
7	H	180	6% 78% 22%

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Mol	Chain	Length	Quality of chain
8	I	148	17% 34% 9% 57%
9	J	162	51% 81% 19%
10	K	139	20% 47% 51%
11	L	145	88% 12%
12	M	122	80% 20%
13	N	145	5% 66% 34%
14	O	138	72% 27%
15	P	121	71% 29%
16	Q	119	79% 19%
17	R	117	5% 72% 27%
18	S	114	74% 26%
19	T	103	5% 76% 24%
20	U	115	83% 17%
21	V	98	5% 81% 19%
22	W	101	13% 65% 34%
23	X	181	19% 69% 30%
24	Y	74	86% 14%
25	Z	91	73% 27%
26	a	65	5% 100%
27	b	100	100%
28	c	81	54% 70% 28%
29	d	59	100%
30	e	51	12% 100%
31	f	50	100%
32	g	66	5% 98%

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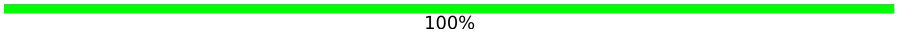
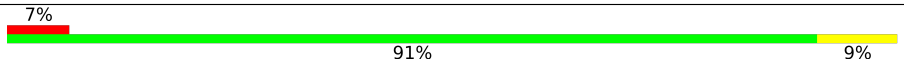
Mol	Chain	Length	Quality of chain
33	h	37	
34	i	46	

2 Entry composition (i)

There are 35 unique types of molecules in this entry. The entry contains 89742 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2762	59248	26483	10866	19137	2762	0	0

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	112	2398	1071	434	781	112	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	277	2156	1354	414	383	5	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	206	1564	995	278	286	5	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	209	1658	1056	301	299	2	0	0

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	182	1439	930	240	265	4	0	0

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	180	Total	C	N	O	S	0	0
			1405	895	249	259	2		

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	63	Total	C	N	O	S	0	0
			411	253	76	81	1		

- Molecule 9 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	J	132	Total	C	N	O	0	0
			528	264	132	132		

- Molecule 10 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	K	68	Total	C	N	O	0	0
			272	136	68	68		

- Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	145	Total	C	N	O	S	0	0
			1171	756	211	202	2		

- Molecule 12 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	122	Total	C	N	O	S	0	0
			942	593	174	170	5		

- Molecule 13 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	145	Total	C	N	O	S	0	0
			1129	716	210	201	2		

- Molecule 14 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	138	Total	C	N	O	S	0	0
			1092	693	204	188	7		

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	121	Total	C	N	O	S	0	0
			1004	643	193	164	4		

- Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	119	Total	C	N	O	S	0	0
			968	613	184	170	1		

- Molecule 17 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	117	Total	C	N	O	S	0	0
			951	613	174	161	3		

- Molecule 18 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	114	Total	C	N	O	S	0	0
			943	597	189	155	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	40	ARG	UNK	conflict	UNP O51206

- Molecule 19 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	103	Total	C	N	O	S	0	0
			859	552	148	157	2		

- Molecule 20 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	115	Total	C	N	O	S	0	0
			918	574	180	158	6		

- Molecule 21 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	98	Total	C	N	O	S	0	0
			784	507	134	140	3		

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	101	Total	C	N	O	S	0	0
			800	501	155	140	4		

- Molecule 23 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	181	Total	C	N	O	S	0	0
			1432	912	245	273	2		

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	Y	74	Total	C	N	O	0	0
			571	359	112	100		

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	91	Total	C	N	O	S	0	0
			705	452	135	115	3		

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	65	Total	C	N	O	S	0	0
			553	352	102	95	4		

- Molecule 27 is a protein called 50S ribosomal protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	100	Total	C	N	O	S	0	0
			814	518	158	133	5		

- Molecule 28 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	58	Total	C	N	O	S	0	0
			466	300	77	87	2		

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	59	Total	C	N	O	S	0	0
			484	300	99	80	5		

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	51	Total	C	N	O	S	0	0
			425	266	80	76	3		

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	50	Total	C	N	O	S	0	0
			422	260	95	64	3		

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	66	Total	C	N	O	S	0	0
			548	346	111	88	3		

- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	37	Total	C	N	O	S	0	0
			305	192	63	46	4		

- Molecule 34 is a protein called 50S ribosomal protein bL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	46	Total	C	N	O	S	0	0
			375	236	72	65	2		

- Molecule 35 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

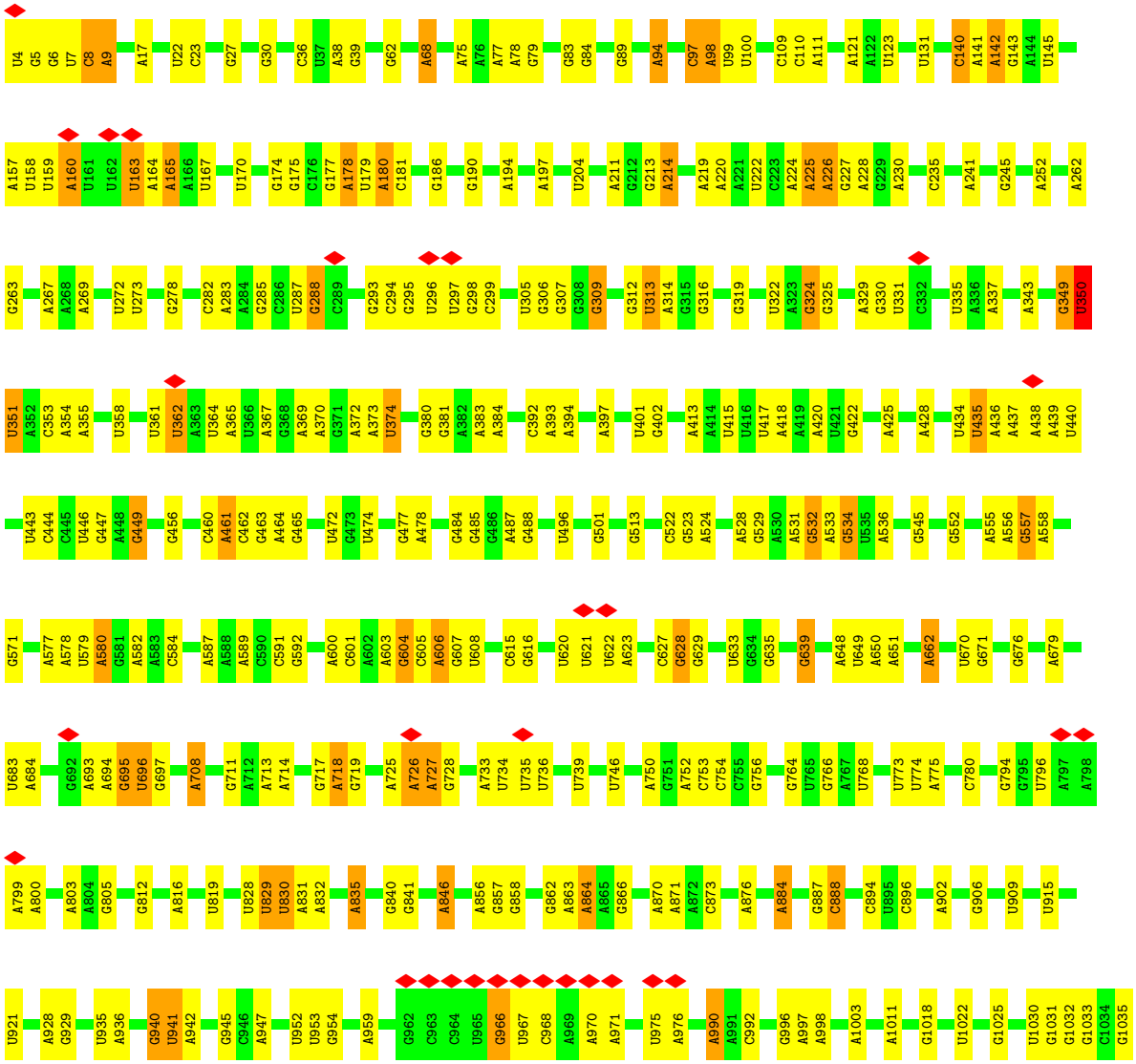
Mol	Chain	Residues	Atoms		AltConf
35	d	1	Total	Zn	0
			1	1	
35	h	1	Total	Zn	0
			1	1	

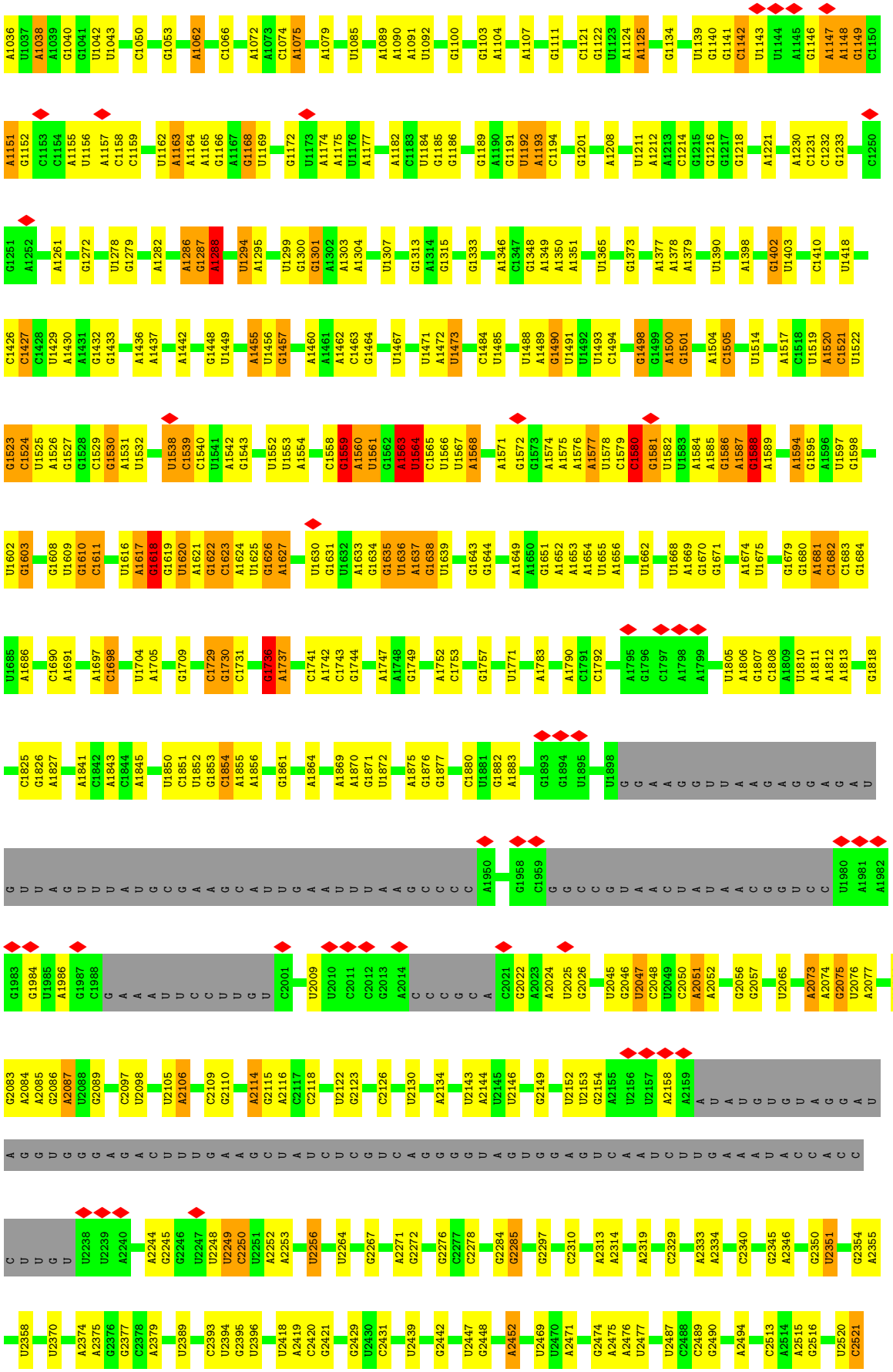
3 Residue-property plots (i)

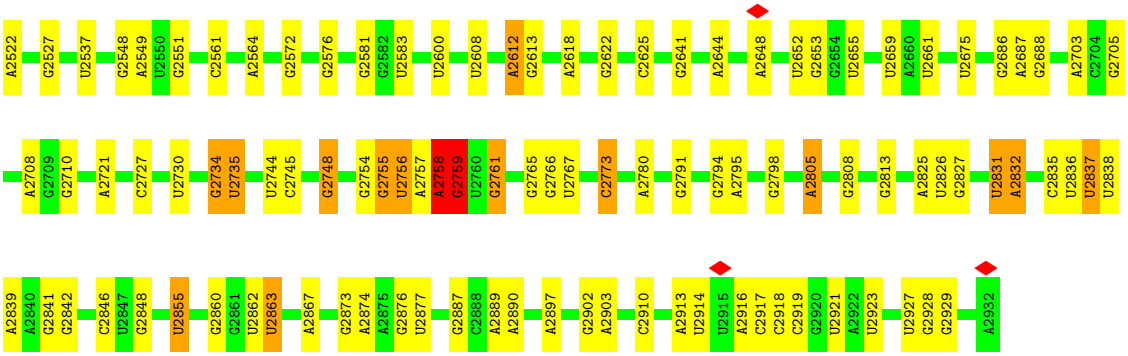
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 23S ribosomal RNA

Chain A:

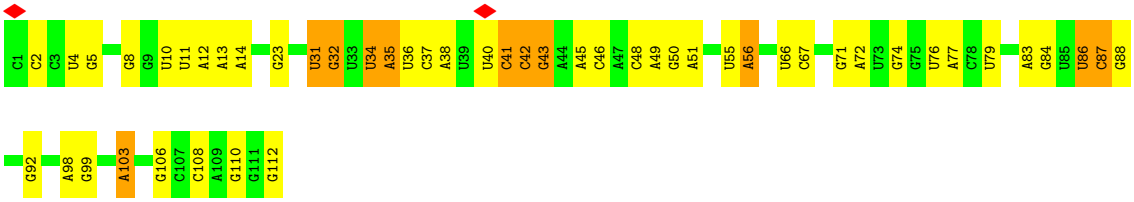






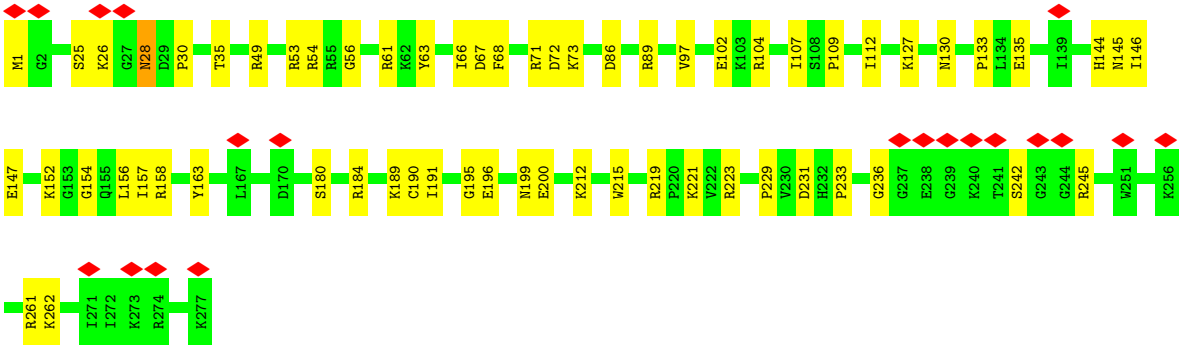
• Molecule 2: 5S ribosomal RNA

Chain B:



• Molecule 3: 50S ribosomal protein L2

Chain D:



• Molecule 4: 50S ribosomal protein L3

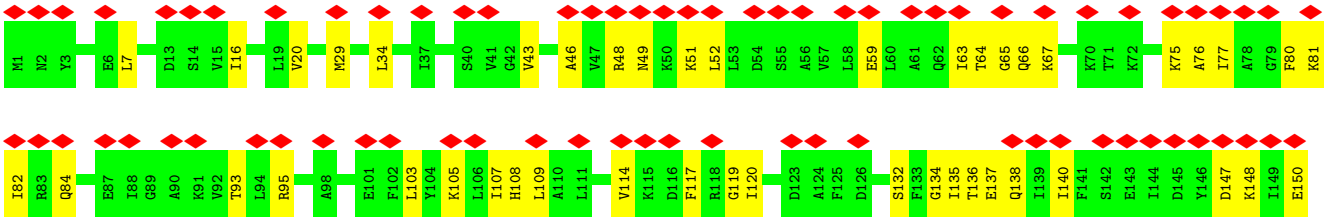
Chain E:

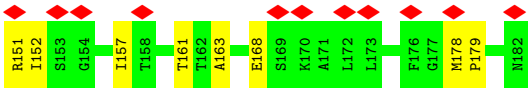
• Molecule 5: 50S ribosomal protein L4

Chain F:

• Molecule 6: 50S ribosomal protein L5

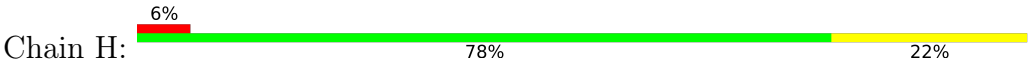
Chain G:

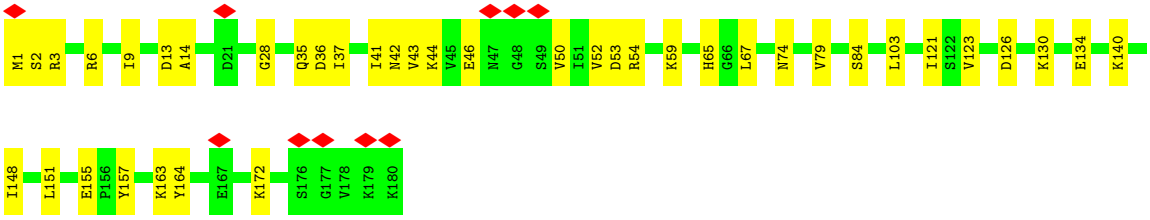




• Molecule 7: 50S ribosomal protein L6

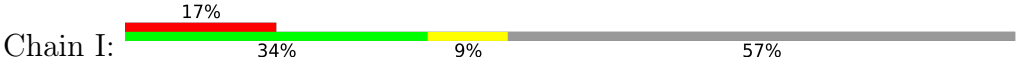
Chain H:

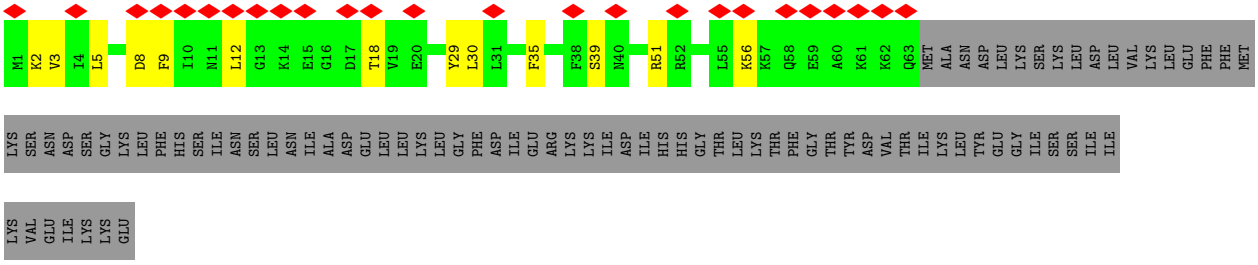




• Molecule 8: 50S ribosomal protein L9

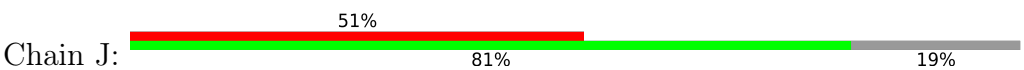
Chain I:

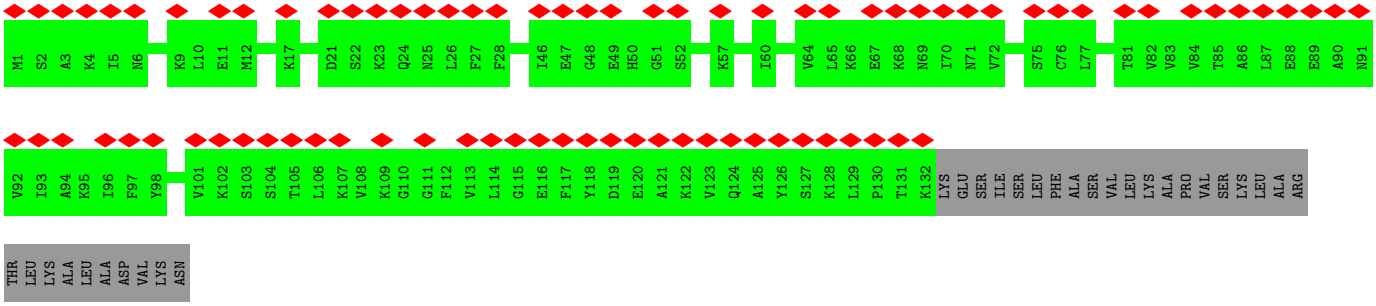




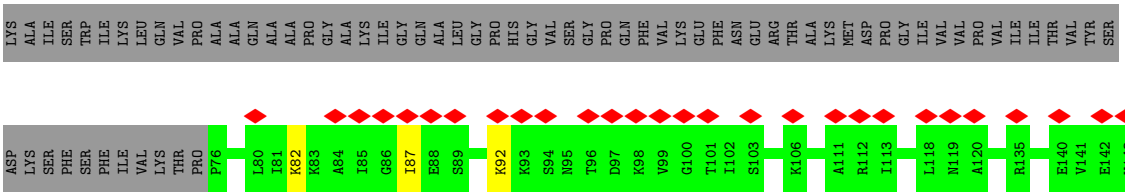
• Molecule 9: 50S ribosomal protein L10

Chain J:

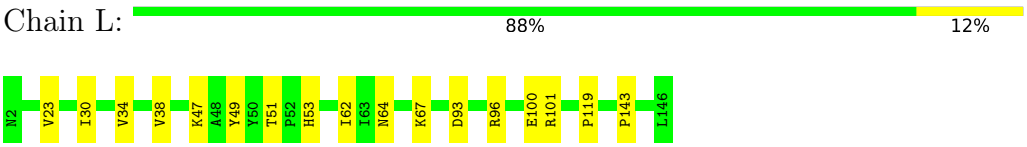




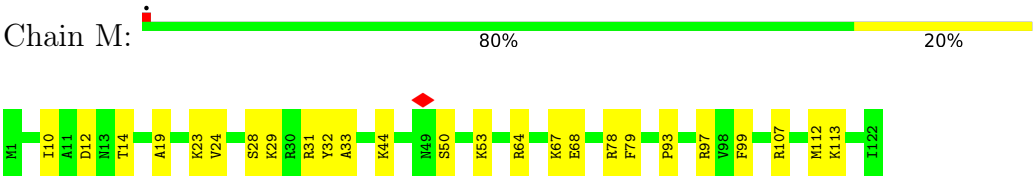
• Molecule 10: 50S ribosomal protein L11



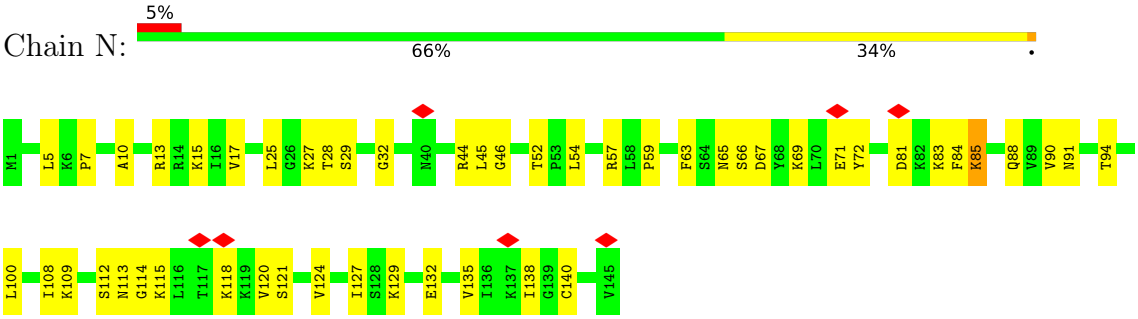
• Molecule 11: 50S ribosomal protein L13



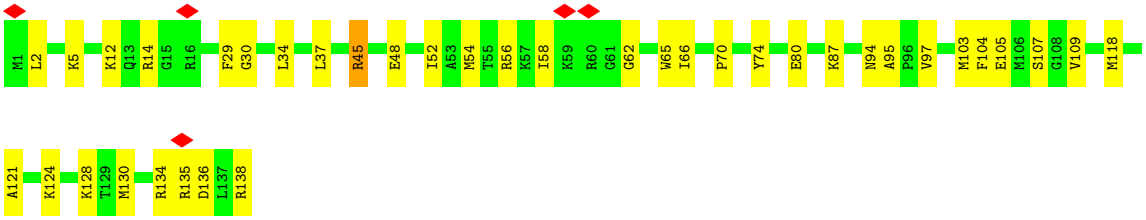
• Molecule 12: 50S ribosomal protein L14



• Molecule 13: 50S ribosomal protein L15



• Molecule 14: 50S ribosomal protein L16

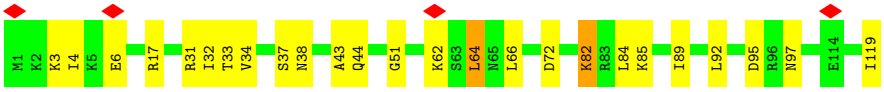


• Molecule 15: 50S ribosomal protein L17

Chain P:

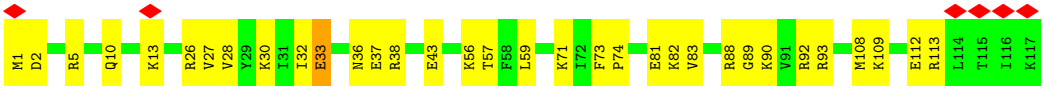
• Molecule 16: 50S ribosomal protein L18

Chain Q:



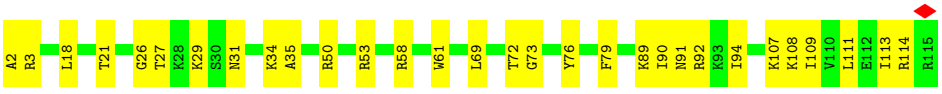
• Molecule 17: 50S ribosomal protein L19

Chain R:



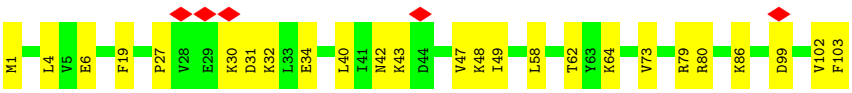
• Molecule 18: 50S ribosomal protein L20

Chain S:



• Molecule 19: 50S ribosomal protein L21

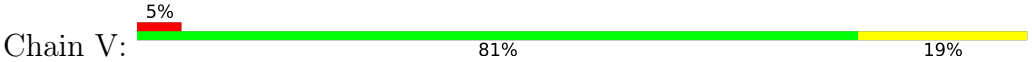
Chain T:

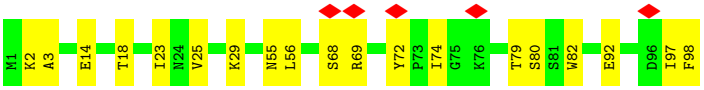


• Molecule 20: 50S ribosomal protein L22

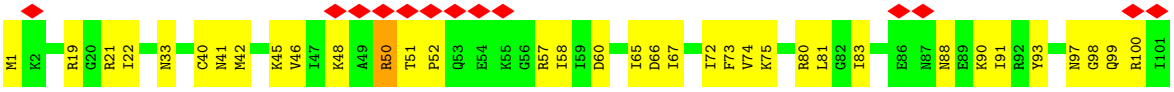
Chain U:

• Molecule 21: 50S ribosomal protein L23

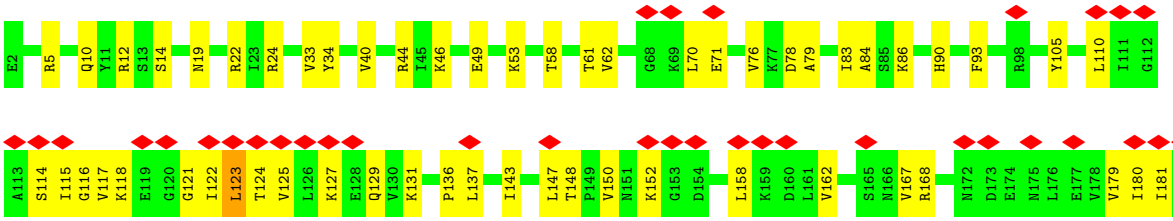




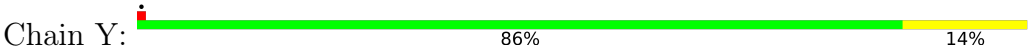
• Molecule 22: 50S ribosomal protein L24

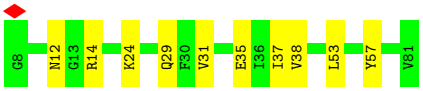


• Molecule 23: 50S ribosomal protein L25



• Molecule 24: 50S ribosomal protein L27



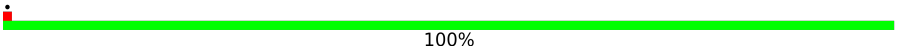


• Molecule 25: 50S ribosomal protein L28

• Molecule 26: 50S ribosomal protein L29

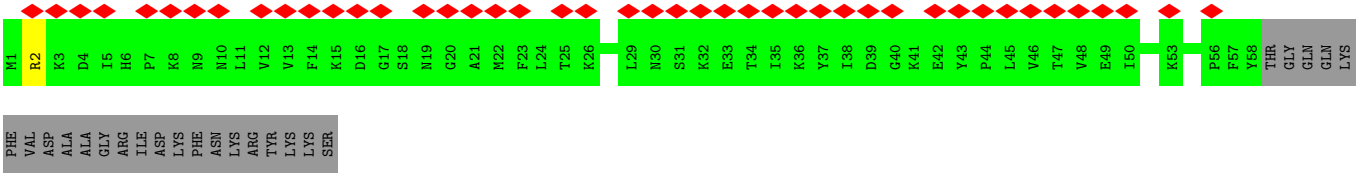
• Molecule 27: 50S ribosomal protein uL30

Chain b:



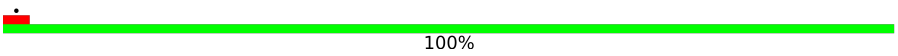
• Molecule 28: 50S ribosomal protein L31 type B

Chain c:



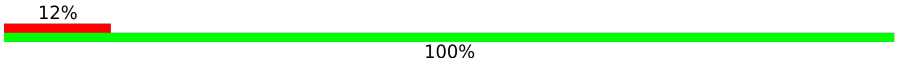
• Molecule 29: 50S ribosomal protein L32

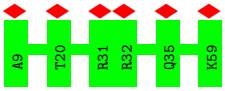
Chain d:



• Molecule 30: 50S ribosomal protein L33

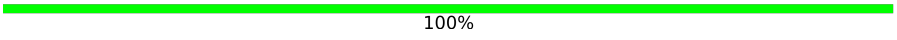
Chain e:





• Molecule 31: 50S ribosomal protein L34

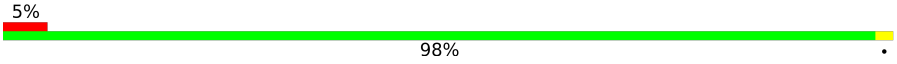
Chain f:

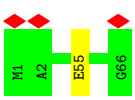


There are no outlier residues recorded for this chain.

• Molecule 32: 50S ribosomal protein L35

Chain g:





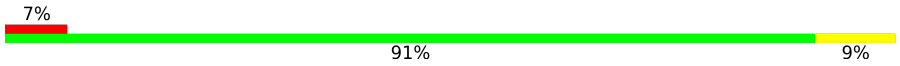
• Molecule 33: 50S ribosomal protein L36

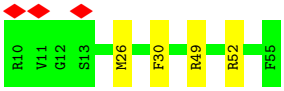
Chain h:

There are no outlier residues recorded for this chain.

• Molecule 34: 50S ribosomal protein bL38

Chain i:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	12449	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	67.527	Depositor
Minimum defocus (nm)	820	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.783	Depositor
Minimum map value	-0.309	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	493.245, 493.245, 493.245	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0961, 1.0961, 1.0961	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.12	0/66391	0.75	140/103525 (0.1%)
2	B	0.11	0/2684	0.65	0/4183
3	D	0.55	0/2196	0.61	1/2935 (0.0%)
4	E	0.54	0/1588	0.59	0/2122
5	F	0.52	0/1682	0.56	1/2249 (0.0%)
6	G	0.37	0/1460	0.58	1/1955 (0.1%)
7	H	0.40	0/1422	0.51	0/1903
8	I	0.36	0/416	0.55	0/548
9	J	0.23	0/527	0.44	0/657
10	K	0.23	0/271	0.43	0/337
11	L	0.56	0/1197	0.58	0/1612
12	M	0.58	0/951	0.63	0/1276
13	N	0.51	0/1142	0.61	0/1515
14	O	0.54	0/1110	0.72	2/1480 (0.1%)
15	P	0.54	0/1020	0.59	0/1353
16	Q	0.39	0/979	0.65	2/1299 (0.2%)
17	R	0.63	1/962 (0.1%)	0.66	0/1280
18	S	0.63	0/954	0.65	0/1264
19	T	0.59	0/872	0.60	0/1163
20	U	0.56	0/931	0.62	0/1245
21	V	0.49	0/796	0.58	0/1065
22	W	0.42	0/803	0.57	0/1059
23	X	0.38	0/1451	0.53	1/1955 (0.1%)
24	Y	0.56	0/577	0.55	0/760
25	Z	0.48	0/713	0.57	0/943
26	a	0.45	0/559	0.61	0/739
27	b	0.50	0/818	0.57	0/1079
28	c	0.34	0/476	0.56	0/640
29	d	0.58	0/492	0.55	0/654
30	e	0.47	0/429	0.73	0/568
31	f	0.55	0/425	0.59	0/551
32	g	0.61	0/554	0.64	2/726 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
33	h	0.52	0/306	0.60	0/400
34	i	0.60	1/381 (0.3%)	1.14	4/502 (0.8%)
All	All	0.29	2/97535 (0.0%)	0.71	154/145542 (0.1%)

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
4	E	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	i	30	PHE	CB-CG	-5.71	1.41	1.51
17	R	33	GLU	CB-CG	-5.16	1.42	1.52

The worst 5 of 154 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1559	G	OP1-P-OP2	-27.08	78.99	119.60
1	A	1559	G	O5'-P-OP1	-26.66	78.71	110.70
1	A	1559	G	O5'-P-OP2	15.62	129.44	110.70
1	A	1558	C	OP2-P-O3'	-15.50	71.09	105.20
1	A	1558	C	OP1-P-O3'	14.44	136.97	105.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	E	163	MET	Mainchain

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	59248	0	29718	372	0
2	B	2398	0	1205	21	0
3	D	2156	0	2261	48	0
4	E	1564	0	1651	27	0
5	F	1658	0	1752	28	0
6	G	1439	0	1512	35	0
7	H	1405	0	1494	31	0
8	I	411	0	348	8	0
9	J	528	0	146	0	0
10	K	272	0	77	2	0
11	L	1171	0	1235	12	0
12	M	942	0	1008	18	0
13	N	1129	0	1232	40	0
14	O	1092	0	1163	27	0
15	P	1004	0	1090	22	0
16	Q	968	0	1039	20	0
17	R	951	0	1037	22	0
18	S	943	0	1033	30	0
19	T	859	0	902	23	0
20	U	918	0	975	11	0
21	V	784	0	847	12	0
22	W	800	0	895	26	0
23	X	1432	0	1486	38	0
24	Y	571	0	611	6	0
25	Z	705	0	784	20	0
26	a	553	0	595	0	0
27	b	814	0	922	0	0
28	c	466	0	478	0	0
29	d	484	0	500	0	0
30	e	425	0	456	0	0
31	f	422	0	480	0	0
32	g	548	0	619	0	0
33	h	305	0	357	0	0
34	i	375	0	393	0	0
35	d	1	0	0	0	0
35	h	1	0	0	0	0
All	All	89742	0	60301	791	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 7.

The worst 5 of 791 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)
6:G:66:GLN:NE2	6:G:93:THR:O	2.06	0.88
17:R:90:LYS:HB2	17:R:113:ARG:HG3	1.55	0.88
13:N:81:ASP:OD1	13:N:118:LYS:NZ	2.10	0.85
7:H:121:ILE:HD11	7:H:140:LYS:HB3	1.59	0.82
13:N:44:ARG:NH1	13:N:44:ARG:O	2.13	0.82

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	
3	D	275/277 (99%)	259 (94%)	16 (6%)	0	100	100
4	E	204/206 (99%)	194 (95%)	9 (4%)	1 (0%)	29	61
5	F	207/209 (99%)	197 (95%)	10 (5%)	0	100	100
6	G	180/182 (99%)	167 (93%)	13 (7%)	0	100	100
7	H	178/180 (99%)	170 (96%)	8 (4%)	0	100	100
8	I	61/148 (41%)	52 (85%)	9 (15%)	0	100	100
9	J	130/162 (80%)	123 (95%)	7 (5%)	0	100	100
10	K	66/139 (48%)	65 (98%)	1 (2%)	0	100	100
11	L	143/145 (99%)	136 (95%)	7 (5%)	0	100	100
12	M	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
13	N	143/145 (99%)	116 (81%)	27 (19%)	0	100	100
14	O	136/138 (99%)	119 (88%)	17 (12%)	0	100	100
15	P	119/121 (98%)	111 (93%)	8 (7%)	0	100	100
16	Q	117/119 (98%)	111 (95%)	6 (5%)	0	100	100
17	R	115/117 (98%)	105 (91%)	10 (9%)	0	100	100
18	S	112/114 (98%)	104 (93%)	8 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	T	101/103 (98%)	95 (94%)	6 (6%)	0	100	100
20	U	113/115 (98%)	108 (96%)	5 (4%)	0	100	100
21	V	96/98 (98%)	92 (96%)	4 (4%)	0	100	100
22	W	99/101 (98%)	91 (92%)	8 (8%)	0	100	100
23	X	179/181 (99%)	169 (94%)	10 (6%)	0	100	100
24	Y	72/74 (97%)	69 (96%)	3 (4%)	0	100	100
25	Z	89/91 (98%)	86 (97%)	3 (3%)	0	100	100
26	a	63/65 (97%)	61 (97%)	2 (3%)	0	100	100
27	b	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
28	c	56/81 (69%)	49 (88%)	7 (12%)	0	100	100
29	d	57/59 (97%)	52 (91%)	5 (9%)	0	100	100
30	e	49/51 (96%)	42 (86%)	7 (14%)	0	100	100
31	f	48/50 (96%)	42 (88%)	6 (12%)	0	100	100
32	g	64/66 (97%)	56 (88%)	8 (12%)	0	100	100
33	h	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
34	i	44/46 (96%)	38 (86%)	6 (14%)	0	100	100
All	All	3569/3842 (93%)	3318 (93%)	250 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	164	ALA

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	
3	D	229/229 (100%)	229 (100%)	0	100	100
4	E	168/168 (100%)	168 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	F	181/181 (100%)	180 (99%)	1 (1%)	86 94
6	G	155/155 (100%)	154 (99%)	1 (1%)	86 94
7	H	156/156 (100%)	155 (99%)	1 (1%)	86 94
8	I	34/134 (25%)	34 (100%)	0	100 100
11	L	127/127 (100%)	127 (100%)	0	100 100
12	M	103/103 (100%)	103 (100%)	0	100 100
13	N	124/124 (100%)	123 (99%)	1 (1%)	81 91
14	O	115/115 (100%)	114 (99%)	1 (1%)	78 90
15	P	110/110 (100%)	110 (100%)	0	100 100
16	Q	104/104 (100%)	103 (99%)	1 (1%)	76 88
17	R	103/103 (100%)	103 (100%)	0	100 100
18	S	99/99 (100%)	98 (99%)	1 (1%)	76 88
19	T	96/96 (100%)	96 (100%)	0	100 100
20	U	100/100 (100%)	99 (99%)	1 (1%)	76 88
21	V	88/88 (100%)	88 (100%)	0	100 100
22	W	89/89 (100%)	86 (97%)	3 (3%)	37 65
23	X	163/163 (100%)	163 (100%)	0	100 100
24	Y	60/60 (100%)	60 (100%)	0	100 100
25	Z	76/76 (100%)	76 (100%)	0	100 100
26	a	61/61 (100%)	61 (100%)	0	100 100
27	b	93/93 (100%)	93 (100%)	0	100 100
28	c	54/73 (74%)	53 (98%)	1 (2%)	57 78
29	d	54/54 (100%)	54 (100%)	0	100 100
30	e	48/48 (100%)	48 (100%)	0	100 100
31	f	44/44 (100%)	44 (100%)	0	100 100
32	g	61/61 (100%)	61 (100%)	0	100 100
33	h	36/36 (100%)	36 (100%)	0	100 100
34	i	40/40 (100%)	39 (98%)	1 (2%)	47 72
All	All	2971/3090 (96%)	2958 (100%)	13 (0%)	91 95

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

Mol	Chain	Res	Type
20	U	6	ARG
22	W	50	ARG
34	i	49	ARG
22	W	88	ASN
28	c	2	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
23	X	90	HIS
34	i	32	ASN
13	N	113	ASN
16	Q	52	HIS
16	Q	69	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2756/2929 (94%)	400 (14%)	29 (1%)
2	B	111/112 (99%)	28 (25%)	4 (3%)
All	All	2867/3041 (94%)	428 (14%)	33 (1%)

5 of 428 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	A
1	A	17	A
1	A	27	G
1	A	38	A
1	A	39	G

5 of 33 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2837	U
2	B	31	U
2	B	86	U
1	A	1155	A
1	A	1146	G

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)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

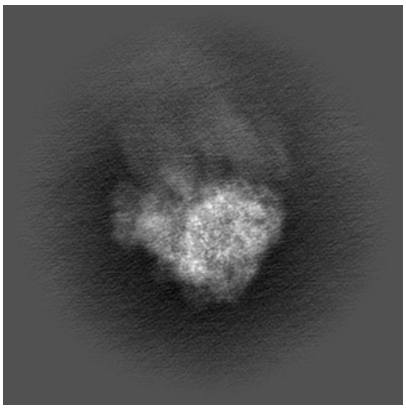
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-29304. These allow visual inspection of the internal detail of the map and identification of artifacts.

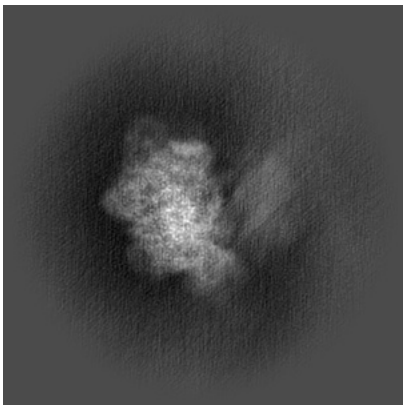
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

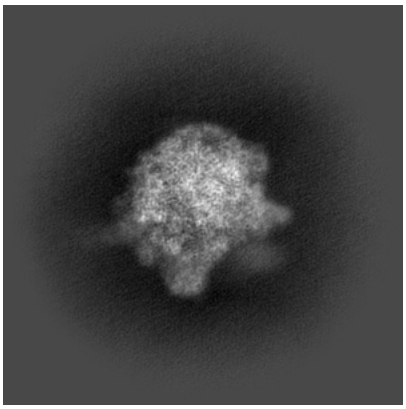
6.1.1 Primary map



X

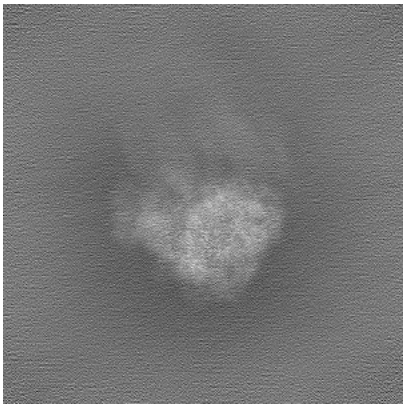


Y

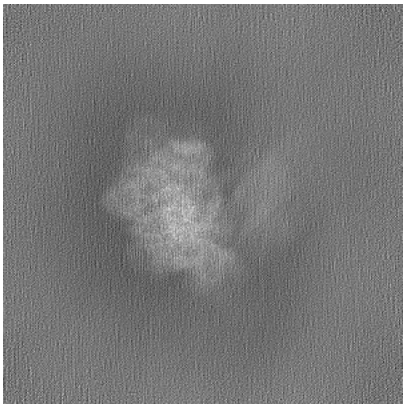


Z

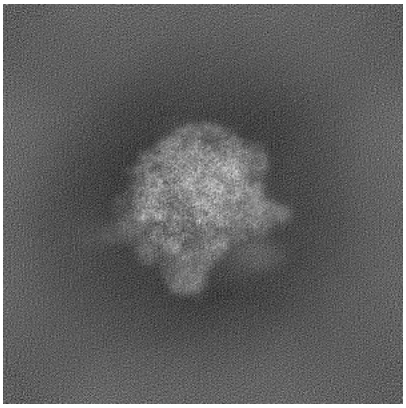
6.1.2 Raw map



X



Y

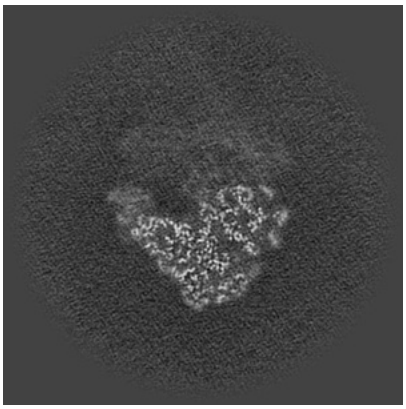


Z

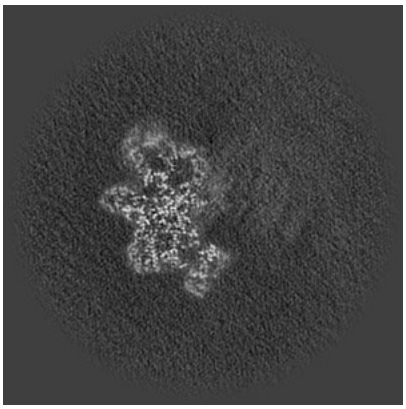
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

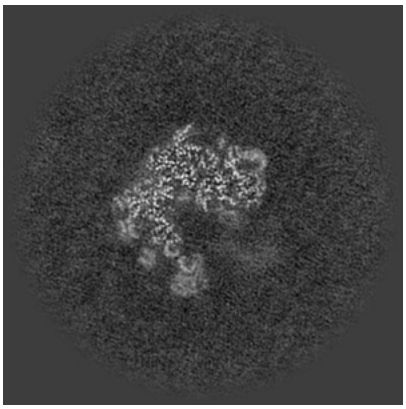
6.2.1 Primary map



X Index: 225

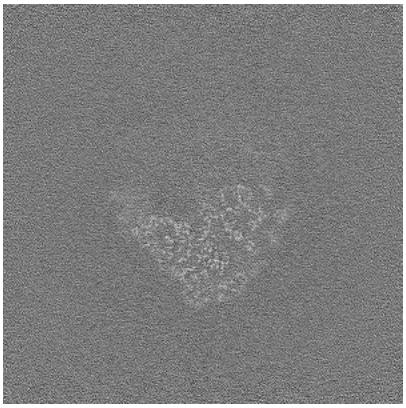


Y Index: 225

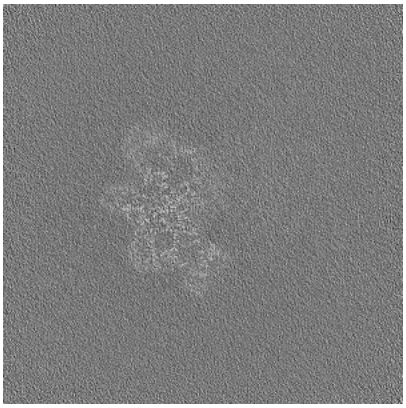


Z Index: 225

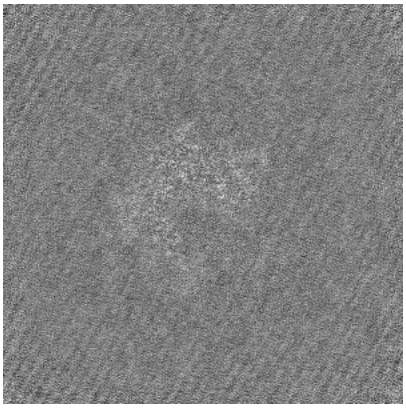
6.2.2 Raw map



X Index: 225



Y Index: 225

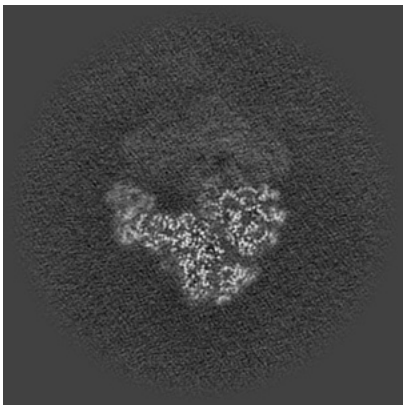


Z Index: 225

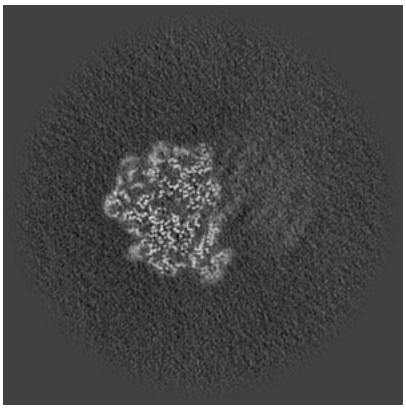
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

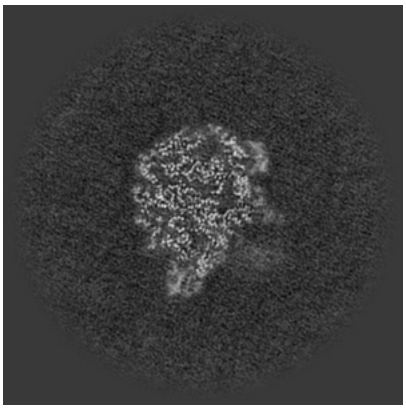
6.3.1 Primary map



X Index: 220

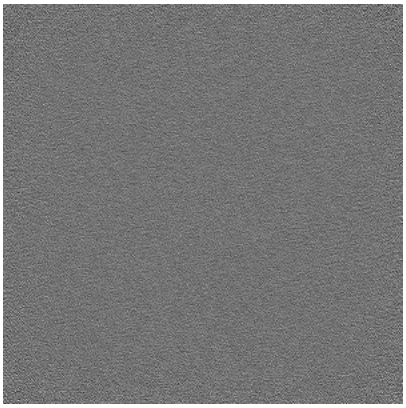


Y Index: 242

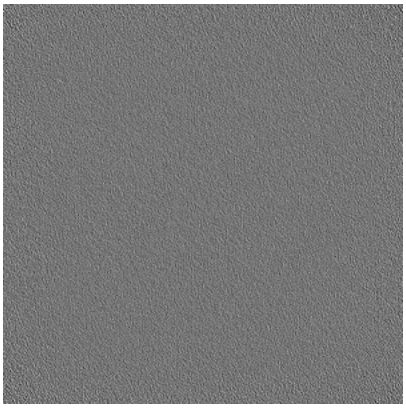


Z Index: 192

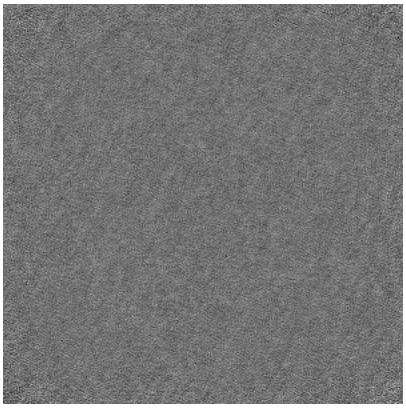
6.3.2 Raw map



X Index: 0



Y Index: 0

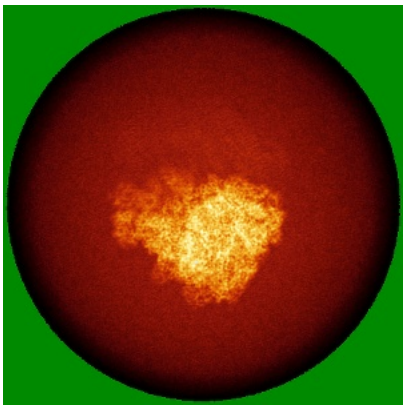


Z Index: 0

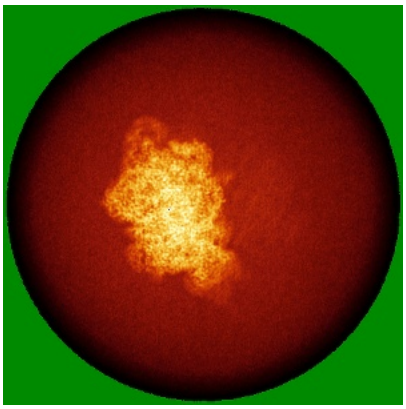
The images above show the largest variance slices of the map in three orthogonal directions.

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

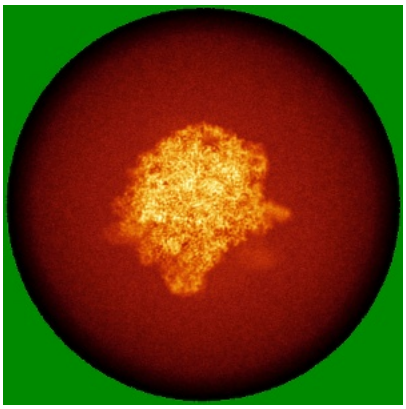
6.4.1 Primary map



X

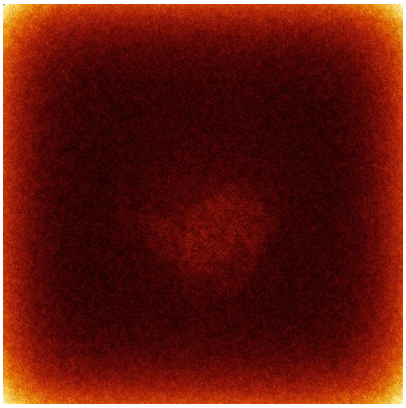


Y

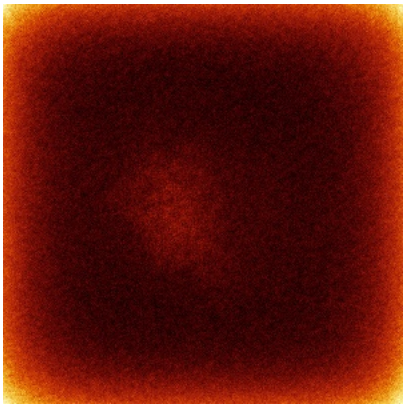


Z

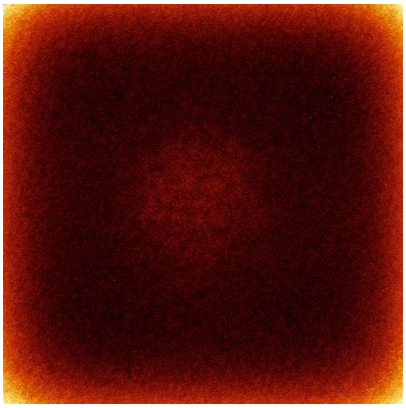
6.4.2 Raw map



X



Y



Z

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

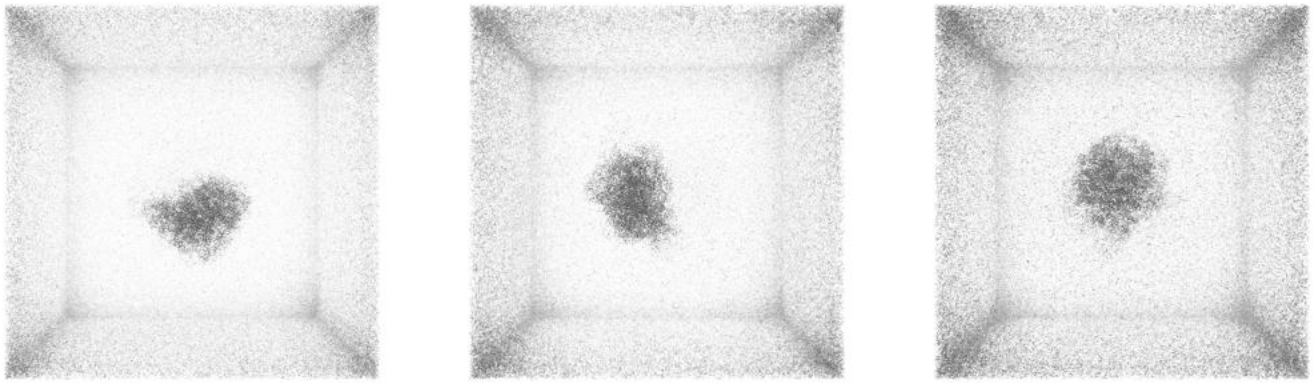
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

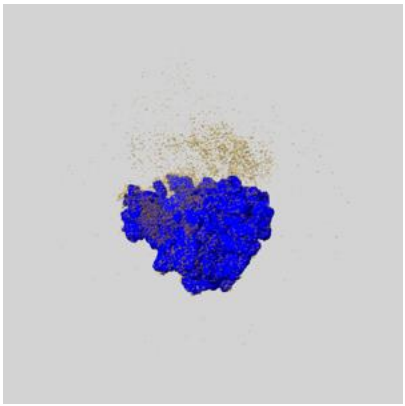
6.6 Mask visualisation

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

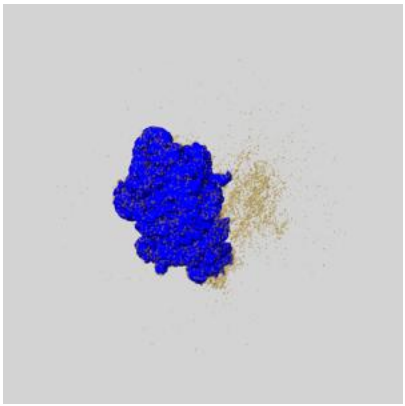
A mask typically either:

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

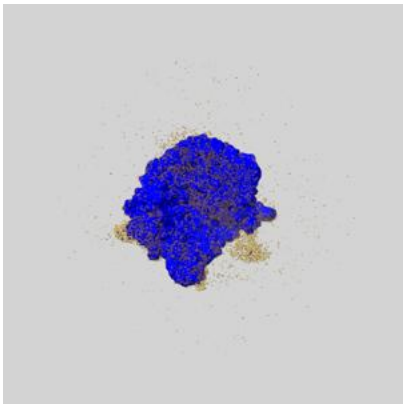
6.6.1 emd_29304_msk_1.map



X



Y

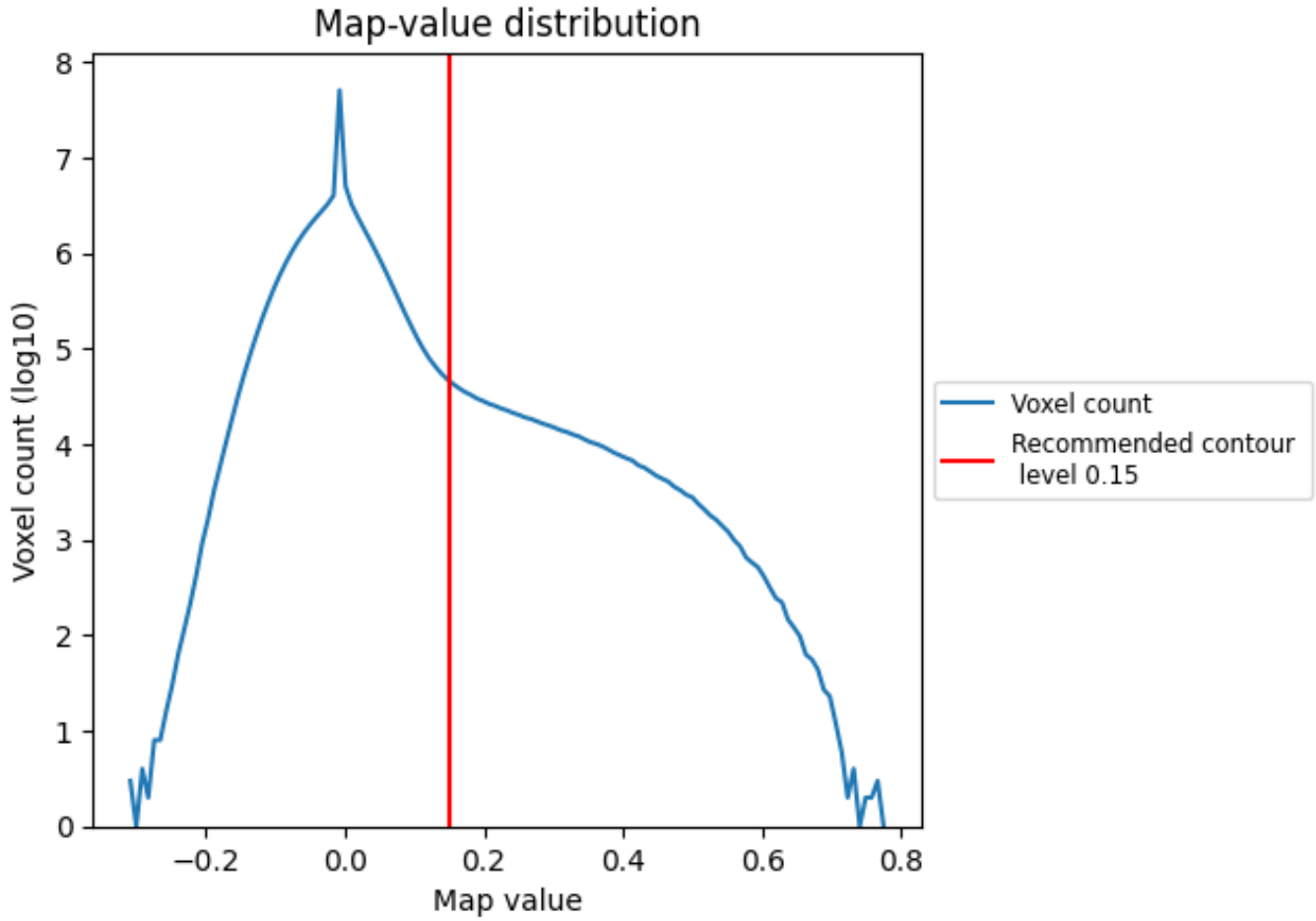


Z

7 Map analysis

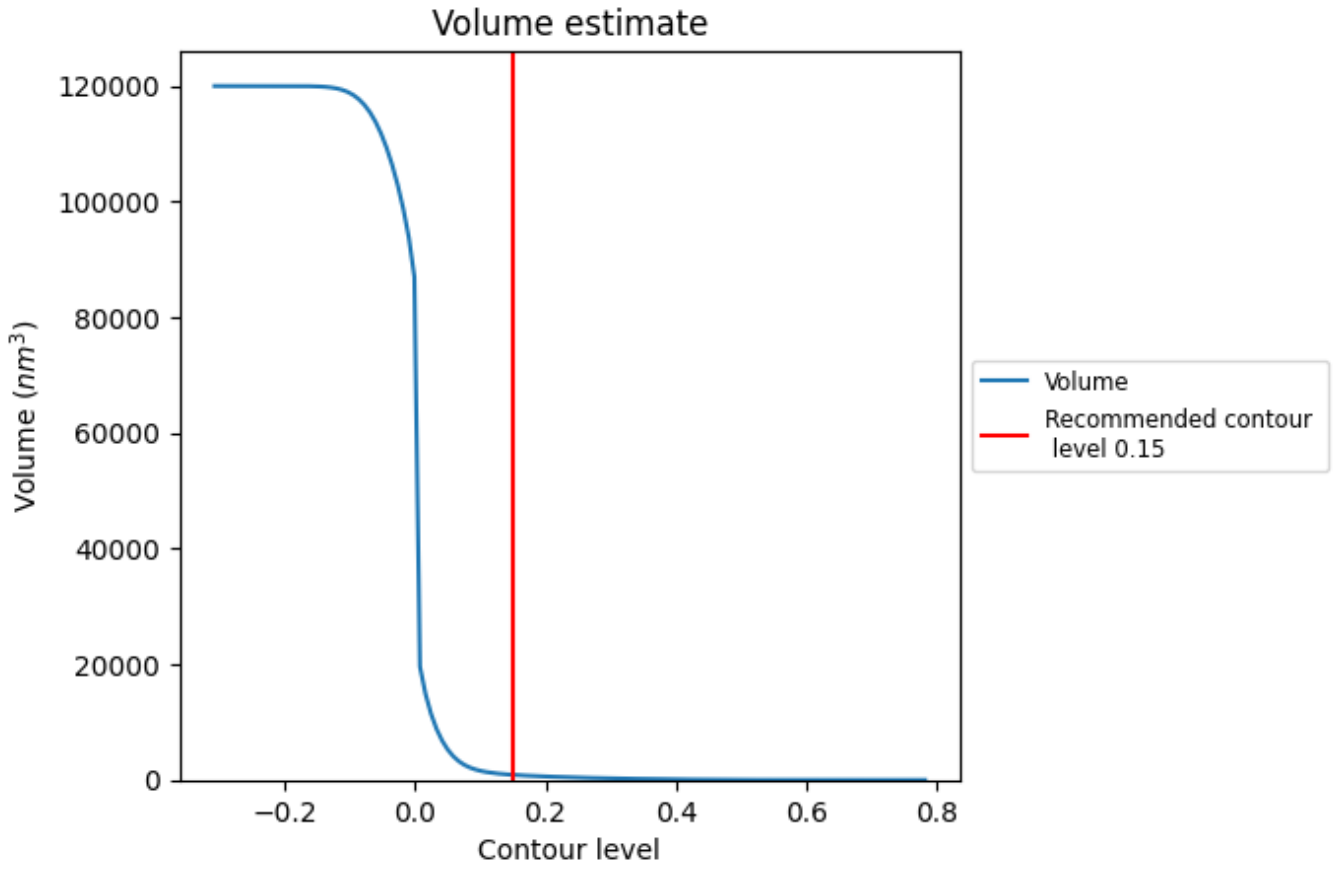
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

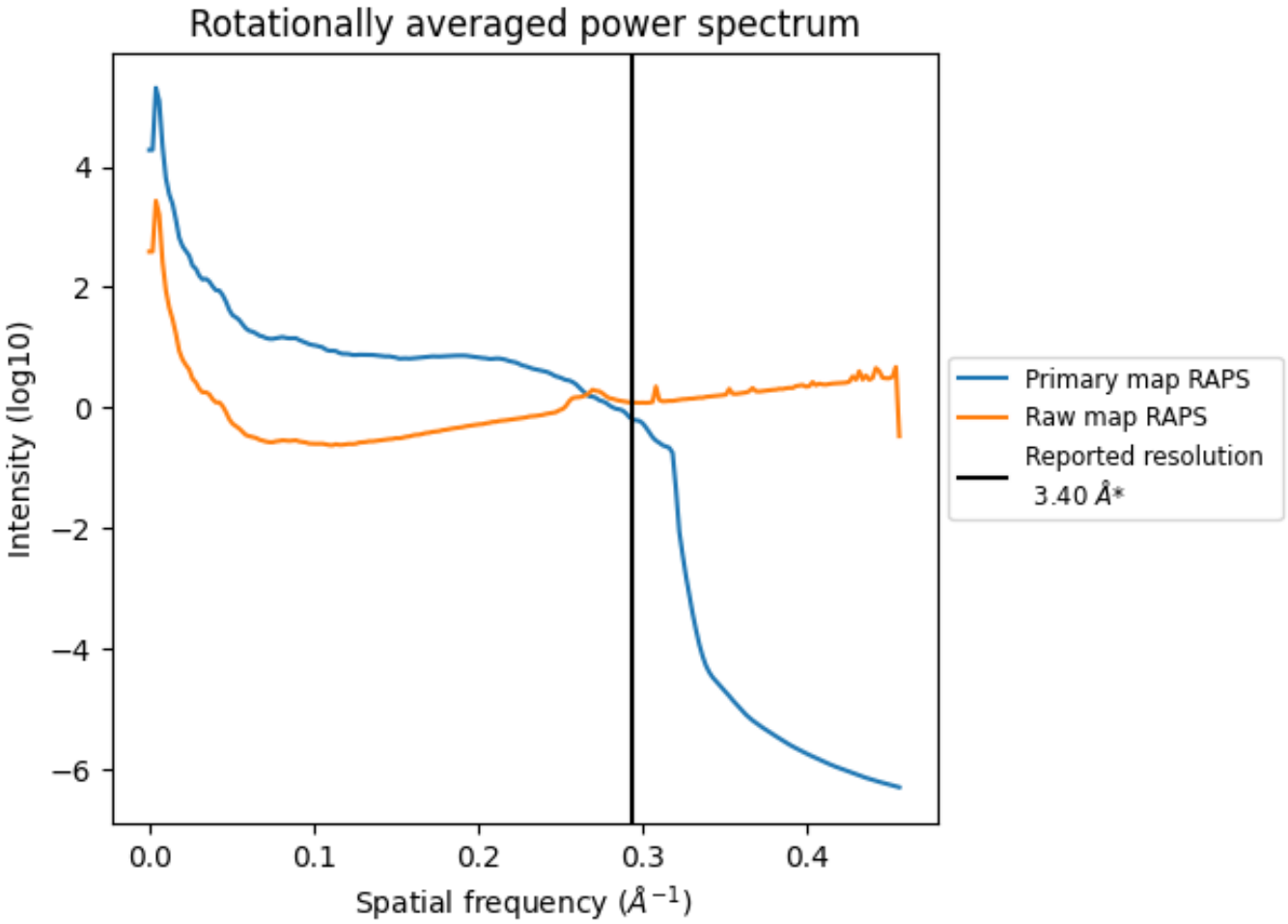
7.2 Volume estimate (i)



The volume at the recommended contour level is 888 nm^3; this corresponds to an approximate mass of 802 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)

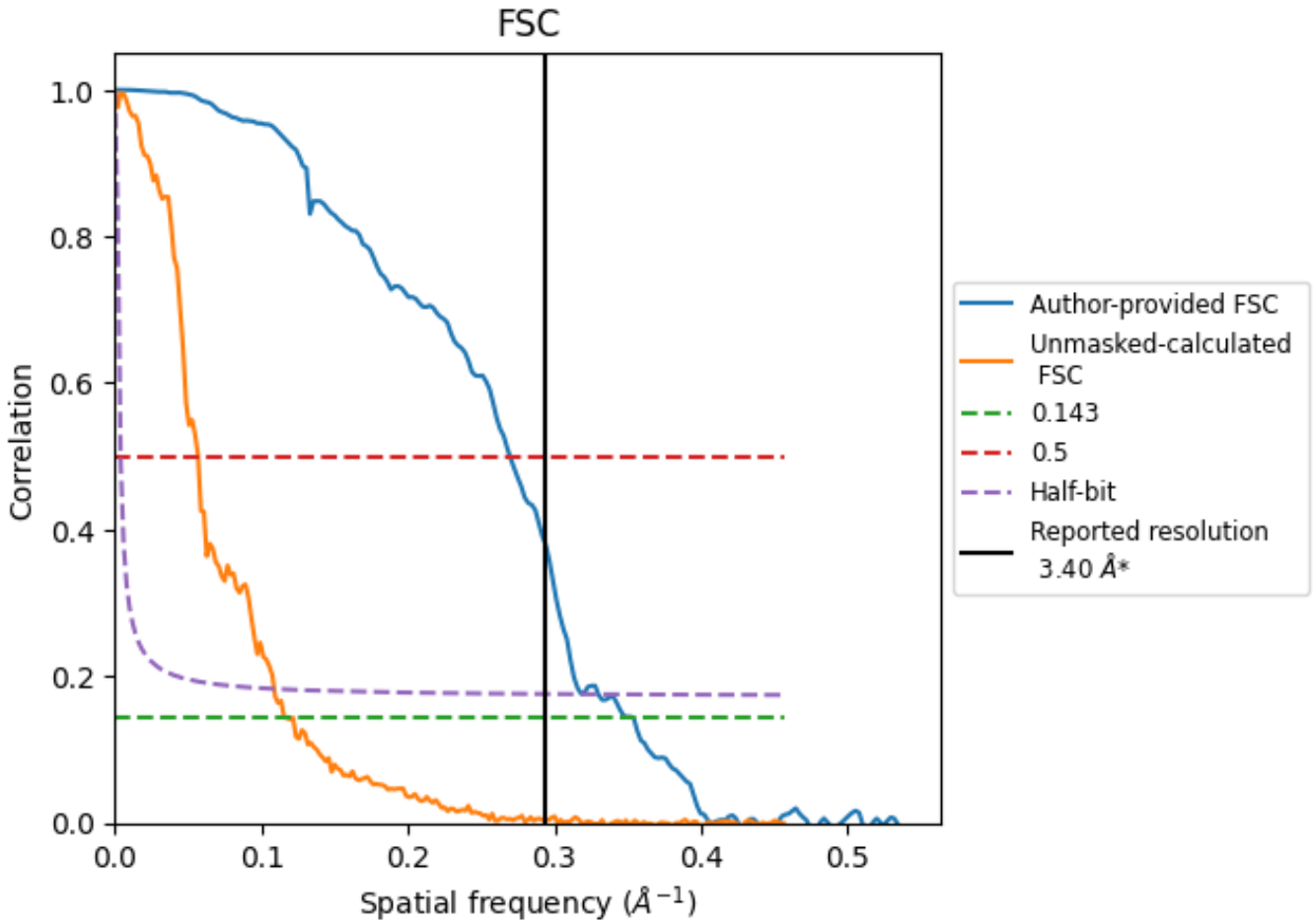


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

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 0.294 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	2.83	3.71	3.03
Unmasked-calculated*	8.56	17.61	9.20

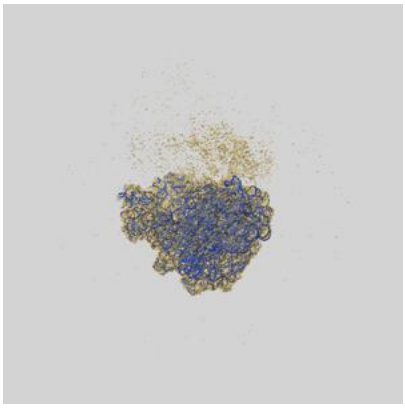
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 2.83 differs from the reported value 3.4 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.56 differs from the reported value 3.4 by more than 10 %

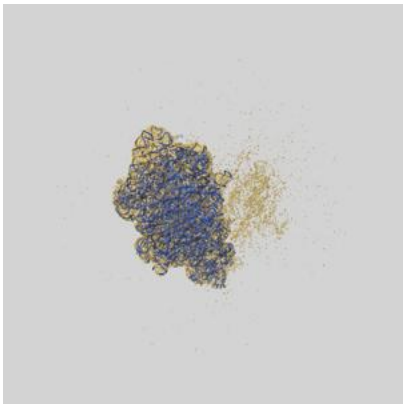
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-29304 and PDB model 8FN2. Per-residue inclusion information can be found in section 3 on page 11.

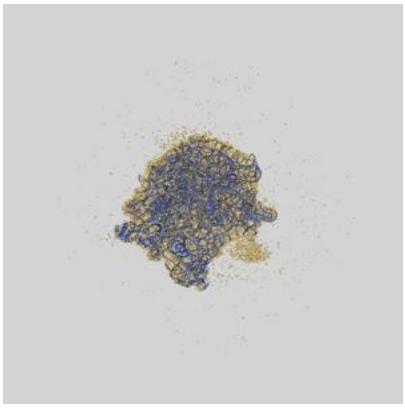
9.1 Map-model overlay



X



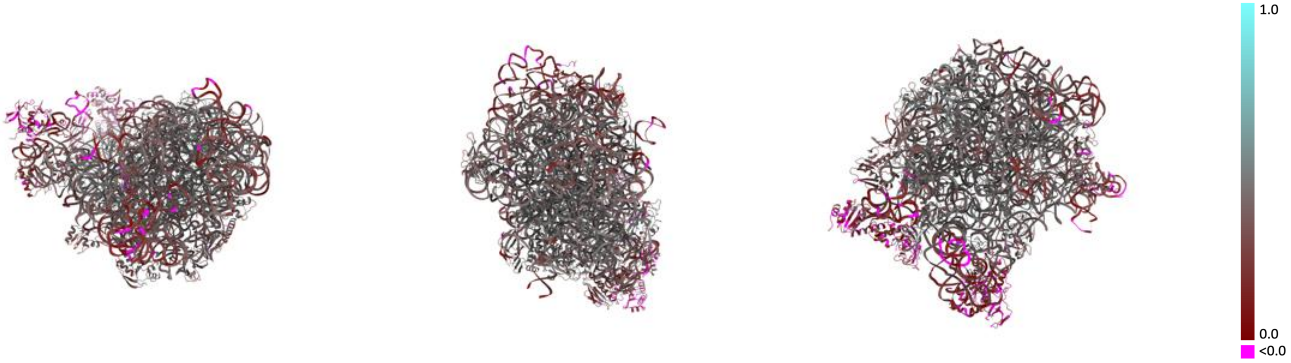
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

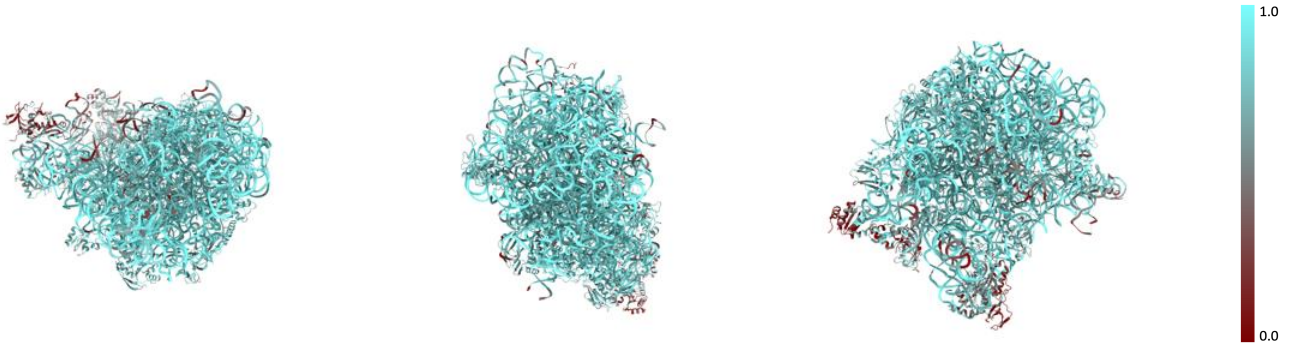
9.2 Q-score mapped to coordinate model



X Y Z

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

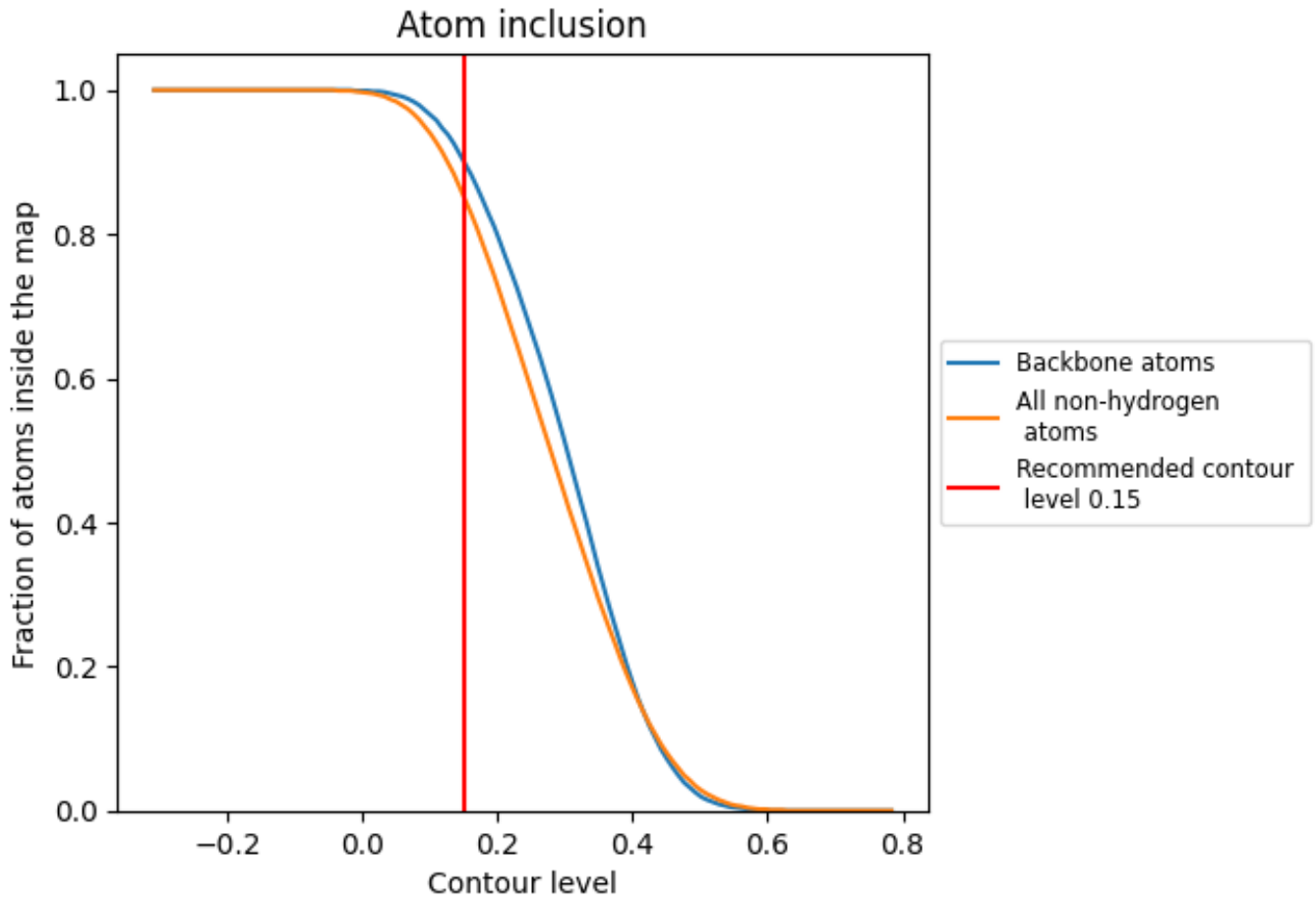
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 85% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8520	0.3790
A	0.9040	0.3840
B	0.8670	0.2810
D	0.7870	0.4120
E	0.8290	0.4580
F	0.8020	0.4350
G	0.4380	0.1240
H	0.7640	0.3160
I	0.4700	0.2440
J	0.3300	0.0820
K	0.4410	0.1380
L	0.8560	0.4610
M	0.8280	0.4500
N	0.7710	0.4030
O	0.7700	0.4310
P	0.8480	0.4660
Q	0.6920	0.2590
R	0.7530	0.4080
S	0.8400	0.4570
T	0.7800	0.4350
U	0.8250	0.4700
V	0.7850	0.4070
W	0.6800	0.3480
X	0.6480	0.2740
Y	0.8410	0.4760
Z	0.7840	0.4240
a	0.7800	0.3520
b	0.8110	0.4600
c	0.2300	0.0510
d	0.8460	0.4530
e	0.6840	0.3580
f	0.8450	0.4940
g	0.8150	0.4720
h	0.8020	0.4450
i	0.8000	0.3120