



## wwPDB EM Validation Summary Report ⓘ

Oct 28, 2024 – 09:59 am GMT

PDB ID : 5GAH  
EMDB ID : EMD-8004  
Title : RNC in complex with SRP with detached NG domain  
Authors : Jomaa, A.; Boehringer, D.; Leibundgut, M.; Ban, N.  
Deposited on : 2015-11-26  
Resolution : 3.80 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](mailto: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:

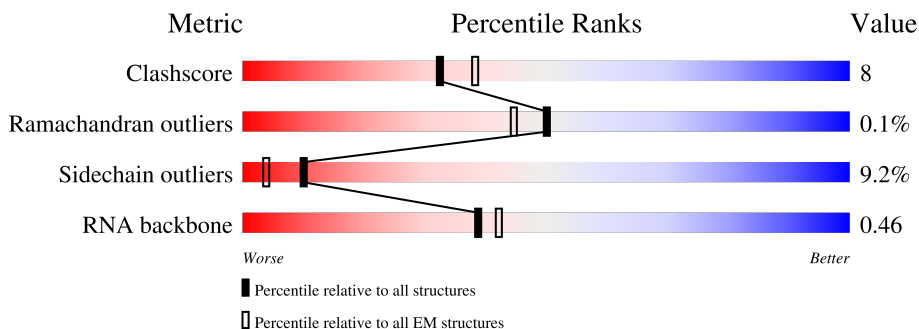
EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 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 3.80 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	210492	15764
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  $\geq 3$ , 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	1	113	
2	2	3	
3	A	2903	
4	B	120	
5	C	273	
6	D	209	
7	E	201	

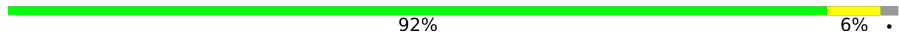
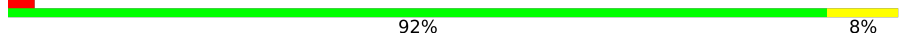


Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	F	179	60% 35%
9	G	177	69% 29%
10	H	149	24% 66% 32%
11	I	165	15% 50% 25% 24%
12	J	142	35% 54% 37% 6%
13	K	142	73% 23%
14	L	123	68% 30%
15	M	144	74% 24%
16	N	136	72% 26%
17	O	127	70% 25%
18	P	117	65% 32%
19	Q	115	74% 24%
20	R	118	74% 21%
21	S	103	70% 28%
22	T	110	78% 20%
23	U	100	71% 23% 5%
24	V	104	68% 29%
25	W	94	74% 24%
26	X	85	59% 28% 11%
27	Y	78	62% 36%
28	Z	63	67% 27% 5%
29	a	59	95%
30	b	57	77% 21%
31	c	55	84% 9% 7%
32	d	46	87% 13%

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
33	e	65	 92% 6%
34	f	38	 92% 8%
35	i	453	 9% 26% 72%
36	k	18	 22% 89% 11%

## 2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 94027 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 SRP 4.5S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	43	926	413	174	296	43	0	0

- Molecule 2 is a RNA chain called tRNA CCAend.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	3	62	28	11	20	3	0	0

- Molecule 3 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	A	2883	61902	27613	11397	20009	2883	0	0

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	B	120	2569	1144	468	837	120	0	0

- Molecule 5 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	C	271	2082	1288	423	364	7	0	0

- Molecule 6 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	D	209	1565	979	288	294	4	0	0

- Molecule 7 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	E	201	1552	974	283	290	5	0	0

- Molecule 8 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	F	177	1410	899	249	256	6	0	0

- Molecule 9 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	G	176	1323	832	243	246	2	0	0

- Molecule 10 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	H	149	1110	699	197	213	1	0	0

- Molecule 11 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	I	125	946	599	169	175	3	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	85	VAL	SER	conflict	UNP P0A7J3
I	86	THR	MET	conflict	UNP P0A7J3

- Molecule 12 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	J	134	979	619	169	185	6	0	0

- Molecule 13 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	K	142	1129	714	212	199	4	0	0

- Molecule 14 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	L	123	946	593	181	166	6	0	0

- Molecule 15 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	M	144	1053	654	207	190	2	0	0

- Molecule 16 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	N	136	1074	686	205	177	6	0	0

- Molecule 17 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	O	125	993	613	202	173	5	0	0

- Molecule 18 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	P	117	900	557	179	163	1	0	0

- Molecule 19 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	Q	114	917	574	179	163	1	0	0

- Molecule 20 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	R	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 21 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 22 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 23 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	95	Total	C	N	O	S	0	0
			756	479	141	135	1		

- Molecule 24 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	V	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 25 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 26 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	76	Total	C	N	O	S	0	0
			580	359	117	103	1		

- Molecule 27 is a protein called 50S ribosomal protein L28.



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	Y	77	625	388	129	106	2	0	0

- Molecule 28 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	Z	62	501	308	98	94	1	0	0

- Molecule 29 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	a	58	449	281	87	79	2	0	0

- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	b	56	444	269	94	80	1	0	0

- Molecule 31 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
31	c	51	414	266	76	72	0	0

- Molecule 32 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	d	46	377	228	90	57	2	0	0

- Molecule 33 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	e	64	504	323	105	74	2	0	0

- Molecule 34 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 35 is a protein called Signal recognition particle protein Ffh.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	126	Total	C	N	O	S	0	0
			916	575	169	161	11		

- Molecule 36 is a protein called 1A9L SS.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	18	Total	C	N	O	S	0	0
			137	94	20	22	1		

- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

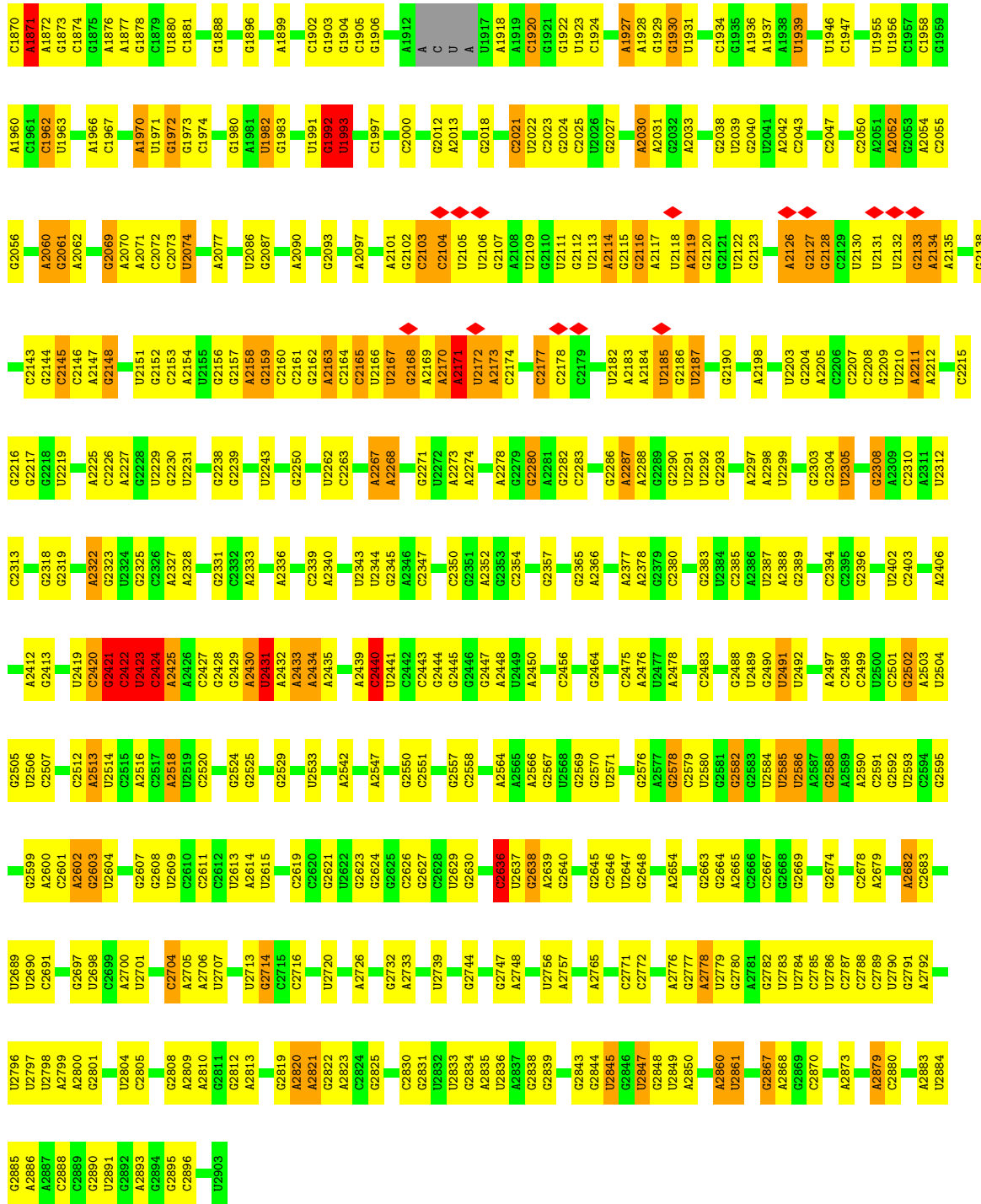
Mol	Chain	Residues	Atoms		AltConf
37	2	1	Total	Mg	0
			1	1	
37	A	412	Total	Mg	0
			412	412	
37	B	11	Total	Mg	0
			11	11	
37	C	2	Total	Mg	0
			2	2	
37	D	1	Total	Mg	0
			1	1	
37	E	1	Total	Mg	0
			1	1	
37	P	1	Total	Mg	0
			1	1	
37	R	1	Total	Mg	0
			1	1	
37	b	1	Total	Mg	0
			1	1	

- Molecule 38 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
38	f	1	Total	Zn	0
			1	1	



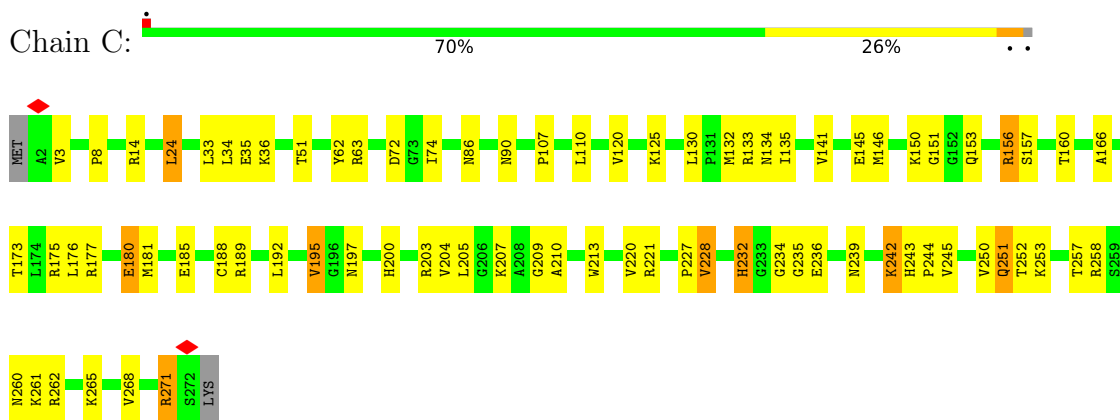




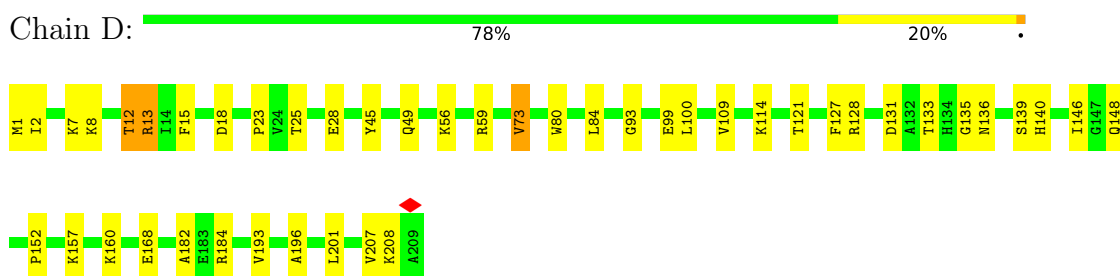
• Molecule 4: 5S rRNA



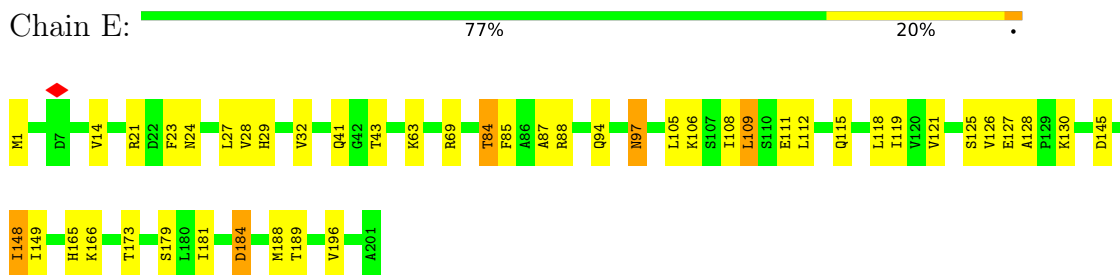
• Molecule 5: 50S ribosomal protein L2



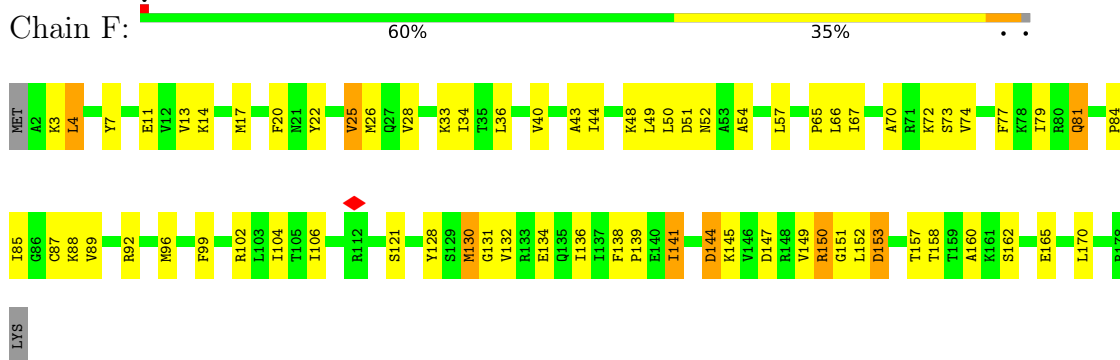
• Molecule 6: 50S ribosomal protein L3



• Molecule 7: 50S ribosomal protein L4

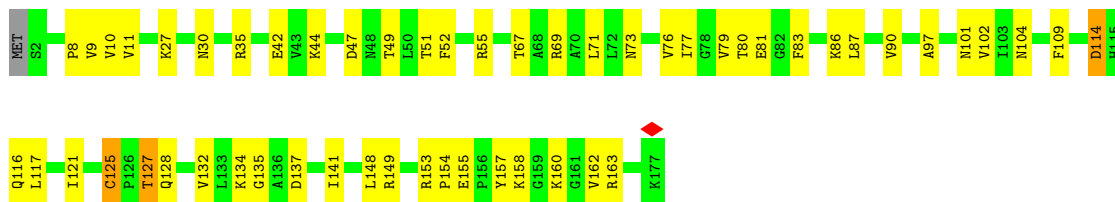


• Molecule 8: 50S ribosomal protein L5

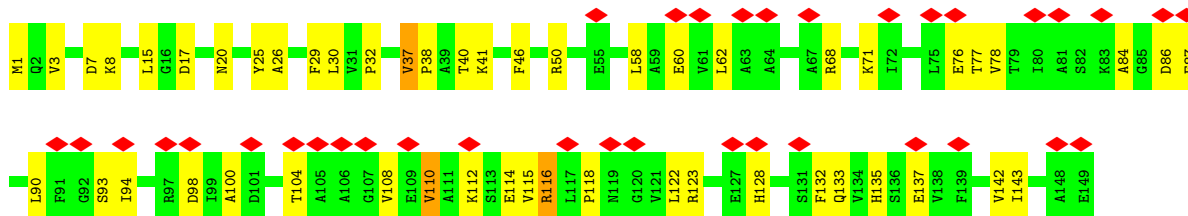


• Molecule 9: 50S ribosomal protein L6

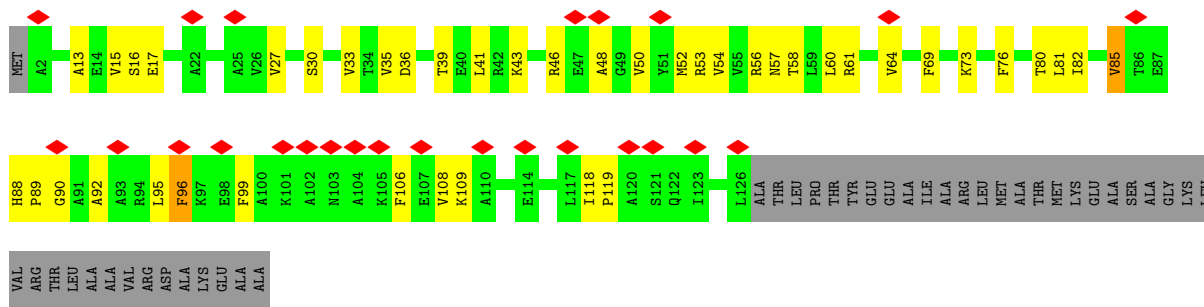




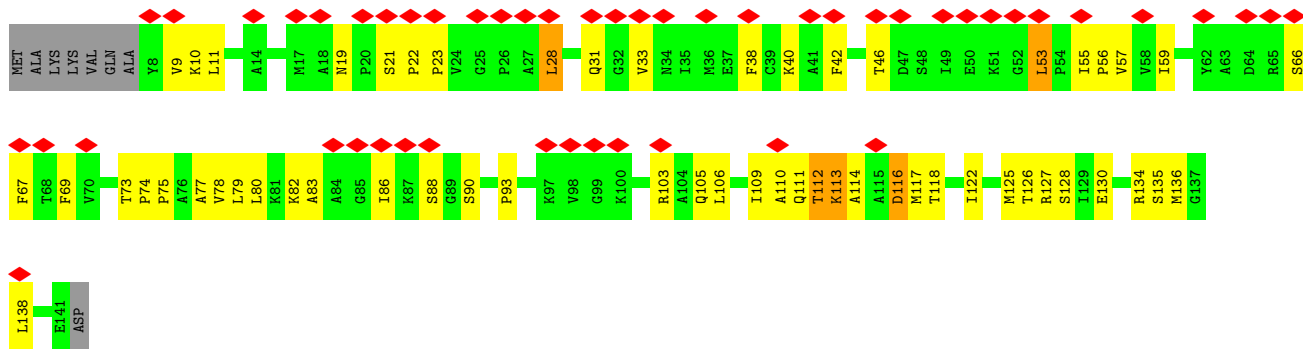
• Molecule 10: 50S ribosomal protein L9



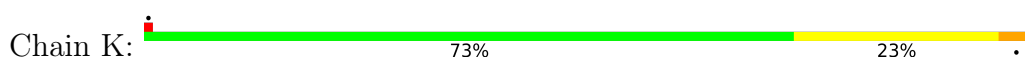
• Molecule 11: 50S ribosomal protein L10

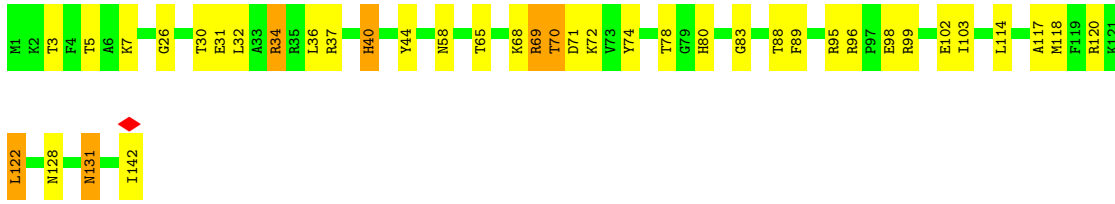


• Molecule 12: 50S ribosomal protein L11

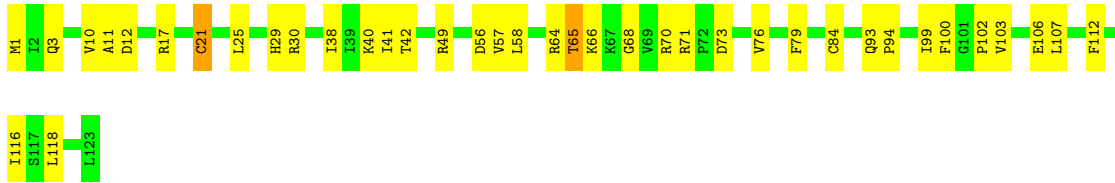


• Molecule 13: 50S ribosomal protein L13

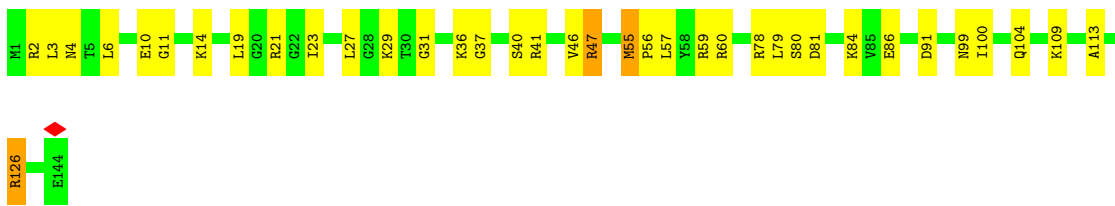
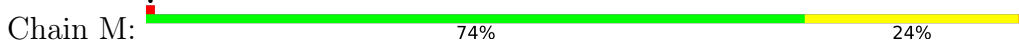




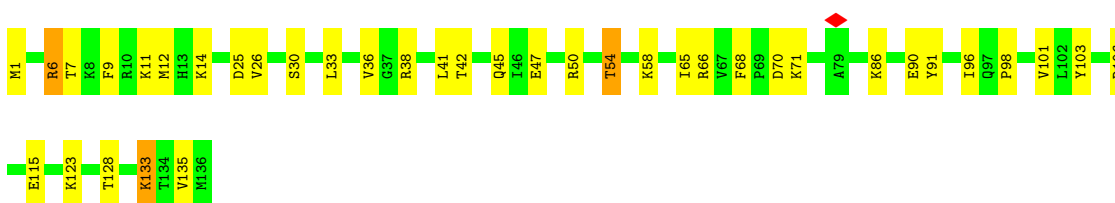
• Molecule 14: 50S ribosomal protein L14



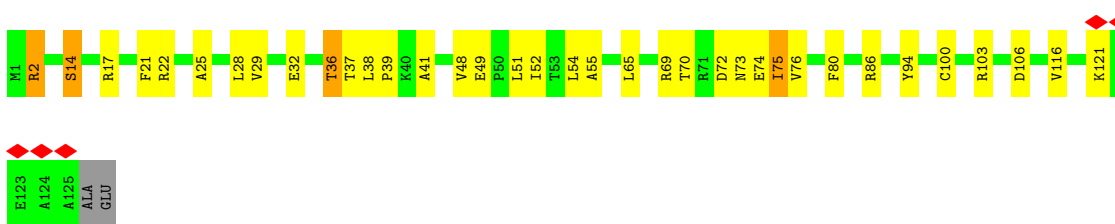
• Molecule 15: 50S ribosomal protein L15



• Molecule 16: 50S ribosomal protein L16



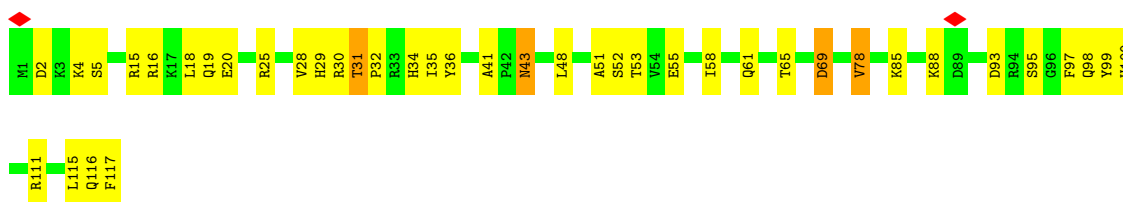
• Molecule 17: 50S ribosomal protein L17




• Molecule 18: 50S ribosomal protein L18



Chain P:  65% 32%



- Molecule 19: 50S ribosomal protein L19

Chain Q:  74% 24%



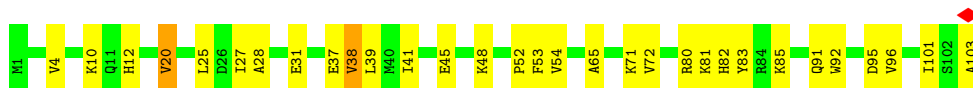
- Molecule 20: 50S ribosomal protein L20

Chain R:  74% 21%




- Molecule 21: 50S ribosomal protein L21

Chain S:  70% 28%



- Molecule 22: 50S ribosomal protein L22

Chain T:  78% 20%



- Molecule 23: 50S ribosomal protein L23

Chain U:  71% 23% 5%

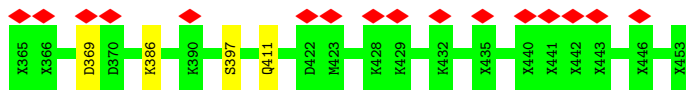


- Molecule 24: 50S ribosomal protein L24

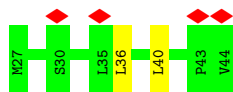
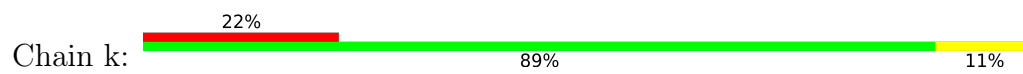
Chain V:  68% 29%







- Molecule 36: 1A9L SS



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	46409	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 ( $e^-/\text{\AA}^2$ )	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.390	Depositor
Minimum map value	-0.215	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.05	Depositor
Map size ( $\text{\AA}$ )	398.88, 398.88, 398.88	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.385, 1.385, 1.385	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, MG

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	1	0.79	0/1037	1.29	7/1616 (0.4%)
2	2	0.57	0/68	1.25	1/103 (1.0%)
3	A	0.68	14/69329 (0.0%)	1.17	187/108152 (0.2%)
4	B	0.51	0/2872	1.04	1/4478 (0.0%)
5	C	0.47	0/2121	0.65	0/2852
6	D	0.47	0/1586	0.63	0/2134
7	E	0.44	0/1571	0.61	1/2113 (0.0%)
8	F	0.39	0/1434	0.56	0/1926
9	G	0.39	0/1343	0.58	0/1816
10	H	0.42	0/1121	0.57	0/1515
11	I	0.48	0/958	0.62	1/1292 (0.1%)
12	J	0.58	0/993	0.69	1/1341 (0.1%)
13	K	0.46	0/1152	0.57	0/1551
14	L	0.45	0/955	0.63	0/1279
15	M	0.47	0/1062	0.64	0/1413
16	N	0.48	0/1093	0.59	0/1460
17	O	0.47	0/1006	0.67	0/1345
18	P	0.41	0/910	0.56	0/1219
19	Q	0.48	0/929	0.60	0/1242
20	R	0.56	0/960	0.59	0/1278
21	S	0.46	0/829	0.62	0/1107
22	T	0.52	0/864	0.71	0/1156
23	U	0.45	0/763	0.61	0/1021
24	V	0.38	0/787	0.54	0/1051
25	W	0.40	0/766	0.57	0/1025
26	X	0.50	0/587	0.60	0/776
27	Y	0.48	0/635	0.61	0/848
28	Z	0.41	0/502	0.54	0/667
29	a	0.38	0/453	0.56	0/605
30	b	0.43	0/450	0.62	0/599
31	c	0.44	0/421	0.61	0/561
32	d	0.51	0/380	0.66	0/498

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	e	0.47	0/513	0.62	0/676
34	f	0.49	0/303	0.58	0/397
35	i	0.44	0/672	0.56	0/883
36	k	0.62	0/137	0.85	0/186
All	All	0.63	14/101562 (0.0%)	1.05	199/152181 (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
5	C	0	1
9	G	0	1
12	J	0	1
All	All	0	3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2542	A	N9-C4	-6.90	1.33	1.37
3	A	1254	A	N9-C4	-6.39	1.34	1.37
3	A	1321	A	N9-C4	6.27	1.41	1.37
3	A	1490	A	N9-C4	6.00	1.41	1.37
3	A	2114	A	N9-C4	5.98	1.41	1.37

The worst 5 of 199 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2423	U	C6-N1-C2	-12.25	113.65	121.00
3	A	1838	C	C6-N1-C2	9.39	124.06	120.30
3	A	2422	C	O4'-C1'-N1	9.31	115.65	108.20
3	A	2423	U	C5-C6-N1	8.80	127.10	122.70
3	A	1584	U	C2-N1-C1'	8.52	127.92	117.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	C	232	HIS	Peptide
9	G	47	ASP	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
12	J	19	ASN	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	926	0	467	10	0
2	2	62	0	34	1	0
3	A	61902	0	31133	683	0
4	B	2569	0	1301	19	0
5	C	2082	0	2154	51	0
6	D	1565	0	1616	32	0
7	E	1552	0	1619	27	0
8	F	1410	0	1444	42	0
9	G	1323	0	1371	35	0
10	H	1110	0	1148	23	0
11	I	946	0	978	31	0
12	J	979	0	1028	39	0
13	K	1129	0	1162	24	0
14	L	946	0	1023	21	0
15	M	1053	0	1129	26	0
16	N	1074	0	1157	23	0
17	O	993	0	1034	25	0
18	P	900	0	935	23	0
19	Q	917	0	962	19	0
20	R	947	0	1019	24	0
21	S	816	0	839	20	0
22	T	857	0	922	14	0
23	U	756	0	817	14	0
24	V	779	0	831	18	0
25	W	753	0	780	14	0
26	X	580	0	594	16	0
27	Y	625	0	652	17	0
28	Z	501	0	531	13	0
29	a	449	0	488	0	0
30	b	444	0	458	0	0
31	c	414	0	442	0	0
32	d	377	0	418	0	0

*Continued on next page...*



Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	e	504	0	572	0	0
34	f	302	0	340	0	0
35	i	916	0	944	0	0
36	k	137	0	168	0	0
37	2	1	0	0	0	0
37	A	412	0	0	0	0
37	B	11	0	0	0	0
37	C	2	0	0	0	0
37	D	1	0	0	0	0
37	E	1	0	0	0	0
37	P	1	0	0	0	0
37	R	1	0	0	0	0
37	b	1	0	0	0	0
38	f	1	0	0	0	0
All	All	94027	0	62510	1167	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 8.

The worst 5 of 1167 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)
3:A:1818:U:OP2	5:C:156:ARG:NH1	2.00	0.95
3:A:1168:G:H1	3:A:1181:U:H3	1.20	0.90
3:A:276:U:O2	3:A:278:A:N6	2.08	0.87
3:A:1827:U:OP2	5:C:221:ARG:NH1	2.08	0.86
10:H:3:VAL:HG12	10:H:38:PRO:HA	1.57	0.86

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	
5	C	269/273 (98%)	261 (97%)	8 (3%)	0	100	100
6	D	207/209 (99%)	201 (97%)	6 (3%)	0	100	100
7	E	199/201 (99%)	190 (96%)	9 (4%)	0	100	100
8	F	175/179 (98%)	166 (95%)	9 (5%)	0	100	100
9	G	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
10	H	147/149 (99%)	138 (94%)	8 (5%)	1 (1%)	19	52
11	I	123/165 (74%)	113 (92%)	9 (7%)	1 (1%)	16	49
12	J	132/142 (93%)	126 (96%)	6 (4%)	0	100	100
13	K	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
14	L	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
15	M	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
16	N	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
17	O	123/127 (97%)	118 (96%)	5 (4%)	0	100	100
18	P	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
19	Q	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
20	R	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
21	S	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
22	T	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
23	U	93/100 (93%)	90 (97%)	3 (3%)	0	100	100
24	V	100/104 (96%)	99 (99%)	1 (1%)	0	100	100
25	W	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
26	X	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
27	Y	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
28	Z	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
29	a	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
30	b	54/57 (95%)	50 (93%)	4 (7%)	0	100	100
31	c	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
32	d	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
33	e	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
34	f	36/38 (95%)	36 (100%)	0	0	100	100
35	i	84/453 (18%)	84 (100%)	0	0	100	100
36	k	16/18 (89%)	12 (75%)	4 (25%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3532/4045 (87%)	3415 (97%)	115 (3%)	2 (0%)	50 79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	H	118	PRO
11	I	108	VAL

### 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
5	C	216/218 (99%)	192 (89%)	24 (11%)	5 21
6	D	164/164 (100%)	154 (94%)	10 (6%)	15 41
7	E	165/165 (100%)	152 (92%)	13 (8%)	10 34
8	F	148/150 (99%)	130 (88%)	18 (12%)	4 19
9	G	137/138 (99%)	129 (94%)	8 (6%)	17 42
10	H	114/114 (100%)	100 (88%)	14 (12%)	4 19
11	I	95/123 (77%)	89 (94%)	6 (6%)	15 40
12	J	104/110 (94%)	93 (89%)	11 (11%)	5 23
13	K	116/116 (100%)	105 (90%)	11 (10%)	7 26
14	L	104/104 (100%)	94 (90%)	10 (10%)	7 26
15	M	103/103 (100%)	94 (91%)	9 (9%)	8 30
16	N	109/109 (100%)	100 (92%)	9 (8%)	9 32
17	O	102/103 (99%)	95 (93%)	7 (7%)	13 37
18	P	87/87 (100%)	75 (86%)	12 (14%)	3 17
19	Q	99/100 (99%)	90 (91%)	9 (9%)	7 28
20	R	89/90 (99%)	82 (92%)	7 (8%)	10 34
21	S	84/84 (100%)	76 (90%)	8 (10%)	7 26
22	T	93/93 (100%)	88 (95%)	5 (5%)	18 43

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	U	82/84 (98%)	77 (94%)	5 (6%)	15	41
24	V	83/85 (98%)	76 (92%)	7 (8%)	9	32
25	W	78/78 (100%)	72 (92%)	6 (8%)	10	34
26	X	57/63 (90%)	51 (90%)	6 (10%)	5	23
27	Y	67/68 (98%)	63 (94%)	4 (6%)	16	41
28	Z	54/55 (98%)	47 (87%)	7 (13%)	3	18
29	a	48/49 (98%)	46 (96%)	2 (4%)	25	49
30	b	47/48 (98%)	35 (74%)	12 (26%)	0	3
31	c	45/49 (92%)	40 (89%)	5 (11%)	5	21
32	d	38/38 (100%)	32 (84%)	6 (16%)	2	13
33	e	51/52 (98%)	47 (92%)	4 (8%)	10	34
34	f	34/34 (100%)	31 (91%)	3 (9%)	8	30
35	i	71/341 (21%)	65 (92%)	6 (8%)	8	31
36	k	17/17 (100%)	15 (88%)	2 (12%)	4	20
All	All	2901/3232 (90%)	2635 (91%)	266 (9%)	10	28

5 of 266 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
30	b	18	SER
30	b	46	ASP
35	i	369	ASP
12	J	55	ILE
12	J	21	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
26	X	46	HIS
35	i	411	GLN
28	Z	39	GLN
32	d	29	GLN
12	J	31	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	42/113 (37%)	13 (30%)	0
2	2	2/3 (66%)	1 (50%)	0
3	A	2878/2903 (99%)	518 (17%)	19 (0%)
4	B	119/120 (99%)	13 (10%)	0
All	All	3041/3139 (96%)	545 (17%)	19 (0%)

5 of 545 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	33	C
1	1	36	U
1	1	37	U
1	1	38	U
1	1	39	A

5 of 19 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	A	2422	C
3	A	2602	A
3	A	2756	U
3	A	2430	A
3	A	1344	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 432 ligands modelled in this entry, 432 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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

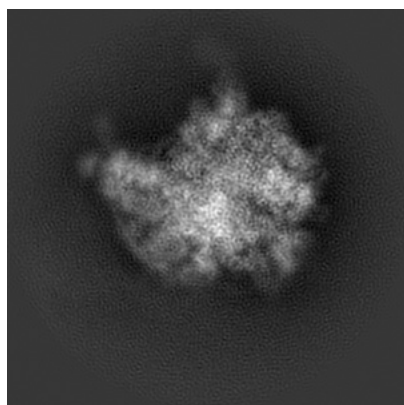
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8004. These allow visual inspection of the internal detail of the map and identification of artifacts.

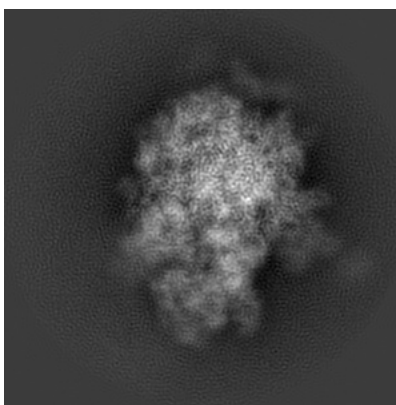
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

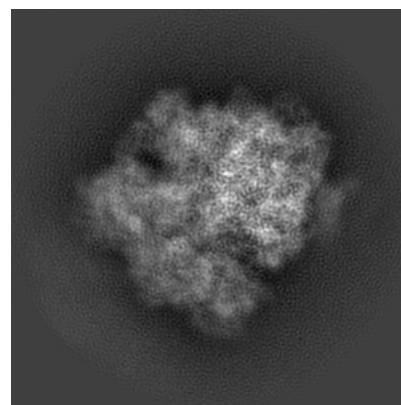
#### 6.1.1 Primary map



X



Y

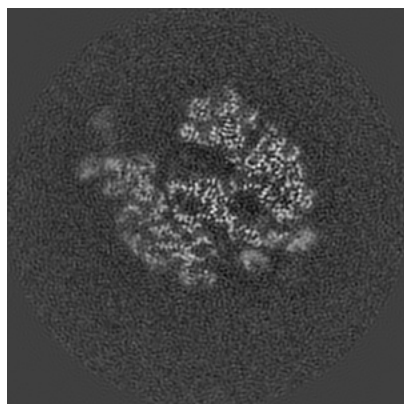


Z

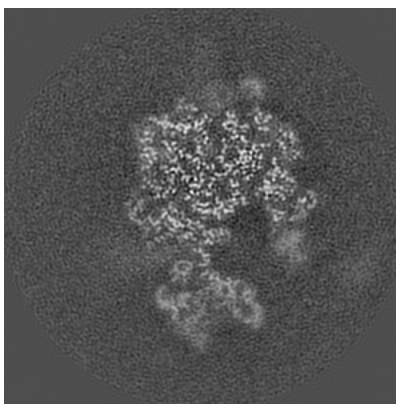
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

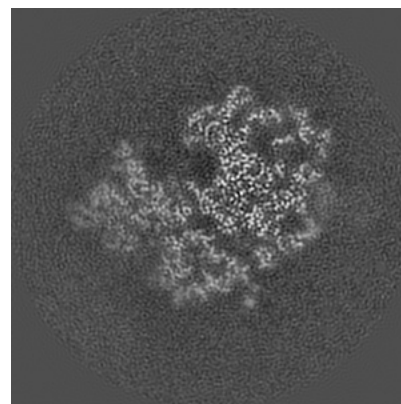
#### 6.2.1 Primary map



X Index: 144



Y Index: 144

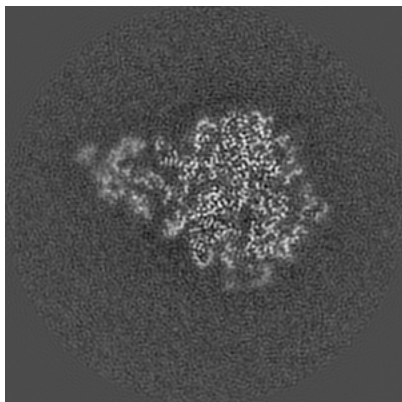


Z Index: 144

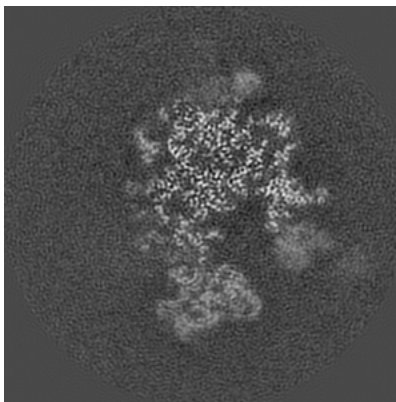
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

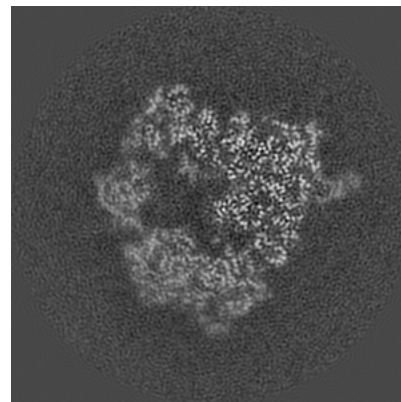
### 6.3.1 Primary map



X Index: 165



Y Index: 150

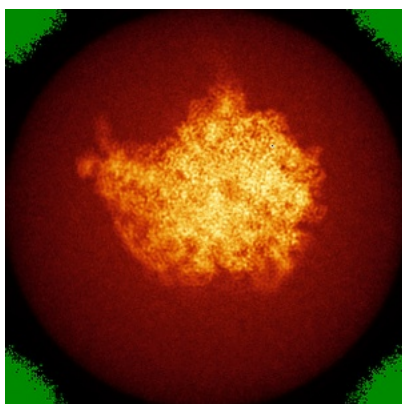


Z Index: 166

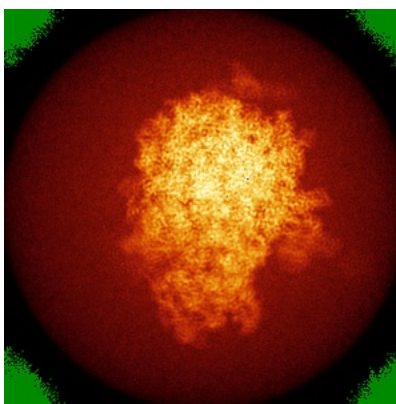
The images above show the largest variance slices of the map in three orthogonal directions.

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

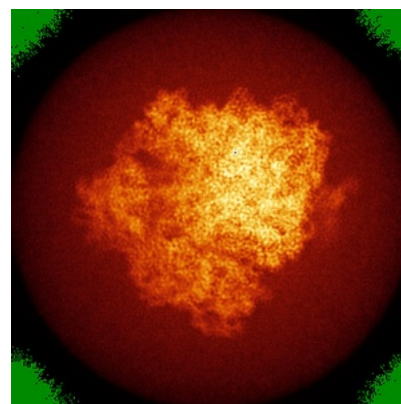
### 6.4.1 Primary map



X



Y



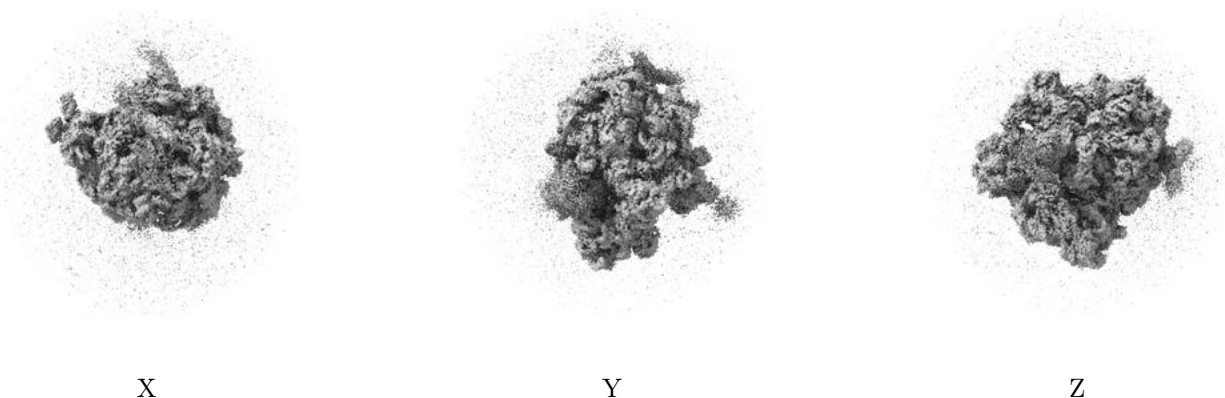
Z

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

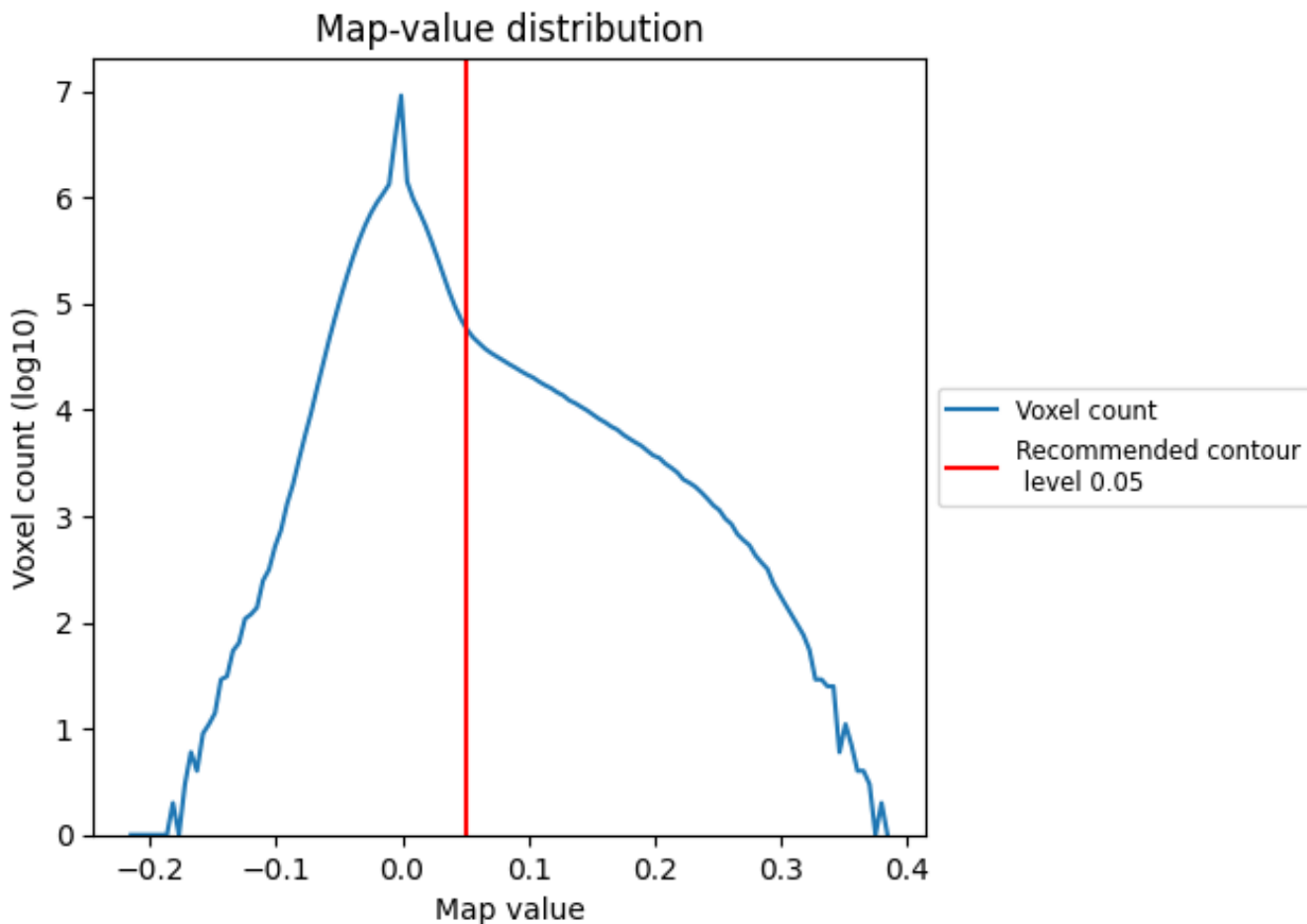
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

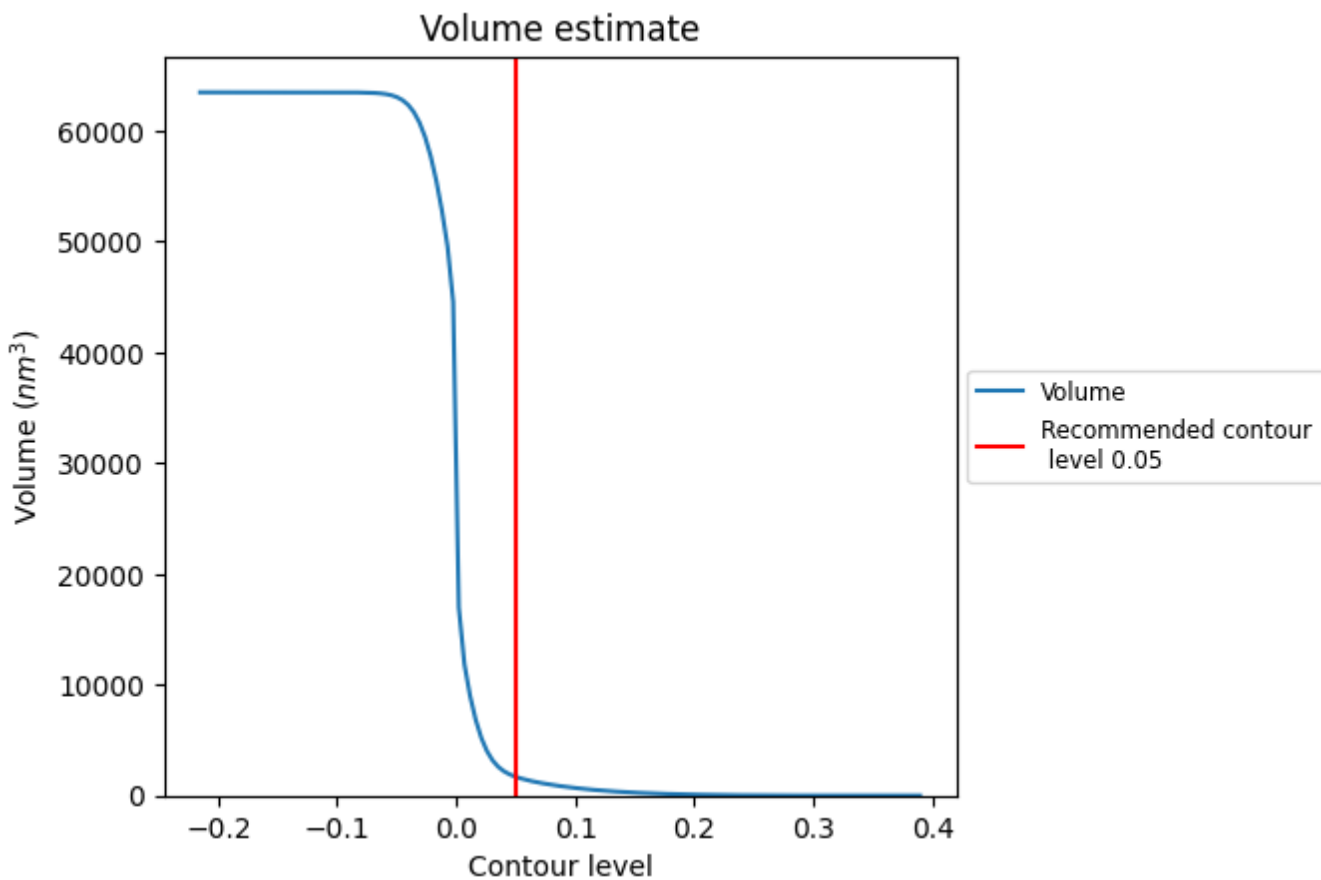
This section contains the results of statistical analysis of the map.

### 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.

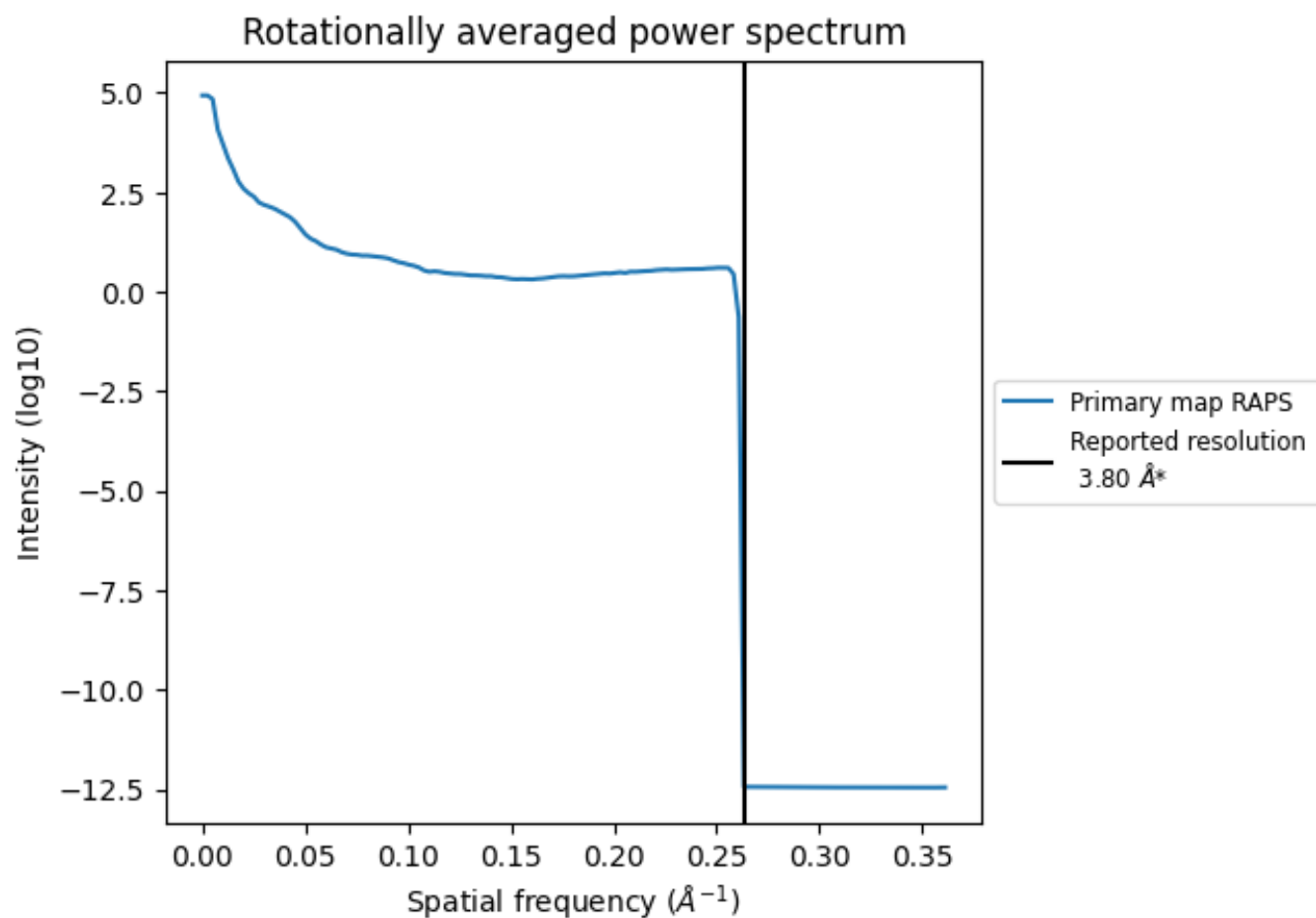
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1693 nm<sup>3</sup>; this corresponds to an approximate mass of 1530 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 0.263 Å<sup>-1</sup>

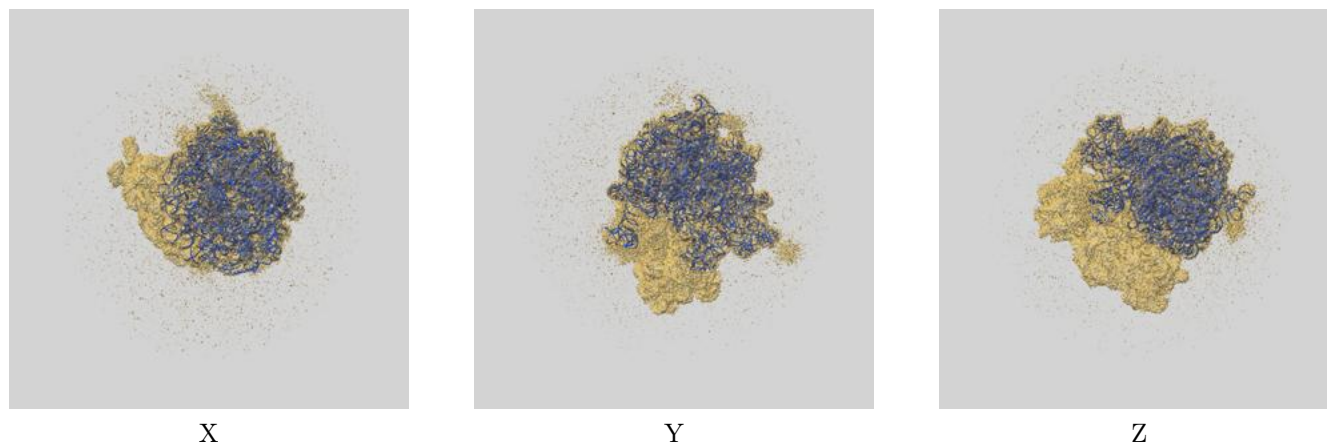
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

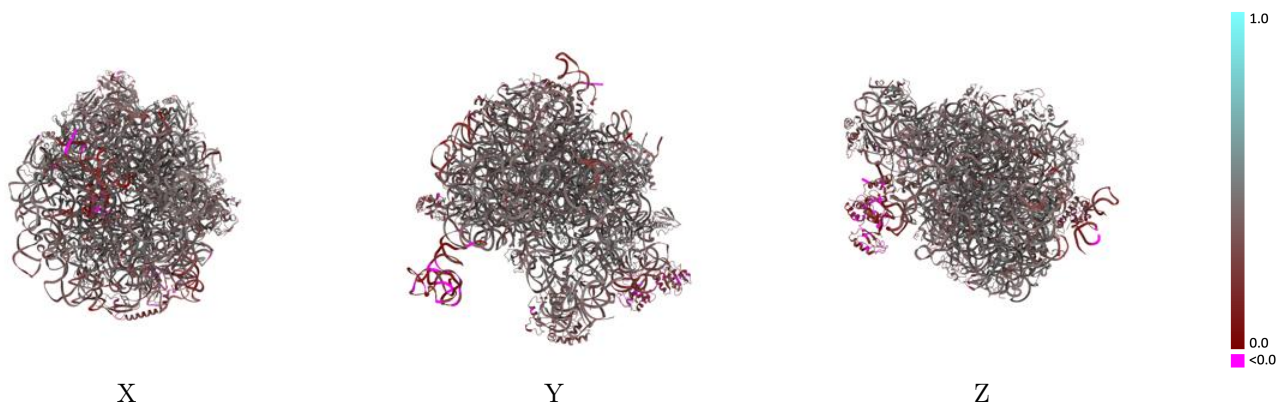
This section contains information regarding the fit between EMDB map EMD-8004 and PDB model 5GAH. Per-residue inclusion information can be found in section [3](#) on page [11](#).

### 9.1 Map-model overlay [i](#)



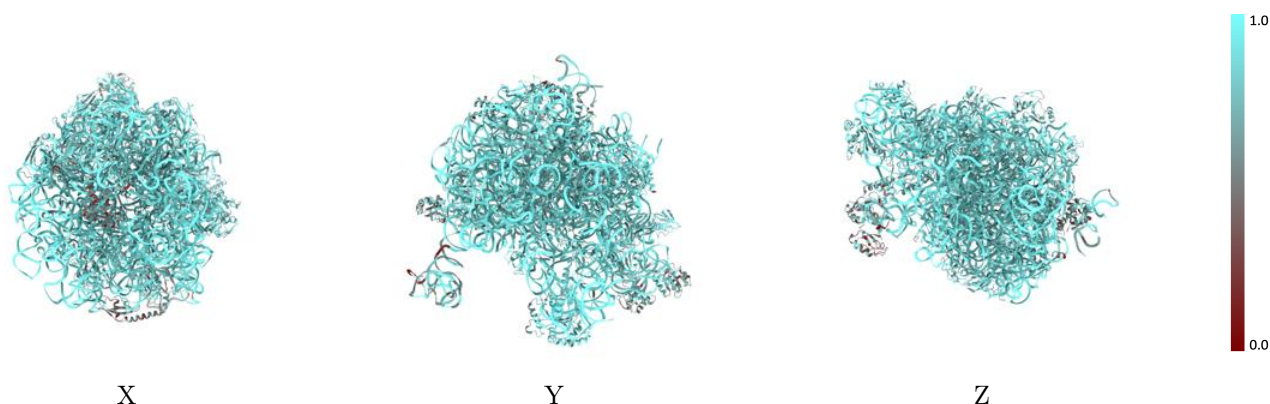
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



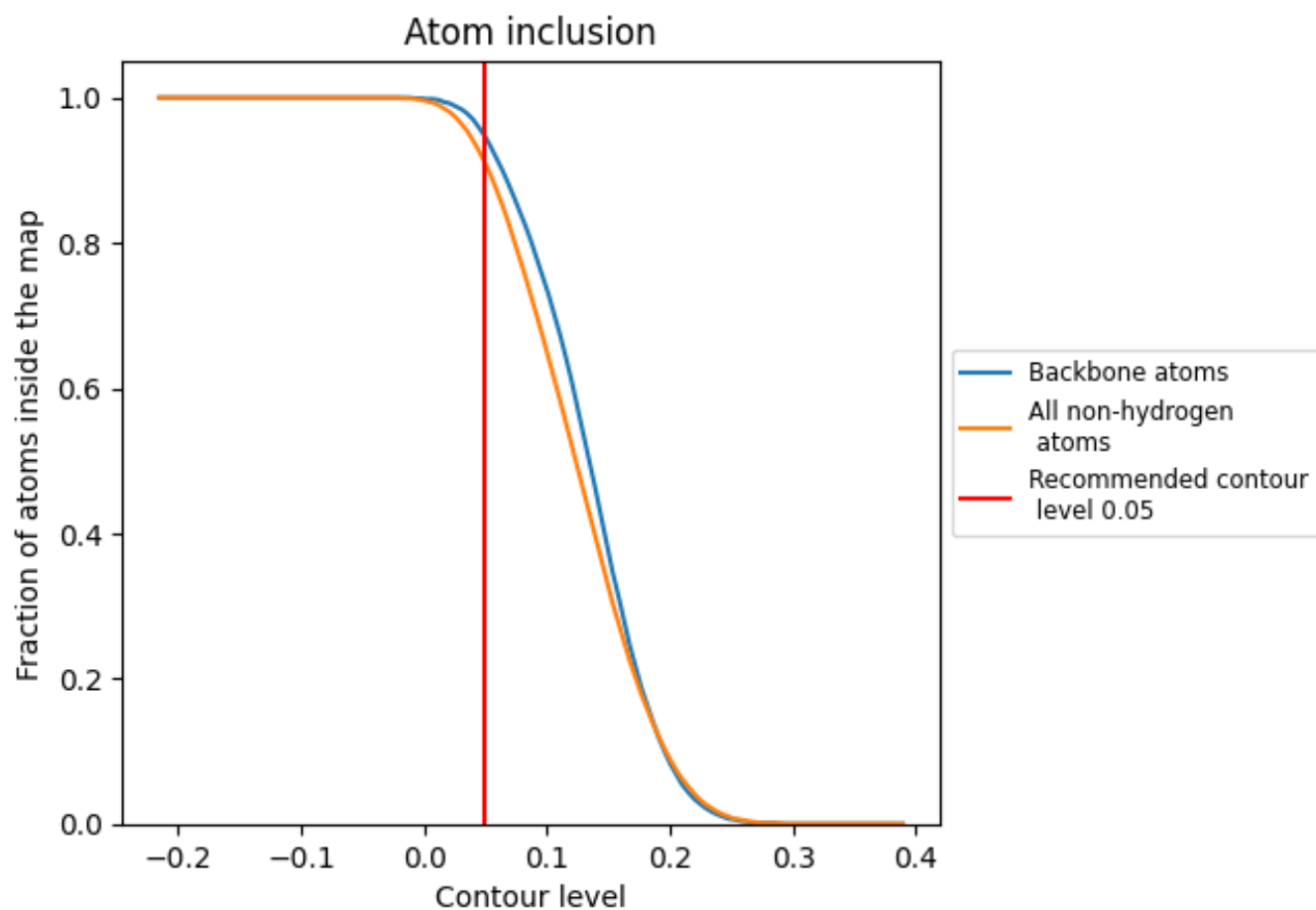
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 95% of all backbone atoms, 91% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9090	 0.3880
1	 0.7850	 0.1610
2	 0.9360	 0.4300
A	 0.9530	 0.3920
B	 0.9820	 0.3990
C	 0.8470	 0.4420
D	 0.8660	 0.4400
E	 0.8250	 0.4010
F	 0.8190	 0.3330
G	 0.8570	 0.3810
H	 0.5880	 0.2850
I	 0.6240	 0.1910
J	 0.5320	 0.1210
K	 0.8750	 0.4340
L	 0.7960	 0.4210
M	 0.8590	 0.4120
N	 0.8560	 0.4350
O	 0.8470	 0.4110
P	 0.8840	 0.4000
Q	 0.8260	 0.4050
R	 0.8740	 0.4190
S	 0.8770	 0.4320
T	 0.8130	 0.4270
U	 0.8080	 0.3860
V	 0.8360	 0.4030
W	 0.8740	 0.4250
X	 0.8650	 0.4480
Y	 0.8470	 0.4240
Z	 0.8020	 0.3690
a	 0.8700	 0.4200
b	 0.8390	 0.4110
c	 0.8180	 0.3950
d	 0.8650	 0.4380
e	 0.8720	 0.4570
f	 0.8800	 0.4360



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
i	 0.5820	 0.2390
k	 0.5330	 0.1660