



## wwPDB EM Validation Summary Report ⓘ

Sep 1, 2025 – 03:27 PM EDT

PDB ID : 9B51 / pdb\_00009b51  
EMDB ID : EMD-44194  
Title : E. coli 70S ribosome complex (N1-methylated 16S A1408 + G418)  
Authors : Mattingly, J.M.; Dey, D.; Zelinskaya, N.; Dunham, C.M.; Conn, G.L.  
Deposited on : 2024-03-21  
Resolution : 2.40 Å(reported)  
Based on initial models : 5JTE, 7K00

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>.

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

EMDB validation analysis : 0.0.1.dev126  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
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) : 2.45.1

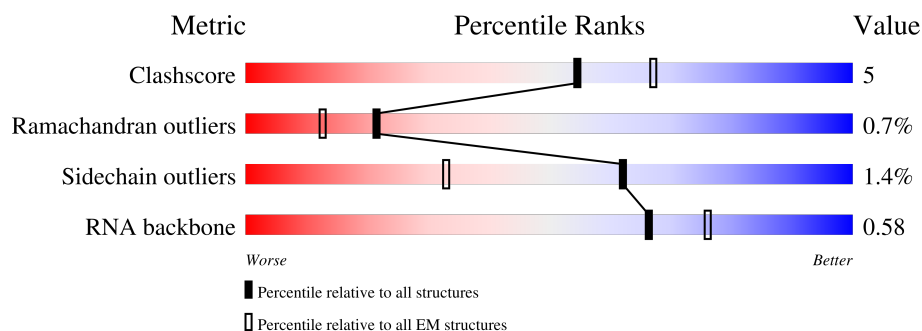
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.40 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.








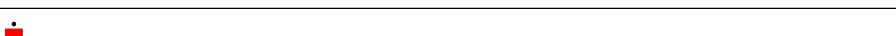
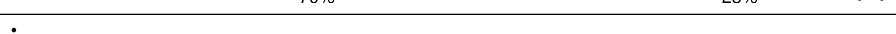
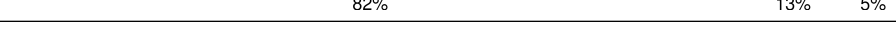
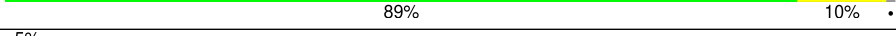






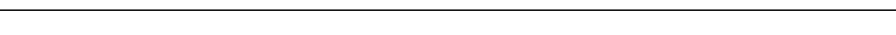

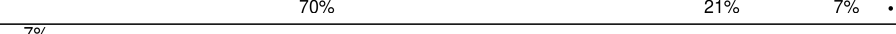







Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	AA	1539	
2	AB	240	
3	AC	233	
4	AD	206	
5	AE	167	
6	AF	135	
7	AG	179	














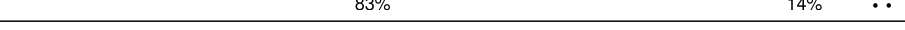







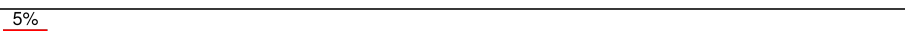


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Mol	Chain	Length	Quality of chain
8	AH	130	
9	AI	130	
10	AJ	103	
11	AK	129	
12	AL	124	
13	AM	118	
14	AN	101	
15	AO	89	
16	AP	82	
17	AQ	84	
18	AR	75	
19	AS	92	
20	AT	87	
21	AU	71	
22	AV	89	
23	AW	76	
23	AY	76	
24	AX	77	
25	B0	57	
26	B1	55	
27	B2	46	
28	B3	65	
29	B4	38	
30	B5	70	
31	BA	2903	

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Mol	Chain	Length	Quality of chain
32	BB	120	 81% 17% ..
33	BC	273	 87% 11% ..
34	BD	209	 87% 12% .
35	BE	201	 92% 8%
36	BF	179	 87% 11% ..
37	BG	177	 92% 7% .
38	BH	149	 8% 25% 5% 68%
39	BJ	142	 94% 6%
40	BK	123	 84% 15% ..
41	BL	144	 79% 19% ..
42	BM	136	 91% 9%
43	BN	127	 83% 10% 6%
44	BO	117	 81% 18% .
45	BP	115	 83% 14% ..
46	BQ	118	 92% 8% .
47	BR	103	 86% 14% .
48	BS	110	 85% 14% .
49	BT	100	 80% 12% 7%
50	BU	104	 74% 22% ..
51	BV	94	 94% 6%
52	BW	85	 78% 11% 12%
53	BX	78	 87% 12% .
54	BY	63	 5% 90% 10%
55	BZ	59	 88% 10% .

## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 146485 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	1539	Total	C	N	O	P	0	0
			33016	14726	6052	10699	1539		

- Molecule 2 is a protein called 30S ribosomal protein S2.

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

- Molecule 3 is a protein called 30S ribosomal protein S3.

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

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

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

- Molecule 6 is a protein called 30S ribosomal protein S6.

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

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

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

- Molecule 11 is a protein called 30S ribosomal protein S11.

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

- Molecule 12 is a protein called 30S ribosomal protein S12.

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

- Molecule 13 is a protein called 30S ribosomal protein S13.

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

- Molecule 14 is a protein called 30S ribosomal protein S14.

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0
			710	437	143	129	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

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

- Molecule 17 is a protein called 30S ribosomal protein S17.

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

- Molecule 18 is a protein called 30S ribosomal protein S18.

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

- Molecule 19 is a protein called 30S ribosomal protein S19.

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

- Molecule 20 is a protein called 30S ribosomal protein S20.

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

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AU	51	Total	C	N	O	S	0	0
			425	265	86	73	1		

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AV	10	Total	C	N	O	P	0	0
			218	98	44	66	10		

- Molecule 23 is a RNA chain called tRNA-Val.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	AW	74	Total 1581	C 707	N 288	O 512	P 73	S 1	0	0
23	AY	74	Total 1581	C 707	N 288	O 512	P 73	S 1	0	0

- Molecule 24 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AX	77	Total	C	N	O	P	0	0
			1643	732	297	537	77		

- Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	B0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 26 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	B1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 27 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 28 is a protein called 50S ribosomal protein L35.



Mol	Chain	Residues	Atoms					AltConf	Trace
28	B3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 29 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	B4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 30 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B5	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 31 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BA	2897	Total	C	N	O	P	0	0
			62195	27745	11446	20107	2897		

- Molecule 32 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BB	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	120	A	U	conflict	GB 1370526515

- Molecule 33 is a protein called 50S ribosomal protein L2.

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

- Molecule 34 is a protein called 50S ribosomal protein L3.

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

- Molecule 35 is a protein called 50S ribosomal protein L4.

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

- Molecule 36 is a protein called 50S ribosomal protein L5.

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

- Molecule 37 is a protein called 50S ribosomal protein L6.

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

- Molecule 38 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BH	47	Total	C	N	O	S	0	0
			359	233	62	63	1		

- Molecule 39 is a protein called 50S ribosomal protein L13.

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

- Molecule 40 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BK	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 41 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BL	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 42 is a protein called 50S ribosomal protein L16.

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

- Molecule 43 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BN	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 44 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BO	116	Total	C	N	O		0	0
			892	552	178	162			

- Molecule 45 is a protein called 50S ribosomal protein L19.

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

- Molecule 46 is a protein called 50S ribosomal protein L20.

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

- Molecule 47 is a protein called 50S ribosomal protein L21.

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

- Molecule 48 is a protein called 50S ribosomal protein L22.

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

- Molecule 49 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BT	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

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

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

- Molecule 51 is a protein called 50S ribosomal protein L25.

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

- Molecule 52 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BW	75	Total	C	N	O	S	0	0
			569	353	113	102	1		

- Molecule 53 is a protein called 50S ribosomal protein L28.

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

- Molecule 54 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BY	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

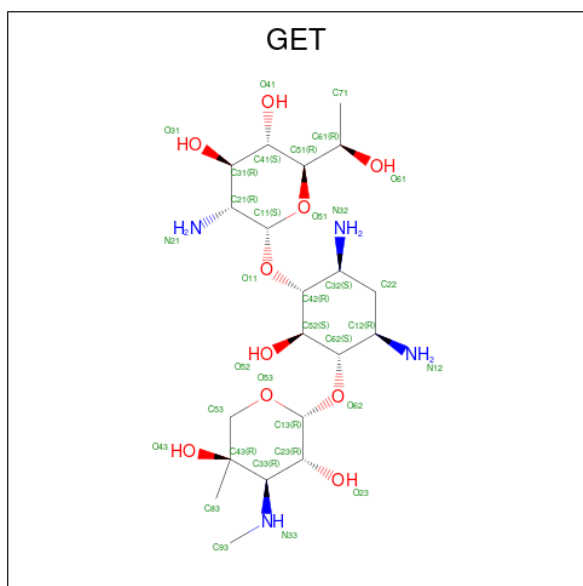
- Molecule 55 is a protein called 50S ribosomal protein L30.

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

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	AA	93	Total	Mg	0
			93	93	
56	B0	2	Total	Mg	0
			2	2	
56	BA	209	Total	Mg	0
			209	209	
56	BB	5	Total	Mg	0
			5	5	

- Molecule 57 is GENETICIN (CCD ID: GET) (formula: C<sub>20</sub>H<sub>40</sub>N<sub>4</sub>O<sub>10</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
57	AA	1	Total	C	N	O	0
			34	20	4	10	
57	AA	1	Total	C	N	O	0
			34	20	4	10	

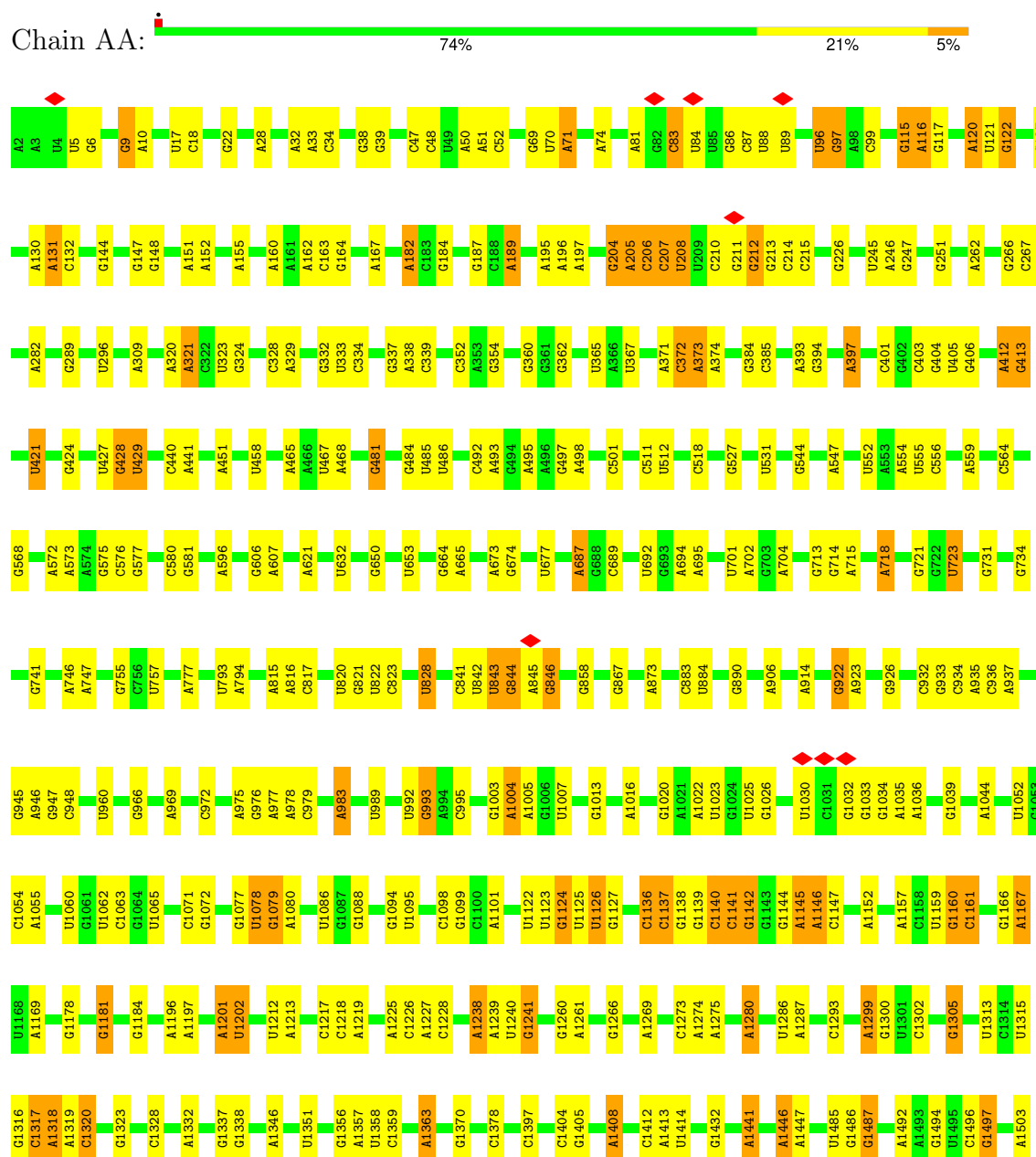
- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
58	B4	1	Total 1	Zn 1	0
58	B5	1	Total 1	Zn 1	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

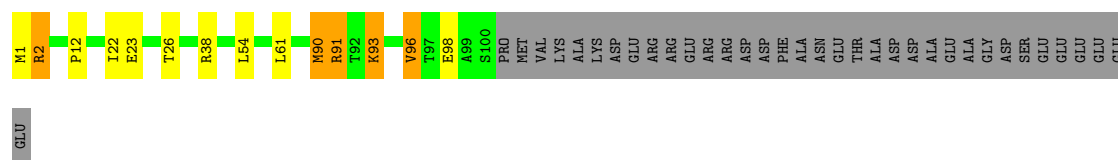
#### • Molecule 1: 16S ribosomal RNA





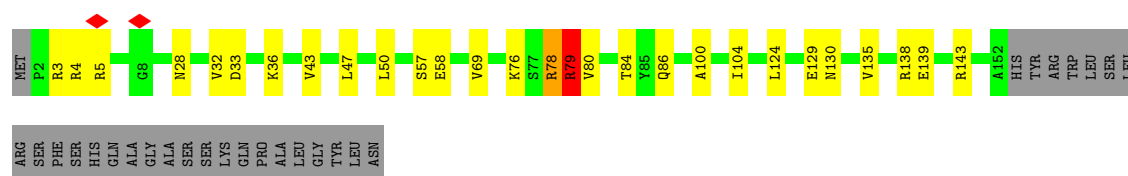


Chain AF: 




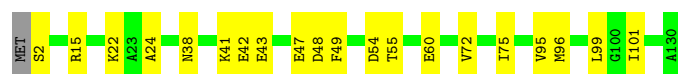
- Molecule 7: 30S ribosomal protein S7

Chain AG: 



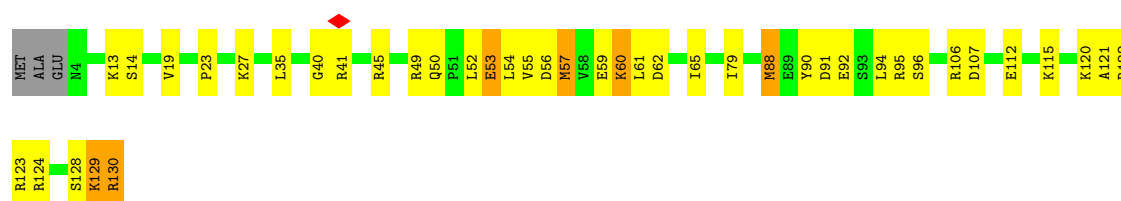
- Molecule 8: 30S ribosomal protein S8

Chain AH: 



- Molecule 9: 30S ribosomal protein S9

Chain AI: 




- Molecule 10: 30S ribosomal protein S10

Chain AJ: 




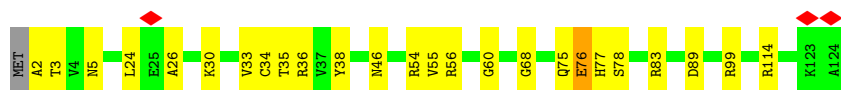
- Molecule 11: 30S ribosomal protein S11

Chain AK: 



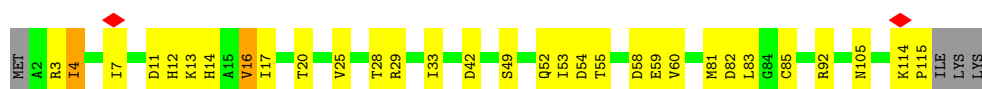
- Molecule 12: 30S ribosomal protein S12

Chain AL:  79% 19% ..




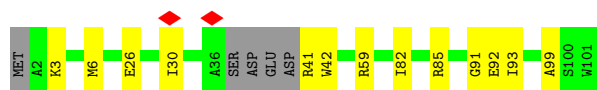
- Molecule 13: 30S ribosomal protein S13

Chain AM:  70% 25% . .



- Molecule 14: 30S ribosomal protein S14

Chain AN:  82% 13% 5%



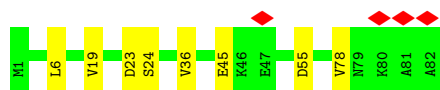
- Molecule 15: 30S ribosomal protein S15

Chain AO:  89% 10% .



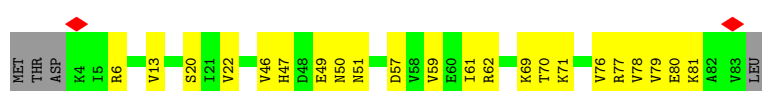
- Molecule 16: 30S ribosomal protein S16

Chain AP:  90% 10% 5%



- Molecule 17: 30S ribosomal protein S17

Chain AQ:  69% 26% 5%



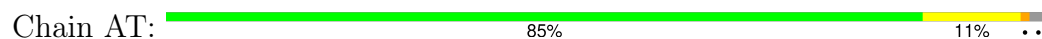
- Molecule 18: 30S ribosomal protein S18

Chain AR:  69% 27%

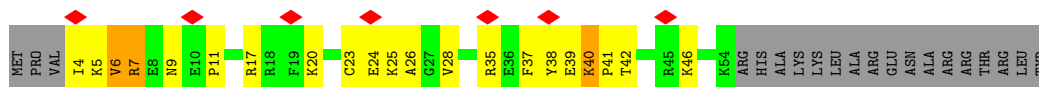
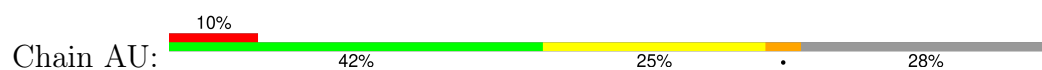
- Molecule 19: 30S ribosomal protein S19



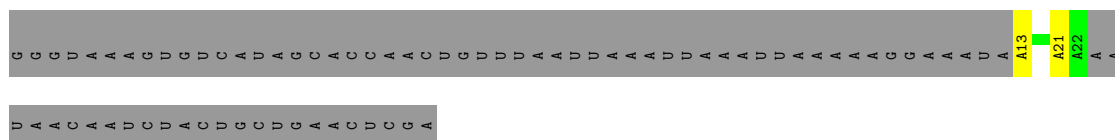
- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein S21



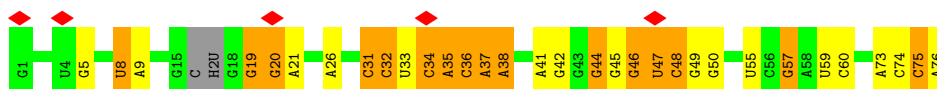
- Molecule 22: mRNA



- Molecule 23: tRNA-Val



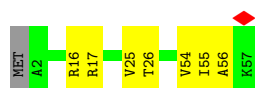
- Molecule 23: tRNA-Val



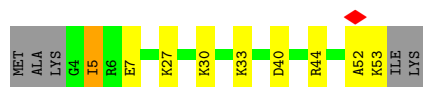
- Molecule 24: tRNA-fMet



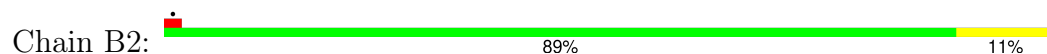
- Molecule 25: 50S ribosomal protein L32



- Molecule 26: 50S ribosomal protein L33



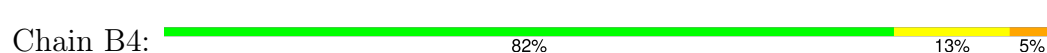
- Molecule 27: 50S ribosomal protein L34



- Molecule 28: 50S ribosomal protein L35



- Molecule 29: 50S ribosomal protein L36

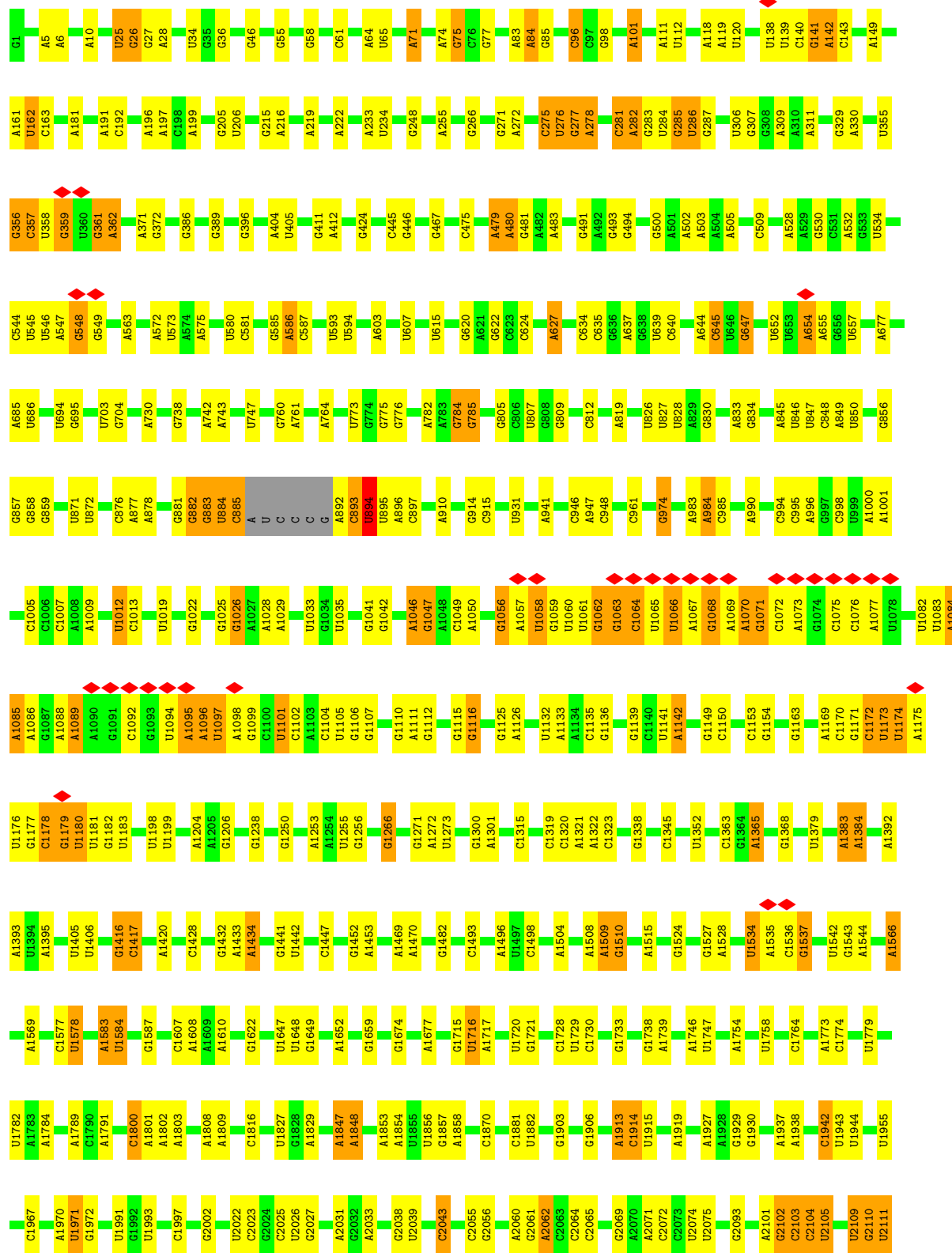


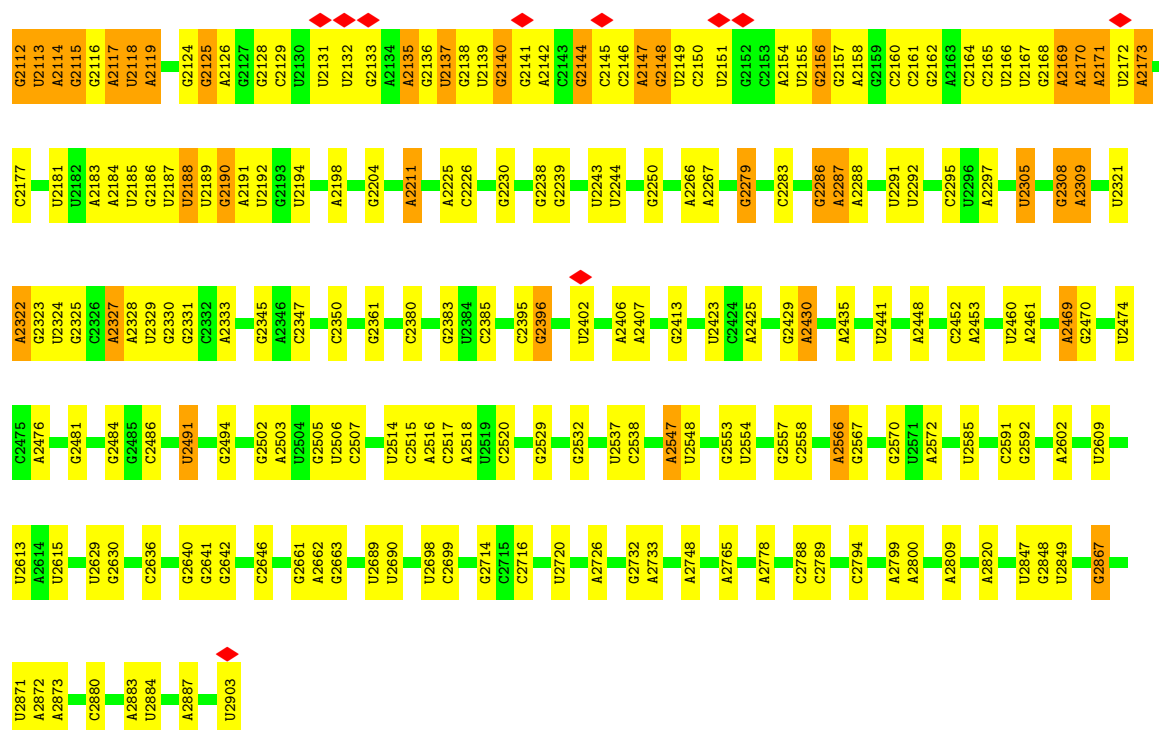
- Molecule 30: 50S ribosomal protein L31



- Molecule 31: 23S ribosomal RNA

Chain BA:







- Molecule 36: 50S ribosomal protein L5

Chain BF: 87% 11% ..



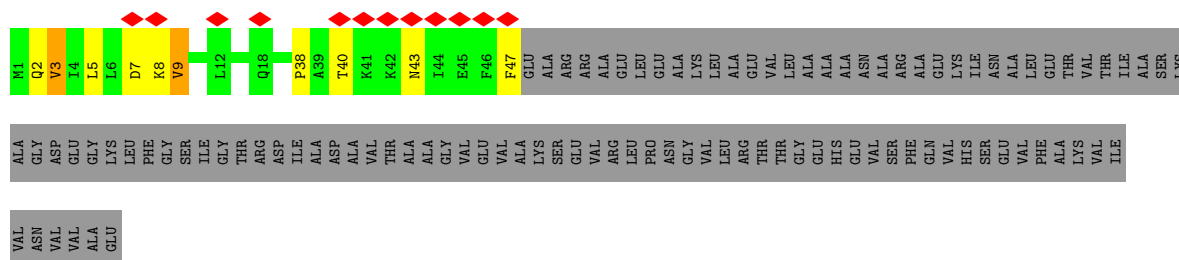
- Molecule 37: 50S ribosomal protein L6

Chain BG: 92% 7% .



- Molecule 38: 50S ribosomal protein L9

Chain BH: 8% 25% 5% 68%



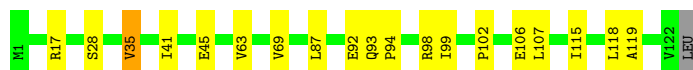
- Molecule 39: 50S ribosomal protein L13

Chain BJ: 94% 6%



- Molecule 40: 50S ribosomal protein L14

Chain BK: 84% 15% ..



- Molecule 41: 50S ribosomal protein L15

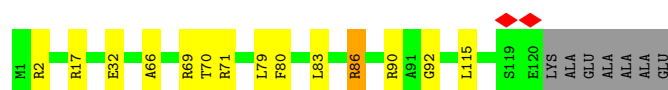
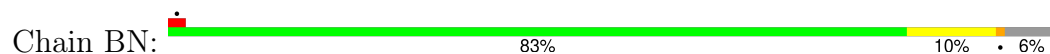
Chain BL: 79% 19% ..



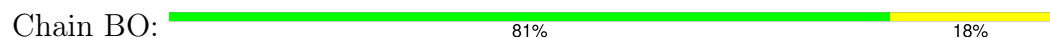
- Molecule 42: 50S ribosomal protein L16



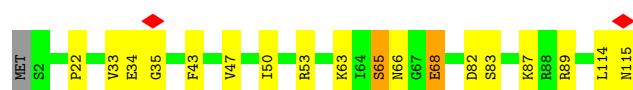
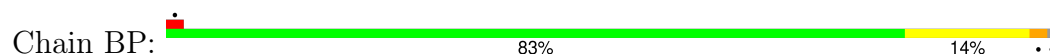
- Molecule 43: 50S ribosomal protein L17



- Molecule 44: 50S ribosomal protein L18



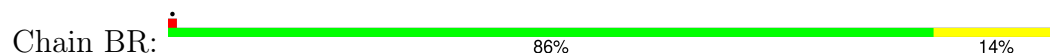
- Molecule 45: 50S ribosomal protein L19



- Molecule 46: 50S ribosomal protein L20




- Molecule 47: 50S ribosomal protein L21




- Molecule 48: 50S ribosomal protein L22



Chain BS:  85% 14% .




- Molecule 49: 50S ribosomal protein L23

Chain BT:  80% 12% 7%



- Molecule 50: 50S ribosomal protein L24

Chain BU:  74% 22% . .




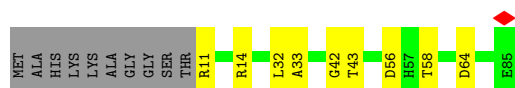
- Molecule 51: 50S ribosomal protein L25

Chain BV:  94% 6%



- Molecule 52: 50S ribosomal protein L27

Chain BW:  78% 11% 12%




- Molecule 53: 50S ribosomal protein L28

Chain BX:  87% 12% .

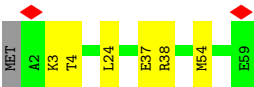
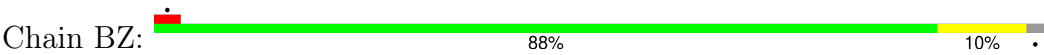


- Molecule 54: 50S ribosomal protein L29

Chain BY:  5% 90% 10%



- Molecule 55: 50S ribosomal protein L30



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	197194	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	28.546	Depositor
Minimum map value	-7.985	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.7	Depositor
Map size (Å)	416.768, 416.768, 416.768	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.814, 0.814, 0.814	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 4SU, 7MG, MG, GET, ZN, 5MU, PSU, 1MA

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	AA	0.18	0/36941	0.27	0/57627
2	AB	0.28	0/1735	0.40	0/2338
3	AC	0.22	0/1651	0.31	0/2225
4	AD	0.25	0/1665	0.44	1/2227 (0.0%)
5	AE	0.16	0/1118	0.35	0/1504
6	AF	0.50	2/835 (0.2%)	0.53	2/1128 (0.2%)
7	AG	0.23	0/1195	0.36	0/1602
8	AH	0.14	0/989	0.30	0/1326
9	AI	0.51	0/1034	0.57	1/1375 (0.1%)
10	AJ	0.32	0/796	0.48	0/1077
11	AK	0.34	0/893	0.45	1/1205 (0.1%)
12	AL	0.28	0/969	0.39	0/1300
13	AM	0.29	0/892	0.40	0/1193
14	AN	0.15	0/785	0.34	0/1043
15	AO	0.20	0/718	0.28	0/959
16	AP	0.15	0/659	0.32	0/884
17	AQ	0.15	0/657	0.35	0/881
18	AR	0.48	0/462	0.41	0/621
19	AS	0.36	0/652	0.43	0/877
20	AT	0.36	0/671	0.37	0/888
21	AU	0.26	0/430	0.60	0/570
22	AV	0.17	0/245	0.21	0/380
23	AW	0.23	0/1672	0.33	0/2604
23	AY	0.23	0/1672	0.40	0/2604
24	AX	0.18	0/1835	0.32	1/2859 (0.0%)
25	B0	0.41	0/450	0.42	0/599
26	B1	0.32	0/416	0.37	0/554
27	B2	0.19	0/380	0.27	0/498
28	B3	0.17	0/513	0.26	0/676
29	B4	0.56	0/303	0.47	0/397
30	B5	0.14	0/488	0.34	0/649
31	BA	0.21	0/69659	0.30	1/108672 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	BB	0.18	0/2828	0.25	0/4410
33	BC	0.26	0/2121	0.38	0/2852
34	BD	0.32	0/1586	0.44	3/2134 (0.1%)
35	BE	0.35	0/1571	0.38	0/2113
36	BF	0.31	0/1434	0.39	0/1926
37	BG	0.12	0/1343	0.23	0/1816
38	BH	0.15	0/364	0.41	0/490
39	BJ	0.18	0/1152	0.25	0/1551
40	BK	0.30	0/947	0.40	0/1268
41	BL	0.17	0/1054	0.36	0/1403
42	BM	0.19	0/1093	0.31	0/1460
43	BN	0.31	0/973	0.38	0/1301
44	BO	0.30	0/902	0.39	0/1209
45	BP	0.29	0/929	0.37	0/1242
46	BQ	0.18	0/960	0.24	0/1278
47	BR	0.18	0/829	0.33	0/1107
48	BS	0.31	0/864	0.38	0/1156
49	BT	0.26	0/744	0.33	0/994
50	BU	0.38	0/787	0.48	1/1051 (0.1%)
51	BV	0.16	0/766	0.26	0/1025
52	BW	0.16	0/576	0.26	0/762
53	BX	0.17	0/635	0.26	0/848
54	BY	0.33	0/510	0.34	0/677
55	BZ	0.14	0/453	0.25	0/605
All	All	0.22	2/158801 (0.0%)	0.31	11/238020 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	AF	1	MET	C-N	7.58	1.43	1.33
6	AF	2	ARG	C-N	5.32	1.40	1.33

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AD	39	GLY	N-CA-C	12.17	124.46	112.04
34	BD	151	THR	CA-C-N	-8.14	110.50	118.97
34	BD	151	THR	C-N-CA	-8.14	110.50	118.97
50	BU	6	ARG	N-CA-C	7.68	120.53	108.79
9	AI	53	GLU	N-CA-C	-6.48	103.84	111.03

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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	AA	33016	0	16618	183	0
2	AB	1704	0	1732	35	0
3	AC	1624	0	1696	15	0
4	AD	1643	0	1707	33	0
5	AE	1105	0	1148	21	0
6	AF	817	0	808	11	0
7	AG	1181	0	1238	25	0
8	AH	979	0	1031	13	0
9	AI	1022	0	1070	32	0
10	AJ	786	0	828	28	0
11	AK	877	0	887	16	0
12	AL	955	0	1016	16	0
13	AM	883	0	941	27	0
14	AN	774	0	824	10	0
15	AO	710	0	728	3	0
16	AP	649	0	666	7	0
17	AQ	648	0	691	16	0
18	AR	455	0	478	2	0
19	AS	637	0	665	16	0
20	AT	665	0	714	9	0
21	AU	425	0	449	23	0
22	AV	218	0	109	3	0
23	AW	1581	0	811	8	0
23	AY	1581	0	811	33	0
24	AX	1643	0	836	13	0
25	B0	444	0	458	6	0
26	B1	409	0	440	5	0
27	B2	377	0	418	4	0
28	B3	504	0	572	3	0
29	B4	302	0	340	6	0
30	B5	480	0	478	11	0
31	BA	62195	0	31280	362	0
32	BB	2529	0	1281	10	0
33	BC	2082	0	2154	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	BD	1565	0	1616	19	0
35	BE	1552	0	1619	10	0
36	BF	1410	0	1444	16	0
37	BG	1323	0	1371	7	0
38	BH	359	0	381	9	0
39	BJ	1129	0	1162	12	0
40	BK	938	0	1012	13	0
41	BL	1045	0	1117	21	0
42	BM	1074	0	1157	11	0
43	BN	960	0	1000	8	0
44	BO	892	0	923	12	0
45	BP	917	0	962	12	0
46	BQ	947	0	1019	9	0
47	BR	816	0	839	10	0
48	BS	857	0	922	9	0
49	BT	738	0	807	7	0
50	BU	779	0	831	17	0
51	BV	753	0	780	4	0
52	BW	569	0	581	8	0
53	BX	625	0	652	6	0
54	BY	509	0	543	7	0
55	BZ	449	0	488	4	0
56	AA	93	0	0	0	0
56	B0	2	0	0	0	0
56	BA	209	0	0	0	0
56	BB	5	0	0	0	0
57	AA	68	0	80	6	0
58	B4	1	0	0	0	0
58	B5	1	0	0	0	0
All	All	146485	0	97229	1146	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 5.

The worst 5 of 1146 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)
31:BA:2110:G:H5'	31:BA:2118:U:H3	1.25	0.98
23:AY:34:C:H3'	23:AY:35:A:H8	1.30	0.95
23:AY:37:A:H3'	23:AY:38:A:H8	1.30	0.93
7:AG:79:ARG:HB2	7:AG:84:THR:HA	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AI:130:ARG:NH2	24:AX:34:U:H3'	1.92	0.85

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	216/240 (90%)	193 (89%)	21 (10%)	2 (1%)	14	22
3	AC	204/233 (88%)	184 (90%)	18 (9%)	2 (1%)	13	20
4	AD	203/206 (98%)	184 (91%)	15 (7%)	4 (2%)	6	8
5	AE	148/167 (89%)	128 (86%)	19 (13%)	1 (1%)	19	29
6	AF	98/135 (73%)	86 (88%)	12 (12%)	0	100	100
7	AG	149/179 (83%)	141 (95%)	7 (5%)	1 (1%)	19	29
8	AH	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
9	AI	125/130 (96%)	103 (82%)	19 (15%)	3 (2%)	5	5
10	AJ	96/103 (93%)	81 (84%)	13 (14%)	2 (2%)	5	7
11	AK	115/129 (89%)	105 (91%)	10 (9%)	0	100	100
12	AL	121/124 (98%)	101 (84%)	18 (15%)	2 (2%)	7	10
13	AM	112/118 (95%)	102 (91%)	9 (8%)	1 (1%)	14	22
14	AN	92/101 (91%)	82 (89%)	9 (10%)	1 (1%)	12	18
15	AO	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	5	6
16	AP	80/82 (98%)	70 (88%)	10 (12%)	0	100	100
17	AQ	78/84 (93%)	67 (86%)	11 (14%)	0	100	100
18	AR	53/75 (71%)	50 (94%)	3 (6%)	0	100	100
19	AS	77/92 (84%)	71 (92%)	6 (8%)	0	100	100
20	AT	83/87 (95%)	78 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	AU	49/71 (69%)	39 (80%)	9 (18%)	1 (2%)	6	8
25	B0	54/57 (95%)	49 (91%)	5 (9%)	0	100	100
26	B1	48/55 (87%)	44 (92%)	3 (6%)	1 (2%)	5	7
27	B2	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
28	B3	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
29	B4	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
30	B5	56/70 (80%)	49 (88%)	6 (11%)	1 (2%)	7	9
33	BC	269/273 (98%)	248 (92%)	18 (7%)	3 (1%)	12	18
34	BD	207/209 (99%)	197 (95%)	9 (4%)	1 (0%)	25	38
35	BE	199/201 (99%)	191 (96%)	7 (4%)	1 (0%)	25	38
36	BF	175/179 (98%)	162 (93%)	13 (7%)	0	100	100
37	BG	174/177 (98%)	165 (95%)	9 (5%)	0	100	100
38	BH	45/149 (30%)	33 (73%)	10 (22%)	2 (4%)	2	1
39	BJ	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
40	BK	120/123 (98%)	110 (92%)	9 (8%)	1 (1%)	16	26
41	BL	141/144 (98%)	121 (86%)	18 (13%)	2 (1%)	9	13
42	BM	134/136 (98%)	126 (94%)	8 (6%)	0	100	100
43	BN	118/127 (93%)	107 (91%)	11 (9%)	0	100	100
44	BO	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
45	BP	112/115 (97%)	103 (92%)	9 (8%)	0	100	100
46	BQ	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
47	BR	101/103 (98%)	94 (93%)	7 (7%)	0	100	100
48	BS	108/110 (98%)	99 (92%)	8 (7%)	1 (1%)	14	22
49	BT	91/100 (91%)	85 (93%)	5 (6%)	1 (1%)	12	18
50	BU	100/104 (96%)	87 (87%)	11 (11%)	2 (2%)	6	8
51	BV	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
52	BW	73/85 (86%)	72 (99%)	1 (1%)	0	100	100
53	BX	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
54	BY	61/63 (97%)	55 (90%)	6 (10%)	0	100	100
55	BZ	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
All	All	5432/5912 (92%)	4978 (92%)	416 (8%)	38 (1%)	21	29

5 of 38 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	34	ALA
4	AD	153	SER
12	AL	76	GLU
15	AO	88	ARG
21	AU	40	LYS

### 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	
2	AB	180/198 (91%)	178 (99%)	2 (1%)	70	84
3	AC	170/190 (90%)	170 (100%)	0	100	100
4	AD	172/173 (99%)	166 (96%)	6 (4%)	31	51
5	AE	113/126 (90%)	113 (100%)	0	100	100
6	AF	87/116 (75%)	83 (95%)	4 (5%)	23	39
7	AG	124/147 (84%)	122 (98%)	2 (2%)	58	76
8	AH	104/105 (99%)	104 (100%)	0	100	100
9	AI	105/107 (98%)	97 (92%)	8 (8%)	11	18
10	AJ	86/90 (96%)	78 (91%)	8 (9%)	7	11
11	AK	90/99 (91%)	89 (99%)	1 (1%)	70	84
12	AL	103/104 (99%)	101 (98%)	2 (2%)	52	72
13	AM	92/96 (96%)	91 (99%)	1 (1%)	70	84
14	AN	79/84 (94%)	79 (100%)	0	100	100
15	AO	75/77 (97%)	74 (99%)	1 (1%)	65	81
16	AP	65/65 (100%)	65 (100%)	0	100	100
17	AQ	74/78 (95%)	74 (100%)	0	100	100
18	AR	48/65 (74%)	48 (100%)	0	100	100
19	AS	70/79 (89%)	66 (94%)	4 (6%)	17	29
20	AT	65/66 (98%)	64 (98%)	1 (2%)	60	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	AU	44/61 (72%)	42 (96%)	2 (4%)	23	40
25	B0	47/48 (98%)	47 (100%)	0	100	100
26	B1	45/49 (92%)	44 (98%)	1 (2%)	47	67
27	B2	38/38 (100%)	38 (100%)	0	100	100
28	B3	51/52 (98%)	51 (100%)	0	100	100
29	B4	34/34 (100%)	31 (91%)	3 (9%)	8	13
30	B5	55/62 (89%)	55 (100%)	0	100	100
33	BC	216/218 (99%)	216 (100%)	0	100	100
34	BD	164/164 (100%)	163 (99%)	1 (1%)	84	92
35	BE	165/165 (100%)	164 (99%)	1 (1%)	84	92
36	BF	148/150 (99%)	145 (98%)	3 (2%)	50	70
37	BG	137/138 (99%)	137 (100%)	0	100	100
38	BH	38/114 (33%)	38 (100%)	0	100	100
39	BJ	116/116 (100%)	116 (100%)	0	100	100
40	BK	103/104 (99%)	102 (99%)	1 (1%)	73	86
41	BL	102/103 (99%)	102 (100%)	0	100	100
42	BM	109/109 (100%)	109 (100%)	0	100	100
43	BN	100/103 (97%)	99 (99%)	1 (1%)	73	86
44	BO	86/87 (99%)	84 (98%)	2 (2%)	45	66
45	BP	99/100 (99%)	97 (98%)	2 (2%)	50	70
46	BQ	89/90 (99%)	89 (100%)	0	100	100
47	BR	84/84 (100%)	84 (100%)	0	100	100
48	BS	93/93 (100%)	91 (98%)	2 (2%)	47	67
49	BT	80/84 (95%)	78 (98%)	2 (2%)	42	63
50	BU	83/85 (98%)	82 (99%)	1 (1%)	67	82
51	BV	78/78 (100%)	78 (100%)	0	100	100
52	BW	56/63 (89%)	56 (100%)	0	100	100
53	BX	67/68 (98%)	67 (100%)	0	100	100
54	BY	55/55 (100%)	55 (100%)	0	100	100
55	BZ	48/49 (98%)	48 (100%)	0	100	100
All	All	4532/4829 (94%)	4470 (99%)	62 (1%)	62	79

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	AJ	87	LEU
45	BP	65	SER
19	AS	11	ILE
44	BO	116	GLN
49	BT	1	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
48	BS	61	ASN
49	BT	70	HIS
54	BY	25	GLN
33	BC	134	ASN
26	B1	19	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1538/1539 (99%)	199 (12%)	11 (0%)
22	AV	9/89 (10%)	0	0
23	AW	72/76 (94%)	13 (18%)	2 (2%)
23	AY	72/76 (94%)	24 (33%)	0
24	AX	76/77 (98%)	19 (25%)	1 (1%)
31	BA	2895/2903 (99%)	409 (14%)	23 (0%)
32	BB	117/120 (97%)	10 (8%)	0
All	All	4779/4880 (97%)	674 (14%)	37 (0%)

5 of 674 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	9	G
1	AA	22	G
1	AA	32	A
1	AA	39	G

5 of 37 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
31	BA	1913	A
31	BA	2308	G
31	BA	2109	U
31	BA	2147	A
23	AW	46	7MG

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

9 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z  > 2$
23	7MG	AW	46	23	23,26,27	1.43	4 (17%)	27,39,42	2.62	7 (25%)
23	5MU	AW	54	23	19,22,23	0.42	0	27,32,35	0.56	0
23	5MU	AY	54	23	19,22,23	0.35	0	27,32,35	0.60	0
23	PSU	AW	55	23	18,21,22	1.09	1 (5%)	21,30,33	1.98	5 (23%)
23	7MG	AY	46	23	23,26,27	1.11	1 (4%)	27,39,42	0.87	2 (7%)
23	4SU	AY	8	23	18,21,22	3.93	8 (44%)	25,30,33	2.31	4 (16%)
23	4SU	AW	8	23	18,21,22	3.87	8 (44%)	25,30,33	2.28	5 (20%)
1	1MA	AA	1408	1	17,25,26	0.96	2 (11%)	17,37,40	1.11	2 (11%)
23	PSU	AY	55	23	18,21,22	1.13	1 (5%)	21,30,33	1.88	4 (19%)

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
23	7MG	AW	46	23	-	0/7/37/38	0/3/3/3
23	5MU	AW	54	23	-	0/7/25/26	0/2/2/2
23	5MU	AY	54	23	-	0/7/25/26	0/2/2/2
23	PSU	AW	55	23	-	0/7/25/26	0/2/2/2
23	7MG	AY	46	23	-	3/7/37/38	0/3/3/3
23	4SU	AY	8	23	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	4SU	AW	8	23	-	0/7/25/26	0/2/2/2
1	1MA	AA	1408	1	-	0/3/25/26	0/3/3/3
23	PSU	AY	55	23	-	0/7/25/26	0/2/2/2

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AY	8	4SU	C4-N3	8.52	1.46	1.37
23	AW	8	4SU	C4-N3	8.33	1.46	1.37
23	AY	8	4SU	C2-N3	7.25	1.50	1.38
23	AW	8	4SU	C2-N3	7.10	1.50	1.38
23	AY	8	4SU	C2-N1	6.96	1.49	1.38

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AW	46	7MG	N9-C4-N3	8.49	137.90	125.46
23	AY	8	4SU	C4-N3-C2	-7.90	119.74	127.31
23	AW	8	4SU	C4-N3-C2	-7.89	119.75	127.31
23	AW	46	7MG	N9-C8-N7	-6.08	94.76	103.37
23	AW	8	4SU	C5-C4-N3	5.45	119.82	114.75

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	AY	46	7MG	C4'-C5'-O5'-P
23	AY	46	7MG	C2'-C1'-N9-C8
23	AY	46	7MG	O4'-C1'-N9-C8

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	AY	8	4SU	2	0
1	AA	1408	1MA	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 313 ligands modelled in this entry, 311 are monoatomic - leaving 2 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
57	GET	AA	1695	-	35,36,36	1.91	9 (25%)	43,55,55	2.66	14 (32%)
57	GET	AA	1694	-	35,36,36	0.57	0	43,55,55	1.67	6 (13%)

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
57	GET	AA	1695	-	-	6/13/74/74	0/3/3/3
57	GET	AA	1694	-	-	1/13/74/74	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	AA	1695	GET	O43-C43	-4.79	1.36	1.44
57	AA	1695	GET	C31-C21	-4.07	1.48	1.53
57	AA	1695	GET	O53-C53	-3.28	1.39	1.43
57	AA	1695	GET	C23-C33	-3.13	1.47	1.53
57	AA	1695	GET	C42-C32	-2.66	1.47	1.53

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	AA	1695	GET	C93-N33-C33	-9.90	100.85	114.47
57	AA	1694	GET	C93-N33-C33	-6.96	104.89	114.47
57	AA	1695	GET	C11-O11-C42	-5.71	104.44	117.98
57	AA	1695	GET	C41-C51-C61	-5.11	105.36	113.33
57	AA	1695	GET	O51-C51-C41	4.80	114.73	107.94

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	AA	1695	GET	C21-C11-O11-C42
57	AA	1695	GET	C41-C51-C61-O61
57	AA	1695	GET	C41-C51-C61-C71
57	AA	1695	GET	O51-C51-C61-O61
57	AA	1695	GET	C23-C33-N33-C93

There are no ring outliers.

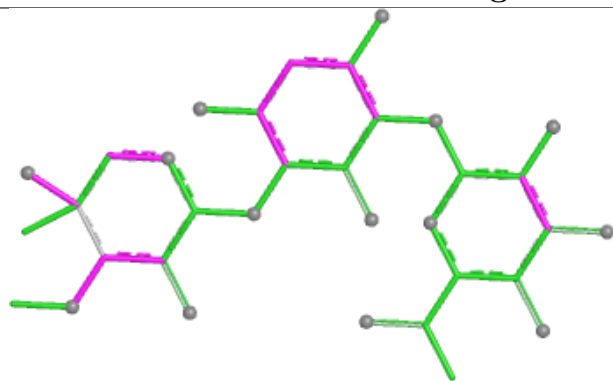
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	AA	1695	GET	3	0
57	AA	1694	GET	3	0

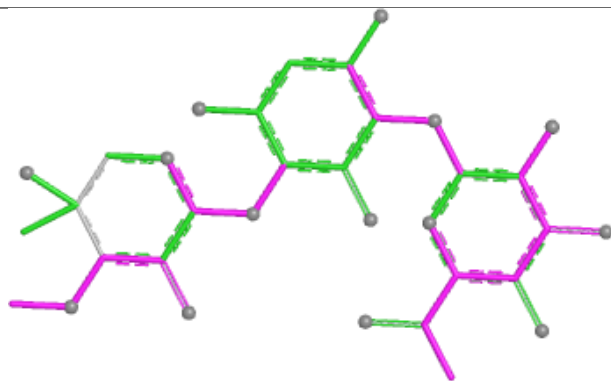
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



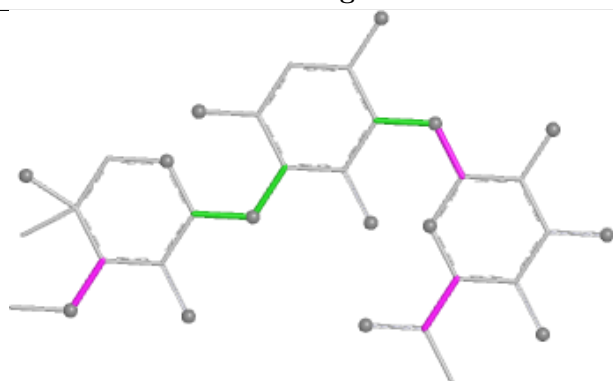
## Ligand GET AA 1695



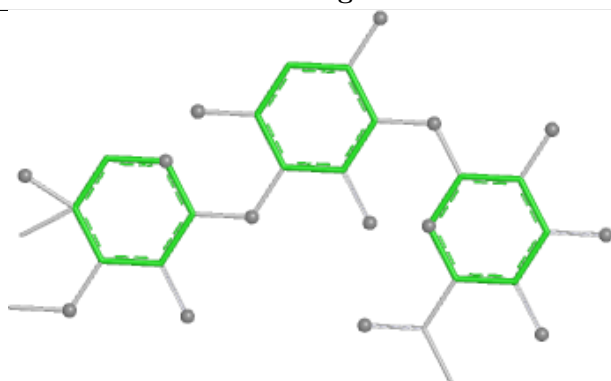
Bond lengths



Bond angles

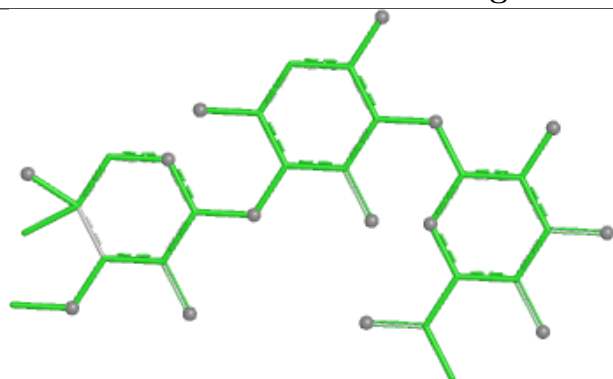


Torsions

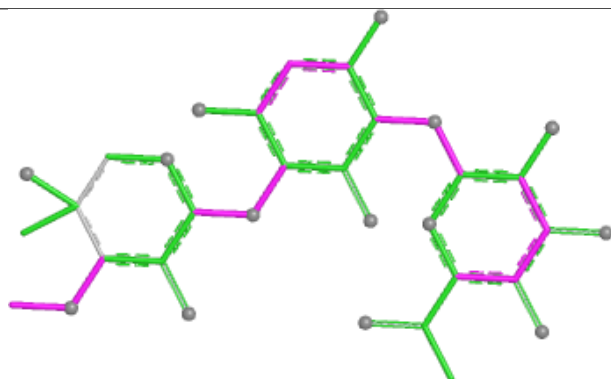


Rings

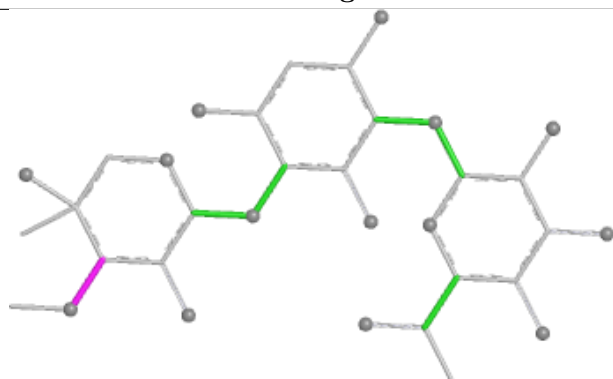
## Ligand GET AA 1694



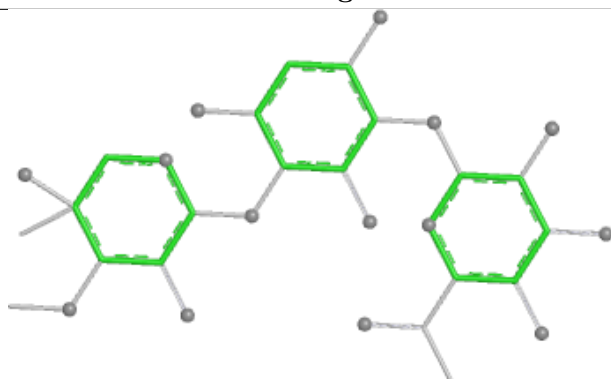
Bond lengths



Bond angles



Torsions



Rings

## 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.

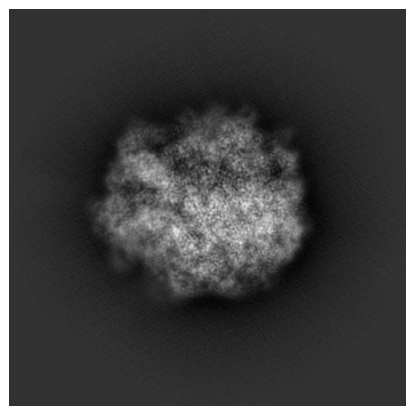
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44194. These allow visual inspection of the internal detail of the map and identification of artifacts.

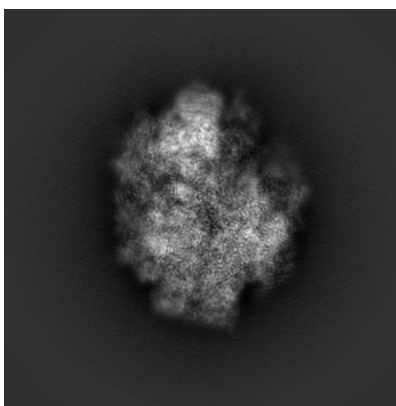
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

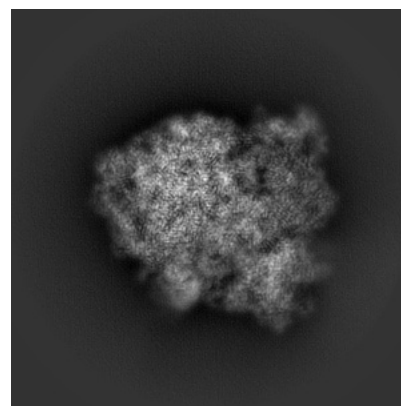
#### 6.1.1 Primary map



X

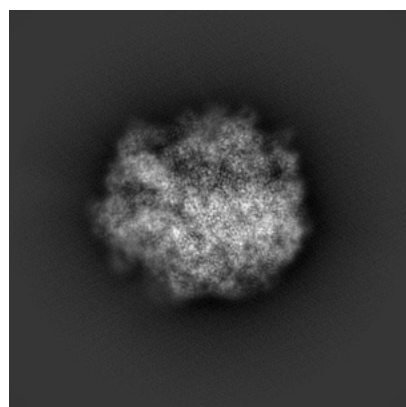


Y

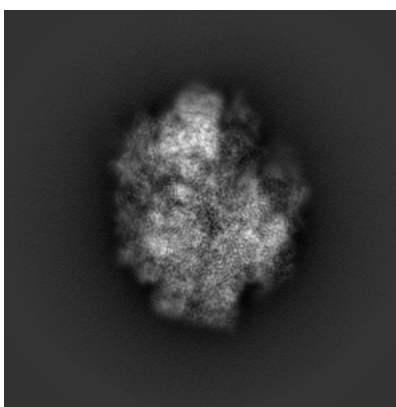


Z

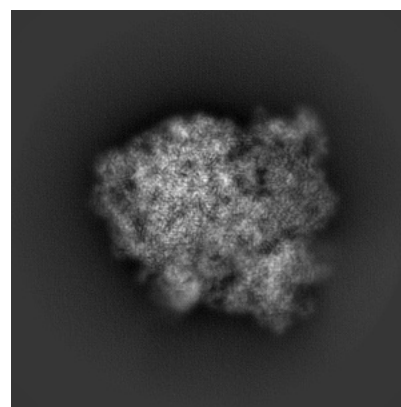
#### 6.1.2 Raw map



X



Y

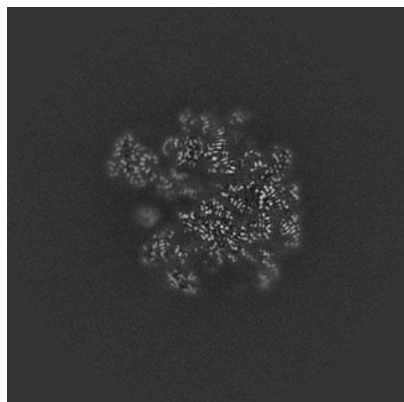


Z

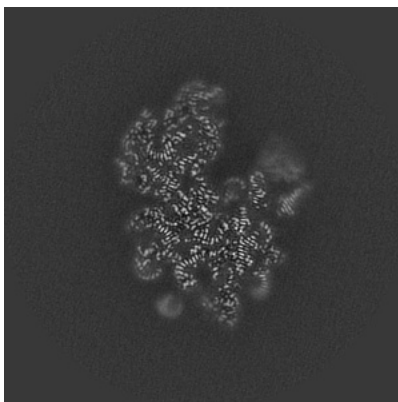
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

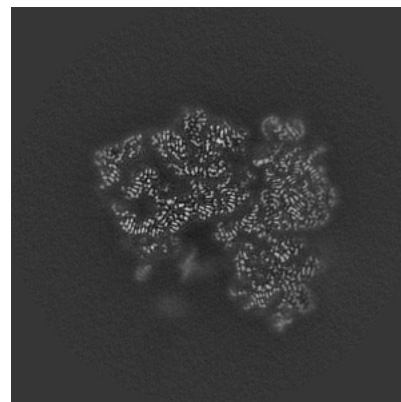
### 6.2.1 Primary map



X Index: 256

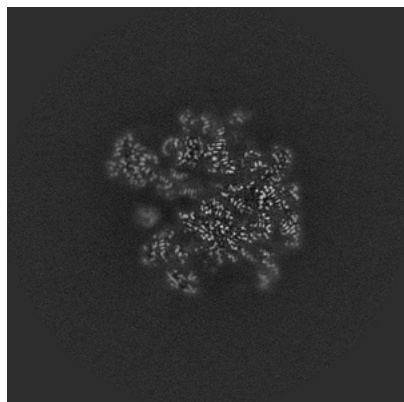


Y Index: 256

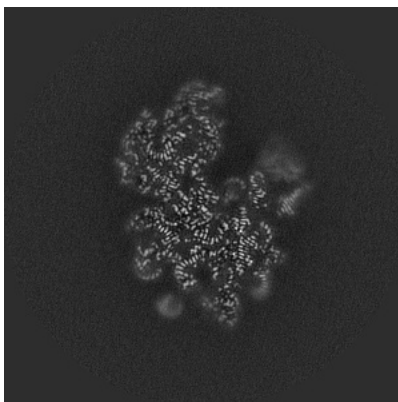


Z Index: 256

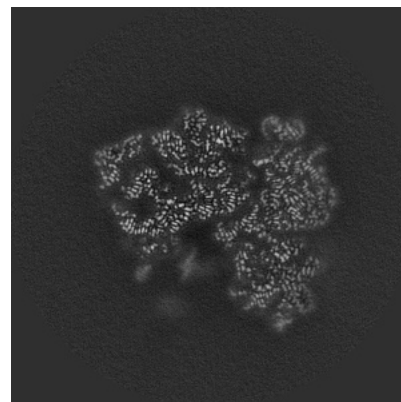
### 6.2.2 Raw map



X Index: 256



Y Index: 256

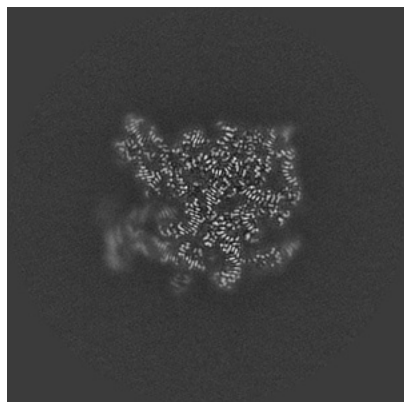


Z Index: 256

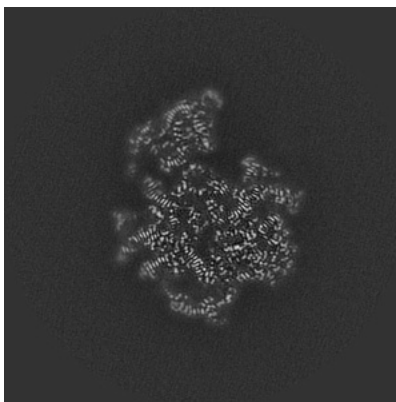
The images above show central slices of the map in three orthogonal directions.

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

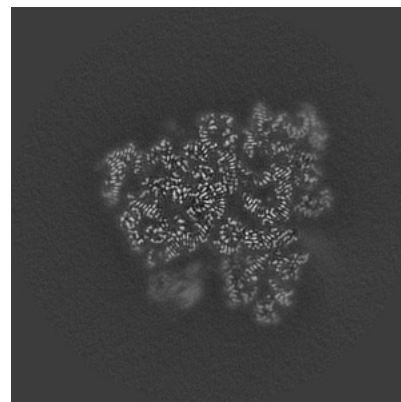
### 6.3.1 Primary map



X Index: 215

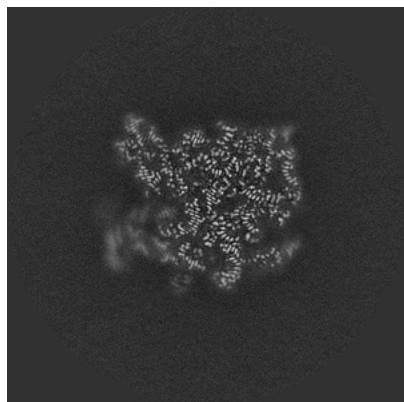


Y Index: 289

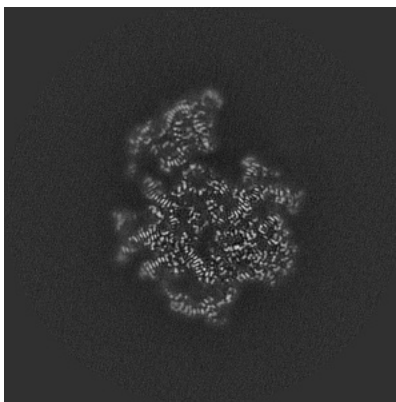


Z Index: 228

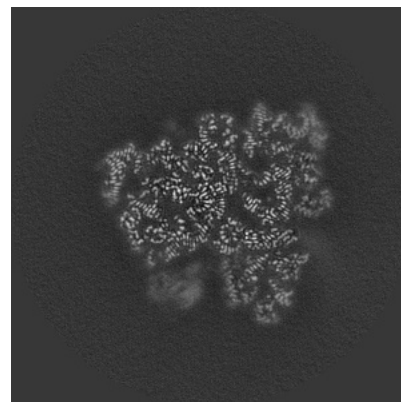
### 6.3.2 Raw map



X Index: 215



Y Index: 289



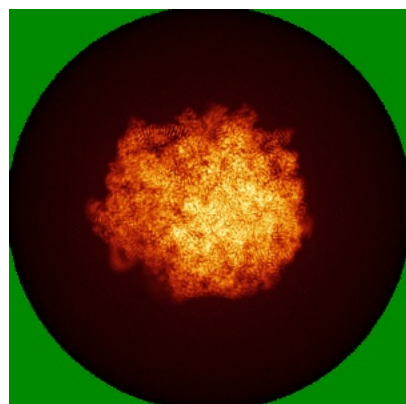
Z Index: 228

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

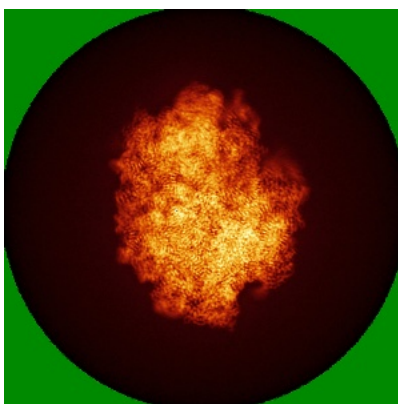


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

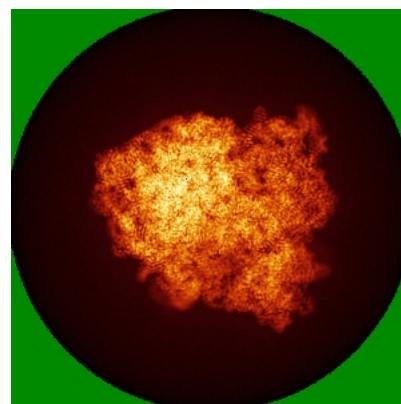
### 6.4.1 Primary map



X

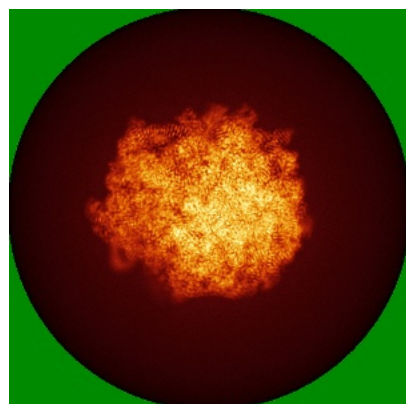


Y

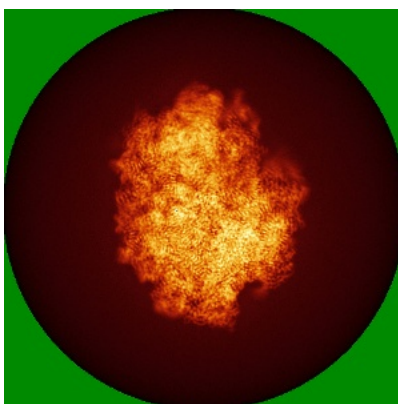


Z

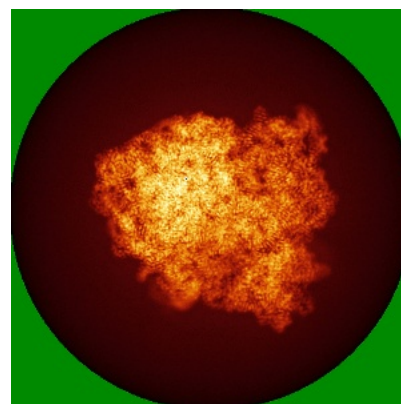
### 6.4.2 Raw map



X



Y

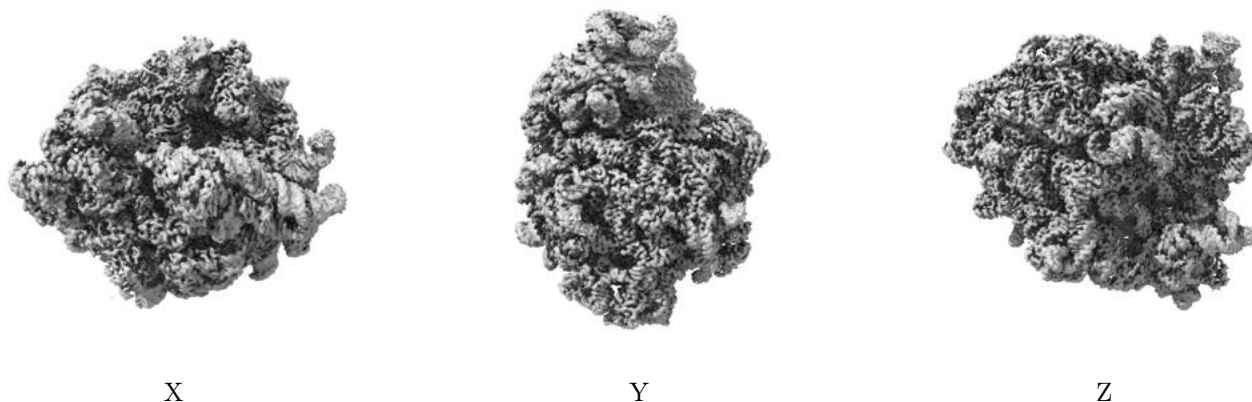


Z

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 2.7. 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.

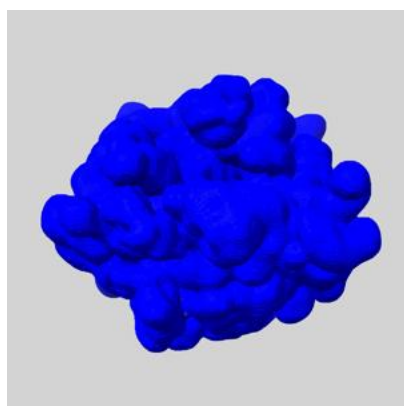
## 6.6 Mask visualisation [i](#)

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

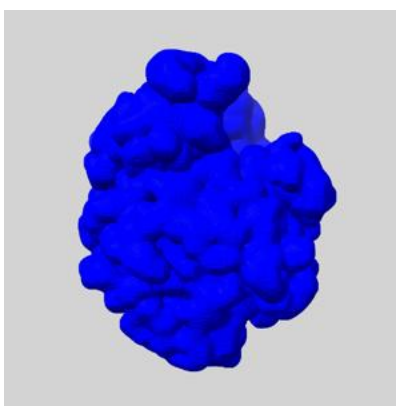
A mask typically either:

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

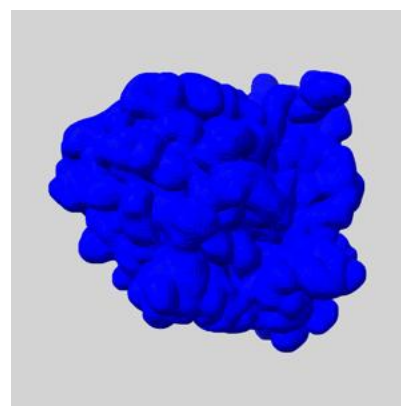
### 6.6.1 emd\_44194\_msk\_1.map [i](#)



X



Y



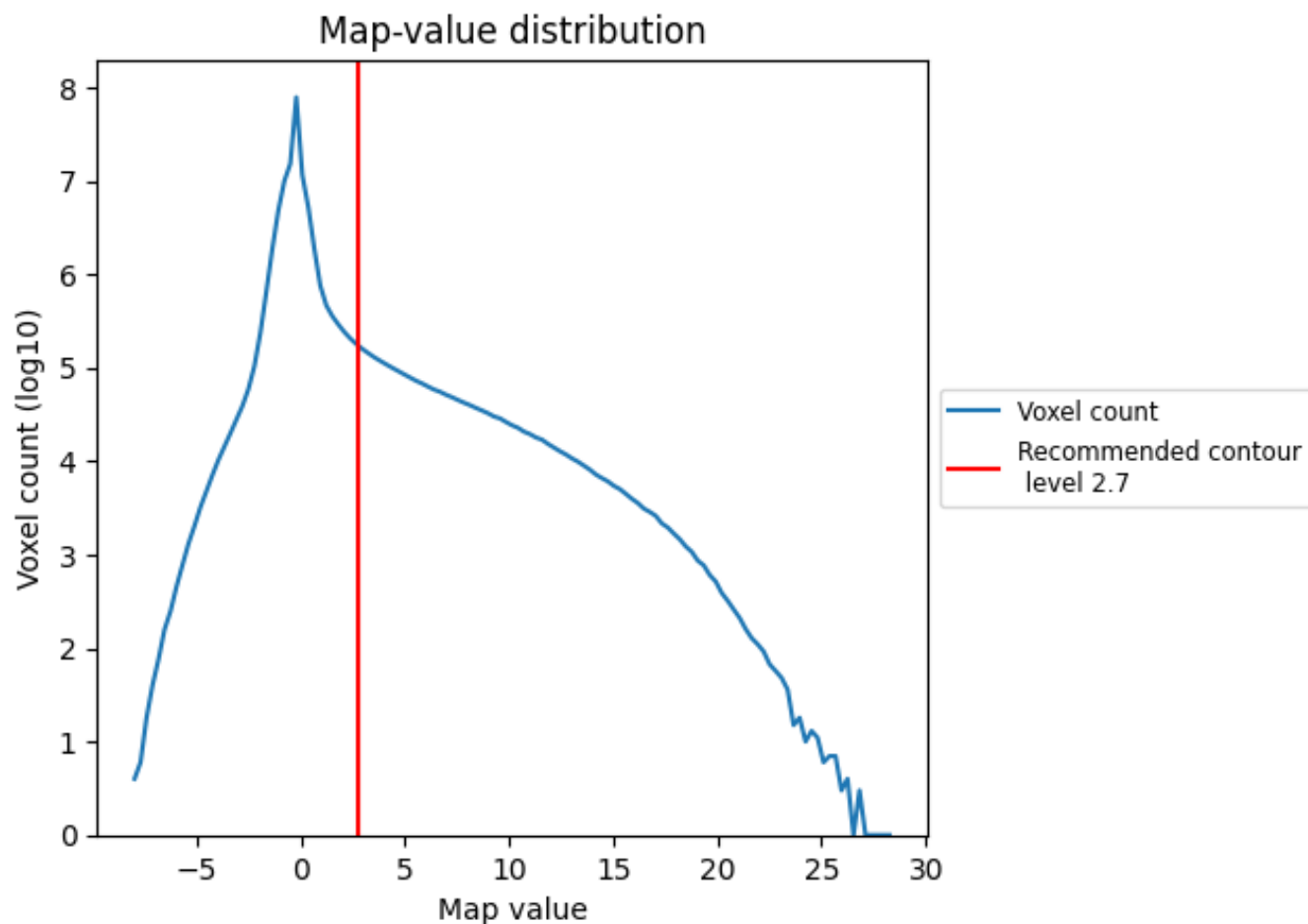
Z



## 7 Map analysis [i](#)

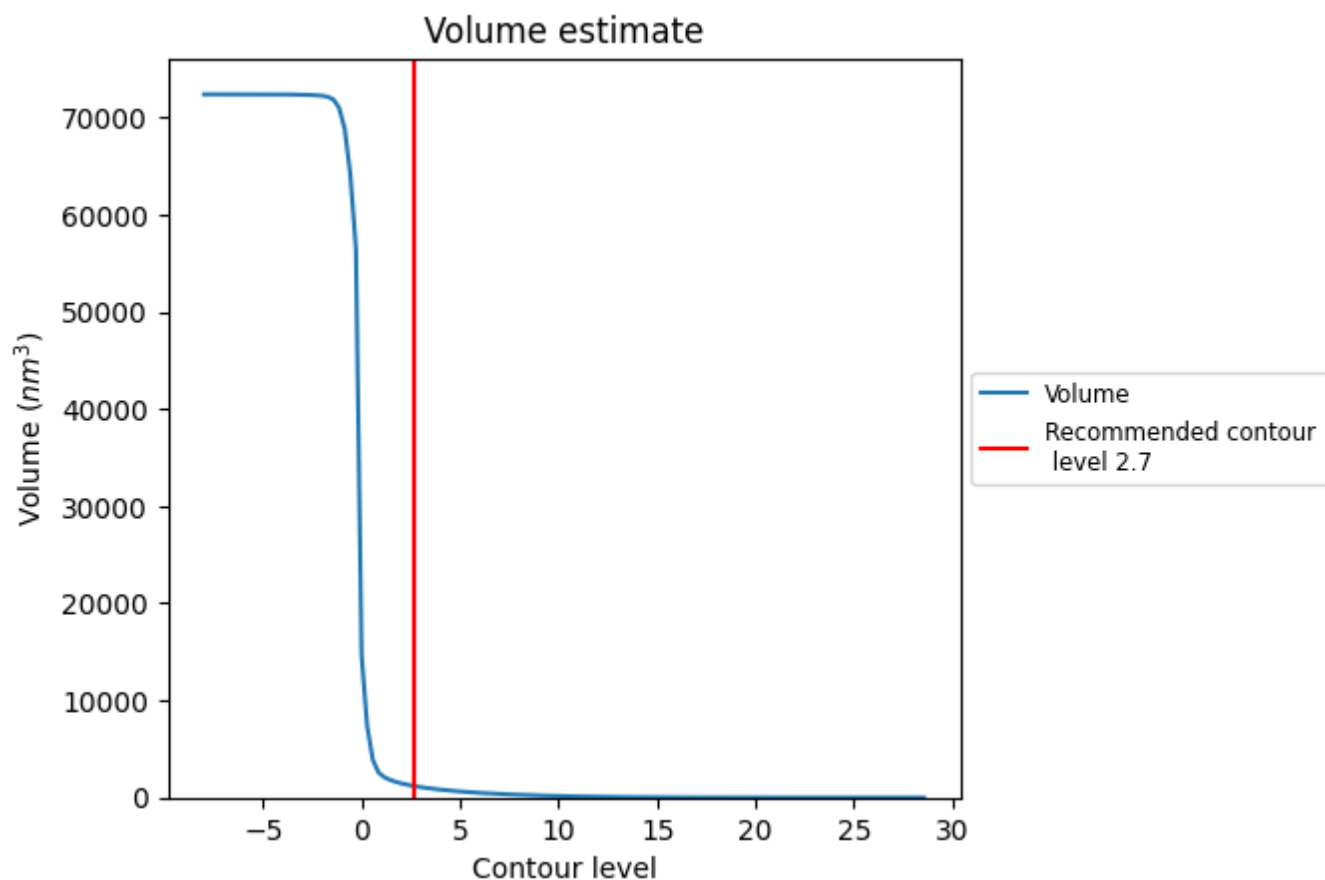
This section contains the results of statistical analysis of the map.

### 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.

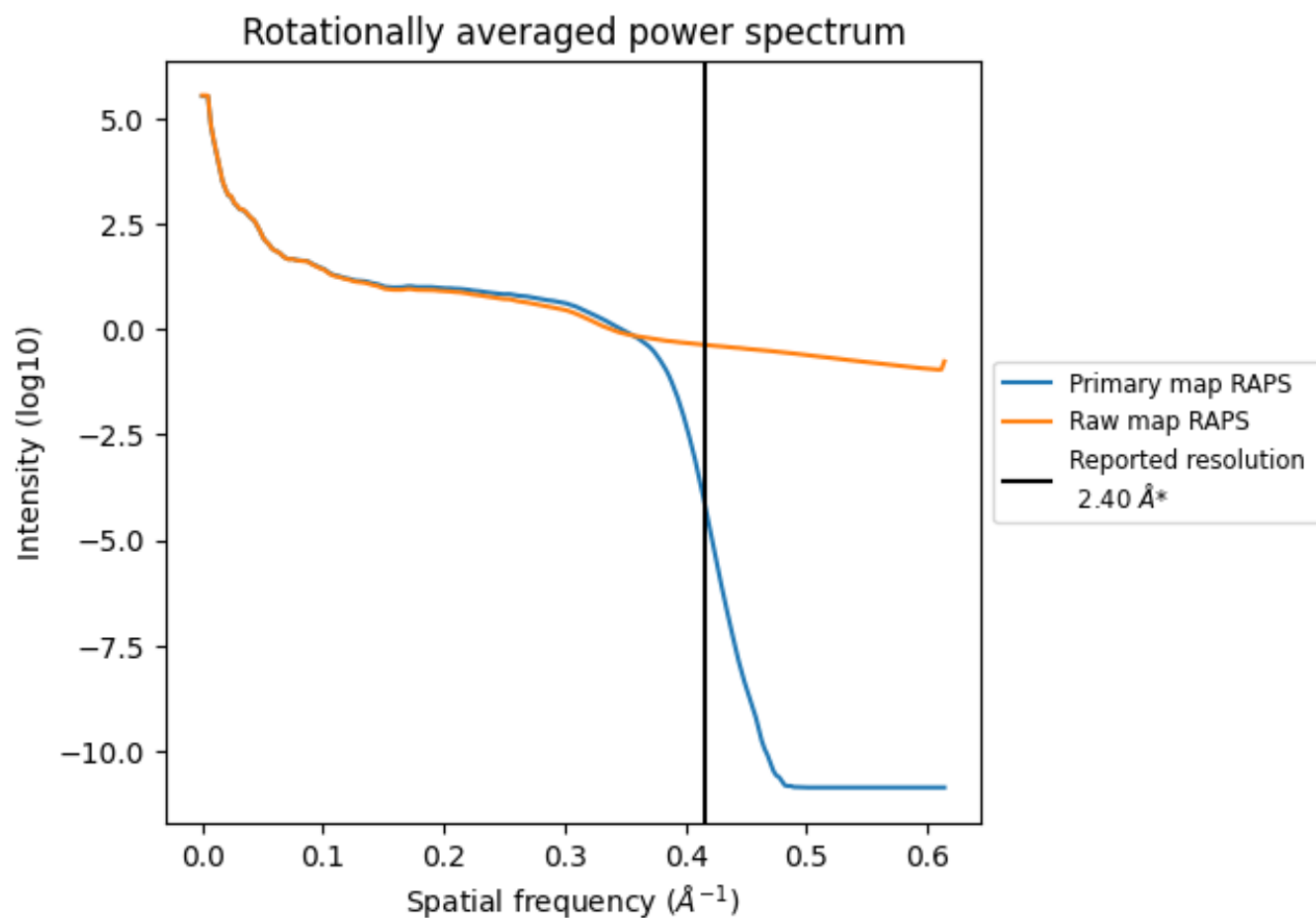
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1175 nm<sup>3</sup>; this corresponds to an approximate mass of 1061 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 ⓘ

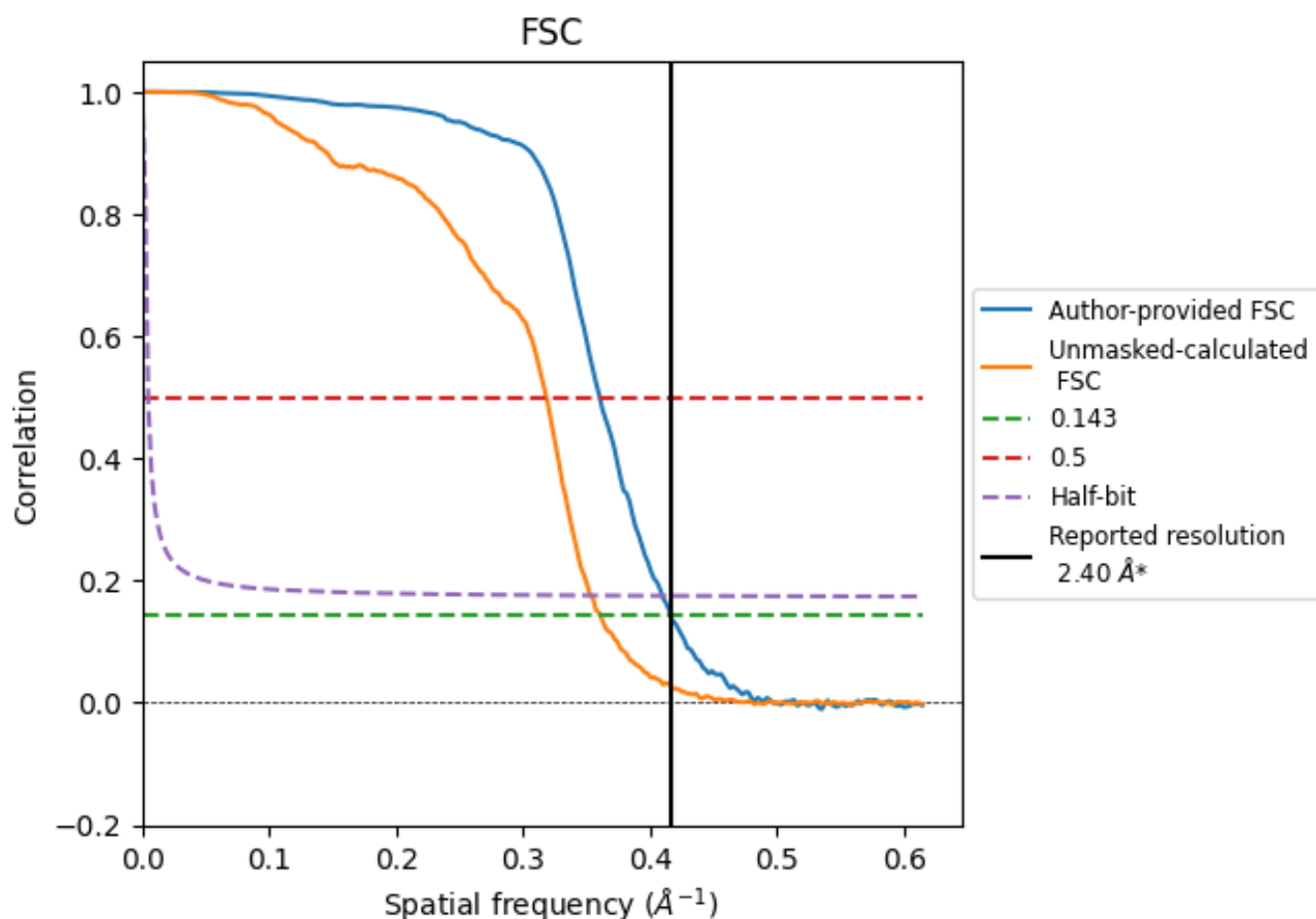


\*Reported resolution corresponds to spatial frequency of 0.417 Å<sup>-1</sup>

## 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 0.417  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

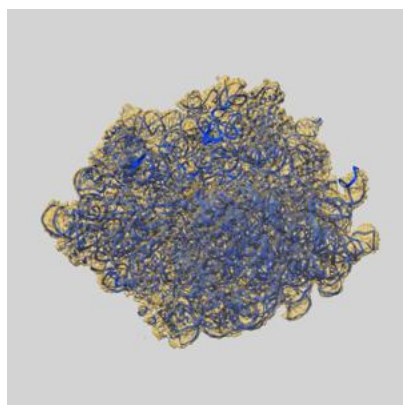
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.40	2.77	2.44
Unmasked-calculated*	2.77	3.14	2.83

\*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 2.77 differs from the reported value 2.4 by more than 10 %

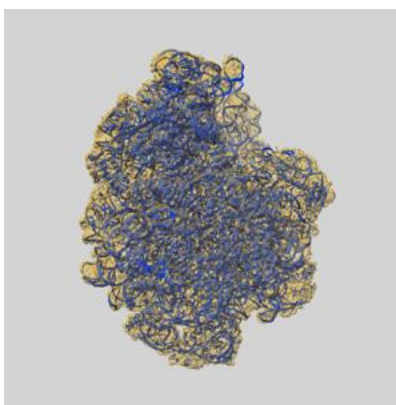
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44194 and PDB model 9B51. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

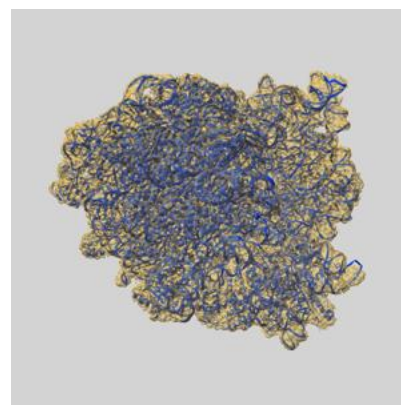
### 9.1 Map-model overlay [i](#)



X



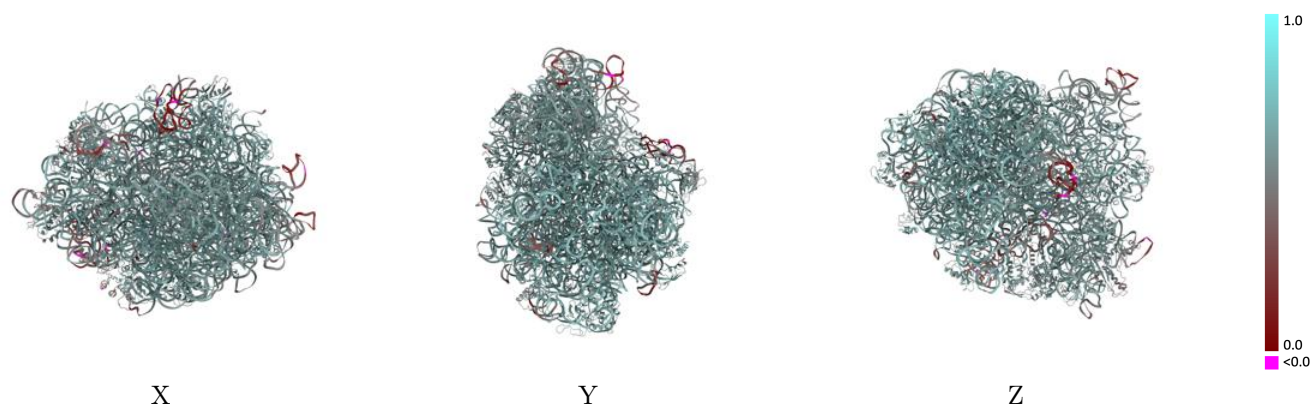
Y



Z

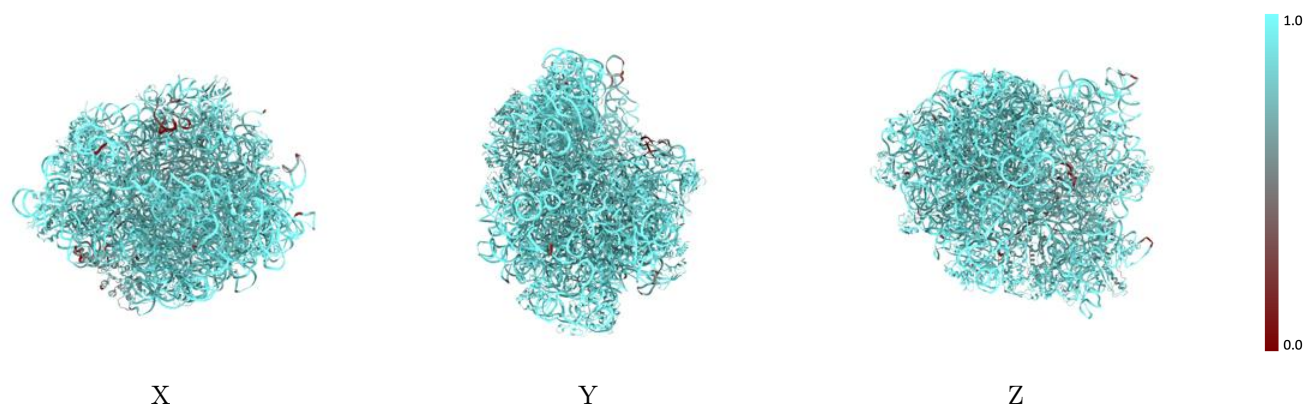
The images above show the 3D surface view of the map at the recommended contour level 2.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



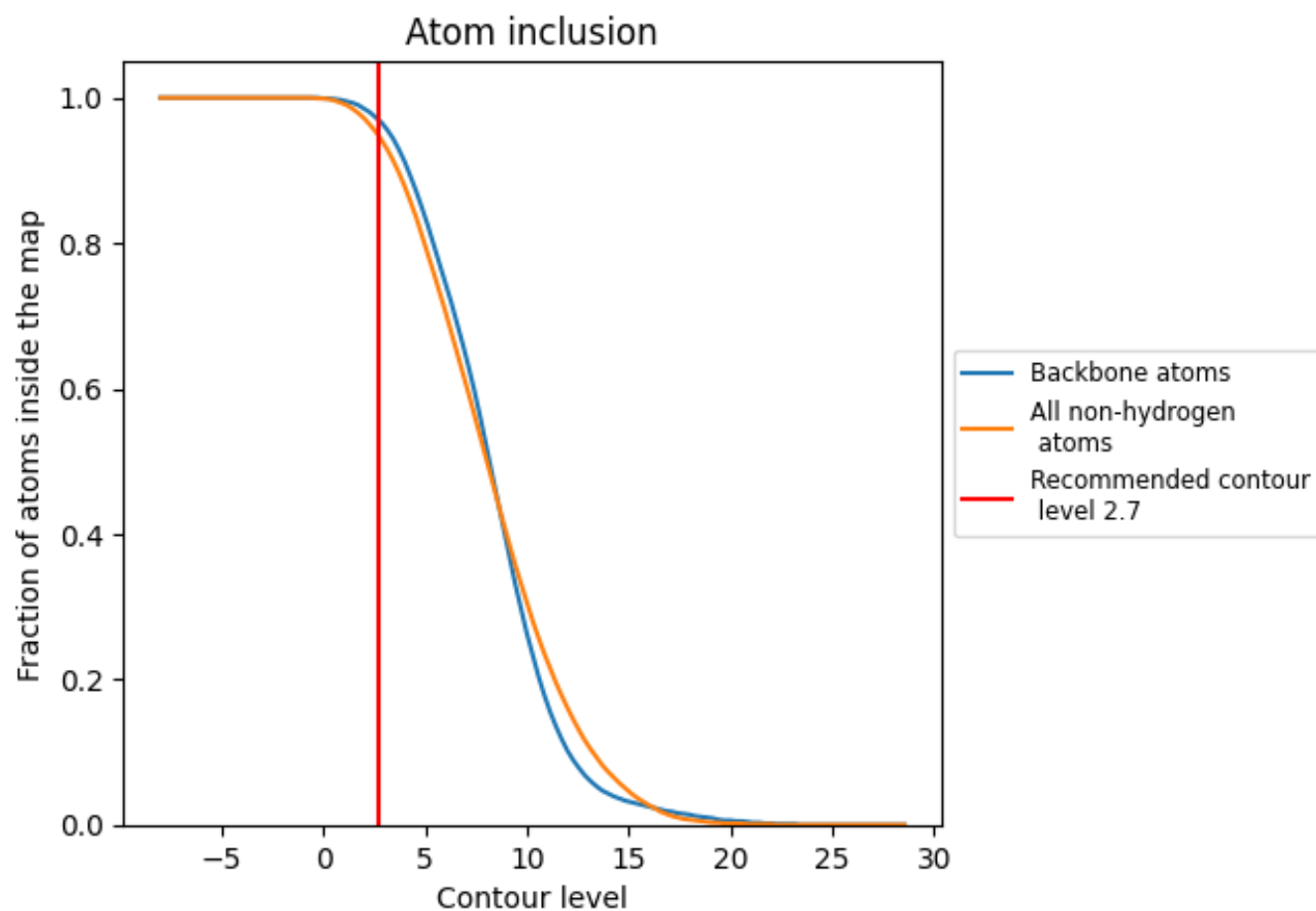
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.7).

## 9.4 Atom inclusion ⓘ









































































At the recommended contour level, 97% of all backbone atoms, 95% 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 (2.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9490	 0.5960
AA	 0.9790	 0.5950
AB	 0.6380	 0.4940
AC	 0.8920	 0.5780
AD	 0.8700	 0.5480
AE	 0.9160	 0.5840
AF	 0.9040	 0.5680
AG	 0.8630	 0.5430
AH	 0.9280	 0.6000
AI	 0.9140	 0.5670
AJ	 0.8420	 0.5200
AK	 0.9160	 0.5770
AL	 0.8990	 0.5900
AM	 0.9080	 0.5560
AN	 0.9180	 0.5570
AO	 0.9140	 0.5960
AP	 0.8820	 0.5500
AQ	 0.8770	 0.5610
AR	 0.9220	 0.5930
AS	 0.9050	 0.5660
AT	 0.8920	 0.5610
AU	 0.6580	 0.3970
AV	 0.9820	 0.6060
AW	 0.8990	 0.5700
AX	 0.8920	 0.5560
AY	 0.6880	 0.3050
B0	 0.9400	 0.6270
B1	 0.9000	 0.5980
B2	 0.9550	 0.6500
B3	 0.9720	 0.6540
B4	 0.9560	 0.6270
B5	 0.8670	 0.5340
BA	 0.9730	 0.6090
BB	 0.9910	 0.6150
BC	 0.9470	 0.6420



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Chain	Atom inclusion	Q-score
BD	 0.9470	 0.6350
BE	 0.9320	 0.6130
BF	 0.8970	 0.5720
BG	 0.8980	 0.5630
BH	 0.6380	 0.4600
BJ	 0.9440	 0.6360
BK	 0.9280	 0.6240
BL	 0.9360	 0.6160
BM	 0.9450	 0.6380
BN	 0.9610	 0.6350
BO	 0.9470	 0.5960
BP	 0.9120	 0.6210
BQ	 0.9810	 0.6540
BR	 0.9220	 0.5950
BS	 0.9270	 0.6210
BT	 0.9060	 0.5870
BU	 0.9180	 0.5790
BV	 0.9120	 0.6070
BW	 0.9420	 0.6430
BX	 0.9520	 0.6380
BY	 0.8710	 0.5390
BZ	 0.9290	 0.6240