



## wwPDB EM Validation Summary Report ⓘ

Oct 6, 2024 – 10:06 am BST

PDB ID : 7PJT  
EMDB ID : EMD-13459  
Title : Structure of the 70S ribosome with tRNAs in hybrid state 1 (H1)  
Authors : Petrychenko, V.; Peng, B.Z.; Schwarzer, A.C.; Peske, F.; Rodnina, M.V.;  
Fischer, N.  
Deposited on : 2021-08-24  
Resolution : 6.00 Å (reported)  
Based on initial models : 6YSS, 4AQY, 5LZD

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.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
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) : 2.39

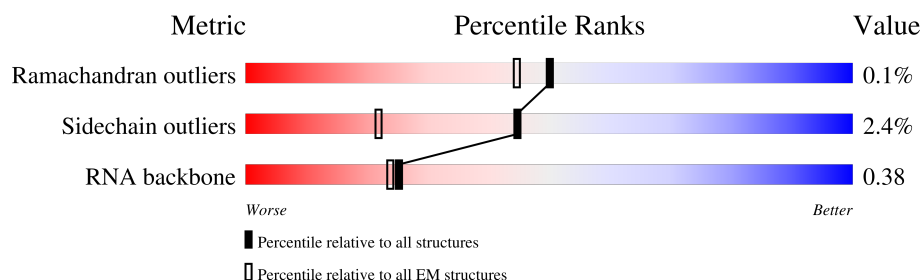
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



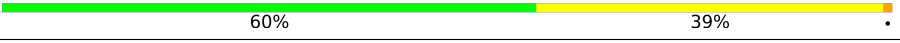
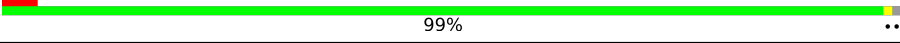
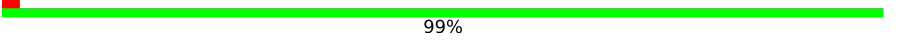
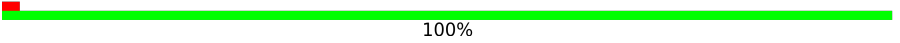
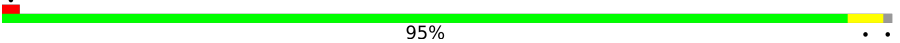
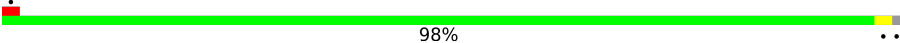
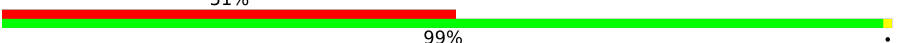

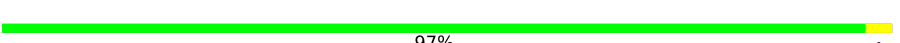
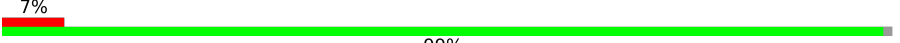

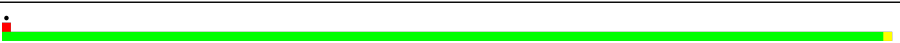



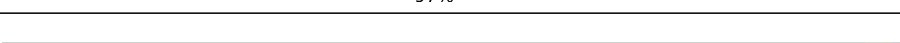
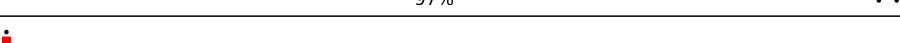
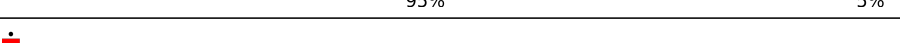
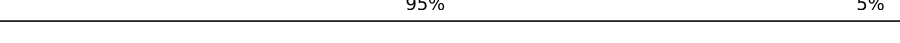

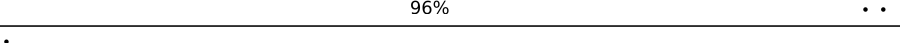
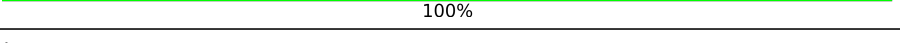

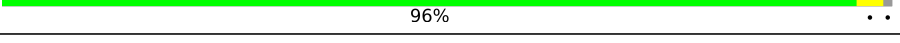
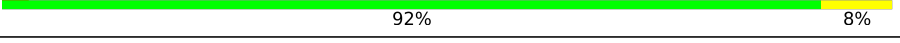
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	0	57	
2	1	55	
3	2	46	
4	3	65	
5	4	38	
6	5	165	
7	6	70	
8	A	2903	




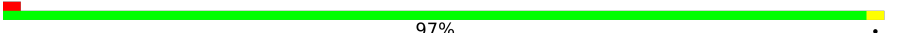











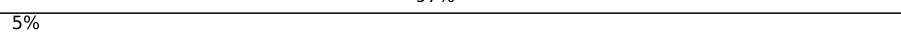
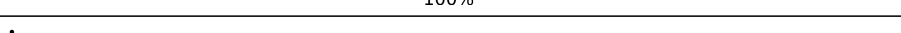
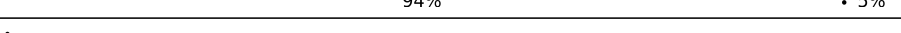


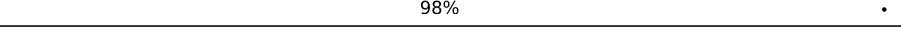



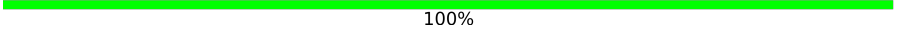
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Mol	Chain	Length	Quality of chain
9	B	120	
10	C	273	
11	D	209	
12	E	201	
13	F	179	
14	G	177	
15	H	149	
16	I	142	
17	J	142	
18	K	123	
19	L	144	
20	M	136	
21	N	127	
22	O	117	
23	P	115	
24	Q	118	
25	R	103	
26	S	110	
27	T	100	
28	U	104	
29	V	94	
30	W	85	
31	X	78	
32	Y	63	
33	Z	59	

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Mol	Chain	Length	Quality of chain
34	a	1542	
35	b	240	
36	c	233	
37	d	206	
38	e	167	
39	f	135	
40	g	179	
41	h	130	
42	i	130	
43	j	103	
44	k	129	
45	l	124	
46	m	118	
47	n	102	
48	o	89	
49	p	82	
50	q	84	
51	r	75	
52	s	92	
53	t	87	
54	u	71	
55	v	77	
56	w	76	
57	y	2	
58	z	33	

## 2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 147222 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L32.

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

- Molecule 2 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 3 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 4 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 5 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 6 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	5	131	Total	C	N	O	0	0
			647	385	131	131		

- Molecule 7 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 8 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	2902	Total	C	N	O	P	0	0
			62317	27806	11469	20140	2902		

- Molecule 9 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	120	Total	C	N	O	P	0	0
			2570	1144	468	838	120		

- Molecule 10 is a protein called 50S ribosomal protein L2.

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

- Molecule 11 is a protein called 50S ribosomal protein L3.

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

- Molecule 12 is a protein called 50S ribosomal protein L4.

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

- Molecule 13 is a protein called 50S ribosomal protein L5.

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

- Molecule 14 is a protein called 50S ribosomal protein L6.

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

- Molecule 15 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 16 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	141	Total	C	N	O	S	0	0
			693	411	141	141			

- Molecule 17 is a protein called 50S ribosomal protein L13.

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

- Molecule 18 is a protein called 50S ribosomal protein L14.

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

- Molecule 19 is a protein called 50S ribosomal protein L15.

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

- Molecule 20 is a protein called 50S ribosomal protein L16.

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

- Molecule 21 is a protein called 50S ribosomal protein L17.

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

- Molecule 22 is a protein called 50S ribosomal protein L18.

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

- Molecule 23 is a protein called 50S ribosomal protein L19.

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

- Molecule 24 is a protein called 50S ribosomal protein L20.

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

- Molecule 25 is a protein called 50S ribosomal protein L21.

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

- Molecule 26 is a protein called 50S ribosomal protein L22.

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

- Molecule 27 is a protein called 50S ribosomal protein L23.

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

- Molecule 28 is a protein called 50S ribosomal protein L24.



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

- Molecule 29 is a protein called 50S ribosomal protein L25.

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

- Molecule 30 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	W	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 31 is a protein called 50S ribosomal protein L28.

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

- Molecule 32 is a protein called 50S ribosomal protein L29.

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

- Molecule 33 is a protein called 50S ribosomal protein L30.

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

- Molecule 34 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	1540	Total	C	N	O	P	0	0
			33050	14748	6057	10705	1540		

- Molecule 35 is a protein called 30S ribosomal protein S2.

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

- Molecule 36 is a protein called 30S ribosomal protein S3.

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

- Molecule 37 is a protein called 30S ribosomal protein S4.

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

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	157	Total	C	N	O	S	0	0
			1141	709	218	208	6		

- Molecule 39 is a protein called 30S ribosomal protein S6.

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

- Molecule 40 is a protein called 30S ribosomal protein S7.

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

- Molecule 41 is a protein called 30S ribosomal protein S8.

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

- Molecule 42 is a protein called 30S ribosomal protein S9.

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

- Molecule 43 is a protein called 30S ribosomal protein S10.

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

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	k	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 45 is a protein called 30S ribosomal protein S12.

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

- Molecule 46 is a protein called 30S ribosomal protein S13.

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

- Molecule 47 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	n	101	Total	C	N	O	S	0	0
			799	498	165	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP C3SR07

- Molecule 48 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	o	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 49 is a protein called 30S ribosomal protein S16.

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

- Molecule 50 is a protein called 30S ribosomal protein S17.

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

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	r	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s	82	Total	C	N	O	S	0	0
			658	421	125	110	2		

- Molecule 53 is a protein called 30S ribosomal protein S20.

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

- Molecule 54 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	u	65	Total	C	N	O	S	0	0
			506	313	105	87	1		

- Molecule 55 is a RNA chain called P-site tRNA(fMet).

Mol	Chain	Residues	Atoms						AltConf	Trace
55	v	77	Total	C	N	O	P	S	0	0
			1642	733	297	534	77	1		

- Molecule 56 is a RNA chain called P-site fMet-Phe-tRNA(Phe).

Mol	Chain	Residues	Atoms						AltConf	Trace
56	w	76	Total	C	N	O	P	S	0	0
			1631	731	291	531	76	2		

- Molecule 57 is a protein called Dipeptide (FME-PHE).

Mol	Chain	Residues	Atoms					AltConf	Trace
57	y	2	Total	C	N	O	S	0	0
			21	15	2	3	1		

- Molecule 58 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	z	11	Total	C	N	O	P	0	0
			230	103	35	81	11		

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
59	4	1	Total	Zn	0
			1	1	
59	6	1	Total	Zn	0
			1	1	

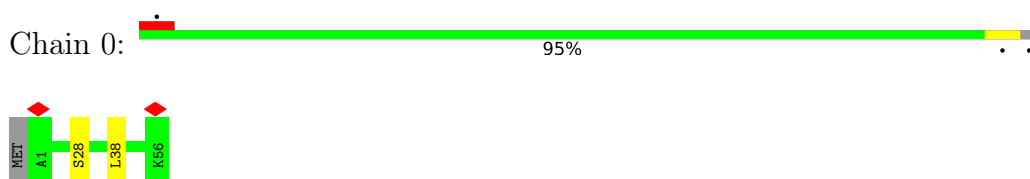
- Molecule 60 is APRAMYCIN (three-letter code: AM2) (formula: C<sub>21</sub>H<sub>41</sub>N<sub>5</sub>O<sub>11</sub>).



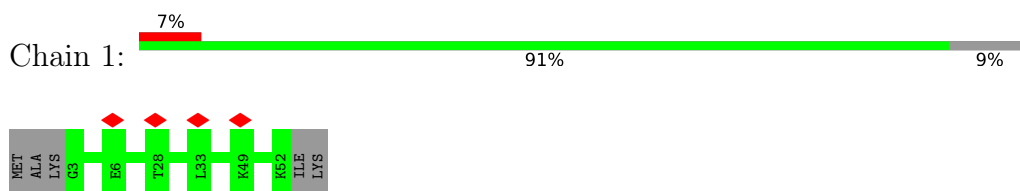
### 3 Residue-property plots [i](#)

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

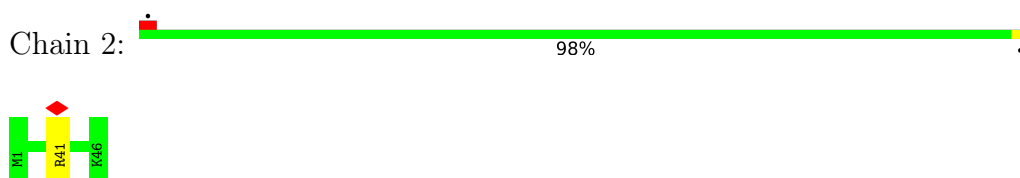
- Molecule 1: 50S ribosomal protein L32



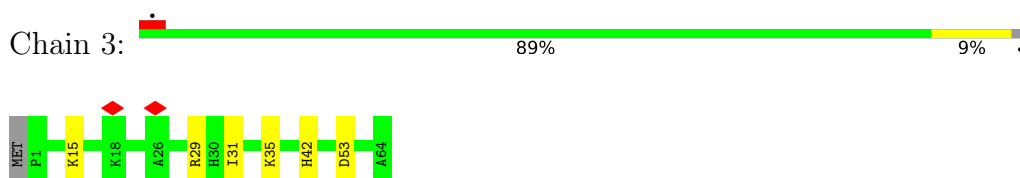
- Molecule 2: 50S ribosomal protein L33



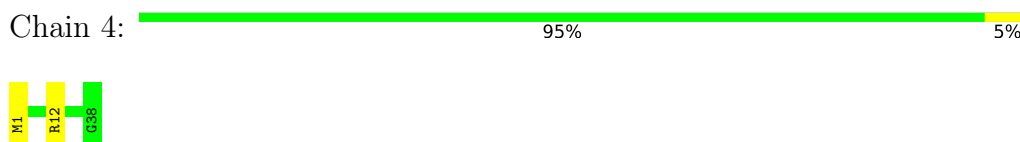
- Molecule 3: 50S ribosomal protein L34



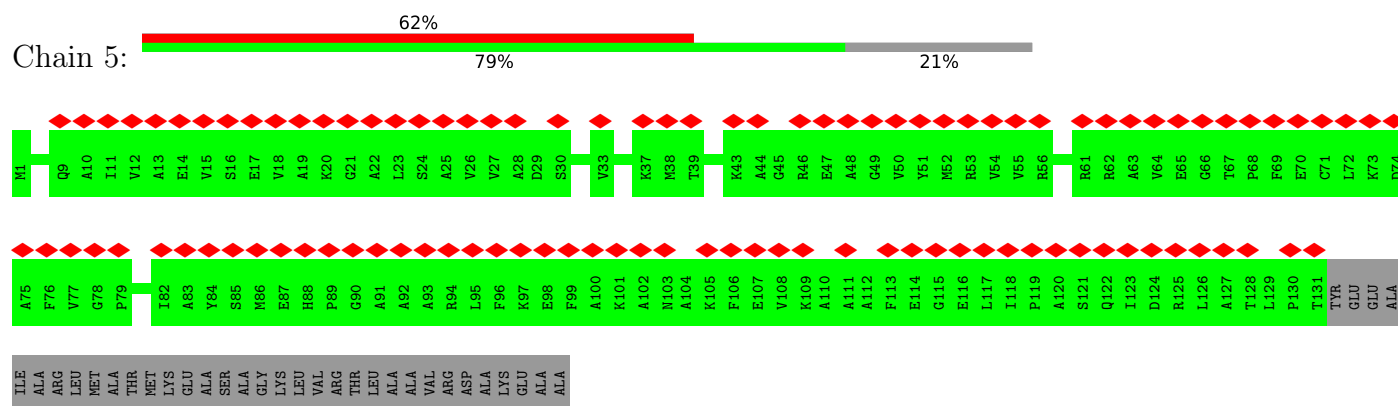
- Molecule 4: 50S ribosomal protein L35



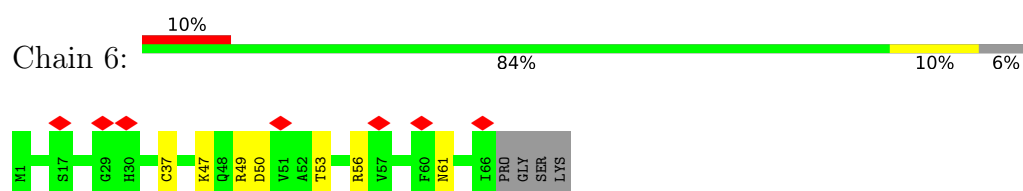
- Molecule 5: 50S ribosomal protein L36



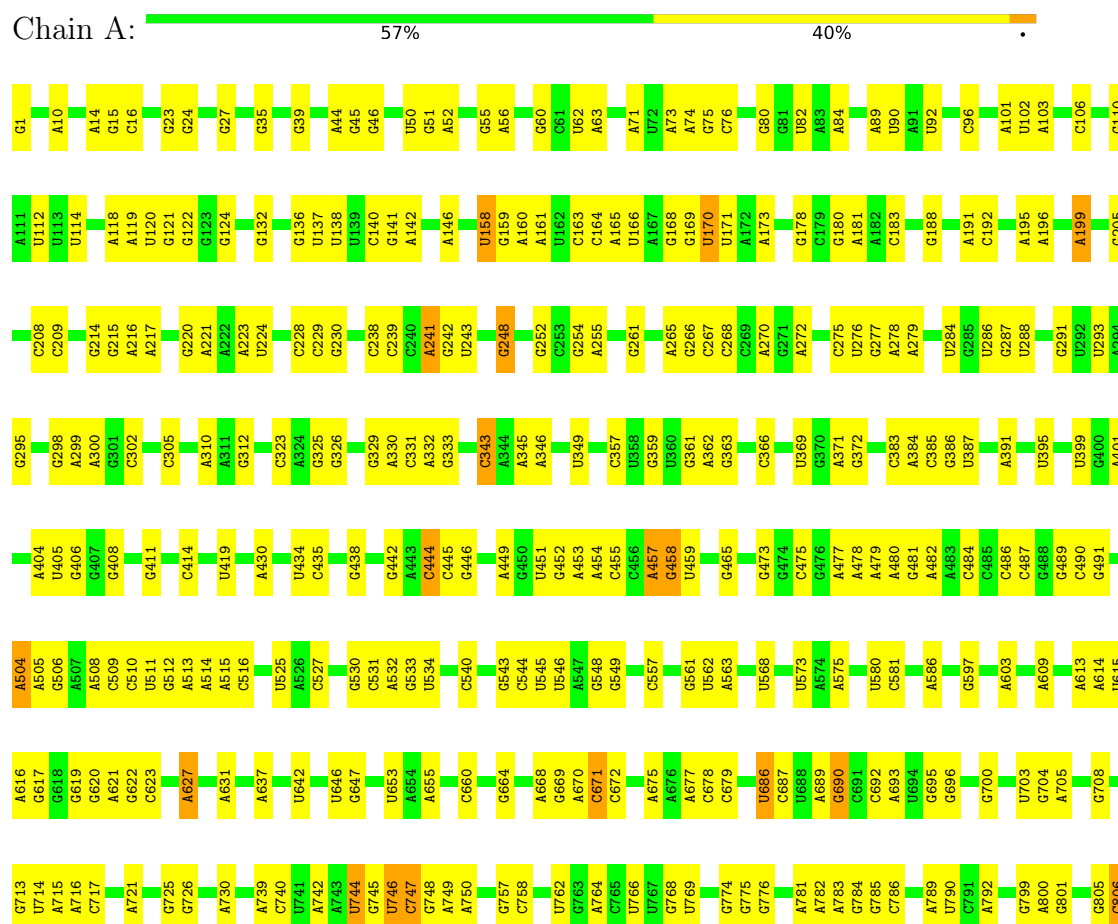
- Molecule 6: 50S ribosomal protein L10



- Molecule 7: 50S ribosomal protein L31

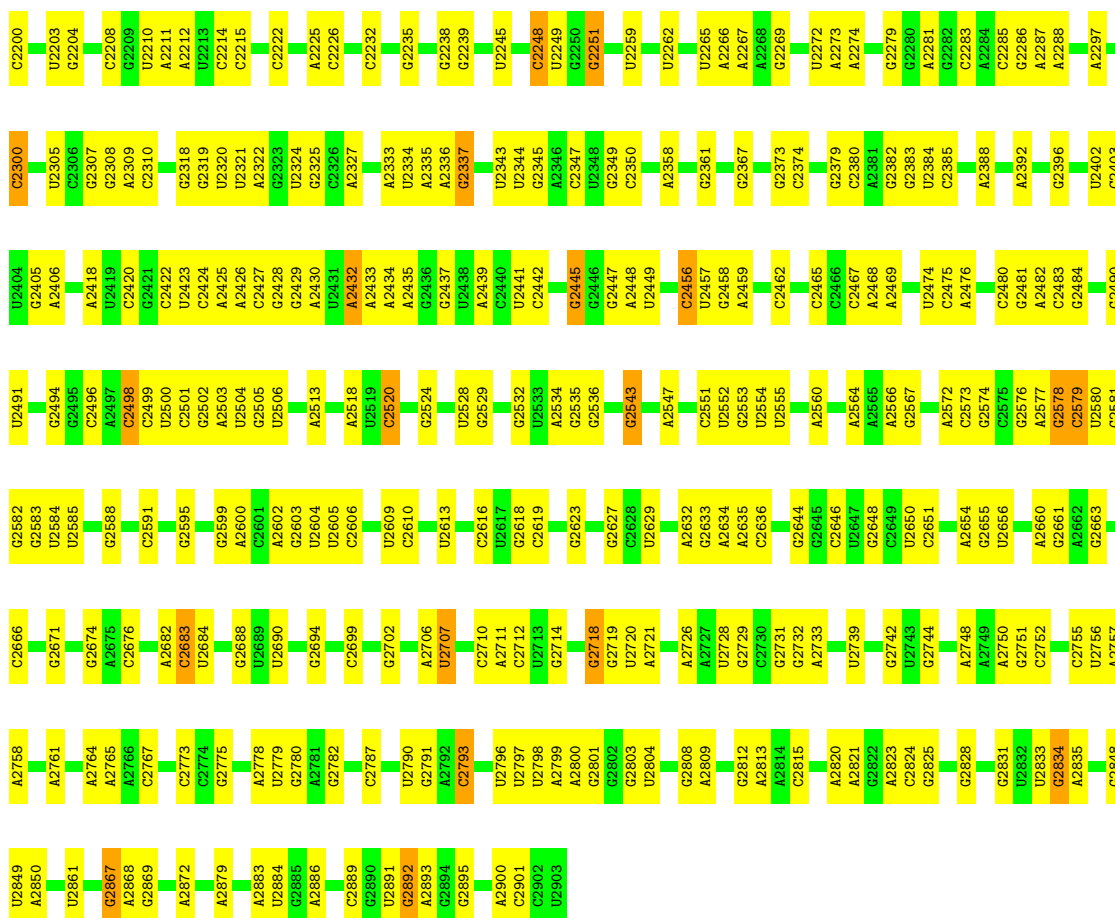


- Molecule 8: 23S ribosomal RNA



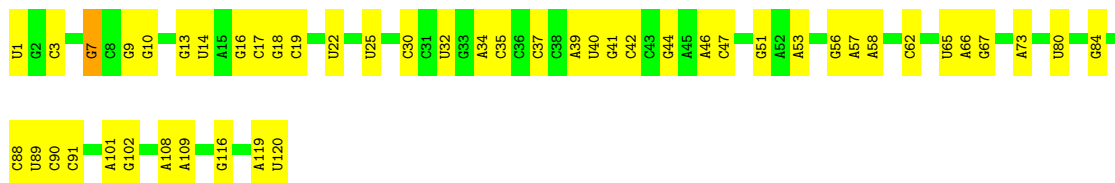


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U2131	U1782	A1668	A1577	G1482	C1376	G1256	A1156	U1080	G1003	C898	U811
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G2049	A1763	G1674	U1578	U1484	U1379	A1268	C1170	U1083	C1005	U901	U813
G2050	A1765	C1675	U1584	U1488	G1380	A1269	G1171	A1084	U1006	C902	C814
A2051	A1766	C1691	U1585	C1489	A1383	G1270	U1173	A1086	A1010	C903	A819
A2052	A1767	C1692	U1591	C1490	A1384	A1284	U1174	G1087	G1012	G907	A820
C2055	C1767	U1691	A1594	G1491	A1385	A1286	U1175	A1088	U1011	A910	U826
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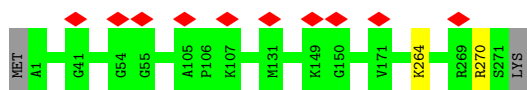
• Molecule 9: 5S ribosomal RNA

Chain B: 60% 39%



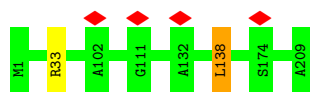
• Molecule 10: 50S ribosomal protein L2

Chain C: 99%

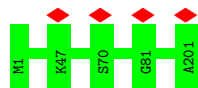


• Molecule 11: 50S ribosomal protein L3

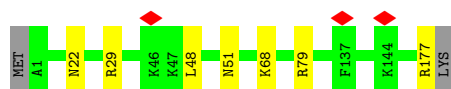
Chain D: 99%



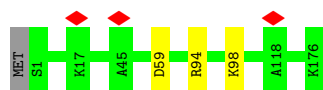
- Molecule 12: 50S ribosomal protein L4



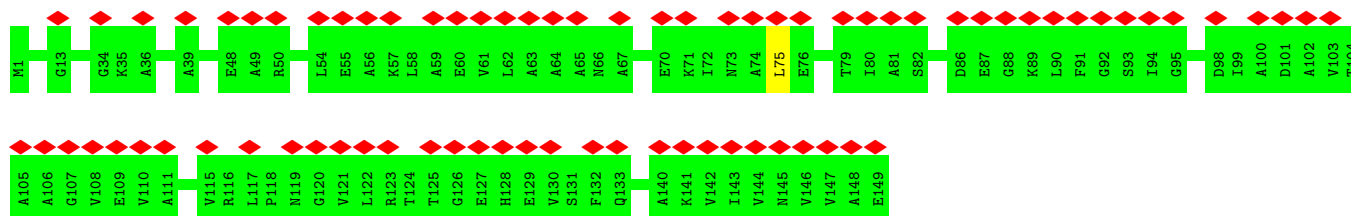
- Molecule 13: 50S ribosomal protein L5



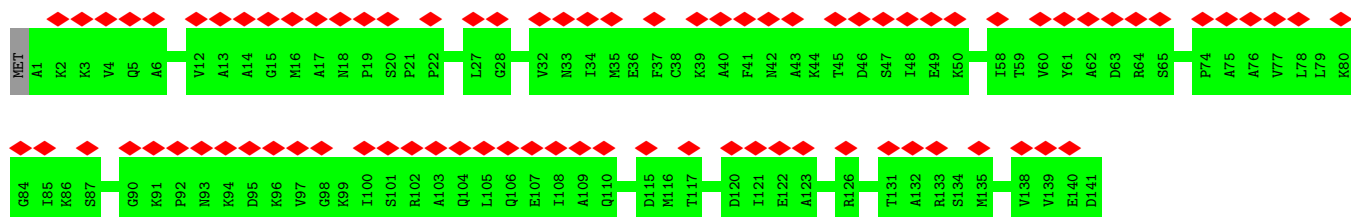
- Molecule 14: 50S ribosomal protein L6



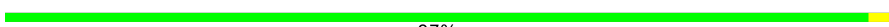
- Molecule 15: 50S ribosomal protein L9



- Molecule 16: 50S ribosomal protein L11



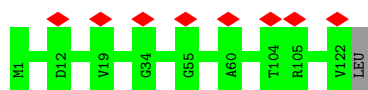
- Molecule 17: 50S ribosomal protein L13

Chain J:  97% .



- Molecule 18: 50S ribosomal protein L14

Chain K:  99% .



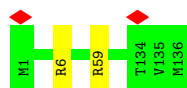
- Molecule 19: 50S ribosomal protein L15

Chain L:  97% ..



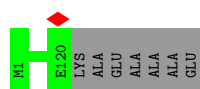
- Molecule 20: 50S ribosomal protein L16

Chain M:  99% .



- Molecule 21: 50S ribosomal protein L17

Chain N:  94% 6%



- Molecule 22: 50S ribosomal protein L18

Chain O:  95% ..



- Molecule 23: 50S ribosomal protein L19

Chain P:  97% ..



- Molecule 24: 50S ribosomal protein L20

Chain Q:  97% ..



- Molecule 25: 50S ribosomal protein L21

Chain R:  95% 5%




- Molecule 26: 50S ribosomal protein L22

Chain S:  95% 5%



- Molecule 27: 50S ribosomal protein L23

Chain T:  91% 7%



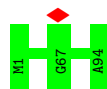
- Molecule 28: 50S ribosomal protein L24

Chain U:  96% ..



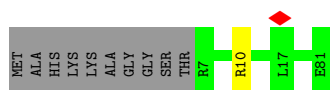
- Molecule 29: 50S ribosomal protein L25

Chain V:  100%



- Molecule 30: 50S ribosomal protein L27

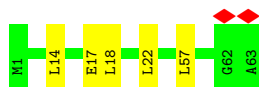
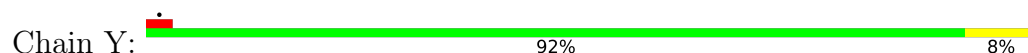
Chain W:  87% 12%



- Molecule 31: 50S ribosomal protein L28



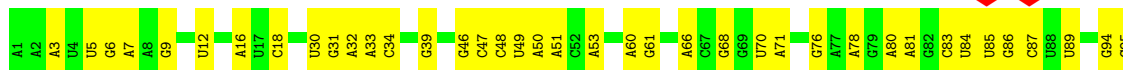
- Molecule 32: 50S ribosomal protein L29

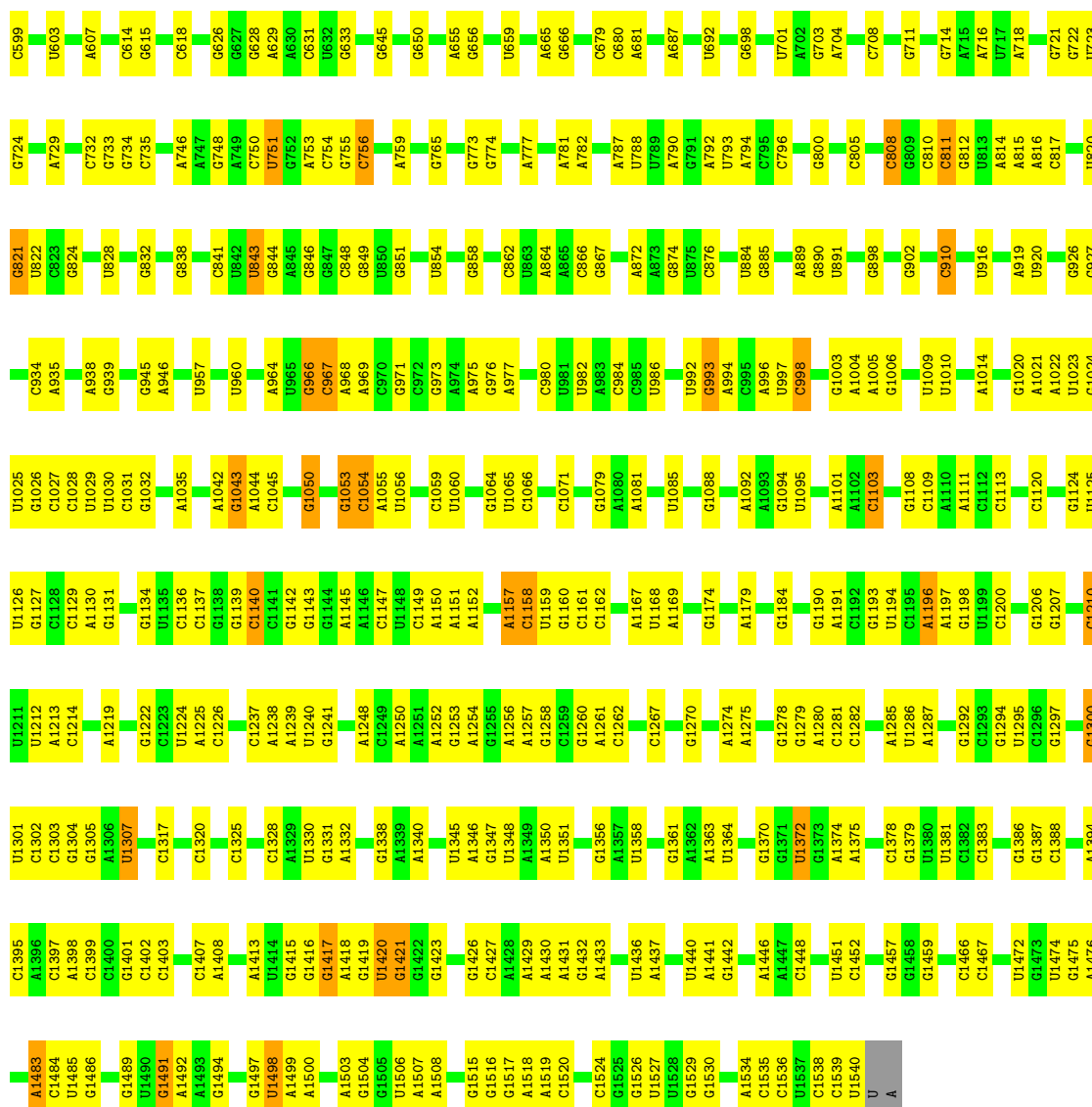


- Molecule 33: 50S ribosomal protein L30

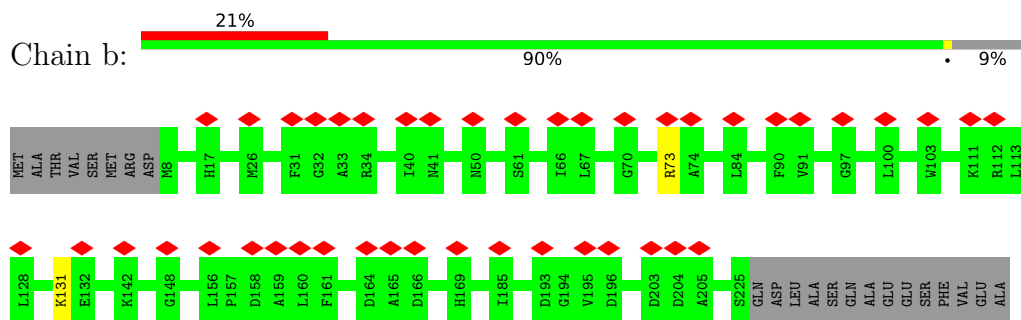


- Molecule 34: 16S ribosomal RNA

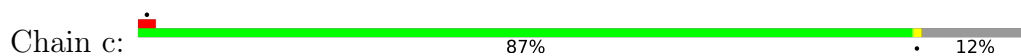




• Molecule 35: 30S ribosomal protein S2

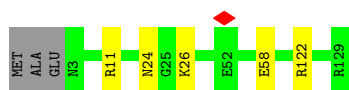


• Molecule 36: 30S ribosomal protein S3

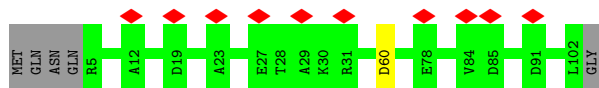
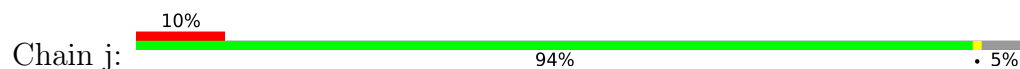




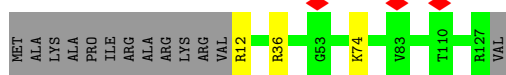
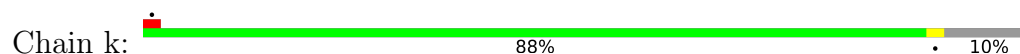




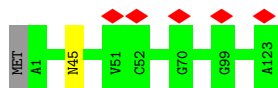
- Molecule 43: 30S ribosomal protein S10



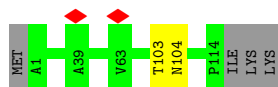
- Molecule 44: 30S ribosomal protein S11



- Molecule 45: 30S ribosomal protein S12



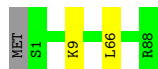
- Molecule 46: 30S ribosomal protein S13



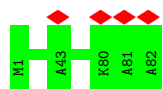
- Molecule 47: 30S ribosomal protein S14



- Molecule 48: 30S ribosomal protein S15



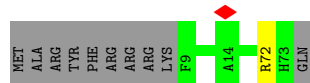
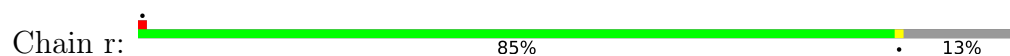
- Molecule 49: 30S ribosomal protein S16



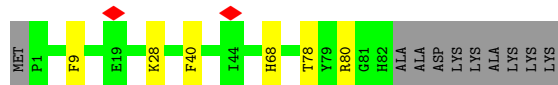
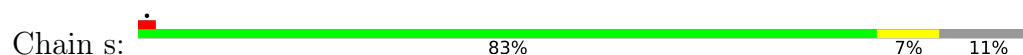
- Molecule 50: 30S ribosomal protein S17



- Molecule 51: 30S ribosomal protein S18



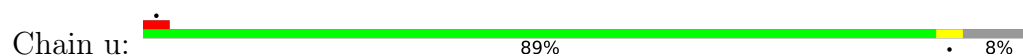
- Molecule 52: 30S ribosomal protein S19



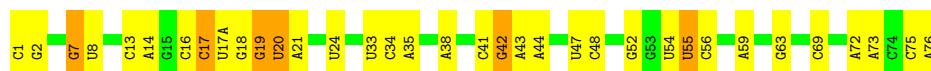
- Molecule 53: 30S ribosomal protein S20



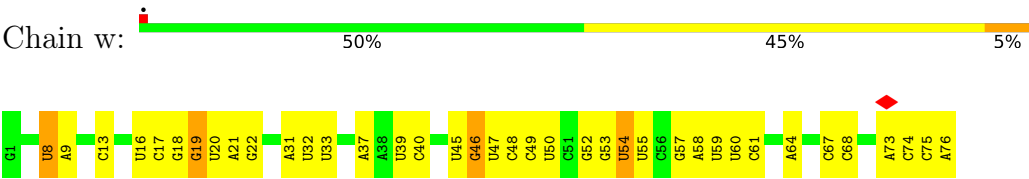
- Molecule 54: 30S ribosomal protein S21



- Molecule 55: P-site tRNA(fMet)



● Molecule 56: P-site fMet-Phe-tRNA(Phe)

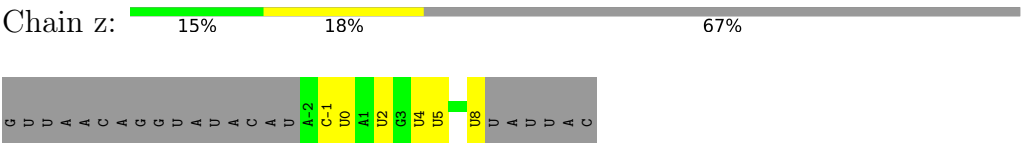


● Molecule 57: Dipeptide (FME-PHE)



There are no outlier residues recorded for this chain.

● Molecule 58: mRNA



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6937	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 ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	11.607	Depositor
Minimum map value	-7.178	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.5	Depositor
Map size (Å)	334.08, 334.08, 334.08	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMG, OMC, FME, 2MA, 6MZ, 2MG, OMU, PSU, H2U, G7M, 1MG, 4OC, ZN, 4SU, 5MU, UR3, MA6, AM2, 5MC, MIA

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	0	0.53	0/450	0.60	0/599
2	1	0.39	0/416	0.52	0/554
3	2	0.46	0/380	0.66	0/498
4	3	0.50	0/513	0.69	0/676
5	4	0.43	0/303	0.60	0/397
6	5	0.26	0/646	0.51	0/898
7	6	0.49	0/531	0.73	0/709
8	A	1.04	22/69266 (0.0%)	1.20	242/108055 (0.2%)
9	B	0.87	2/2873 (0.1%)	1.10	1/4478 (0.0%)
10	C	0.48	0/2121	0.62	0/2852
11	D	0.47	0/1586	0.62	0/2134
12	E	0.46	0/1571	0.60	0/2113
13	F	0.43	0/1434	0.59	0/1926
14	G	0.40	0/1343	0.57	0/1816
15	H	0.38	0/1122	0.61	0/1515
16	I	0.26	0/692	0.50	0/960
17	J	0.50	0/1152	0.55	0/1551
18	K	0.43	0/947	0.61	0/1268
19	L	0.48	0/1054	0.69	1/1403 (0.1%)
20	M	0.46	0/1093	0.57	0/1460
21	N	0.42	0/973	0.62	0/1301
22	O	0.43	0/902	0.61	0/1209
23	P	0.47	0/929	0.63	2/1242 (0.2%)
24	Q	0.50	0/960	0.60	1/1278 (0.1%)
25	R	0.47	0/829	0.64	0/1107
26	S	0.44	0/864	0.61	0/1156
27	T	0.42	0/744	0.62	0/994
28	U	0.46	0/787	0.61	0/1051
29	V	0.46	0/766	0.57	0/1025
30	W	0.45	0/582	0.63	0/769
31	X	0.44	0/635	0.66	1/848 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	Y	0.41	0/510	0.64	0/677
33	Z	0.40	0/453	0.55	0/605
34	a	0.91	3/36725 (0.0%)	1.17	121/57285 (0.2%)
35	b	0.37	0/1735	0.57	0/2338
36	c	0.43	0/1651	0.56	1/2225 (0.0%)
37	d	0.39	0/1665	0.59	0/2227
38	e	0.42	0/1154	0.58	0/1554
39	f	0.38	0/835	0.56	0/1128
40	g	0.37	0/1195	0.54	0/1602
41	h	0.41	0/989	0.59	0/1326
42	i	0.42	0/1034	0.60	0/1375
43	j	0.37	0/796	0.62	0/1077
44	k	0.43	0/885	0.61	0/1195
45	l	0.44	0/969	0.60	0/1300
46	m	0.37	0/892	0.60	0/1193
47	n	0.45	0/811	0.69	0/1081
48	o	0.40	0/722	0.63	1/964 (0.1%)
49	p	0.40	0/659	0.58	0/884
50	q	0.41	0/657	0.59	0/881
51	r	0.42	0/544	0.60	0/731
52	s	0.46	0/675	0.69	0/908
53	t	0.38	0/671	0.51	0/888
54	u	0.40	0/512	0.56	0/683
55	v	0.83	1/1745 (0.1%)	1.17	7/2716 (0.3%)
56	w	0.69	0/1650	1.17	5/2569 (0.2%)
57	y	0.63	0/11	0.43	0/13
58	z	0.53	0/255	0.95	0/394
All	All	0.86	28/158864 (0.0%)	1.07	383/237661 (0.2%)

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	v	1	C	OP3-P	-10.75	1.48	1.61
9	B	1	U	OP3-P	-10.74	1.48	1.61
8	A	1	G	OP3-P	-10.73	1.48	1.61
8	A	1786	A	N9-C4	-7.76	1.33	1.37
8	A	195	A	N9-C4	-6.71	1.33	1.37

The worst 5 of 383 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1054	C	O5'-P-OP1	14.14	127.67	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1196	A	C2'-C3'-O3'	9.93	131.35	109.50
34	a	1053	G	O3'-P-O5'	-9.74	85.50	104.00
34	a	1421	G	N9-C4-C5	9.61	109.24	105.40
34	a	1421	G	C8-N9-C1'	9.46	139.30	127.00

There are no chirality outliers.

There are no planarity outliers.

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

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

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	54/57 (95%)	42 (78%)	12 (22%)	0	100	100
2	1	48/55 (87%)	38 (79%)	10 (21%)	0	100	100
3	2	44/46 (96%)	27 (61%)	17 (39%)	0	100	100
4	3	62/65 (95%)	48 (77%)	14 (23%)	0	100	100
5	4	36/38 (95%)	28 (78%)	8 (22%)	0	100	100
6	5	129/165 (78%)	100 (78%)	29 (22%)	0	100	100
7	6	64/70 (91%)	54 (84%)	10 (16%)	0	100	100
10	C	269/273 (98%)	213 (79%)	56 (21%)	0	100	100
11	D	207/209 (99%)	172 (83%)	34 (16%)	1 (0%)	25	65
12	E	199/201 (99%)	165 (83%)	34 (17%)	0	100	100
13	F	175/179 (98%)	153 (87%)	22 (13%)	0	100	100
14	G	174/177 (98%)	149 (86%)	25 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	H	147/149 (99%)	117 (80%)	30 (20%)	0	100	100
16	I	139/142 (98%)	104 (75%)	35 (25%)	0	100	100
17	J	140/142 (99%)	109 (78%)	31 (22%)	0	100	100
18	K	120/123 (98%)	101 (84%)	19 (16%)	0	100	100
19	L	141/144 (98%)	108 (77%)	33 (23%)	0	100	100
20	M	134/136 (98%)	109 (81%)	24 (18%)	1 (1%)	19	57
21	N	118/127 (93%)	87 (74%)	31 (26%)	0	100	100
22	O	114/117 (97%)	101 (89%)	13 (11%)	0	100	100
23	P	112/115 (97%)	98 (88%)	14 (12%)	0	100	100
24	Q	115/118 (98%)	102 (89%)	13 (11%)	0	100	100
25	R	101/103 (98%)	87 (86%)	14 (14%)	0	100	100
26	S	108/110 (98%)	89 (82%)	19 (18%)	0	100	100
27	T	91/100 (91%)	74 (81%)	17 (19%)	0	100	100
28	U	100/104 (96%)	81 (81%)	19 (19%)	0	100	100
29	V	92/94 (98%)	79 (86%)	13 (14%)	0	100	100
30	W	73/85 (86%)	56 (77%)	17 (23%)	0	100	100
31	X	75/78 (96%)	63 (84%)	12 (16%)	0	100	100
32	Y	61/63 (97%)	49 (80%)	12 (20%)	0	100	100
33	Z	56/59 (95%)	51 (91%)	5 (9%)	0	100	100
35	b	216/240 (90%)	184 (85%)	32 (15%)	0	100	100
36	c	204/233 (88%)	181 (89%)	23 (11%)	0	100	100
37	d	203/206 (98%)	160 (79%)	42 (21%)	1 (0%)	25	65
38	e	155/167 (93%)	119 (77%)	36 (23%)	0	100	100
39	f	98/135 (73%)	88 (90%)	10 (10%)	0	100	100
40	g	149/179 (83%)	130 (87%)	19 (13%)	0	100	100
41	h	127/130 (98%)	107 (84%)	20 (16%)	0	100	100
42	i	125/130 (96%)	98 (78%)	27 (22%)	0	100	100
43	j	96/103 (93%)	76 (79%)	19 (20%)	1 (1%)	13	49
44	k	114/129 (88%)	92 (81%)	22 (19%)	0	100	100
45	l	121/124 (98%)	96 (79%)	25 (21%)	0	100	100
46	m	112/118 (95%)	99 (88%)	13 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	n	99/102 (97%)	87 (88%)	12 (12%)	0	100	100
48	o	86/89 (97%)	74 (86%)	12 (14%)	0	100	100
49	p	80/82 (98%)	61 (76%)	19 (24%)	0	100	100
50	q	78/84 (93%)	68 (87%)	10 (13%)	0	100	100
51	r	63/75 (84%)	49 (78%)	14 (22%)	0	100	100
52	s	80/92 (87%)	70 (88%)	10 (12%)	0	100	100
53	t	83/87 (95%)	66 (80%)	17 (20%)	0	100	100
54	u	63/71 (89%)	50 (79%)	13 (21%)	0	100	100
All	All	5850/6220 (94%)	4809 (82%)	1037 (18%)	4 (0%)	50	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
43	j	60	ASP
37	d	144	ILE
11	D	138	LEU
20	M	59	ARG

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	47/48 (98%)	45 (96%)	2 (4%)	25	46
2	1	45/49 (92%)	45 (100%)	0	100	100
3	2	38/38 (100%)	37 (97%)	1 (3%)	41	59
4	3	51/52 (98%)	45 (88%)	6 (12%)	4	16
5	4	34/34 (100%)	32 (94%)	2 (6%)	16	38
7	6	59/62 (95%)	52 (88%)	7 (12%)	4	16
10	C	216/218 (99%)	214 (99%)	2 (1%)	75	83
11	D	164/164 (100%)	162 (99%)	2 (1%)	67	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	E	165/165 (100%)	165 (100%)	0	100	100
13	F	148/150 (99%)	141 (95%)	7 (5%)	22	44
14	G	137/138 (99%)	134 (98%)	3 (2%)	47	65
15	H	114/114 (100%)	113 (99%)	1 (1%)	75	83
17	J	116/116 (100%)	112 (97%)	4 (3%)	32	51
18	K	103/104 (99%)	103 (100%)	0	100	100
19	L	102/103 (99%)	100 (98%)	2 (2%)	50	68
20	M	109/109 (100%)	108 (99%)	1 (1%)	75	83
21	N	100/103 (97%)	100 (100%)	0	100	100
22	O	86/87 (99%)	81 (94%)	5 (6%)	17	38
23	P	99/100 (99%)	98 (99%)	1 (1%)	73	82
24	Q	89/90 (99%)	87 (98%)	2 (2%)	47	65
25	R	84/84 (100%)	79 (94%)	5 (6%)	16	37
26	S	93/93 (100%)	88 (95%)	5 (5%)	18	40
27	T	80/84 (95%)	78 (98%)	2 (2%)	42	61
28	U	83/85 (98%)	81 (98%)	2 (2%)	44	62
29	V	78/78 (100%)	78 (100%)	0	100	100
30	W	57/63 (90%)	56 (98%)	1 (2%)	54	71
31	X	67/68 (98%)	66 (98%)	1 (2%)	60	75
32	Y	55/55 (100%)	50 (91%)	5 (9%)	7	24
33	Z	48/49 (98%)	48 (100%)	0	100	100
35	b	180/198 (91%)	178 (99%)	2 (1%)	70	80
36	c	170/190 (90%)	168 (99%)	2 (1%)	67	79
37	d	172/173 (99%)	168 (98%)	4 (2%)	45	64
38	e	114/126 (90%)	113 (99%)	1 (1%)	75	83
39	f	87/116 (75%)	85 (98%)	2 (2%)	45	64
40	g	124/147 (84%)	121 (98%)	3 (2%)	44	62
41	h	104/105 (99%)	102 (98%)	2 (2%)	52	69
42	i	105/107 (98%)	100 (95%)	5 (5%)	21	43
43	j	86/90 (96%)	86 (100%)	0	100	100
44	k	89/99 (90%)	86 (97%)	3 (3%)	32	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	l	103/104 (99%)	102 (99%)	1 (1%)	73	82
46	m	92/96 (96%)	90 (98%)	2 (2%)	47	65
47	n	79/84 (94%)	75 (95%)	4 (5%)	20	41
48	o	76/77 (99%)	75 (99%)	1 (1%)	65	77
49	p	65/65 (100%)	65 (100%)	0	100	100
50	q	74/78 (95%)	73 (99%)	1 (1%)	62	75
51	r	56/65 (86%)	55 (98%)	1 (2%)	54	71
52	s	72/79 (91%)	66 (92%)	6 (8%)	9	27
53	t	65/66 (98%)	65 (100%)	0	100	100
54	u	46/61 (75%)	44 (96%)	2 (4%)	25	46
57	y	1/1 (100%)	1 (100%)	0	100	100
All	All	4627/4830 (96%)	4516 (98%)	111 (2%)	45	62

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	S	104	THR
54	u	37	TYR
36	c	167	TYR
54	u	15	LEU
47	n	63	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
32	Y	45	GLN
41	h	75	GLN
35	b	17	HIS
39	f	3	HIS
44	k	80	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	a	1536/1542 (99%)	575 (37%)	0
55	v	76/77 (98%)	30 (39%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
56	w	74/76 (97%)	32 (43%)	0
58	z	10/33 (30%)	6 (60%)	0
8	A	2897/2903 (99%)	1092 (37%)	86 (2%)
9	B	119/120 (99%)	46 (38%)	2 (1%)
All	All	4712/4751 (99%)	1781 (37%)	88 (1%)

5 of 1781 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	A	10	A
8	A	14	A
8	A	15	G
8	A	16	C
8	A	23	G

5 of 88 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	A	1921	G
8	A	2405	G
8	A	2015	A
8	A	2192	U
8	A	2474	U

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

45 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	$\# Z  > 2$
8	PSU	A	2504	8	18,21,22	1.10	3 (16%)	22,30,33	2.17	5 (22%)
8	PSU	A	955	8	18,21,22	1.05	1 (5%)	22,30,33	1.88	5 (22%)
8	2MG	A	2445	8	18,26,27	2.45	7 (38%)	16,38,41	1.59	4 (25%)
56	G7M	w	46	56	20,26,27	2.31	7 (35%)	17,39,42	1.26	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	2MG	a	1207	34	18,26,27	2.40	7 (38%)	16,38,41	1.44	3 (18%)
8	6MZ	A	2030	8	18,25,26	4.06	8 (44%)	16,36,39	2.60	4 (25%)
8	PSU	A	2604	8	18,21,22	1.06	2 (11%)	22,30,33	2.03	5 (22%)
55	PSU	v	55	55	18,21,22	1.11	1 (5%)	22,30,33	1.80	4 (18%)
34	2MG	a	966	34	18,26,27	2.57	7 (38%)	16,38,41	1.49	3 (18%)
8	OMC	A	2498	8	19,22,23	0.95	1 (5%)	26,31,34	1.49	2 (7%)
8	PSU	A	1911	8	18,21,22	1.07	2 (11%)	22,30,33	2.15	6 (27%)
8	2MA	A	2503	8	17,25,26	2.19	5 (29%)	17,37,40	1.36	3 (17%)
56	PSU	w	39	56	18,21,22	1.10	1 (5%)	22,30,33	1.74	3 (13%)
8	1MG	A	745	8	18,26,27	2.57	4 (22%)	19,39,42	1.42	3 (15%)
55	5MU	v	54	55	19,22,23	4.80	7 (36%)	28,32,35	3.54	11 (39%)
34	UR3	a	1498	34	19,22,23	2.48	6 (31%)	26,32,35	1.27	1 (3%)
8	2MG	A	1835	8	18,26,27	2.51	7 (38%)	16,38,41	1.49	3 (18%)
34	5MC	a	967	34	18,22,23	3.66	7 (38%)	26,32,35	1.18	3 (11%)
55	H2U	v	20	55	18,21,22	2.95	5 (27%)	21,30,33	2.17	5 (23%)
8	PSU	A	2580	8	18,21,22	1.32	2 (11%)	22,30,33	2.23	7 (31%)
56	PSU	w	55	56	18,21,22	1.43	3 (16%)	22,30,33	1.89	7 (31%)
8	5MC	A	747	8	18,22,23	3.51	7 (38%)	26,32,35	1.50	2 (7%)
8	PSU	A	2605	8	18,21,22	1.00	1 (5%)	22,30,33	2.05	4 (18%)
34	2MG	a	1516	34	18,26,27	2.46	7 (38%)	16,38,41	1.32	3 (18%)
56	5MU	w	54	56	19,22,23	1.45	6 (31%)	28,32,35	2.26	7 (25%)
8	PSU	A	746	8	18,21,22	1.09	1 (5%)	22,30,33	1.78	4 (18%)
56	4SU	w	8	56	18,21,22	3.57	8 (44%)	26,30,33	2.31	4 (15%)
34	4OC	a	1402	34	20,23,24	2.94	8 (40%)	26,32,35	1.24	5 (19%)
34	MA6	a	1519	34	18,26,27	1.05	1 (5%)	19,38,41	2.66	2 (10%)
56	MIA	w	37	56	24,31,32	2.44	4 (16%)	26,44,47	3.10	9 (34%)
8	PSU	A	1917	8	18,21,22	0.97	1 (5%)	22,30,33	1.88	4 (18%)
34	MA6	a	1518	34	18,26,27	1.11	1 (5%)	19,38,41	1.90	2 (10%)
34	G7M	a	527	34	20,26,27	2.29	7 (35%)	17,39,42	1.37	2 (11%)
34	PSU	a	516	34	18,21,22	1.07	1 (5%)	22,30,33	1.62	3 (13%)
34	5MC	a	1407	34	18,22,23	3.44	7 (38%)	26,32,35	1.18	3 (11%)
8	5MU	A	1939	8	19,22,23	4.76	7 (36%)	28,32,35	3.71	13 (46%)
55	4SU	v	8	55	18,21,22	3.56	7 (38%)	26,30,33	2.08	6 (23%)
8	6MZ	A	1618	8	18,25,26	4.09	8 (44%)	16,36,39	2.40	6 (37%)
8	G7M	A	2069	8	20,26,27	2.25	8 (40%)	17,39,42	1.26	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	PSU	w	32	56	18,21,22	1.06	1 (5%)	22,30,33	1.65	5 (22%)
57	FME	y	101	57	8,9,10	0.90	0	7,9,11	1.14	0
8	PSU	A	2457	8	18,21,22	1.05	2 (11%)	22,30,33	1.99	5 (22%)
8	OMU	A	2552	8	19,22,23	2.90	7 (36%)	26,31,34	1.95	6 (23%)
8	OMG	A	2251	8,56	18,26,27	2.53	8 (44%)	19,38,41	1.60	4 (21%)
8	5MC	A	1962	8	18,22,23	3.49	7 (38%)	26,32,35	1.34	4 (15%)

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
8	PSU	A	2504	8	-	0/7/25/26	0/2/2/2
8	PSU	A	955	8	-	0/7/25/26	0/2/2/2
8	2MG	A	2445	8	-	2/5/27/28	0/3/3/3
56	G7M	w	46	56	-	3/3/25/26	0/3/3/3
34	2MG	a	1207	34	-	0/5/27/28	0/3/3/3
8	6MZ	A	2030	8	-	2/5/27/28	0/3/3/3
8	PSU	A	2604	8	-	0/7/25/26	0/2/2/2
55	PSU	v	55	55	-	3/7/25/26	0/2/2/2
34	2MG	a	966	34	-	1/5/27/28	0/3/3/3
8	OMC	A	2498	8	-	3/9/27/28	0/2/2/2
8	PSU	A	1911	8	-	1/7/25/26	0/2/2/2
8	2MA	A	2503	8	-	3/3/25/26	0/3/3/3
56	PSU	w	39	56	-	5/7/25/26	0/2/2/2
8	1MG	A	745	8	-	0/3/25/26	0/3/3/3
55	5MU	v	54	55	-	2/7/25/26	0/2/2/2
34	UR3	a	1498	34	-	4/7/25/26	0/2/2/2
8	2MG	A	1835	8	-	2/5/27/28	0/3/3/3
34	5MC	a	967	34	-	1/7/25/26	0/2/2/2
55	H2U	v	20	55	-	5/7/38/39	0/2/2/2
8	PSU	A	2580	8	-	2/7/25/26	0/2/2/2
56	PSU	w	55	56	-	1/7/25/26	0/2/2/2
8	5MC	A	747	8	-	2/7/25/26	0/2/2/2
8	PSU	A	2605	8	-	0/7/25/26	0/2/2/2
34	2MG	a	1516	34	-	0/5/27/28	0/3/3/3
56	5MU	w	54	56	-	3/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PSU	A	746	8	-	1/7/25/26	0/2/2/2
56	4SU	w	8	56	-	2/7/25/26	0/2/2/2
34	4OC	a	1402	34	-	3/9/29/30	0/2/2/2
34	MA6	a	1519	34	-	4/7/29/30	0/3/3/3
56	MIA	w	37	56	-	3/11/33/34	0/3/3/3
8	PSU	A	1917	8	-	0/7/25/26	0/2/2/2
34	MA6	a	1518	34	-	3/7/29/30	0/3/3/3
34	G7M	a	527	34	-	1/3/25/26	0/3/3/3
34	PSU	a	516	34	-	1/7/25/26	0/2/2/2
34	5MC	a	1407	34	-	0/7/25/26	0/2/2/2
8	5MU	A	1939	8	-	1/7/25/26	0/2/2/2
55	4SU	v	8	55	-	0/7/25/26	0/2/2/2
8	6MZ	A	1618	8	-	5/5/27/28	0/3/3/3
8	G7M	A	2069	8	-	2/3/25/26	0/3/3/3
56	PSU	w	32	56	-	2/7/25/26	0/2/2/2
57	FME	y	101	57	-	6/7/9/11	-
8	PSU	A	2457	8	-	0/7/25/26	0/2/2/2
8	OMU	A	2552	8	-	6/9/27/28	0/2/2/2
8	OMG	A	2251	8,56	-	3/5/27/28	0/3/3/3
8	5MC	A	1962	8	-	4/7/25/26	0/2/2/2

The worst 5 of 208 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	v	54	5MU	C2-N1	11.24	1.56	1.38
8	A	1939	5MU	C2-N1	11.04	1.56	1.38
55	v	54	5MU	C6-N1	10.29	1.55	1.38
8	A	1939	5MU	C6-N1	10.01	1.55	1.38
55	v	54	5MU	C4-C5	9.91	1.61	1.44

The worst 5 of 192 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1939	5MU	C5-C4-N3	11.77	125.36	115.31
55	v	54	5MU	C5-C4-N3	11.06	124.75	115.31
8	A	1939	5MU	C5-C6-N1	-10.15	112.89	123.34
34	a	1519	MA6	N1-C6-N6	-9.77	106.78	117.06
55	v	54	5MU	C5-C6-N1	-9.01	114.07	123.34

There are no chirality outliers.

5 of 92 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	v	20	H2U	O4'-C1'-N1-C6
55	v	20	H2U	C2'-C1'-N1-C2
55	v	20	H2U	C2'-C1'-N1-C6
8	A	747	5MC	C3'-C4'-C5'-O5'
8	A	1618	6MZ	C5-C6-N6-C9

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\# Z  > 2$
60	AM2	a	2001	-	40,40,40	1.66	10 (25%)	53,60,60	1.71	11 (20%)

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
60	AM2	a	2001	-	-	8/12/84/84	0/4/4/4

The worst 5 of 10 bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	a	2001	AM2	OA4-CA1	4.04	1.52	1.41
60	a	2001	AM2	CB3-CB4	-3.69	1.48	1.53
60	a	2001	AM2	OA5-CA8	3.20	1.50	1.41
60	a	2001	AM2	OA5-CA4	3.08	1.51	1.44
60	a	2001	AM2	OB1-CB1	2.89	1.49	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	a	2001	AM2	CA1-OA1-CC1	-5.36	104.71	117.96
60	a	2001	AM2	CA8-CA7-NA7	-3.99	103.86	111.00
60	a	2001	AM2	CB1-OA8-CA8	-3.84	107.56	114.42
60	a	2001	AM2	CA9-NA7-CA7	-3.31	109.57	114.38
60	a	2001	AM2	OA1-CA1-CA2	3.21	113.61	108.23

There are no chirality outliers.

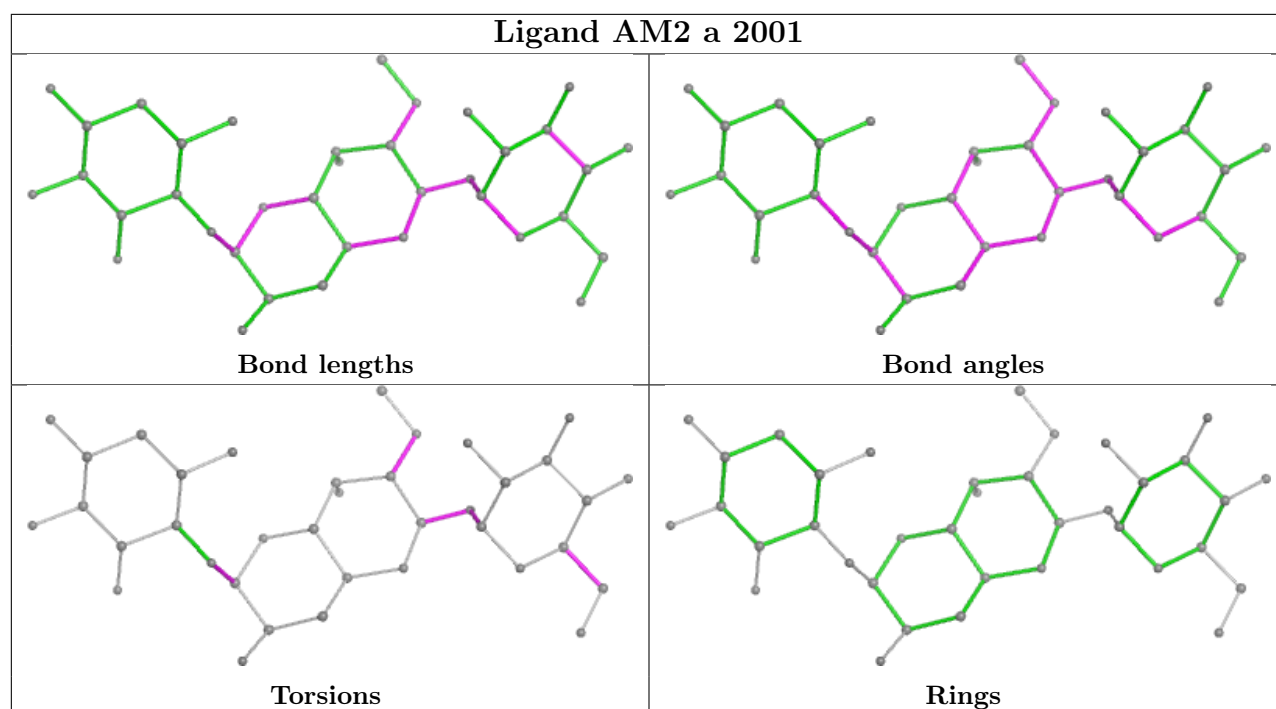
5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	a	2001	AM2	CA7-CA8-OA8-CB1
60	a	2001	AM2	OA5-CA8-OA8-CB1
60	a	2001	AM2	OB1-CB5-CB6-OB6
60	a	2001	AM2	CB4-CB5-CB6-OB6
60	a	2001	AM2	OB1-CB1-OA8-CA8

There are no ring outliers.

No monomer is involved in short contacts.

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.



## 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.

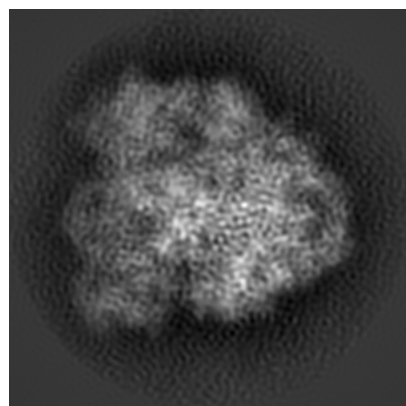
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13459. These allow visual inspection of the internal detail of the map and identification of artifacts.

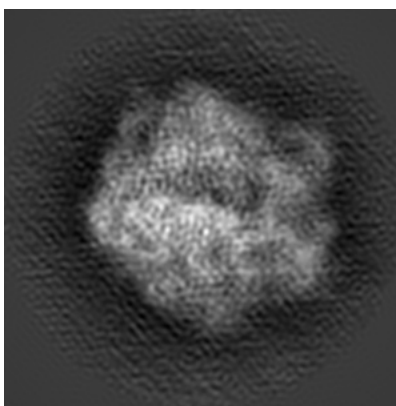
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

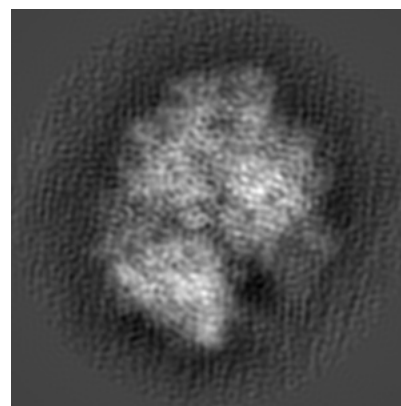
#### 6.1.1 Primary map



X

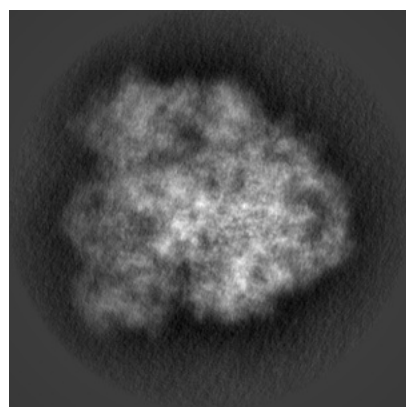


Y

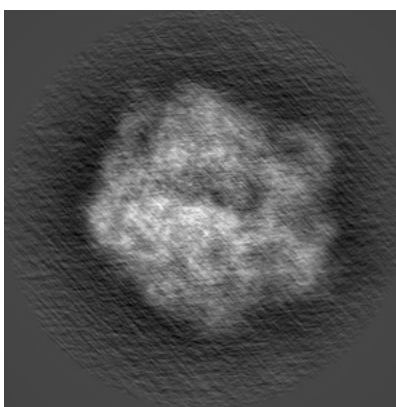


Z

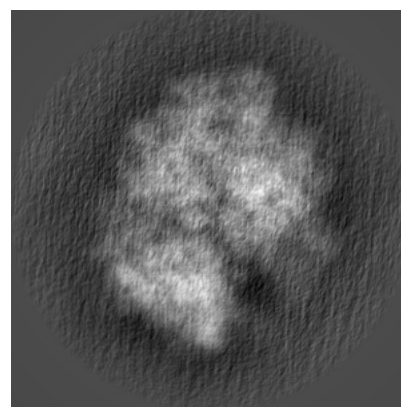
#### 6.1.2 Raw map



X



Y

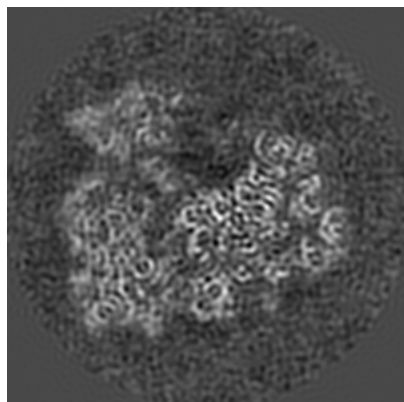


Z

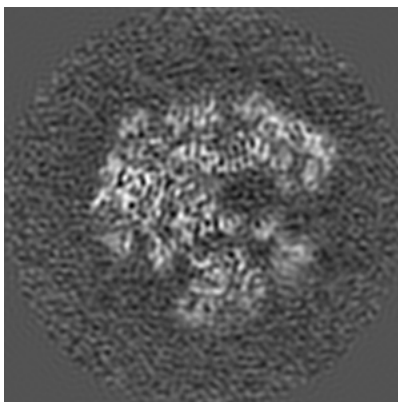
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

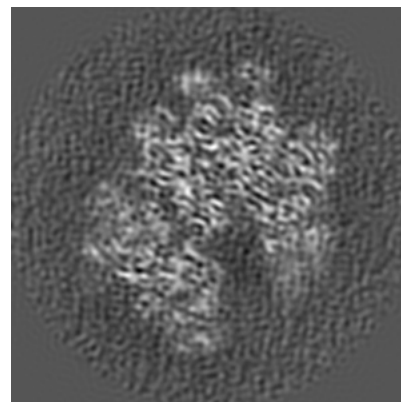
### 6.2.1 Primary map



X Index: 144

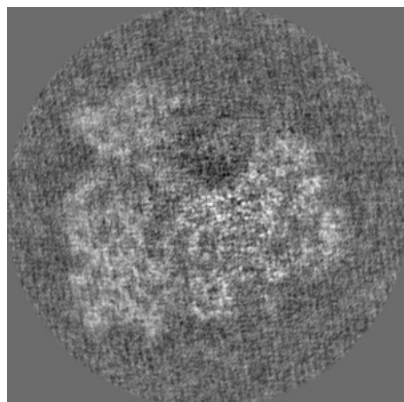


Y Index: 144

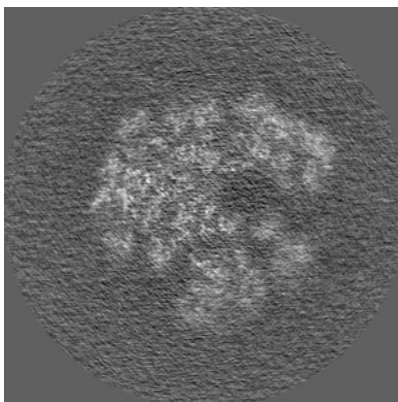


Z Index: 144

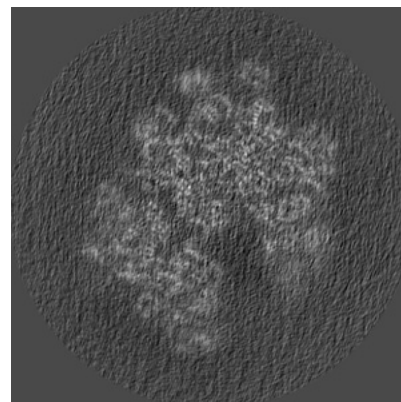
### 6.2.2 Raw map



X Index: 144



Y Index: 144

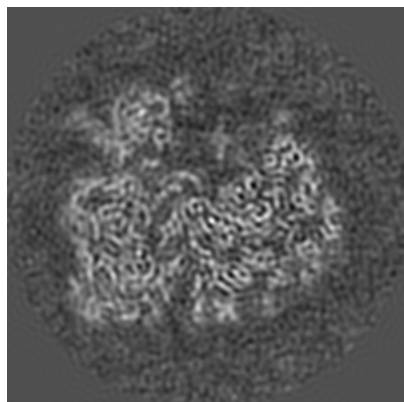


Z Index: 144

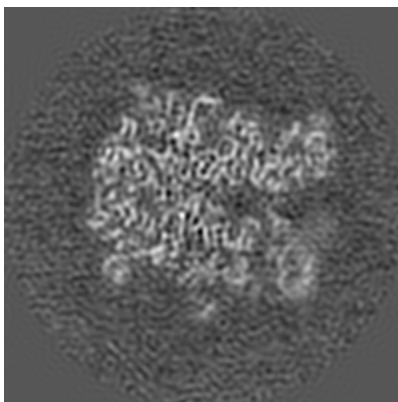
The images above show central slices of the map in three orthogonal directions.

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

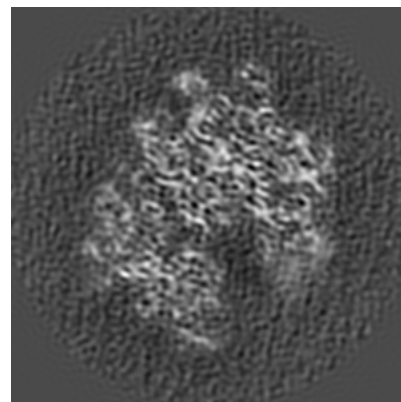
### 6.3.1 Primary map



X Index: 139

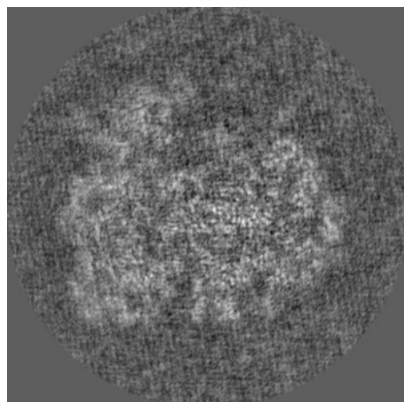


Y Index: 158

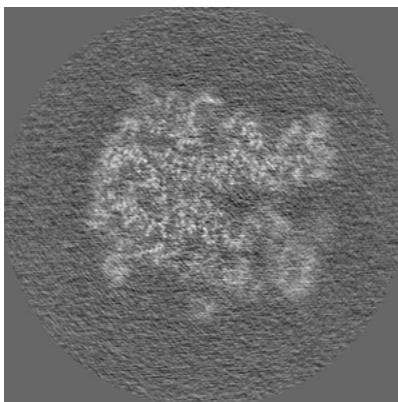


Z Index: 146

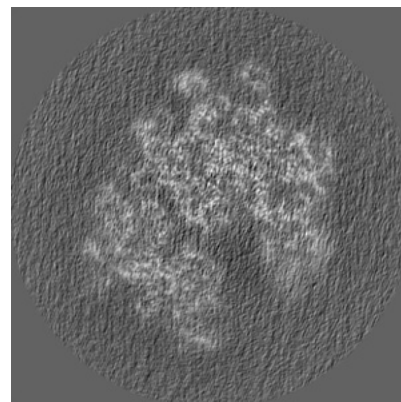
### 6.3.2 Raw map



X Index: 138



Y Index: 157



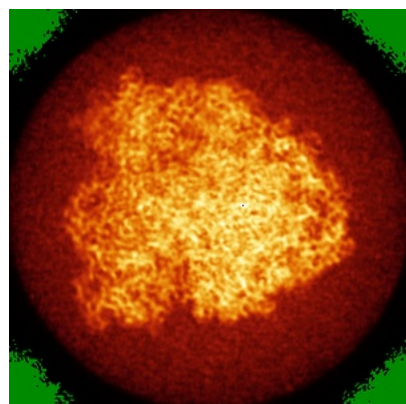
Z Index: 146

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

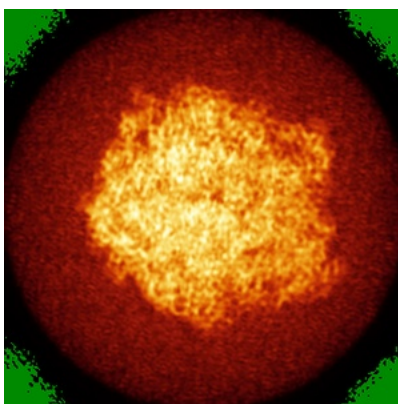


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

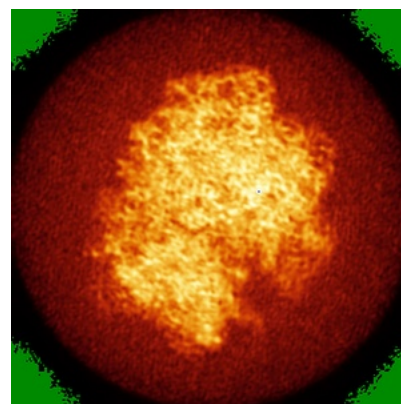
### 6.4.1 Primary map



X

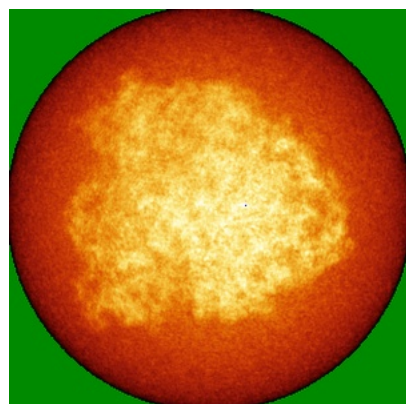


Y

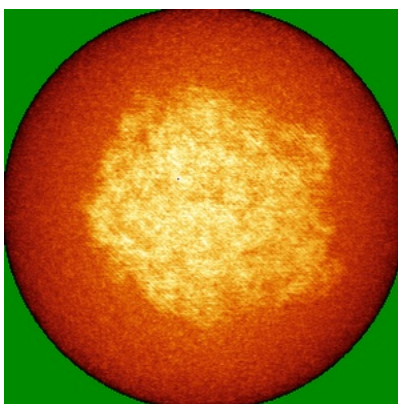


Z

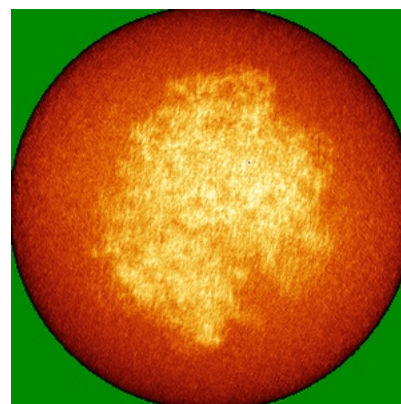
### 6.4.2 Raw map



X



Y

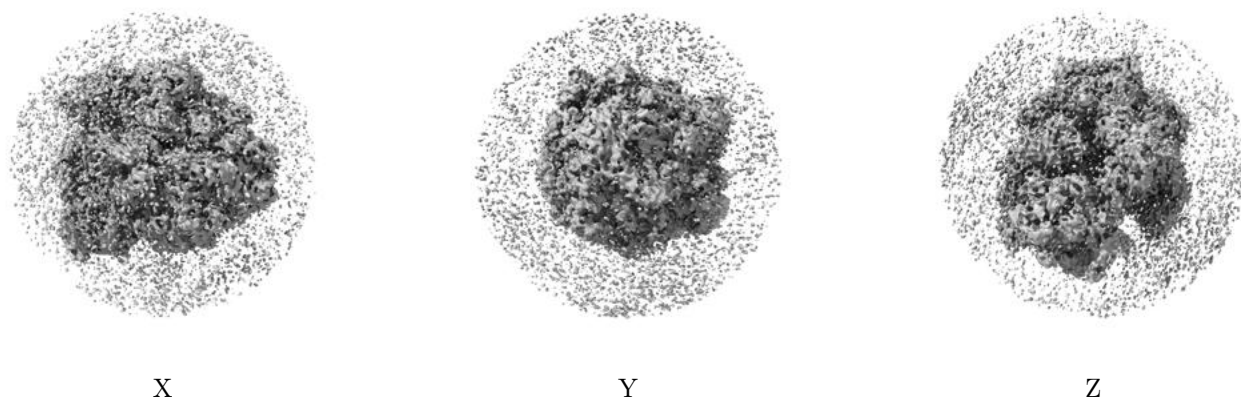


Z

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.

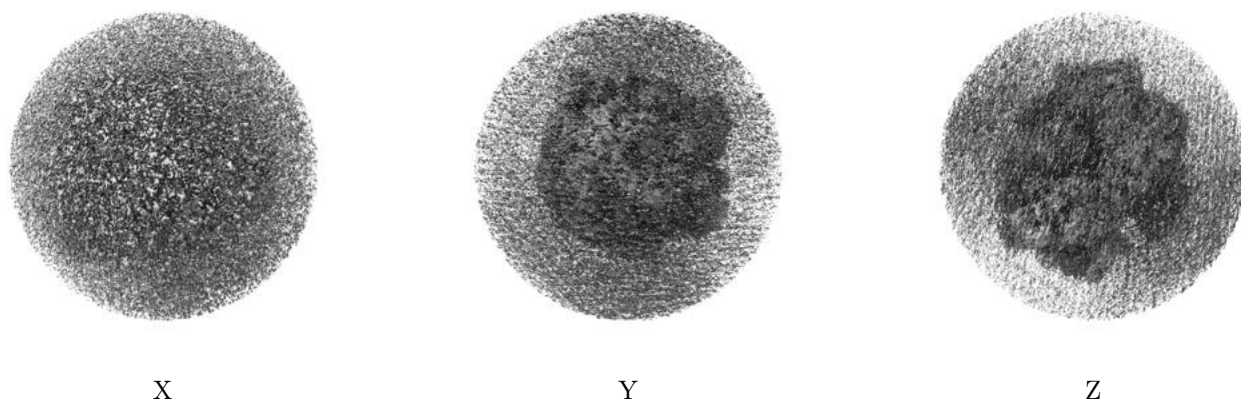
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.5. 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.

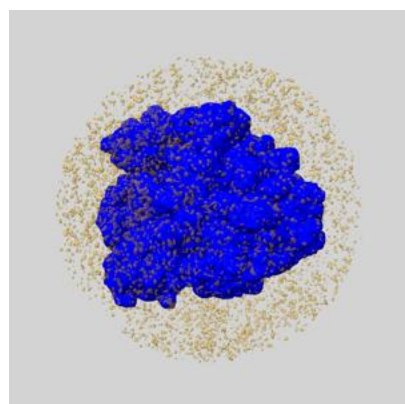
## 6.6 Mask visualisation [i](#)

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

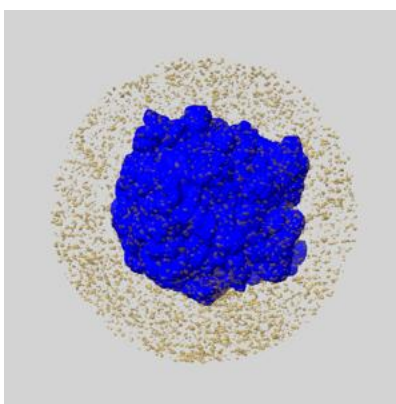
A mask typically either:

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

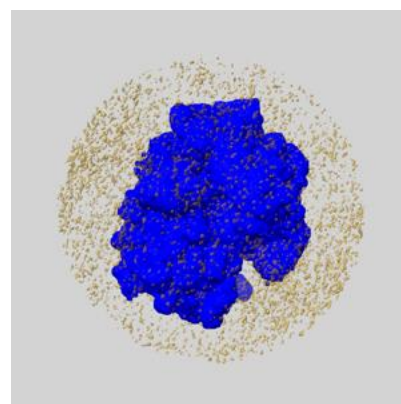
### 6.6.1 emd\_13459\_msk\_1.map [i](#)



X



Y



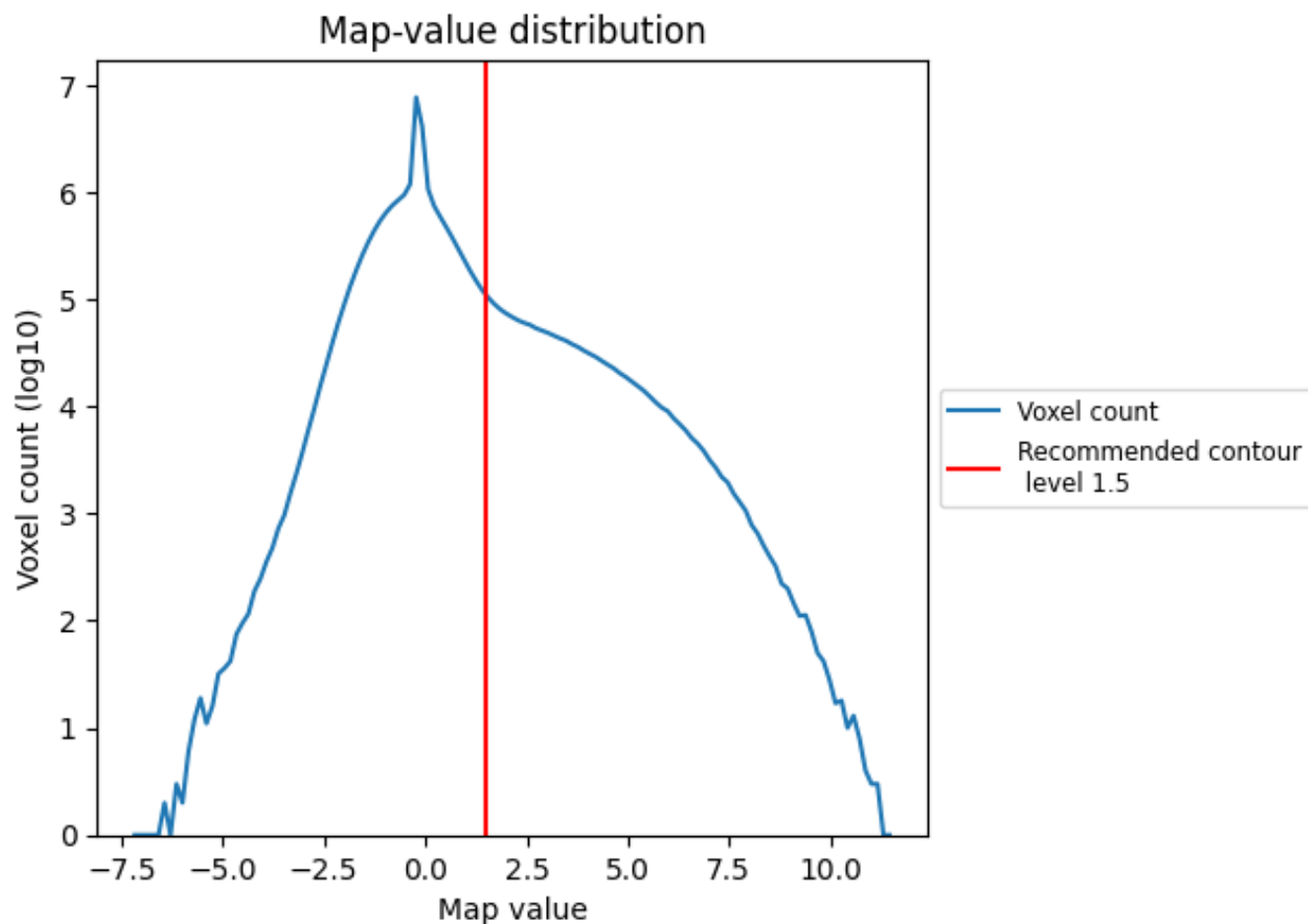
Z



## 7 Map analysis [i](#)

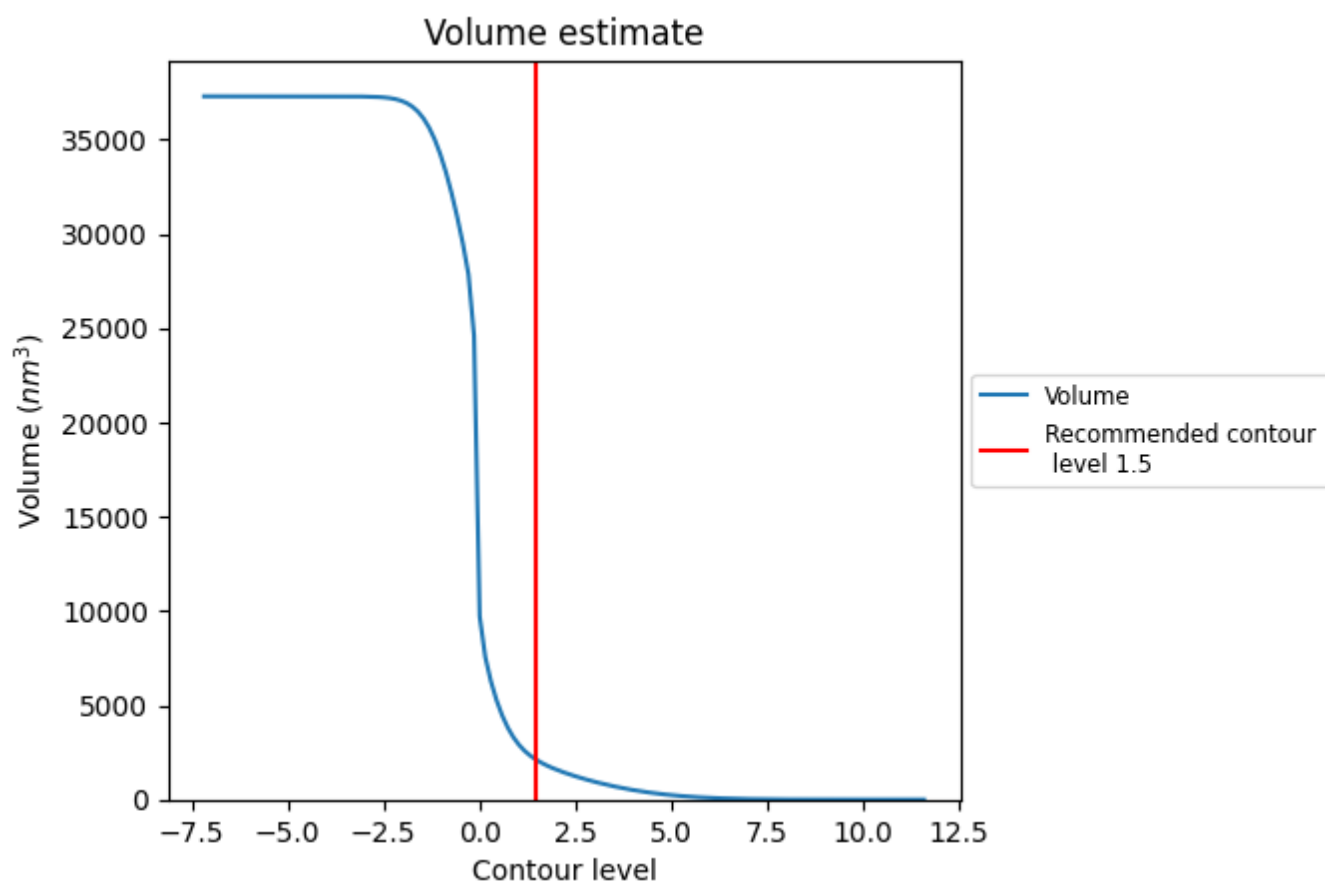
This section contains the results of statistical analysis of the map.

### 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.

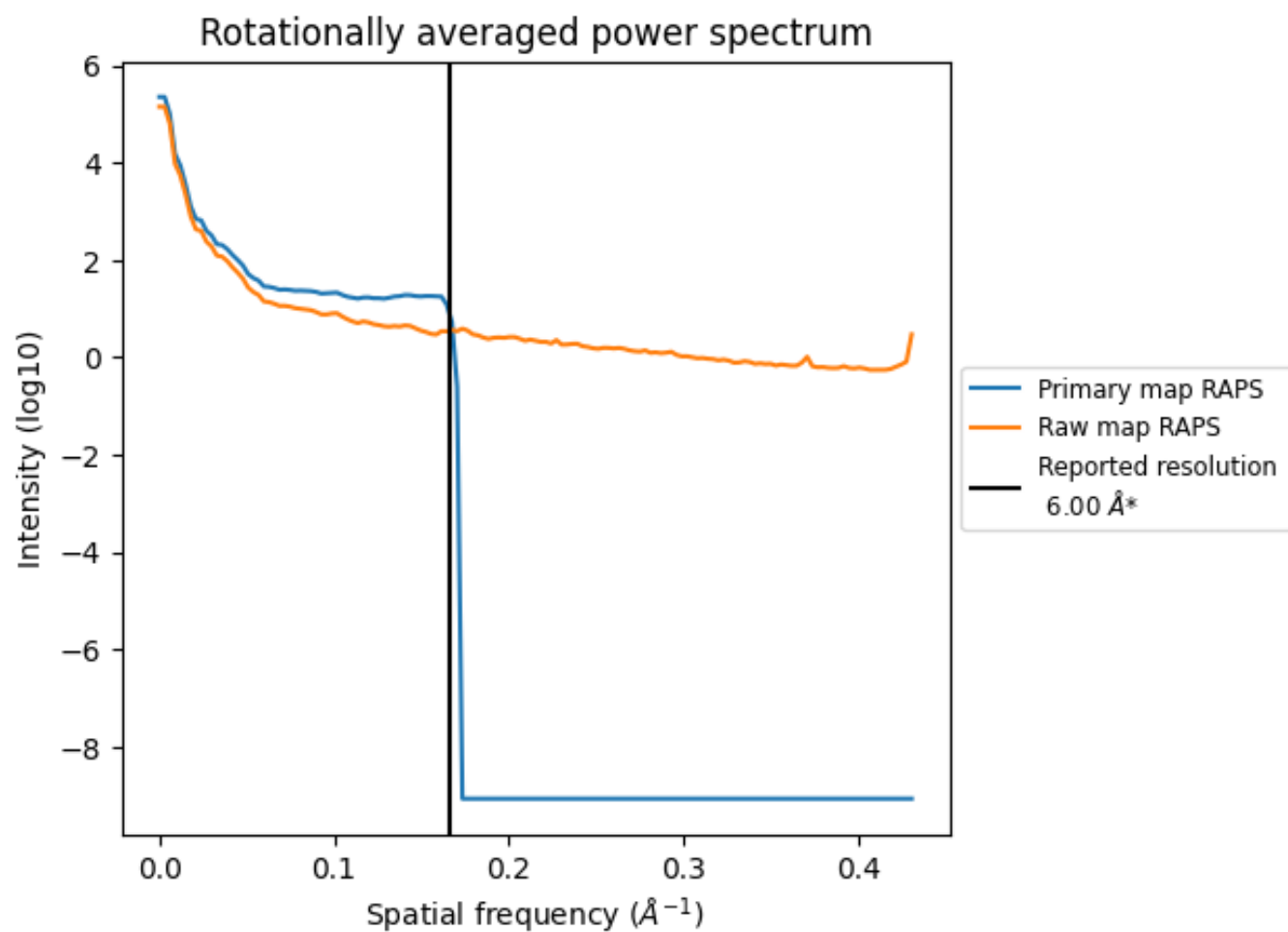
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2098 nm<sup>3</sup>; this corresponds to an approximate mass of 1895 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 ⓘ

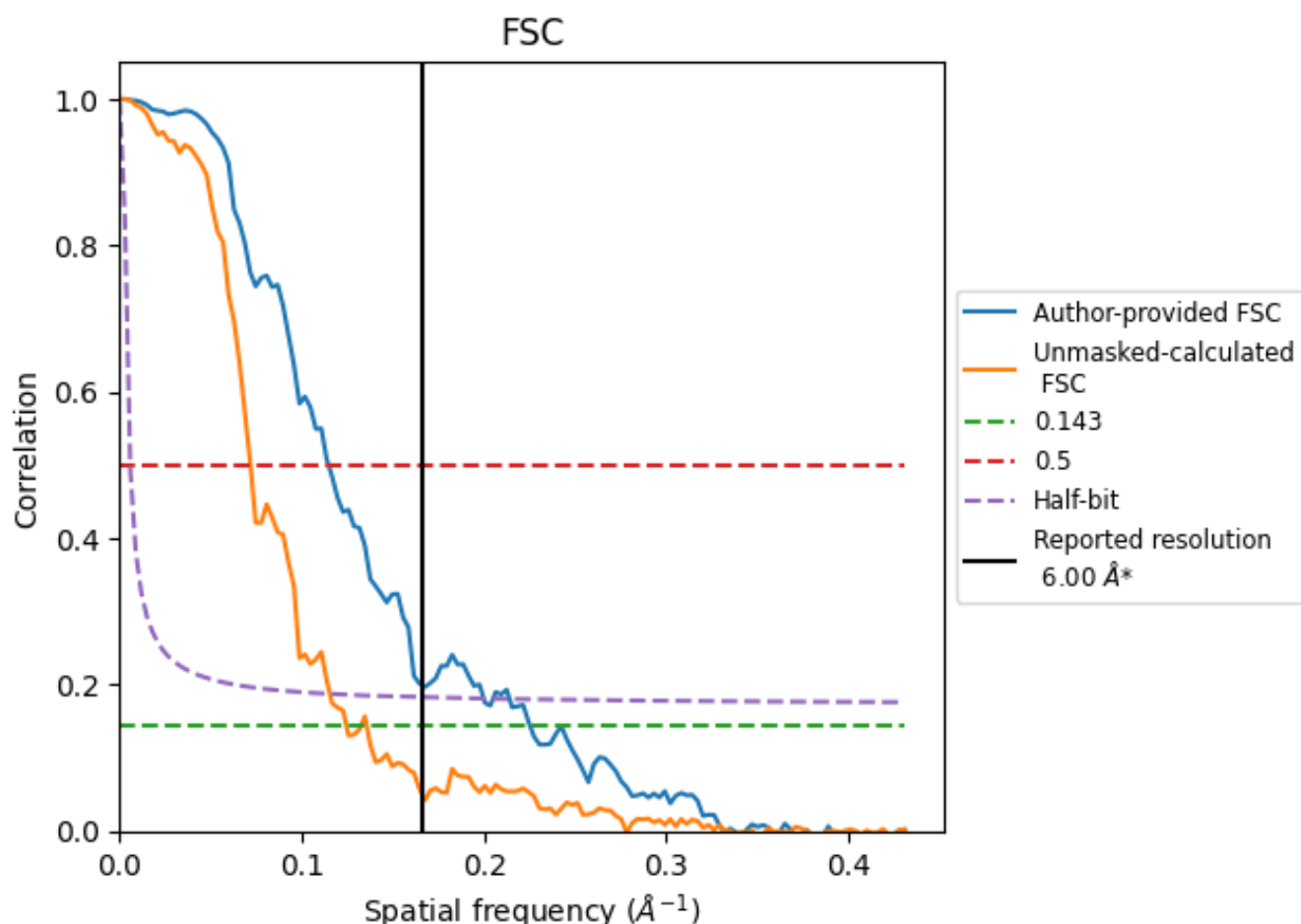


\*Reported resolution corresponds to spatial frequency of 0.167  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.167  $\text{\AA}^{-1}$

## 8.2 Resolution estimates

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.00	-	-
Author-provided FSC curve	4.44	8.72	5.00
Unmasked-calculated*	8.03	13.91	8.65

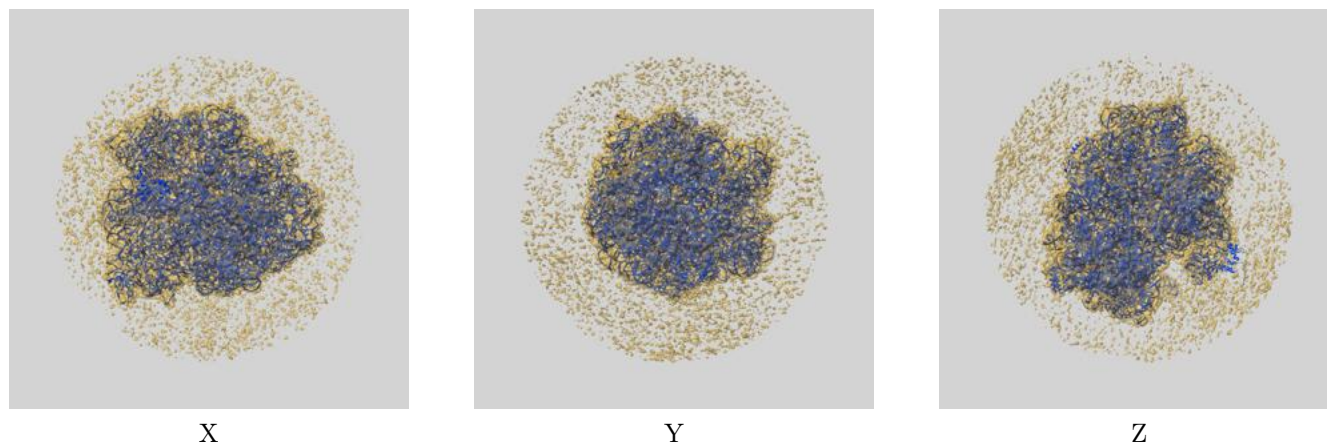
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.44 differs from the reported value 6.0 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.03 differs from the reported value 6.0 by more than 10 %

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

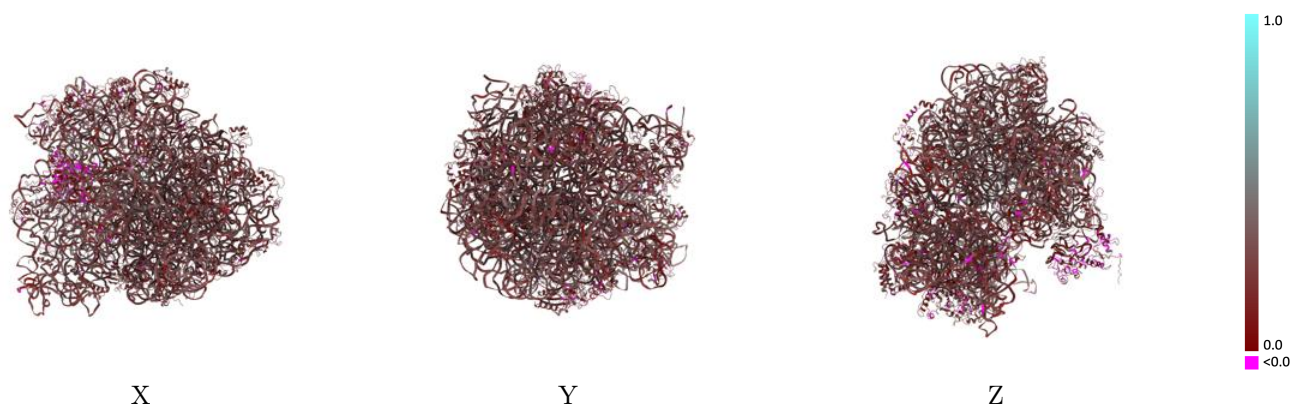
This section contains information regarding the fit between EMDB map EMD-13459 and PDB model 7PJT. Per-residue inclusion information can be found in section [3](#) on page [15](#).

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



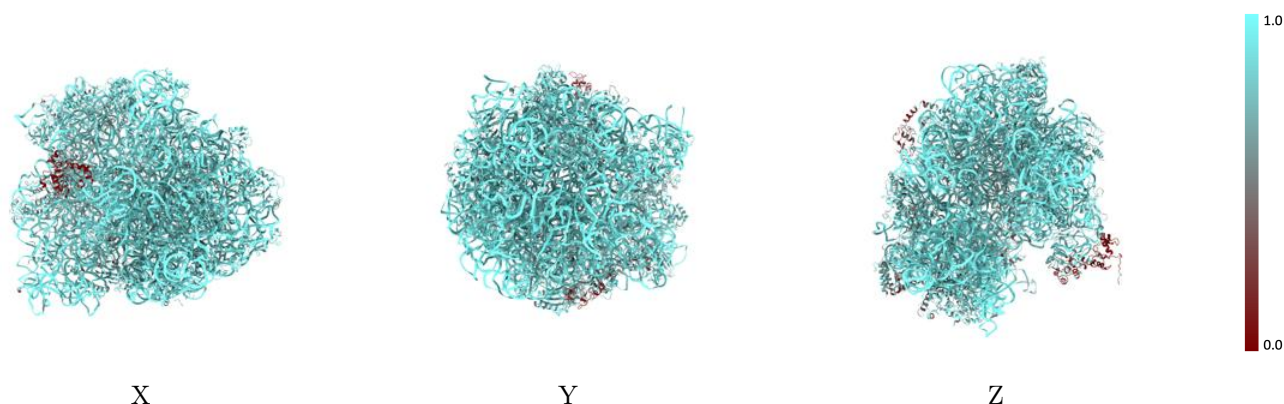
The images above show the 3D surface view of the map at the recommended contour level 1.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



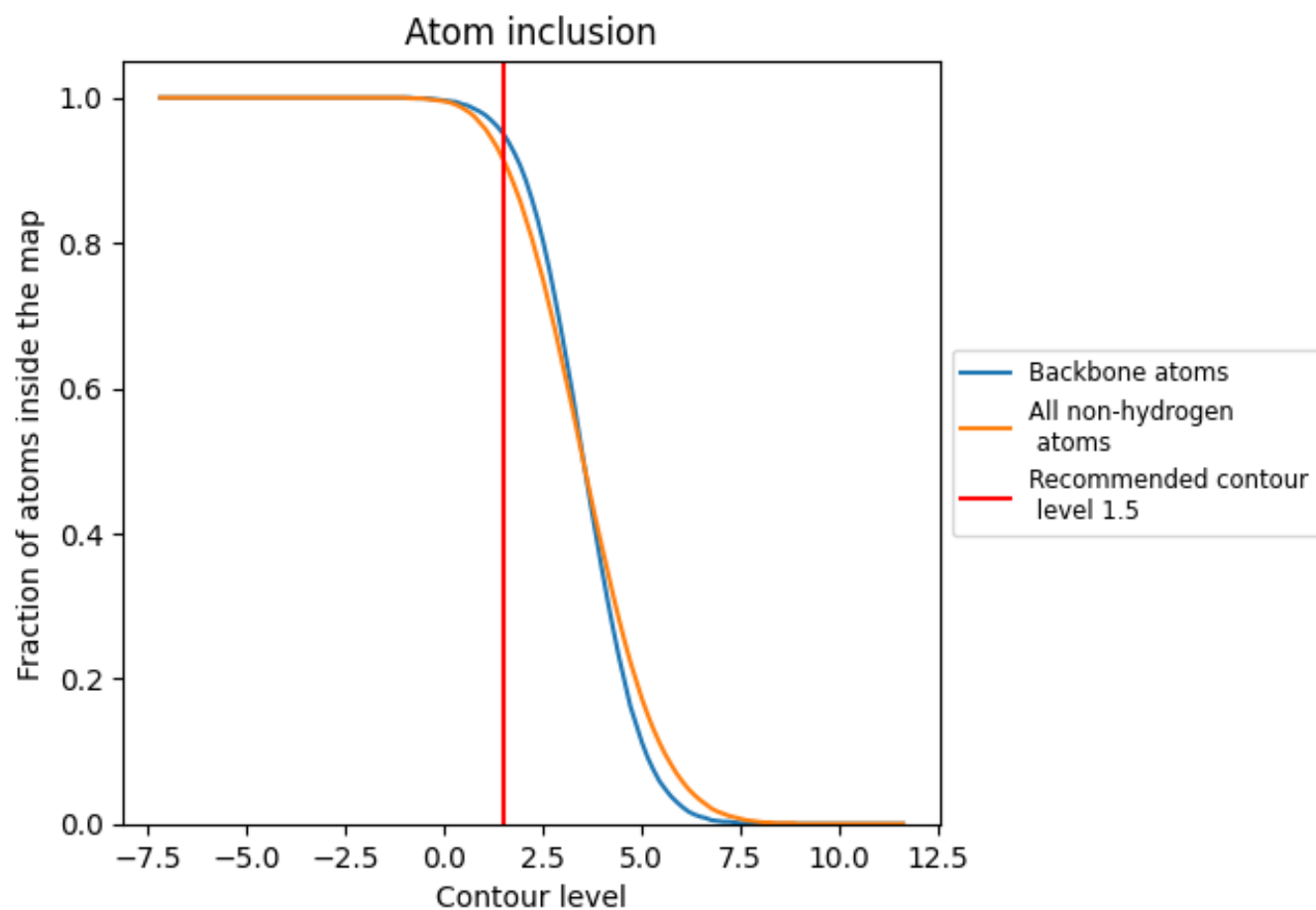
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.5).

## 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 (1.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9140	 0.2680
0	 0.8740	 0.2860
1	 0.8000	 0.2510
2	 0.8170	 0.2680
3	 0.7980	 0.2530
4	 0.8840	 0.2660
5	 0.1980	 0.1440
6	 0.7810	 0.2320
A	 0.9690	 0.2830
B	 0.9860	 0.2740
C	 0.8060	 0.2680
D	 0.8400	 0.2660
E	 0.8160	 0.2690
F	 0.8410	 0.2300
G	 0.8920	 0.2470
H	 0.4410	 0.2090
I	 0.4360	 0.1290
J	 0.8560	 0.2750
K	 0.7630	 0.2690
L	 0.8400	 0.2730
M	 0.8390	 0.2830
N	 0.8670	 0.2420
O	 0.9190	 0.2380
P	 0.8020	 0.2660
Q	 0.8260	 0.2350
R	 0.8520	 0.2590
S	 0.8170	 0.2470
T	 0.8620	 0.2700
U	 0.8970	 0.2540
V	 0.8580	 0.2520
W	 0.8960	 0.2540
X	 0.8450	 0.2770
Y	 0.8590	 0.2100
Z	 0.8510	 0.2590
a	 0.9670	 0.2710



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Chain	Atom inclusion	Q-score
b	 0.6200	 0.2350
c	 0.8220	 0.2430
d	 0.8110	 0.2370
e	 0.7900	 0.2570
f	 0.8480	 0.2490
g	 0.6680	 0.2310
h	 0.8290	 0.2480
i	 0.8430	 0.2380
j	 0.7540	 0.2210
k	 0.8320	 0.2510
l	 0.8210	 0.2770
m	 0.7720	 0.2140
n	 0.8670	 0.2230
o	 0.8800	 0.2490
p	 0.8520	 0.2560
q	 0.8420	 0.2350
r	 0.8600	 0.2450
s	 0.8380	 0.2070
t	 0.8420	 0.2290
u	 0.8060	 0.2540
v	 0.9090	 0.2550
w	 0.8710	 0.2180
y	 0.8090	 0.2520
z	 0.8960	 0.2650