



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 11:52 AM UTC

PDB ID : 6WD9 / pdb_00006wd9
EMDB ID : EMD-21628
Title : Cryo-EM of elongating ribosome with EF-Tu*GTP elucidates tRNA proof-reading (Cognate Structure III-B)
Authors : Loveland, A.B.; Demo, G.; Korostelev, A.A.
Deposited on : 2020-03-31
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

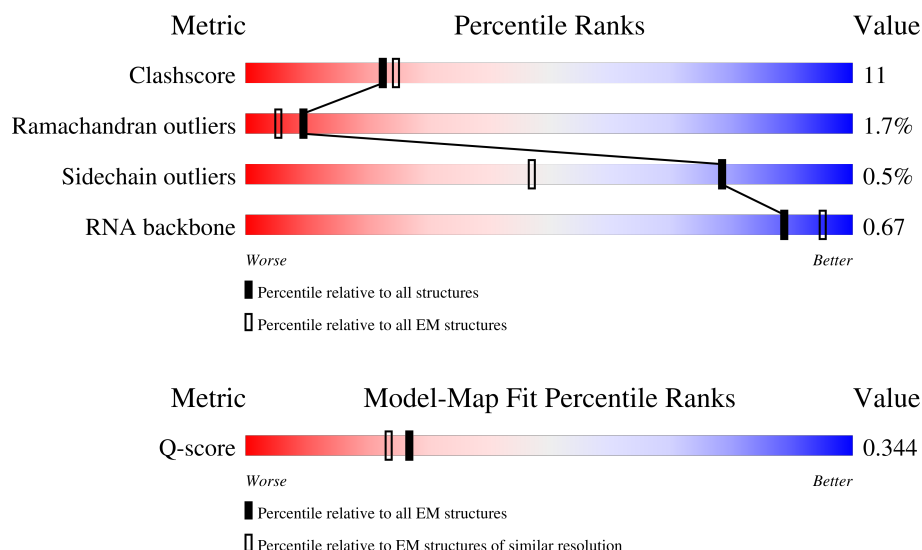
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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.



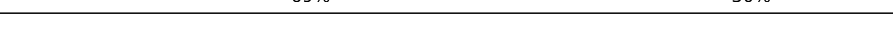
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11569 (3.20 - 4.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	b	271	
2	c	209	
3	d	201	

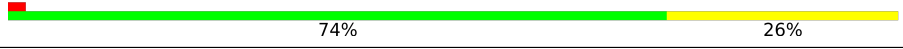
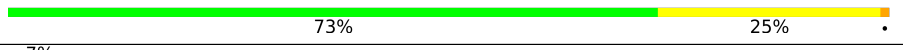
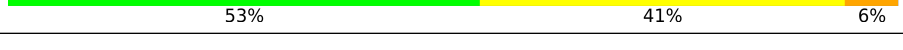
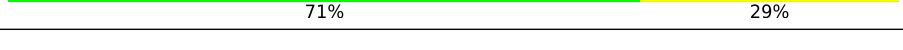
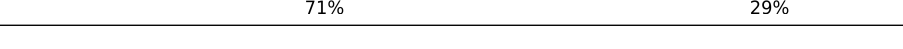
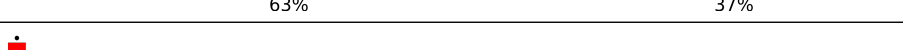
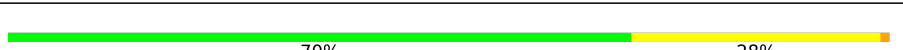
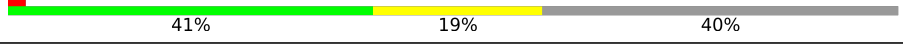
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Mol	Chain	Length	Quality of chain
4	e	177	 67% 33%
5	f	176	 69% 31%
6	g	149	 13% 66% 30%
7	h	131	 18% 49% 44% 6%
8	i	141	 13% 62% 35%
9	j	142	 70% 29%
10	k	122	 62% 33% 5%
11	l	143	 69% 26% 5%
12	m	136	 66% 33%
13	n	120	 66% 33%
14	o	116	 70% 29%
15	p	114	 68% 31%
16	q	117	 76% 21%
17	r	103	 69% 30%
18	s	110	 75% 23%
19	t	93	 77% 22%
20	u	102	 72% 26%
21	v	94	 68% 31%
22	w	75	 68% 31%
23	x	77	 66% 32%
24	y	63	 67% 32%
25	z	58	 78% 22%
26	B	56	 75% 21%
27	C	50	 74% 24%
28	D	46	 67% 30%

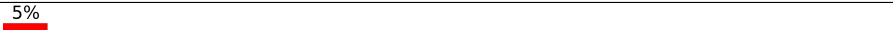
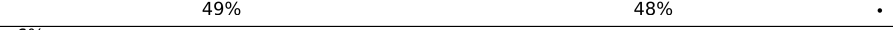
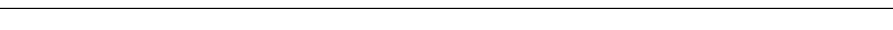
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Mol	Chain	Length	Quality of chain
29	E	64	
30	F	38	
31	G	225	
32	H	206	
33	I	205	
34	J	157	
35	K	100	
36	L	151	
37	M	129	
38	N	127	
39	O	98	
40	P	116	
41	Q	123	
42	R	114	
43	S	100	
44	T	88	
45	U	82	
46	V	80	
47	W	65	
48	X	79	
49	Y	85	
50	Z	65	
51	a	223	
52	3	1539	
53	1	2903	

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Mol	Chain	Length	Quality of chain
54	2	120	 55%38%7%
55	5	77	 53%43%•
55	6	77	 5%49%48%•
56	4	18	 6%50%50%
57	7	76	 49%46%5%
58	8	400	 56%29%•14%

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 152927 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 L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	b	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

- Molecule 2 is a protein called 50S ribosomal protein L3.

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

- Molecule 3 is a protein called 50S ribosomal protein L4.

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

- Molecule 4 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	e	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 5 is a protein called 50S ribosomal protein L6.

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

- Molecule 6 is a protein called 50S ribosomal protein L9.

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

- Molecule 7 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	h	131	Total	C	N	O	S	0	0
			989	625	175	184	5		

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	i	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 9 is a protein called 50S ribosomal protein L13.

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

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	k	122	Total	C	N	O	S	0	0
			939	587	180	166	6		

- Molecule 11 is a protein called 50S ribosomal protein L15.

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

- Molecule 12 is a protein called 50S ribosomal protein L16.

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

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	n	120	Total	C	N	O	S	0	0
			961	593	196	167	5		

- Molecule 14 is a protein called 50S ribosomal protein L18.

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

- Molecule 15 is a protein called 50S ribosomal protein L19.

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

- Molecule 16 is a protein called 50S ribosomal protein L20.

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

- Molecule 17 is a protein called 50S ribosomal protein L21.

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

- Molecule 18 is a protein called 50S ribosomal protein L22.

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

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	t	93	Total	C	N	O	S	0
			739	466	139	132	2	0

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	u	102	Total	C	N	O		0
			780	492	146	142		0

- Molecule 21 is a protein called 50S ribosomal protein L25.

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

- Molecule 22 is a protein called 50S ribosomal protein L27.

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

- Molecule 23 is a protein called 50S ribosomal protein L28.

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

- Molecule 24 is a protein called 50S ribosomal protein L29.

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

- Molecule 25 is a protein called 50S ribosomal protein L30.

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

- Molecule 26 is a protein called 50S ribosomal protein L32.

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

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	C	50	Total	C	N	O	0	0
			410	263	75	72		

- Molecule 28 is a protein called 50S ribosomal protein L34.

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

- Molecule 29 is a protein called 50S ribosomal protein L35.

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

- Molecule 30 is a protein called 50S ribosomal protein L36.

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

- Molecule 31 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	G	225	Total	C	N	O	S	0	0
			1757	1111	315	323	8		

- Molecule 32 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	H	206	Total	C	N	O	S	0	0
			1625	1028	305	289	3		

- Molecule 33 is a protein called 30S ribosomal protein S4.

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

- Molecule 34 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	J	157	Total	C	N	O	S	0	0
			1157	719	218	214	6		

- Molecule 35 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	K	100	Total	C	N	O	S	0	0
			818	515	148	149	6		

- Molecule 36 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	L	151	Total	C	N	O	S	0	0
			1182	735	227	216	4		

- Molecule 37 is a protein called 30S ribosomal protein S8.

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

- Molecule 38 is a protein called 30S ribosomal protein S9.

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

- Molecule 39 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	O	98	Total	C	N	O	S	0	0
			787	493	150	143	1		

- Molecule 40 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	P	116	Total	C	N	O	S	0	0
			870	535	173	159	3		

- Molecule 41 is a protein called 30S ribosomal protein S12.

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

- Molecule 42 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	R	114	Total	C	N	O	S	0	0
			884	546	178	157	3		

- Molecule 43 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	S	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 44 is a protein called 30S ribosomal protein S15.

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

- Molecule 45 is a protein called 30S ribosomal protein S16.

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

- Molecule 46 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	V	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

- Molecule 47 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	W	65	Total	C	N	O	S	0	0
			536	339	100	96	1		

- Molecule 48 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	X	79	Total	C	N	O	S	0	0
			638	408	120	108	2		

- Molecule 49 is a protein called 30S ribosomal protein S20.

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

- Molecule 50 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Z	65	Total	C	N	O	S	0	0
			545	335	117	92	1		

- Molecule 51 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	a	134	Total	C	N	O	S	0	0
			1027	645	186	194	2		

- Molecule 52 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	3	1539	Total	C	N	O	P	0	0
			33012	14725	6052	10697	1538		

- Molecule 53 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	1	2903	Total	C	N	O	P	0	0
			62317	27801	11468	20146	2902		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	747	C	U	conflict	GB 1036415628

- Molecule 54 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	2	120	Total	C	N	O	P	0	0
			2568	1145	471	833	119		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	120	A	-	insertion	GB 1370526515

- Molecule 55 is a RNA chain called tRNA^fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	5	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		
55	6	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 56 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	4	18	Total	C	N	O	P	0	0
			388	175	76	120	17		

- Molecule 57 is a RNA chain called tRNA^{Phe}.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	7	76	Total	C	N	O	P	0	0
			1619	723	290	531	75		

- Molecule 58 is a protein called Elongation factor Tu.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	8	346	Total	C	N	O	S	0	0
			2677	1698	459	508	12		

There are 7 discrepancies between the modelled and reference sequences:

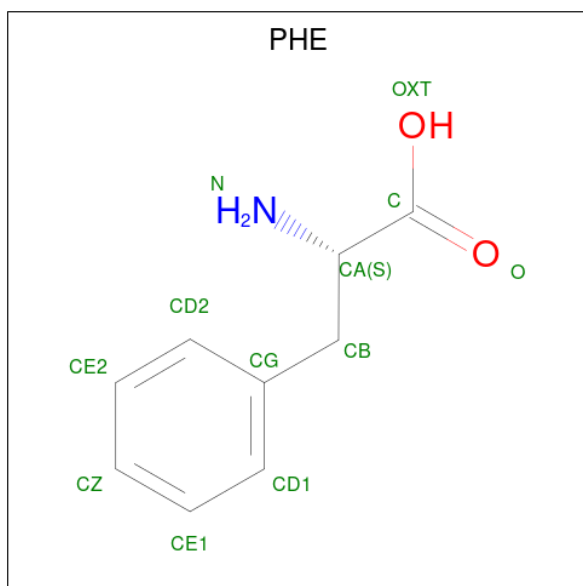
Chain	Residue	Modelled	Actual	Comment	Reference
8	395	SER	-	expression tag	UNP E2QFJ4
8	396	HIS	-	expression tag	UNP E2QFJ4
8	397	HIS	-	expression tag	UNP E2QFJ4
8	398	HIS	-	expression tag	UNP E2QFJ4
8	399	HIS	-	expression tag	UNP E2QFJ4
8	400	HIS	-	expression tag	UNP E2QFJ4
8	401	HIS	-	expression tag	UNP E2QFJ4

- Molecule 59 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: C₆H₁₁NO₃S).



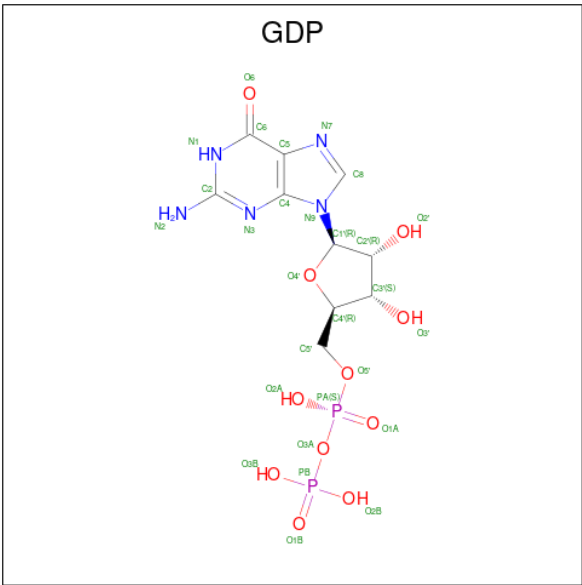
Mol	Chain	Residues	Atoms					AltConf
59	5	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 60 is PHENYLALANINE (CCD ID: PHE) (formula: $C_9H_{11}NO_2$).



Mol	Chain	Residues	Atoms				AltConf
60	7	1	Total	C	N	O	0
			11	9	1	1	

- Molecule 61 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

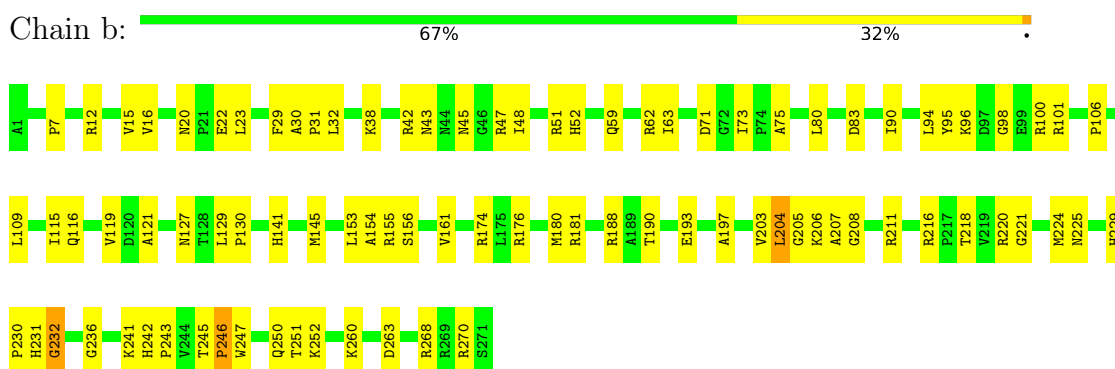


Mol	Chain	Residues	Atoms					AltConf
61	8	1	Total	C	N	O	P	0
			28	10	5	11	2	

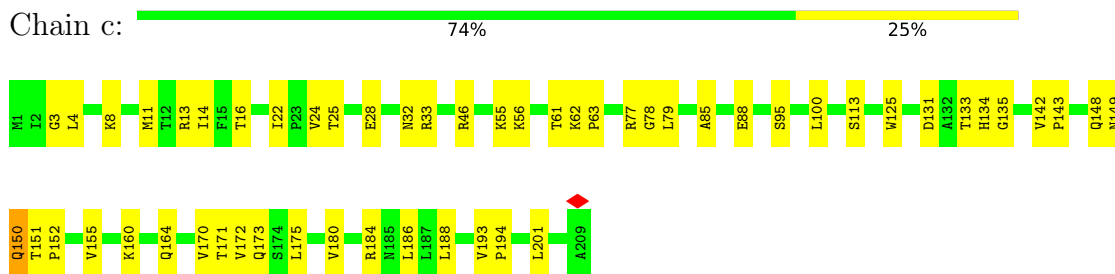
3 Residue-property plots

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.

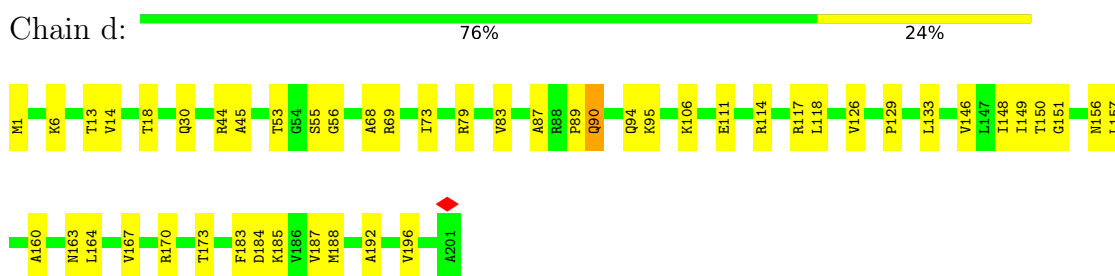
- Molecule 1: 50S ribosomal protein L2



- Molecule 2: 50S ribosomal protein L3

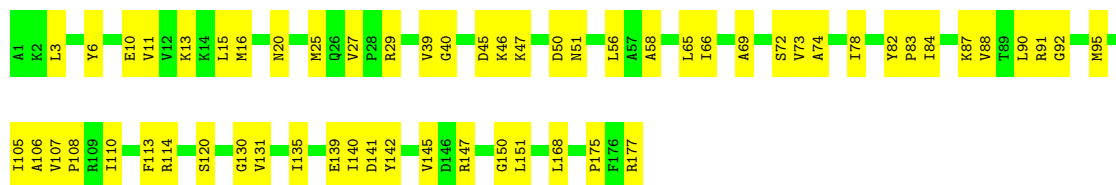


- Molecule 3: 50S ribosomal protein L4



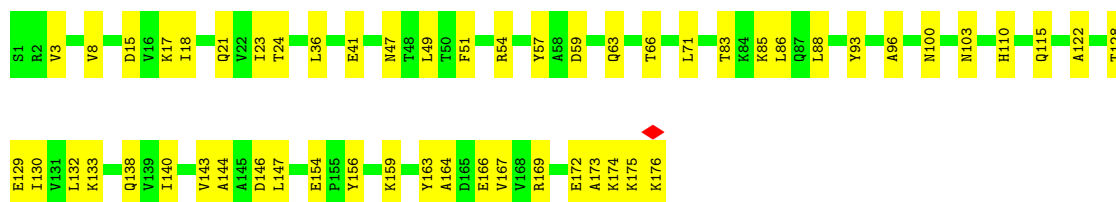
- Molecule 4: 50S ribosomal protein L5

Chain e:  67% 33%



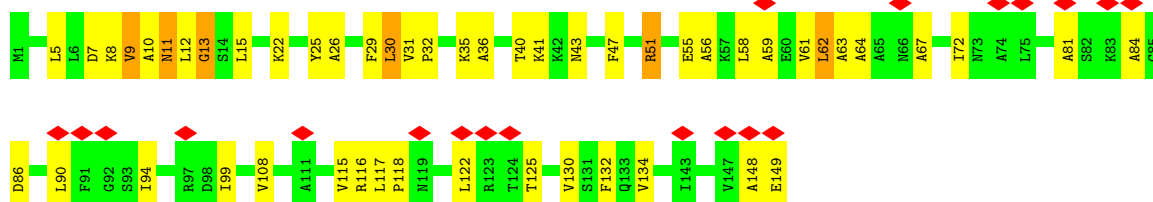
• Molecule 5: 50S ribosomal protein L6

Chain f:  69% 31%



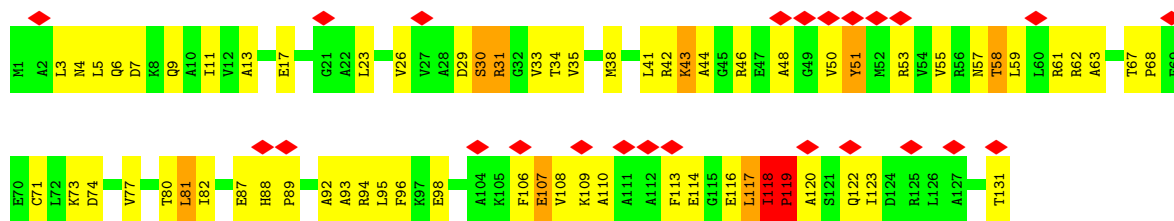
• Molecule 6: 50S ribosomal protein L9

Chain g:  13% 66% 30%



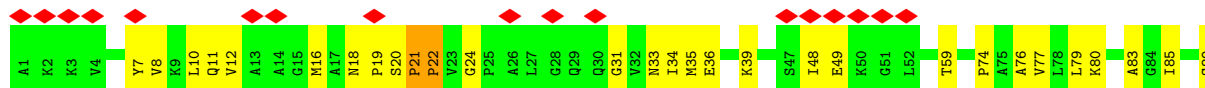
• Molecule 7: 50S ribosomal protein L10

Chain h:  18% 49% 44% 6%



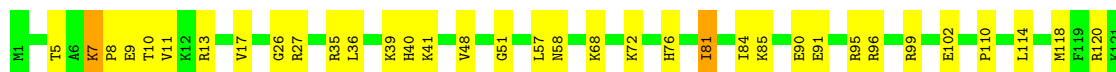
• Molecule 8: 50S ribosomal protein L11

Chain i:  13% 62% 35%





- Molecule 9: 50S ribosomal protein L13



- Molecule 10: 50S ribosomal protein L14



- Molecule 11: 50S ribosomal protein L15

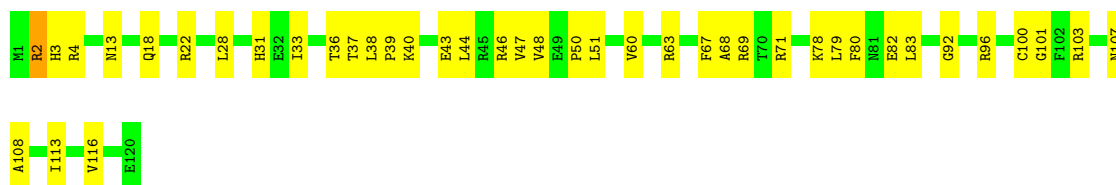


- Molecule 12: 50S ribosomal protein L16



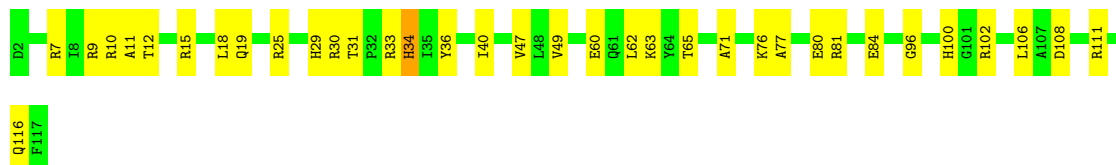
- Molecule 13: 50S ribosomal protein L17





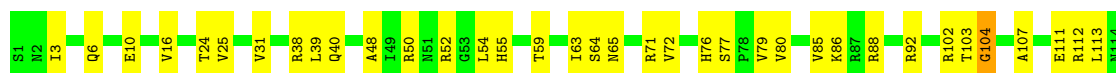
- Molecule 14: 50S ribosomal protein L18

Chain o: 70% 29%



- Molecule 15: 50S ribosomal protein L19

Chain p: 68% 31%



- Molecule 16: 50S ribosomal protein L20

Chain q: 76% 21%



- Molecule 17: 50S ribosomal protein L21

Chain r: 69% 30%



- Molecule 18: 50S ribosomal protein L22

Chain s: 75% 23%

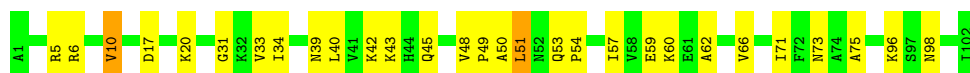


- Molecule 19: 50S ribosomal protein L23

Chain t: 77% 22%



- Molecule 20: 50S ribosomal protein L24



- Molecule 21: 50S ribosomal protein L25



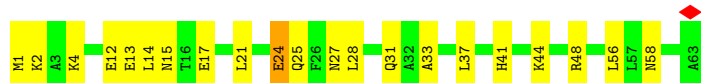
- Molecule 22: 50S ribosomal protein L27



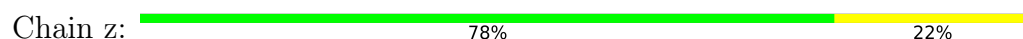
- Molecule 23: 50S ribosomal protein L28



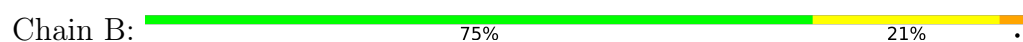
- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30

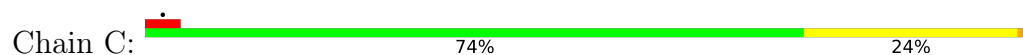


- Molecule 26: 50S ribosomal protein L32

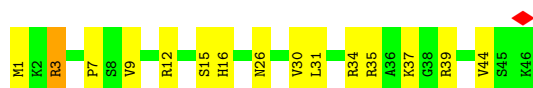




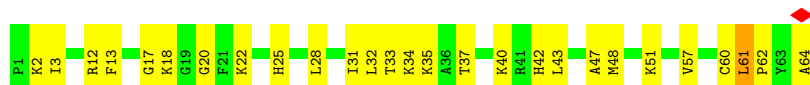
- Molecule 27: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L34



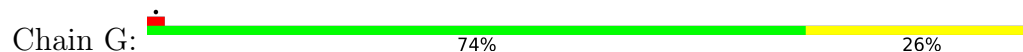
- Molecule 29: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L36

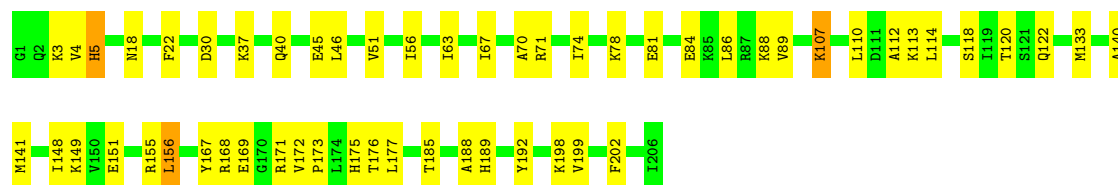


- Molecule 31: 30S ribosomal protein S2

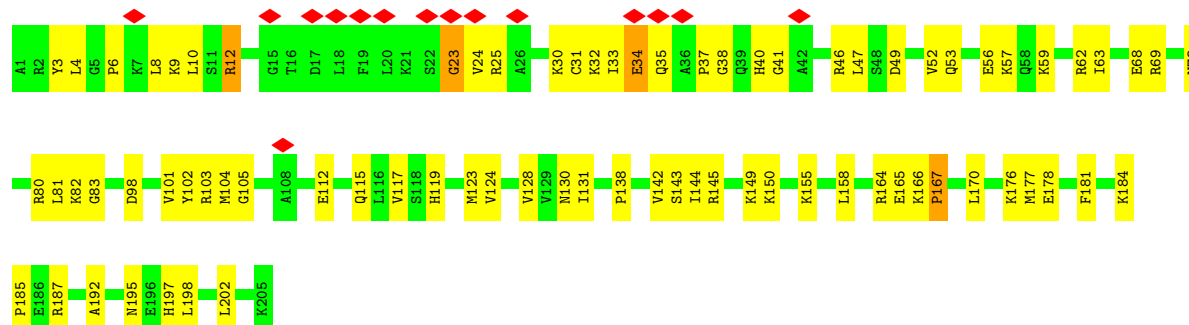


- Molecule 32: 30S ribosomal protein S3

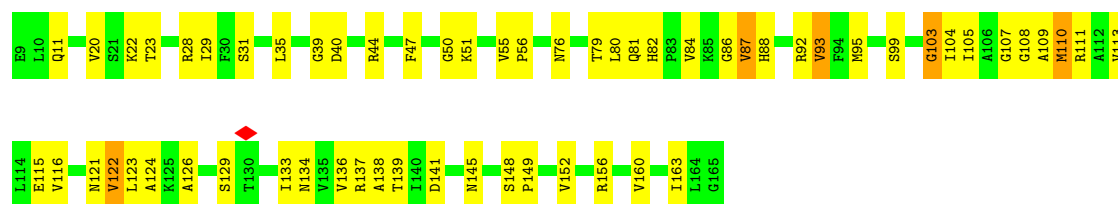




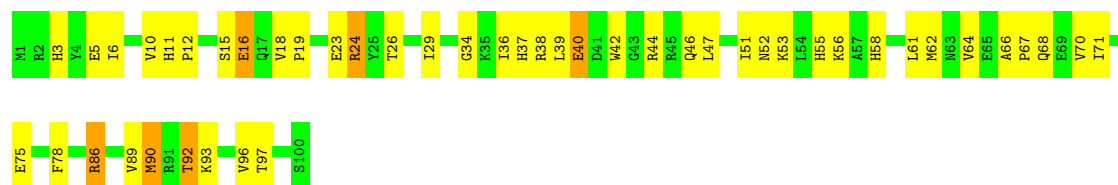
- Molecule 33: 30S ribosomal protein S4



- Molecule 34: 30S ribosomal protein S5



- Molecule 35: 30S ribosomal protein S6



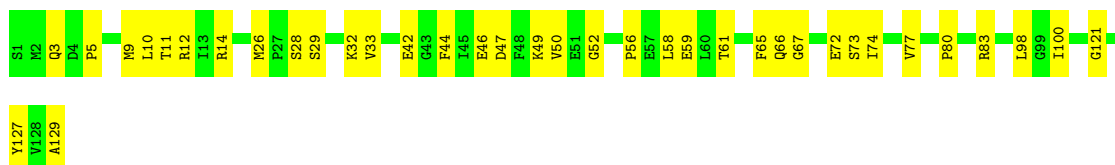
- Molecule 36: 30S ribosomal protein S7





- Molecule 37: 30S ribosomal protein S8

Chain M: 71% 29%



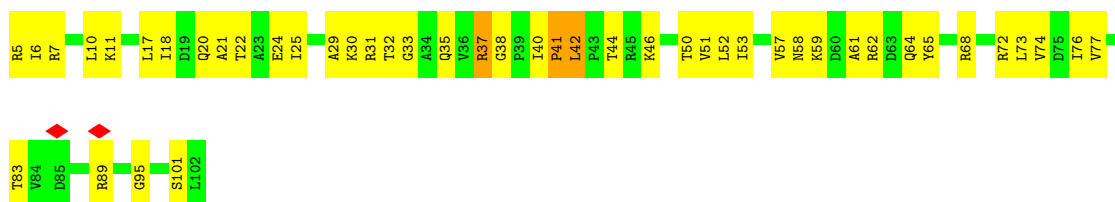
- Molecule 38: 30S ribosomal protein S9

Chain N: 63% 37%



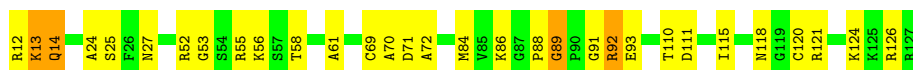
- Molecule 39: 30S ribosomal protein S10

Chain O: 53% 44%



- Molecule 40: 30S ribosomal protein S11

Chain P: 73% 23%



- Molecule 41: 30S ribosomal protein S12

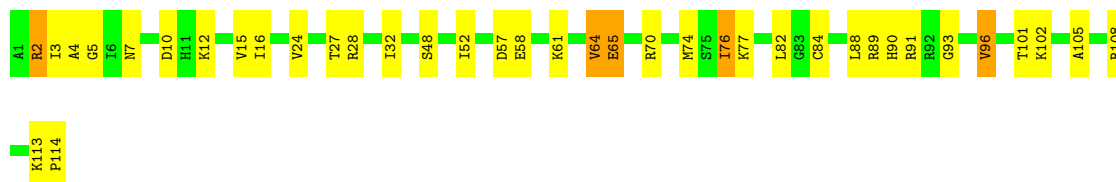
Chain Q: 58% 41%





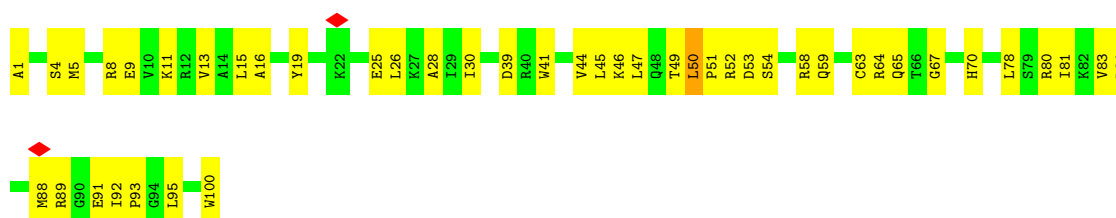
- Molecule 42: 30S ribosomal protein S13

Chain R: 67% 29%



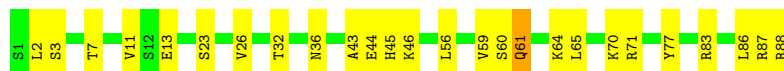
- Molecule 43: 30S ribosomal protein S14

Chain S: 55% 44%



- Molecule 44: 30S ribosomal protein S15

Chain T: 70% 28%



- Molecule 45: 30S ribosomal protein S16

Chain U: 51% 46%



- Molecule 46: 30S ribosomal protein S17

Chain V: 68% 31%



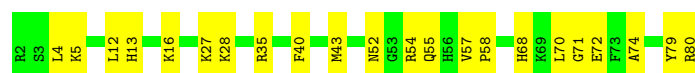
- Molecule 47: 30S ribosomal protein S18

Chain W:  72% 26%



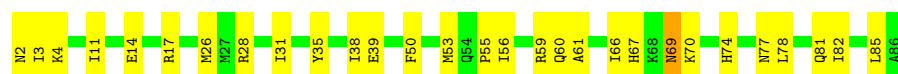
- Molecule 48: 30S ribosomal protein S19

Chain X:  72% 28%



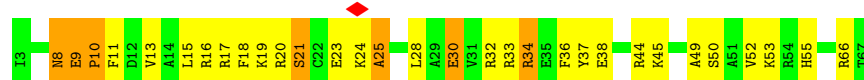
- Molecule 49: 30S ribosomal protein S20

Chain Y:  66% 33%

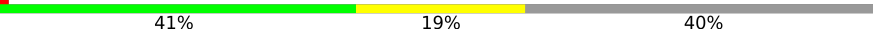


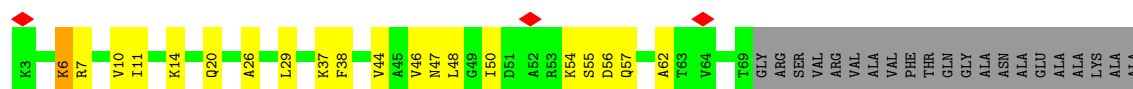
- Molecule 50: 30S ribosomal protein S21

Chain Z:  52% 37% 11%



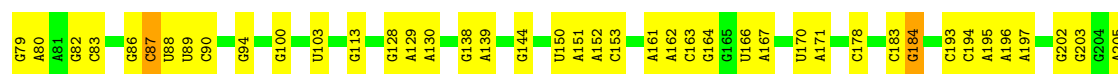
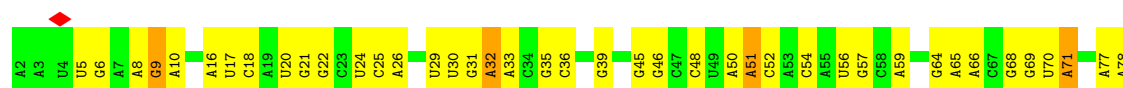
- Molecule 51: 50S ribosomal protein L1

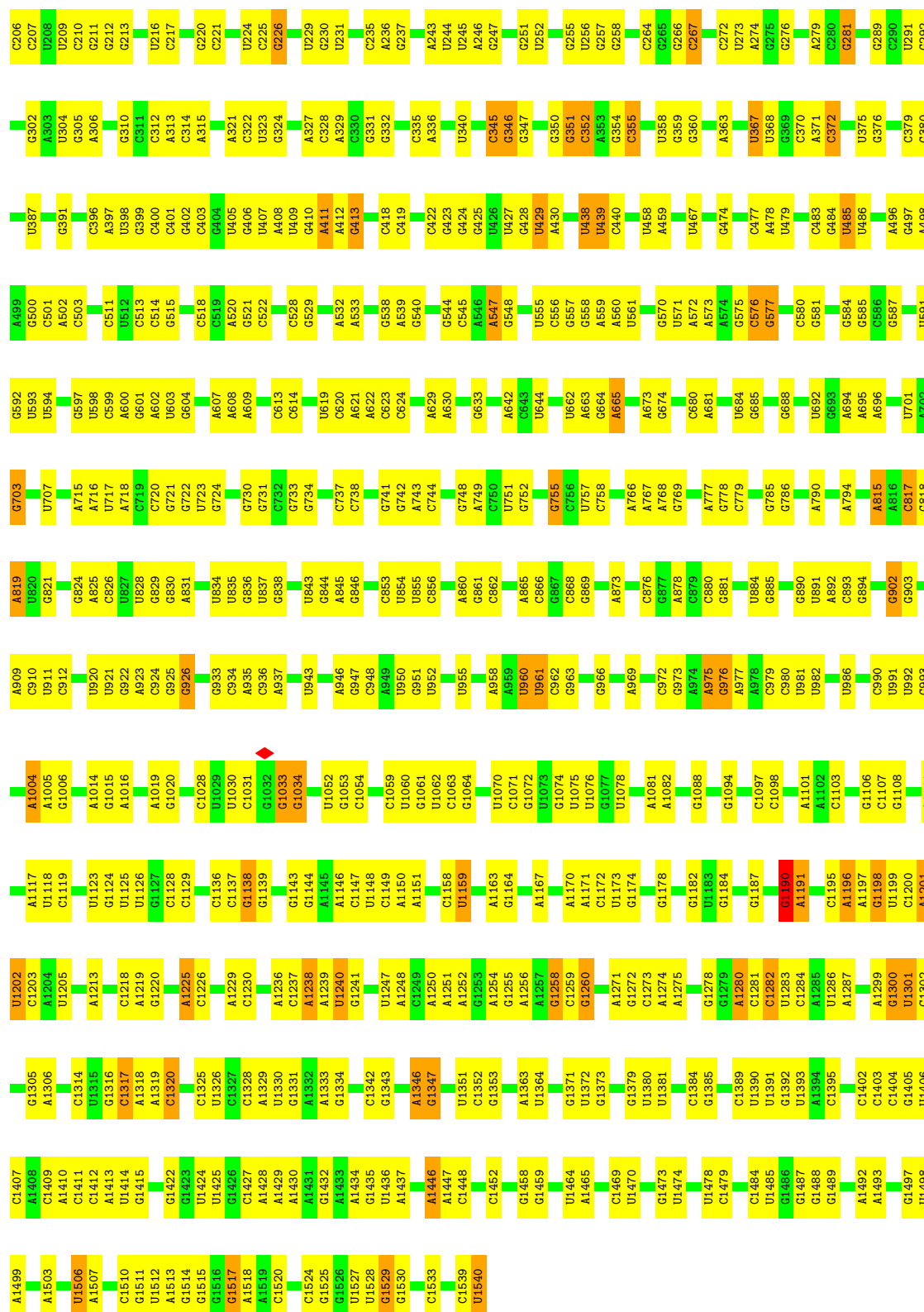
Chain a:  41% 19% 40%



- Molecule 52: 16S ribosomal RNA

Chain 3:  57% 39%





• Molecule 53: 23S ribosomal RNA

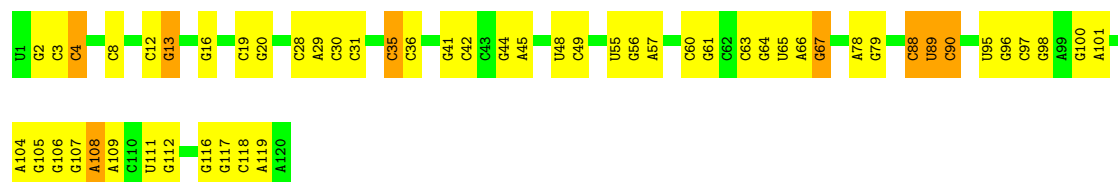


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A1419	C1320	G1202	U1102	C1013	G808	U714	U615	C531	A443	G325	A226	U120	A10
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G1430	A1327	G1210	U1105	A1021	C818	A727	G619	G537	G446	G329	C229	U138	U18
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G1587	C1684	C1684	A1806	A1906	C1996	U2086	U2192	A2278	A2336	A2430	G2503	G2602	C2728	A2820	U2899
G1588	C1685	C1685	G1807	G1907	C1996	U2087	U2193	G2279	G2337	U2431	U2504	A2603	U2729	A2821	G2903
U1589	G1686	G1686	A1808	G1908	C2010	C2091	U2194	A2280	U2338	A2432	G2505	A2604	U2730	G2822	U2903
C1590	G1695	G1695	A1809	G1909	U2011	U2092	U2195	G2281	A2339	A2435	U2514	A2605	U2731	C2830	C2830
A1591	G1696	G1696	A1810	U1911	U2017	U2093	U2196	G2282	U2340	A2441	C2515	A2606	U2732	G2831	G2831
C1592	G1699	G1699	G1811	A1912	A2019	U2094	U2197	G2283	U2341	C2442	C2516	A2607	U2733	U2832	U2832
U1594	U1709	U1709	C1816	C1914	A2020	C2096	U2198	G2284	U2342	C2443	C2517	A2608	A2734	G2833	G2833
C1595	G1710	G1710	G1817	C1915	C2021	C2096	U2199	A2285	U2343	U2444	U2518	A2609	G2737	G2834	U2834
A1596	G1715	G1715	A1818	A1916	U2022	C2096	U2200	G2286	U2344	U2445	U2519	A2610	A2738	A2835	U2835
A1597	C1715	C1715	A1819	A1917	C2023	C2096	U2201	G2287	U2345	U2446	U2520	A2611	U2739	U2836	U2836
A1598	U1729	U1729	U1820	A1918	U2023	C2096	U2202	A2288	U2346	U2447	U2521	A2612	G2740	C2841	C2841
G1601	C1730	C1730	G1823	C1920	U2026	C2096	U2203	G2289	U2347	U2448	U2522	A2613	A2741	G2842	G2842
U1602	U1730	U1730	G1824	C1921	U2027	C2096	U2204	G2290	U2348	U2449	U2523	A2614	A2742	G2843	G2843
A1603	G1738	G1738	G1825	G1921	U2028	C2096	U2205	U2291	U2349	U2450	U2524	A2615	C2752	G2844	G2844
C1604	U1738	U1738	G1826	U1923	A2030	G2125	U2217	U2292	C2368	A2448	U2525	A2616	G2753	U2845	G2845

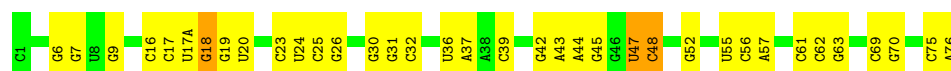
- Molecule 54: 5S ribosomal RNA

Chain 2: 

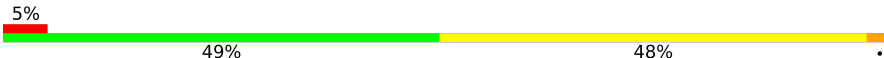


- Molecule 55: tRNA^{fMet}

Chain 5: 



- Molecule 55: tRNA^{fMet}

Chain 6: 



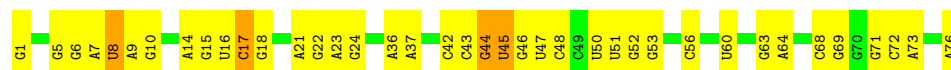
- Molecule 56: mRNA

Chain 4: 



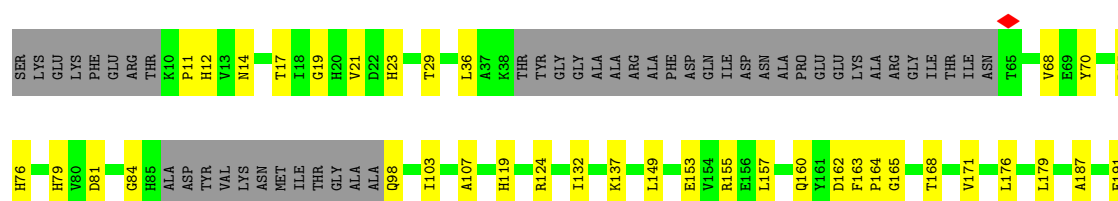
- Molecule 57: tRNA^{Phe}

Chain 7: 



- Molecule 58: Elongation factor Tu

Chain 8: 





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	7974	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 ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	18.424	Depositor
Minimum map value	-10.090	Depositor
Average map value	0.118	Depositor
Map value standard deviation	0.851	Depositor
Recommended contour level	1	Depositor
Map size (Å)	383.904, 383.904, 383.904	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.333, 1.333, 1.333	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	b	0.30	0/2122	0.94	4/2852 (0.1%)
2	c	0.29	0/1586	0.86	3/2134 (0.1%)
3	d	0.28	0/1571	0.86	3/2113 (0.1%)
4	e	0.30	0/1435	0.91	6/1926 (0.3%)
5	f	0.30	0/1343	0.87	4/1816 (0.2%)
6	g	0.32	0/1122	0.96	8/1515 (0.5%)
7	h	0.36	0/1002	1.11	9/1350 (0.7%)
8	i	0.36	0/1046	0.96	4/1410 (0.3%)
9	j	0.29	0/1152	0.88	3/1551 (0.2%)
10	k	0.29	0/948	0.91	1/1268 (0.1%)
11	l	0.30	0/1054	0.93	4/1403 (0.3%)
12	m	0.29	0/1093	0.86	1/1460 (0.1%)
13	n	0.29	0/974	0.91	3/1301 (0.2%)
14	o	0.27	0/902	0.86	2/1209 (0.2%)
15	p	0.29	0/929	0.81	1/1242 (0.1%)
16	q	0.29	0/960	0.91	3/1278 (0.2%)
17	r	0.30	0/829	0.87	4/1107 (0.4%)
18	s	0.29	0/864	0.84	1/1156 (0.1%)
19	t	0.29	0/745	0.87	1/994 (0.1%)
20	u	0.30	0/788	0.94	2/1051 (0.2%)
21	v	0.28	0/766	0.91	2/1025 (0.2%)
22	w	0.27	0/582	0.87	3/769 (0.4%)
23	x	0.27	0/635	0.89	3/848 (0.4%)
24	y	0.26	0/510	0.91	1/677 (0.1%)
25	z	0.28	0/453	0.79	0/605
26	B	0.27	0/450	0.84	1/599 (0.2%)
27	C	0.33	0/417	0.80	0/554
28	D	0.31	0/380	0.96	2/498 (0.4%)
29	E	0.27	0/513	0.91	3/676 (0.4%)
30	F	0.32	0/303	0.82	0/397
31	G	0.29	0/1788	0.88	2/2408 (0.1%)
32	H	0.31	0/1652	0.91	5/2225 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	I	0.30	0/1665	0.92	4/2227 (0.2%)
34	J	0.32	0/1170	1.02	7/1573 (0.4%)
35	K	0.31	0/836	0.93	2/1128 (0.2%)
36	L	0.29	0/1196	0.93	2/1602 (0.1%)
37	M	0.30	0/989	0.88	1/1326 (0.1%)
38	N	0.30	0/1034	0.92	0/1375
39	O	0.33	0/797	0.99	5/1077 (0.5%)
40	P	0.31	0/886	0.90	3/1195 (0.3%)
41	Q	0.33	0/969	1.03	7/1300 (0.5%)
42	R	0.31	0/893	0.96	5/1193 (0.4%)
43	S	0.29	0/817	0.91	3/1088 (0.3%)
44	T	0.28	0/722	0.83	2/964 (0.2%)
45	U	0.32	0/659	0.91	1/884 (0.1%)
46	V	0.30	0/658	0.92	3/881 (0.3%)
47	W	0.32	0/545	0.90	1/731 (0.1%)
48	X	0.31	0/653	0.93	0/877
49	Y	0.29	0/671	0.90	3/888 (0.3%)
50	Z	0.32	0/551	1.04	6/728 (0.8%)
51	a	0.31	0/1034	0.85	1/1387 (0.1%)
52	3	0.41	0/36963	0.47	2/57662 (0.0%)
53	1	0.40	0/69796	0.48	2/108888 (0.0%)
54	2	0.41	0/2872	0.47	0/4479
55	5	0.40	0/1832	0.46	0/2855
55	6	0.41	0/1832	0.47	0/2855
56	4	0.41	0/436	0.46	0/679
57	7	0.39	0/1809	0.47	0/2819
58	8	0.31	0/2726	0.92	7/3689 (0.2%)
All	All	0.37	0/165925	0.62	156/247767 (0.1%)

There are no bond length outliers.

The worst 5 of 156 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	53	VAL	N-CA-C	8.86	119.67	110.72
7	h	117	LEU	N-CA-C	8.36	123.20	109.24
32	H	5	HIS	CA-C-N	7.95	127.51	119.24
32	H	5	HIS	C-N-CA	7.95	127.51	119.24
35	K	24	ARG	N-CA-C	-7.86	103.29	113.12

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	b	2083	0	2157	71	0
2	c	1565	0	1616	43	0
3	d	1552	0	1619	36	0
4	e	1411	0	1447	40	0
5	f	1323	0	1374	37	0
6	g	1111	0	1148	43	0
7	h	989	0	1025	67	0
8	i	1032	0	1088	41	0
9	j	1129	0	1162	36	0
10	k	939	0	1012	42	0
11	l	1045	0	1117	40	0
12	m	1074	0	1157	32	0
13	n	961	0	1000	31	0
14	o	892	0	923	28	0
15	p	917	0	965	33	0
16	q	947	0	1022	26	0
17	r	816	0	839	23	0
18	s	857	0	922	18	0
19	t	739	0	807	19	0
20	u	780	0	834	20	0
21	v	753	0	780	22	0
22	w	575	0	592	20	0
23	x	625	0	655	19	0
24	y	509	0	543	21	0
25	z	449	0	491	9	0
26	B	444	0	461	15	0
27	C	410	0	440	11	0
28	D	377	0	418	12	0
29	E	504	0	574	21	0
30	F	302	0	343	25	0
31	G	1757	0	1787	43	0
32	H	1625	0	1699	39	0
33	I	1643	0	1710	69	0
34	J	1157	0	1199	44	0
35	K	818	0	808	47	0
36	L	1182	0	1240	40	0
37	M	979	0	1034	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	N	1022	0	1070	42	0
39	O	787	0	828	43	0
40	P	870	0	878	25	0
41	Q	955	0	1019	40	0
42	R	884	0	944	35	0
43	S	805	0	847	38	0
44	T	714	0	737	18	0
45	U	649	0	666	38	0
46	V	649	0	691	19	0
47	W	536	0	552	18	0
48	X	638	0	665	17	0
49	Y	665	0	714	20	0
50	Z	545	0	579	27	0
51	a	1027	0	1092	37	0
52	3	33012	0	16618	559	0
53	1	62317	0	31346	941	0
54	2	2568	0	1303	47	0
55	5	1640	0	836	27	0
55	6	1640	0	837	33	0
56	4	388	0	196	5	0
57	7	1619	0	821	29	0
58	8	2677	0	2699	93	0
59	5	10	0	10	0	0
60	7	11	0	8	4	0
61	8	28	0	12	1	0
All	All	152927	0	103976	2898	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 11.

The worst 5 of 2898 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)
52:3:405:U:H3'	52:3:406:G:H5'	1.33	1.10
7:h:73:LYS:HB3	7:h:117:LEU:HD21	1.40	1.04
53:1:1053:C:H2'	53:1:1054:A:H5''	1.45	0.98
45:U:41:PRO:HG2	45:U:42:ILE:HD12	1.45	0.98
52:3:484:G:H4'	52:3:485:U:H5''	1.46	0.97

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	b	269/271 (99%)	238 (88%)	28 (10%)	3 (1%)	11	42
2	c	207/209 (99%)	184 (89%)	22 (11%)	1 (0%)	24	56
3	d	199/201 (99%)	182 (92%)	15 (8%)	2 (1%)	12	43
4	e	175/177 (99%)	156 (89%)	17 (10%)	2 (1%)	11	42
5	f	174/176 (99%)	162 (93%)	12 (7%)	0	100	100
6	g	147/149 (99%)	119 (81%)	25 (17%)	3 (2%)	6	32
7	h	129/131 (98%)	97 (75%)	26 (20%)	6 (5%)	2	18
8	i	139/141 (99%)	117 (84%)	17 (12%)	5 (4%)	2	23
9	j	140/142 (99%)	129 (92%)	9 (6%)	2 (1%)	9	37
10	k	120/122 (98%)	97 (81%)	18 (15%)	5 (4%)	2	20
11	l	141/143 (99%)	112 (79%)	24 (17%)	5 (4%)	3	24
12	m	134/136 (98%)	116 (87%)	15 (11%)	3 (2%)	5	31
13	n	118/120 (98%)	99 (84%)	18 (15%)	1 (1%)	16	48
14	o	114/116 (98%)	110 (96%)	3 (3%)	1 (1%)	14	45
15	p	112/114 (98%)	98 (88%)	13 (12%)	1 (1%)	14	45
16	q	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
17	r	101/103 (98%)	89 (88%)	10 (10%)	2 (2%)	6	32
18	s	108/110 (98%)	95 (88%)	10 (9%)	3 (3%)	4	27
19	t	91/93 (98%)	81 (89%)	9 (10%)	1 (1%)	11	42
20	u	100/102 (98%)	83 (83%)	15 (15%)	2 (2%)	6	32
21	v	92/94 (98%)	85 (92%)	7 (8%)	0	100	100
22	w	73/75 (97%)	64 (88%)	8 (11%)	1 (1%)	9	37
23	x	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
24	y	61/63 (97%)	58 (95%)	2 (3%)	1 (2%)	7	35
25	z	56/58 (97%)	51 (91%)	5 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	B	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
27	C	48/50 (96%)	40 (83%)	7 (15%)	1 (2%)	5	31
28	D	44/46 (96%)	39 (89%)	4 (9%)	1 (2%)	5	30
29	E	62/64 (97%)	54 (87%)	7 (11%)	1 (2%)	7	35
30	F	36/38 (95%)	30 (83%)	5 (14%)	1 (3%)	4	27
31	G	223/225 (99%)	206 (92%)	17 (8%)	0	100	100
32	H	204/206 (99%)	194 (95%)	9 (4%)	1 (0%)	24	56
33	I	203/205 (99%)	174 (86%)	25 (12%)	4 (2%)	6	32
34	J	155/157 (99%)	125 (81%)	24 (16%)	6 (4%)	2	21
35	K	98/100 (98%)	76 (78%)	17 (17%)	5 (5%)	1	17
36	L	149/151 (99%)	131 (88%)	16 (11%)	2 (1%)	9	38
37	M	127/129 (98%)	115 (91%)	11 (9%)	1 (1%)	16	48
38	N	125/127 (98%)	102 (82%)	20 (16%)	3 (2%)	4	29
39	O	96/98 (98%)	77 (80%)	14 (15%)	5 (5%)	1	17
40	P	114/116 (98%)	88 (77%)	21 (18%)	5 (4%)	2	19
41	Q	121/123 (98%)	99 (82%)	17 (14%)	5 (4%)	2	20
42	R	112/114 (98%)	101 (90%)	7 (6%)	4 (4%)	2	23
43	S	98/100 (98%)	81 (83%)	17 (17%)	0	100	100
44	T	86/88 (98%)	79 (92%)	6 (7%)	1 (1%)	10	40
45	U	80/82 (98%)	72 (90%)	7 (9%)	1 (1%)	9	38
46	V	78/80 (98%)	66 (85%)	9 (12%)	3 (4%)	2	22
47	W	63/65 (97%)	57 (90%)	5 (8%)	1 (2%)	7	35
48	X	77/79 (98%)	68 (88%)	8 (10%)	1 (1%)	9	38
49	Y	83/85 (98%)	82 (99%)	1 (1%)	0	100	100
50	Z	63/65 (97%)	43 (68%)	17 (27%)	3 (5%)	2	17
51	a	130/223 (58%)	123 (95%)	6 (5%)	1 (1%)	16	48
58	8	340/400 (85%)	299 (88%)	38 (11%)	3 (1%)	14	45
All	All	6259/6512 (96%)	5480 (88%)	670 (11%)	109 (2%)	9	34

5 of 109 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	b	204	LEU

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Mol	Chain	Res	Type
3	d	83	VAL
6	g	9	VAL
7	h	108	VAL
7	h	118	ILE

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	b	216/216 (100%)	214 (99%)	2 (1%)	70	75
2	c	164/164 (100%)	163 (99%)	1 (1%)	78	79
3	d	165/165 (100%)	164 (99%)	1 (1%)	78	79
4	e	148/148 (100%)	147 (99%)	1 (1%)	76	77
5	f	137/137 (100%)	137 (100%)	0	100	100
6	g	114/114 (100%)	114 (100%)	0	100	100
7	h	100/100 (100%)	98 (98%)	2 (2%)	48	64
8	i	109/109 (100%)	108 (99%)	1 (1%)	70	75
9	j	116/116 (100%)	116 (100%)	0	100	100
10	k	103/103 (100%)	103 (100%)	0	100	100
11	l	102/102 (100%)	101 (99%)	1 (1%)	68	74
12	m	109/109 (100%)	108 (99%)	1 (1%)	70	75
13	n	100/100 (100%)	99 (99%)	1 (1%)	68	74
14	o	86/86 (100%)	86 (100%)	0	100	100
15	p	99/99 (100%)	99 (100%)	0	100	100
16	q	89/89 (100%)	88 (99%)	1 (1%)	65	73
17	r	84/84 (100%)	83 (99%)	1 (1%)	63	72
18	s	93/93 (100%)	93 (100%)	0	100	100
19	t	80/80 (100%)	80 (100%)	0	100	100
20	u	83/83 (100%)	83 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	v	78/78 (100%)	77 (99%)	1 (1%)	61	71
22	w	57/57 (100%)	57 (100%)	0	100	100
23	x	67/67 (100%)	67 (100%)	0	100	100
24	y	55/55 (100%)	55 (100%)	0	100	100
25	z	48/48 (100%)	48 (100%)	0	100	100
26	B	47/47 (100%)	46 (98%)	1 (2%)	47	64
27	C	45/45 (100%)	43 (96%)	2 (4%)	25	50
28	D	38/38 (100%)	38 (100%)	0	100	100
29	E	51/51 (100%)	51 (100%)	0	100	100
30	F	34/34 (100%)	33 (97%)	1 (3%)	37	57
31	G	186/186 (100%)	184 (99%)	2 (1%)	65	73
32	H	170/170 (100%)	170 (100%)	0	100	100
33	I	172/172 (100%)	172 (100%)	0	100	100
34	J	119/119 (100%)	119 (100%)	0	100	100
35	K	87/87 (100%)	86 (99%)	1 (1%)	65	73
36	L	124/124 (100%)	124 (100%)	0	100	100
37	M	104/104 (100%)	104 (100%)	0	100	100
38	N	105/105 (100%)	104 (99%)	1 (1%)	68	74
39	O	86/86 (100%)	86 (100%)	0	100	100
40	P	89/89 (100%)	89 (100%)	0	100	100
41	Q	103/103 (100%)	102 (99%)	1 (1%)	68	74
42	R	92/92 (100%)	92 (100%)	0	100	100
43	S	83/83 (100%)	82 (99%)	1 (1%)	63	72
44	T	76/76 (100%)	76 (100%)	0	100	100
45	U	65/65 (100%)	64 (98%)	1 (2%)	57	68
46	V	74/74 (100%)	74 (100%)	0	100	100
47	W	56/56 (100%)	56 (100%)	0	100	100
48	X	70/70 (100%)	70 (100%)	0	100	100
49	Y	65/65 (100%)	65 (100%)	0	100	100
50	Z	55/55 (100%)	54 (98%)	1 (2%)	51	67
51	a	110/174 (63%)	110 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
58	8	291/332 (88%)	289 (99%)	2 (1%)	76	77
All	All	5199/5304 (98%)	5171 (100%)	28 (0%)	78	80

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	B	8	THR
58	8	293	LEU
30	F	37	GLN
45	U	19	VAL
27	C	46	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 128 such sidechains are listed below:

Mol	Chain	Res	Type
45	U	63	GLN
49	Y	19	HIS
20	u	45	GLN
20	u	39	ASN
49	Y	81	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
52	3	1538/1539 (99%)	136 (8%)	3 (0%)
53	1	2902/2903 (99%)	320 (11%)	10 (0%)
54	2	119/120 (99%)	9 (7%)	1 (0%)
55	5	76/77 (98%)	7 (9%)	0
55	6	76/77 (98%)	8 (10%)	0
56	4	17/18 (94%)	2 (11%)	0
57	7	75/76 (98%)	11 (14%)	1 (1%)
All	All	4803/4810 (99%)	493 (10%)	15 (0%)

5 of 493 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
52	3	6	G
52	3	9	G
52	3	22	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
52	3	32	A
52	3	39	G

5 of 15 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
53	1	1130	U
54	2	88	C
53	1	1475	G
57	7	42	C
53	1	2326	C

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands 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	$\# Z > 2$
59	FME	5	101	55	8,9,10	0.49	0	8,9,11	0.90	0
61	GDP	8	501	-	29,30,30	1.34	2 (6%)	45,47,47	1.90	12 (26%)
60	PHE	7	101	57	10,11,12	0.68	0	8,13,15	0.26	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	FME	5	101	55	-	1/7/9/11	-
61	GDP	8	501	-	-	3/16/32/32	0/3/3/3
60	PHE	7	101	57	-	0/5/6/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	8	501	GDP	PB-O1B	3.62	1.61	1.50
61	8	501	GDP	PA-O3A	2.39	1.62	1.59

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	8	501	GDP	C5-C4-N3	-5.65	119.41	128.39
61	8	501	GDP	C2-N3-C4	5.52	121.81	112.30
61	8	501	GDP	N9-C4-N3	4.28	134.51	125.95
61	8	501	GDP	C8-N7-C5	2.97	109.55	104.26
61	8	501	GDP	O4'-C4'-C3'	2.76	110.63	105.15

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	5	101	FME	O1-CN-N-CA
61	8	501	GDP	PA-O3A-PB-O2B
61	8	501	GDP	PA-O3A-PB-O3B
61	8	501	GDP	PA-O3A-PB-O1B

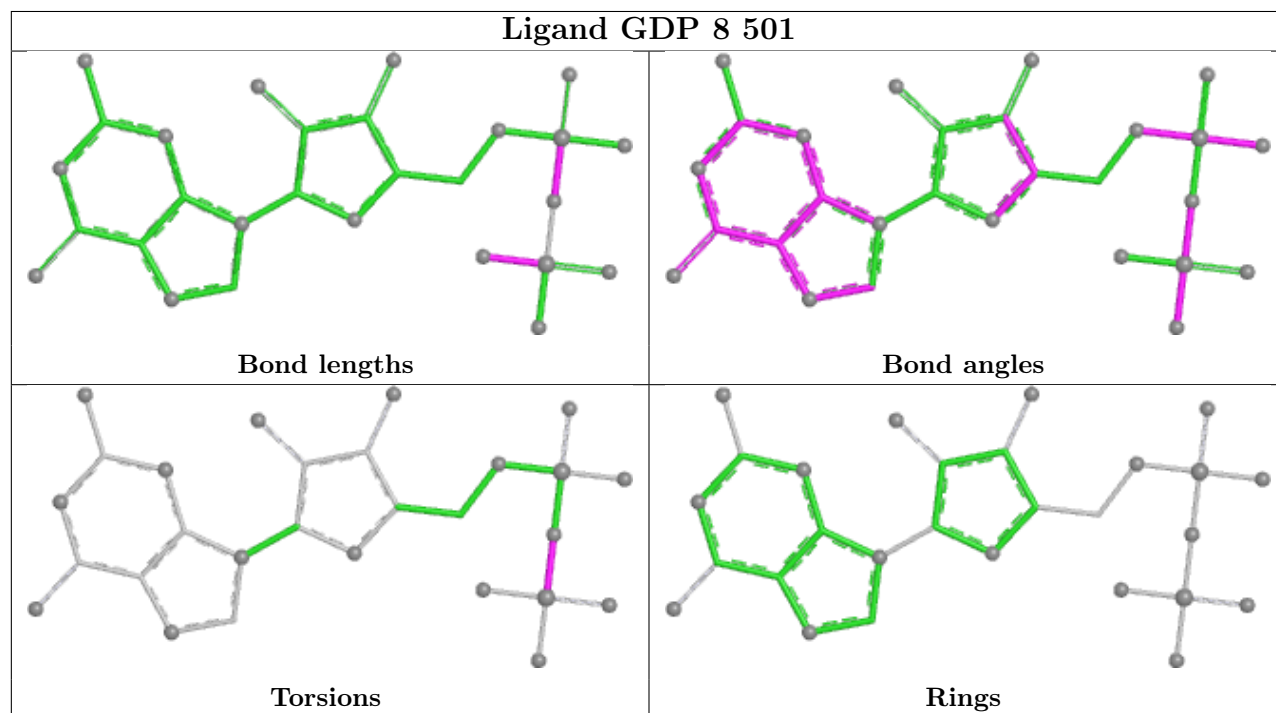
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	8	501	GDP	1	0
60	7	101	PHE	4	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.



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.

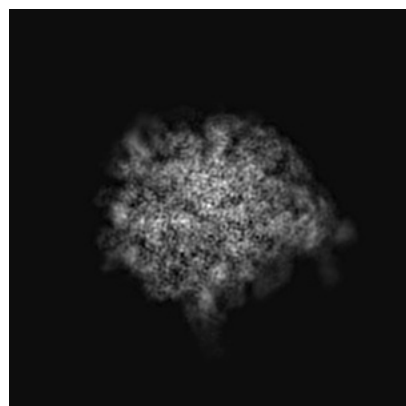
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21628. These allow visual inspection of the internal detail of the map and identification of artifacts.

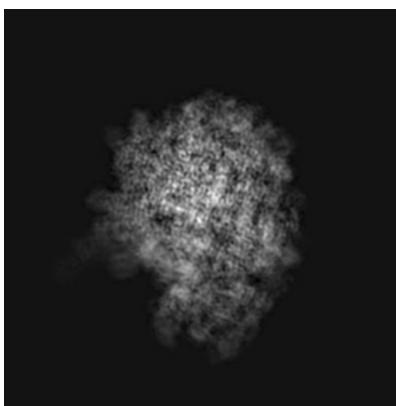
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

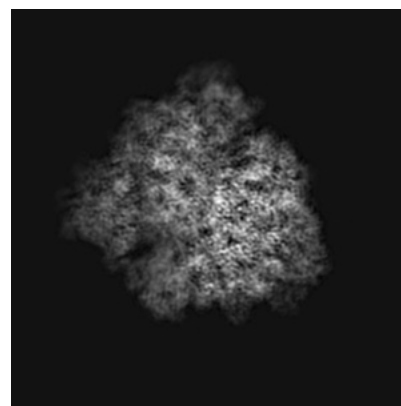
6.1.1 Primary map



X

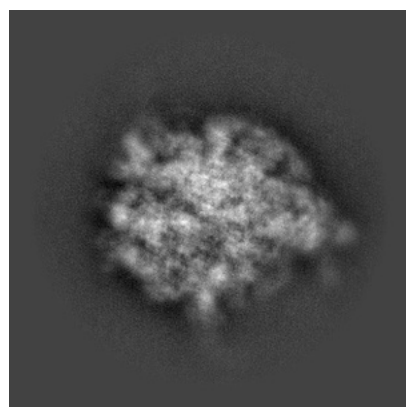


Y

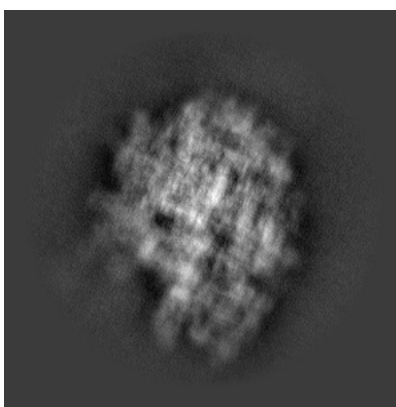


Z

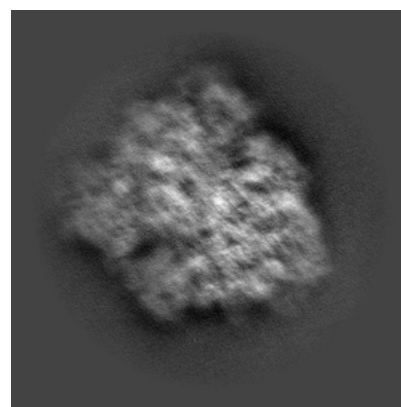
6.1.2 Raw map



X



Y

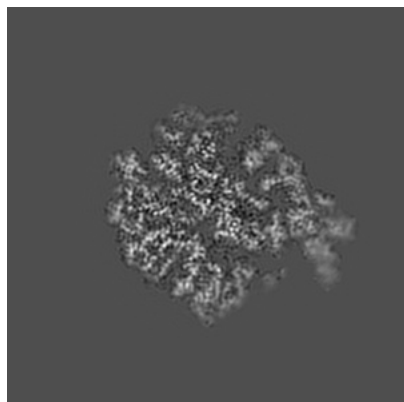


Z

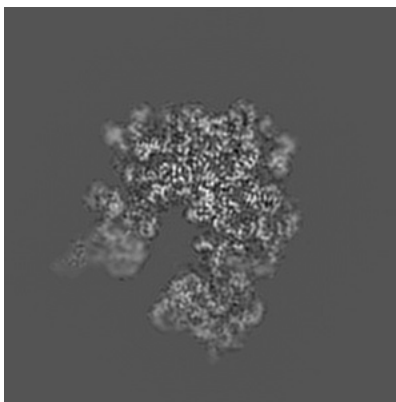
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

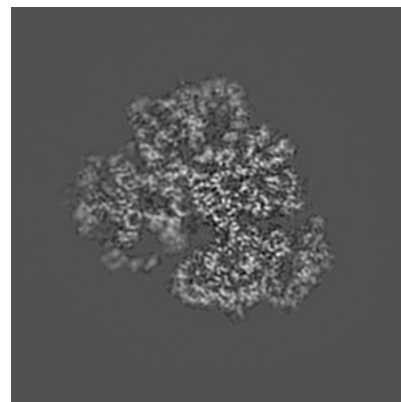
6.2.1 Primary map



X Index: 144

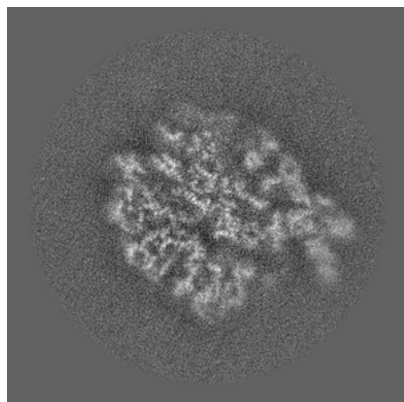


Y Index: 144

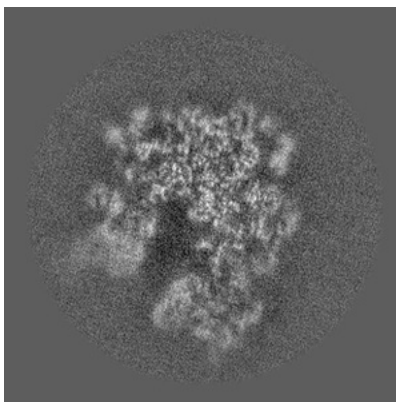


Z Index: 144

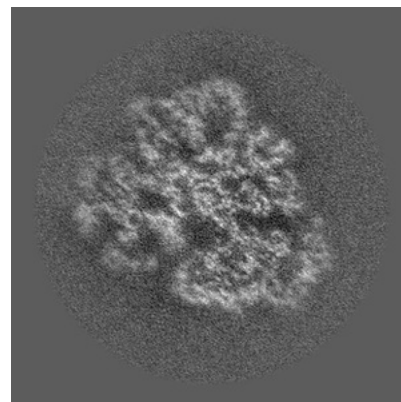
6.2.2 Raw map



X Index: 144



Y Index: 144

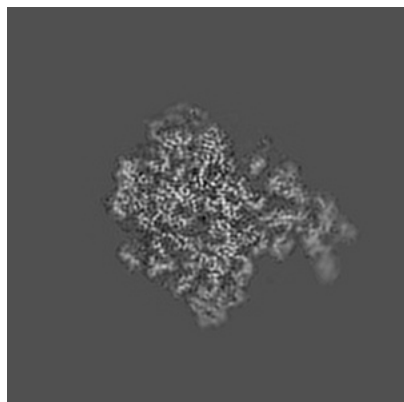


Z Index: 144

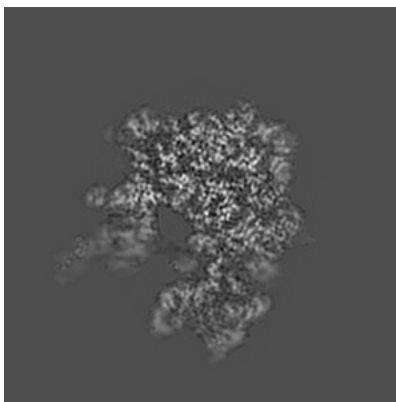
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

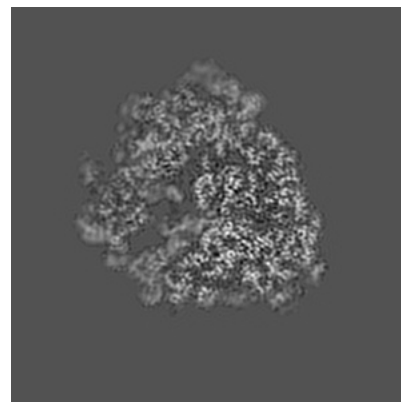
6.3.1 Primary map



X Index: 149

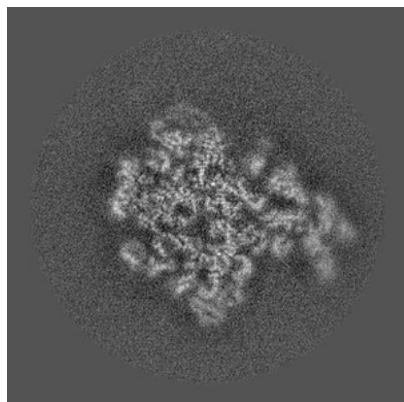


Y Index: 149

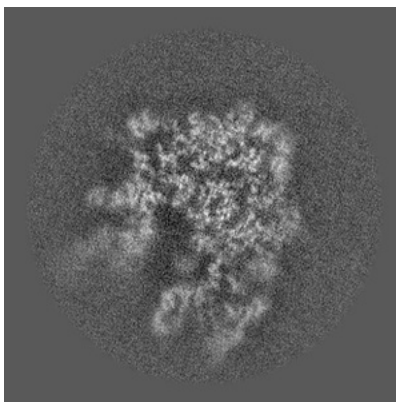


Z Index: 135

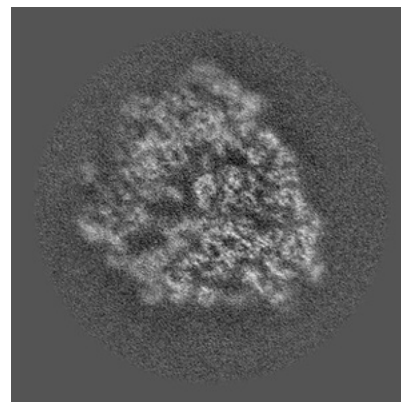
6.3.2 Raw map



X Index: 149



Y Index: 149

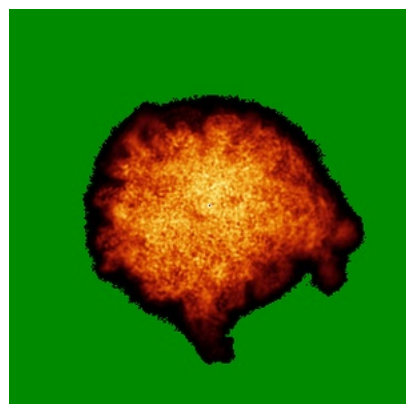


Z Index: 135

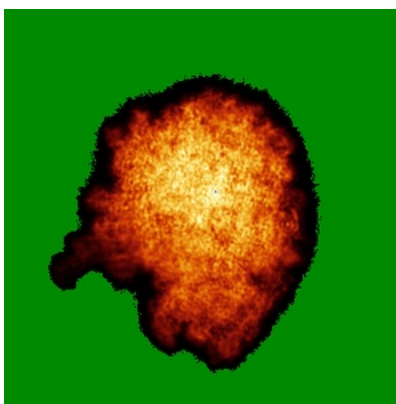
The images above show the largest variance slices of the map in three orthogonal directions.

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

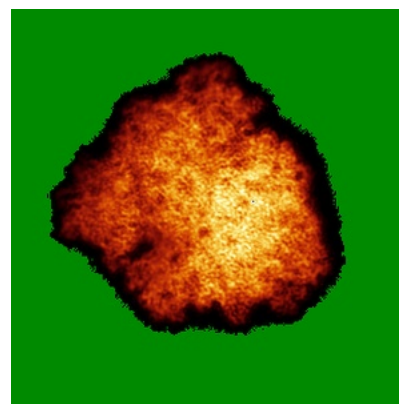
6.4.1 Primary map



X

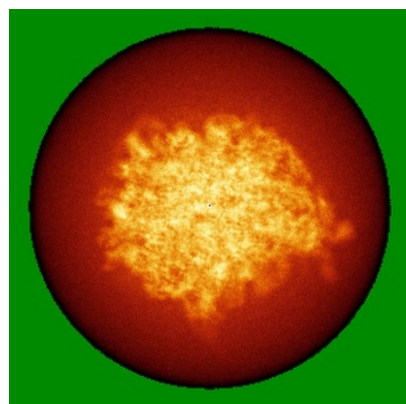


Y

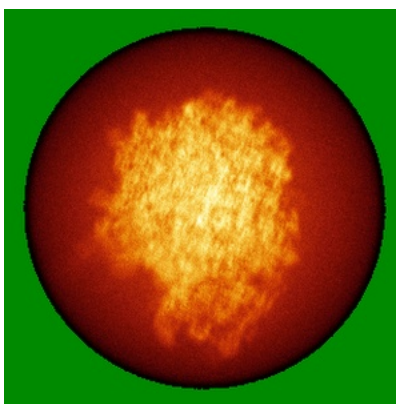


Z

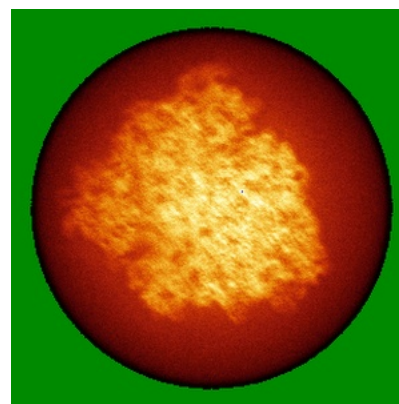
6.4.2 Raw map



X



Y

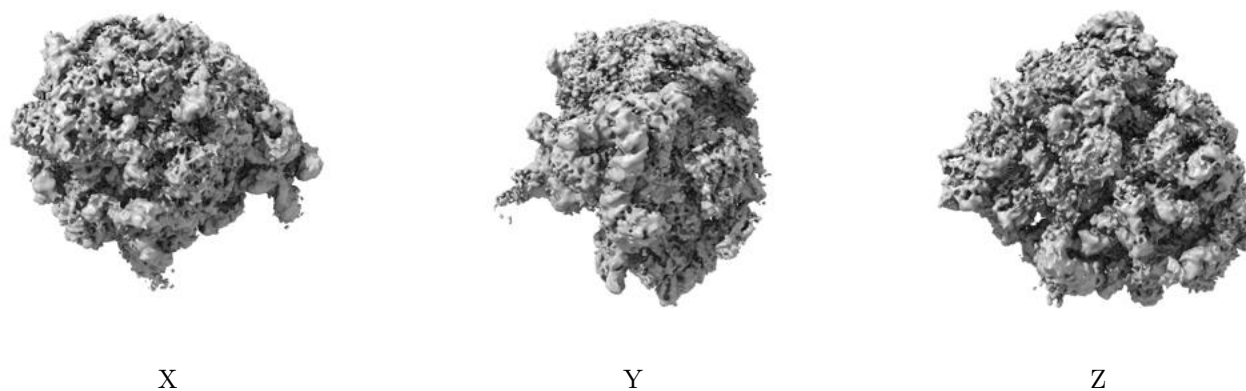


Z

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.

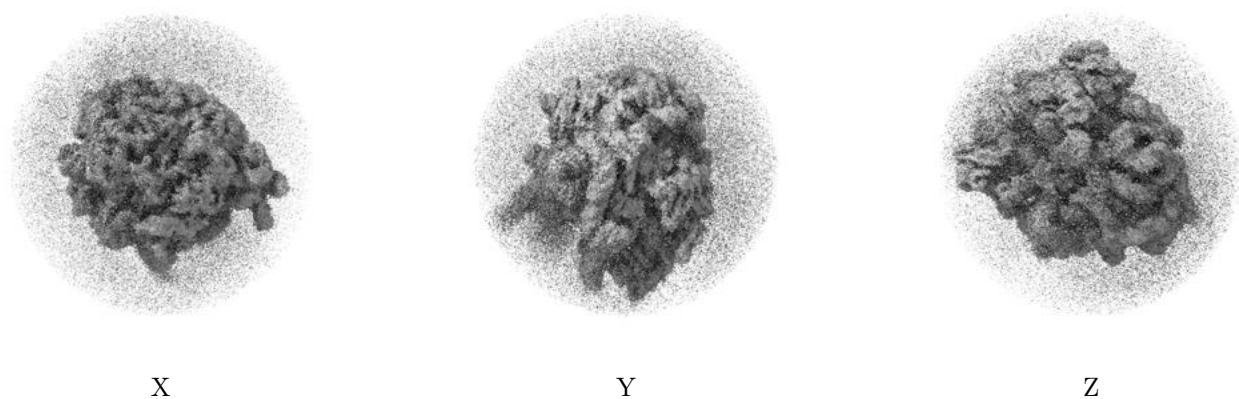
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

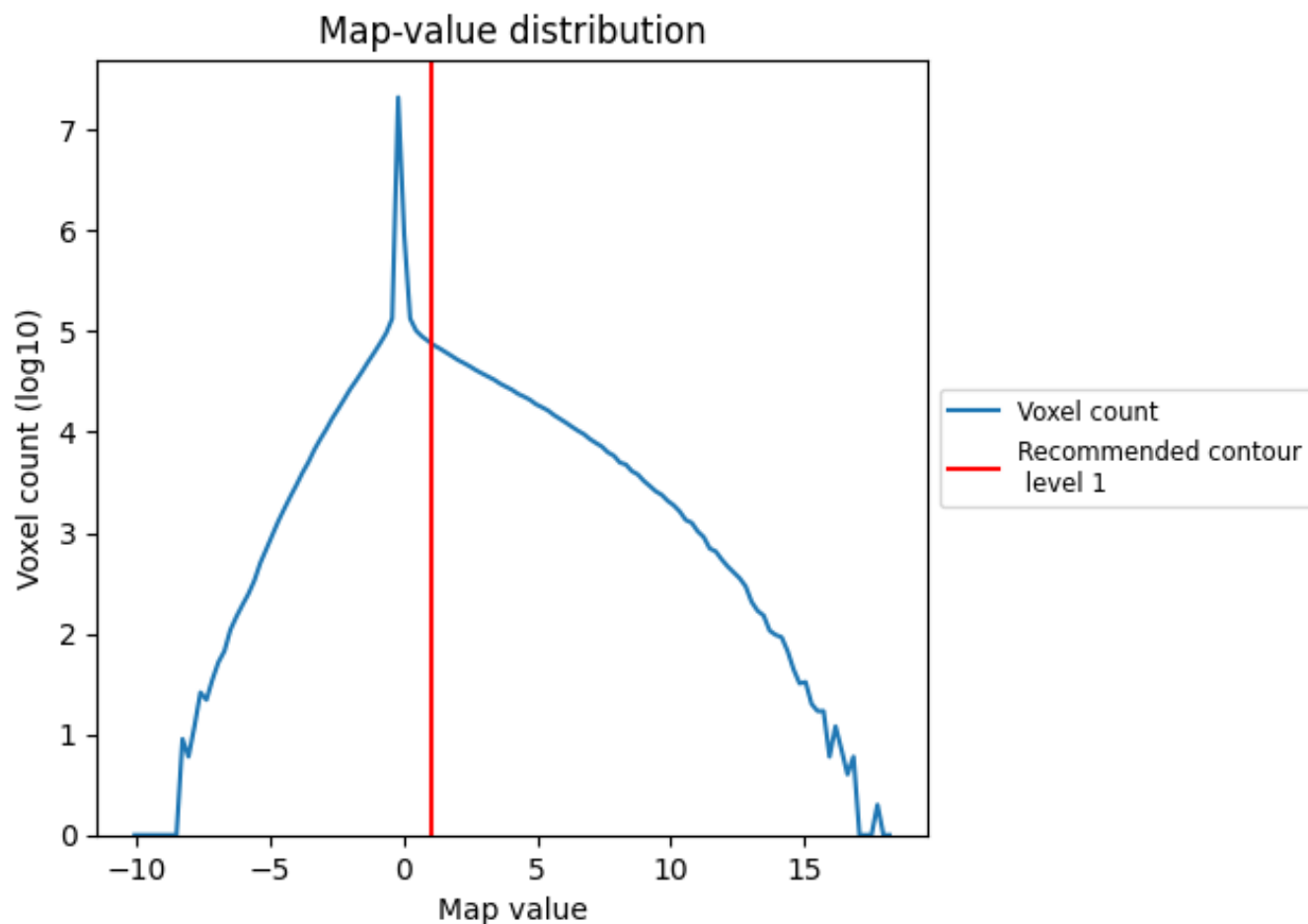
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

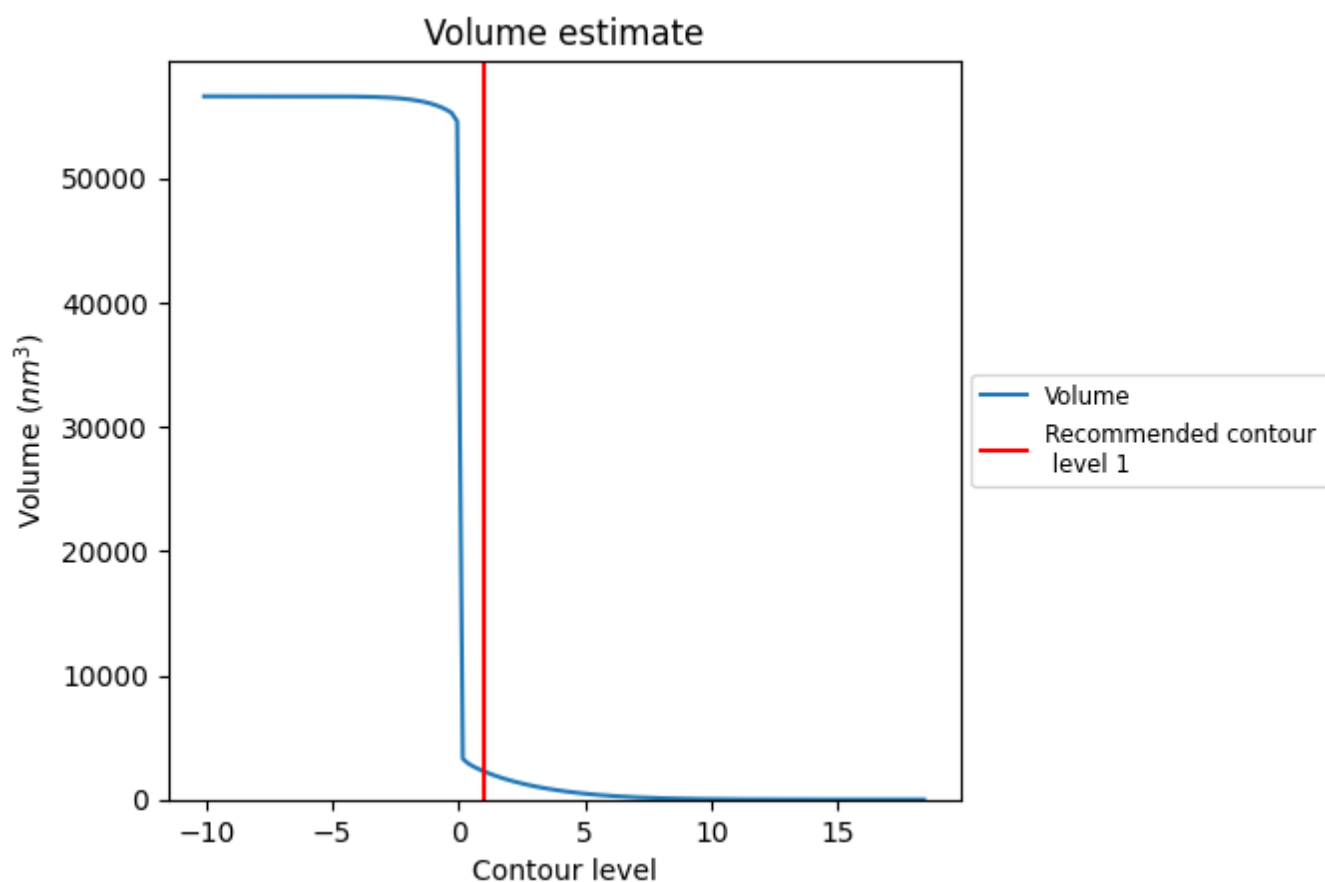
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

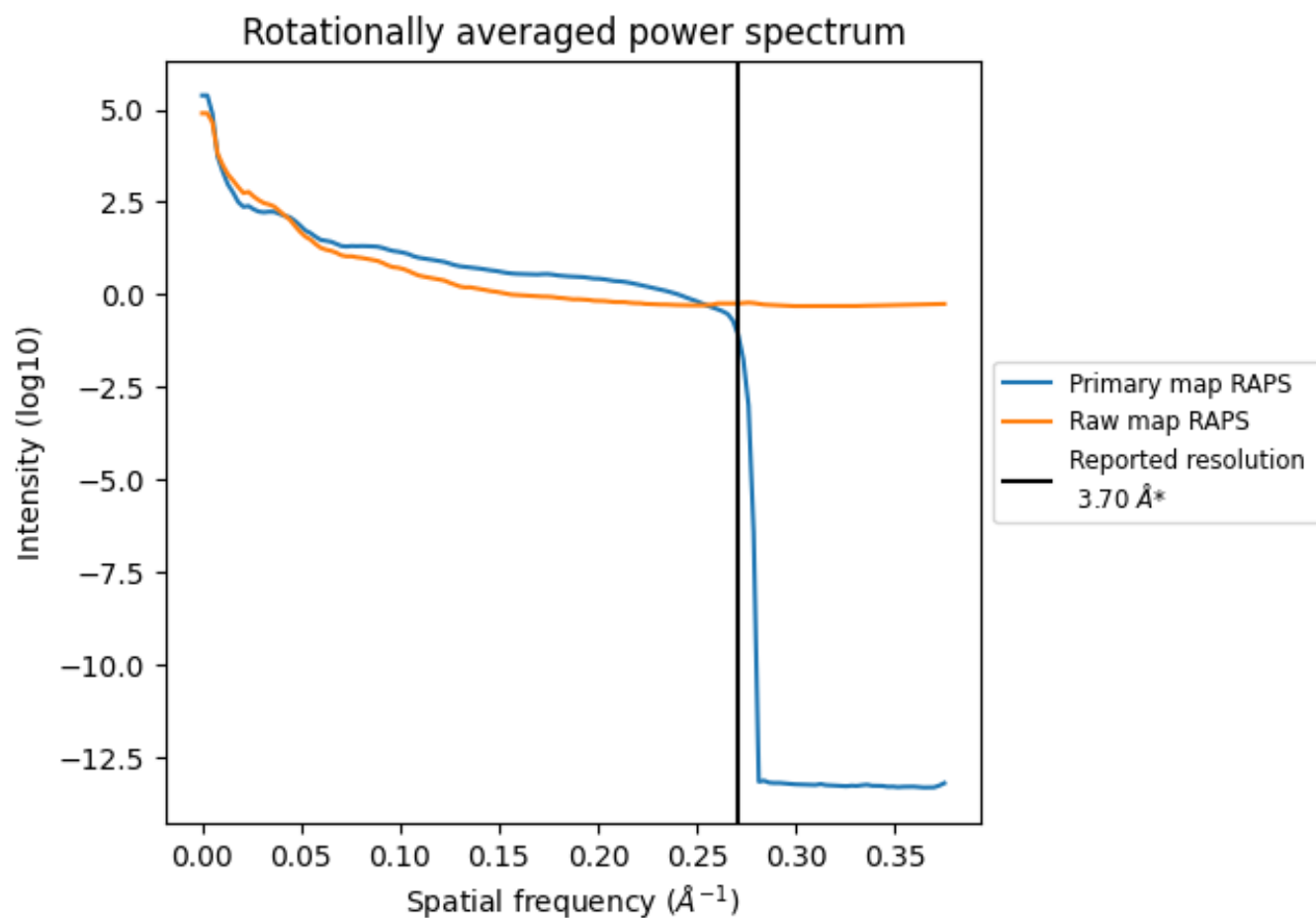
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2262 nm³; this corresponds to an approximate mass of 2043 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 ⓘ

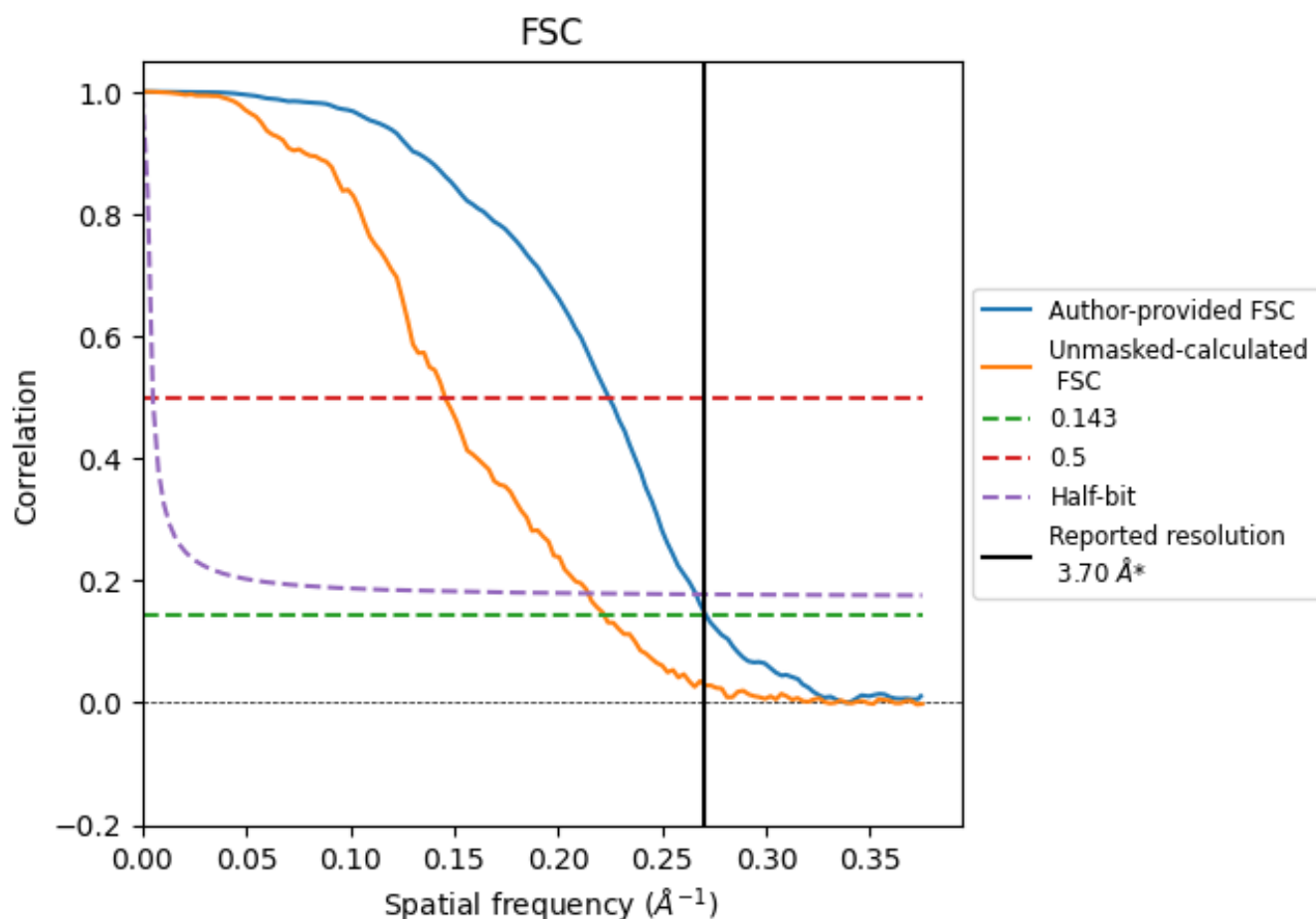


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

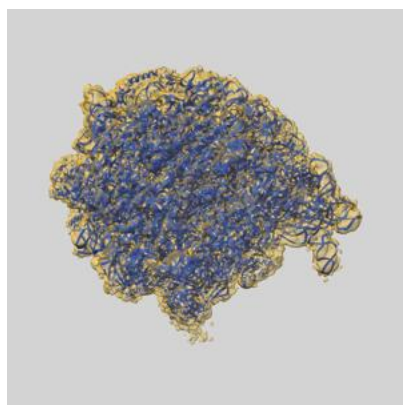
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.69	4.46	3.76
Unmasked-calculated*	4.50	6.87	4.66

*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 4.50 differs from the reported value 3.7 by more than 10 %

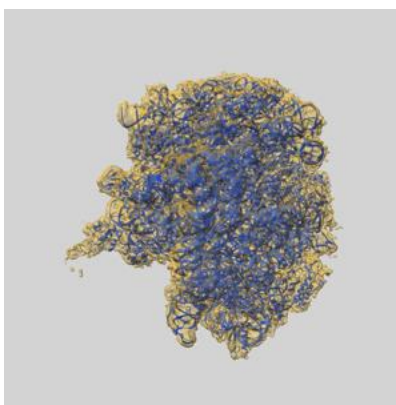
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21628 and PDB model 6WD9. Per-residue inclusion information can be found in section [3](#) on page [17](#).

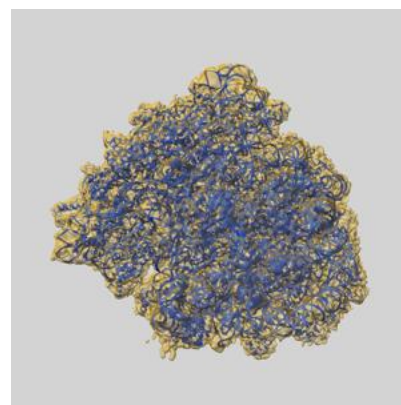
9.1 Map-model overlay [i](#)



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.0 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](#)

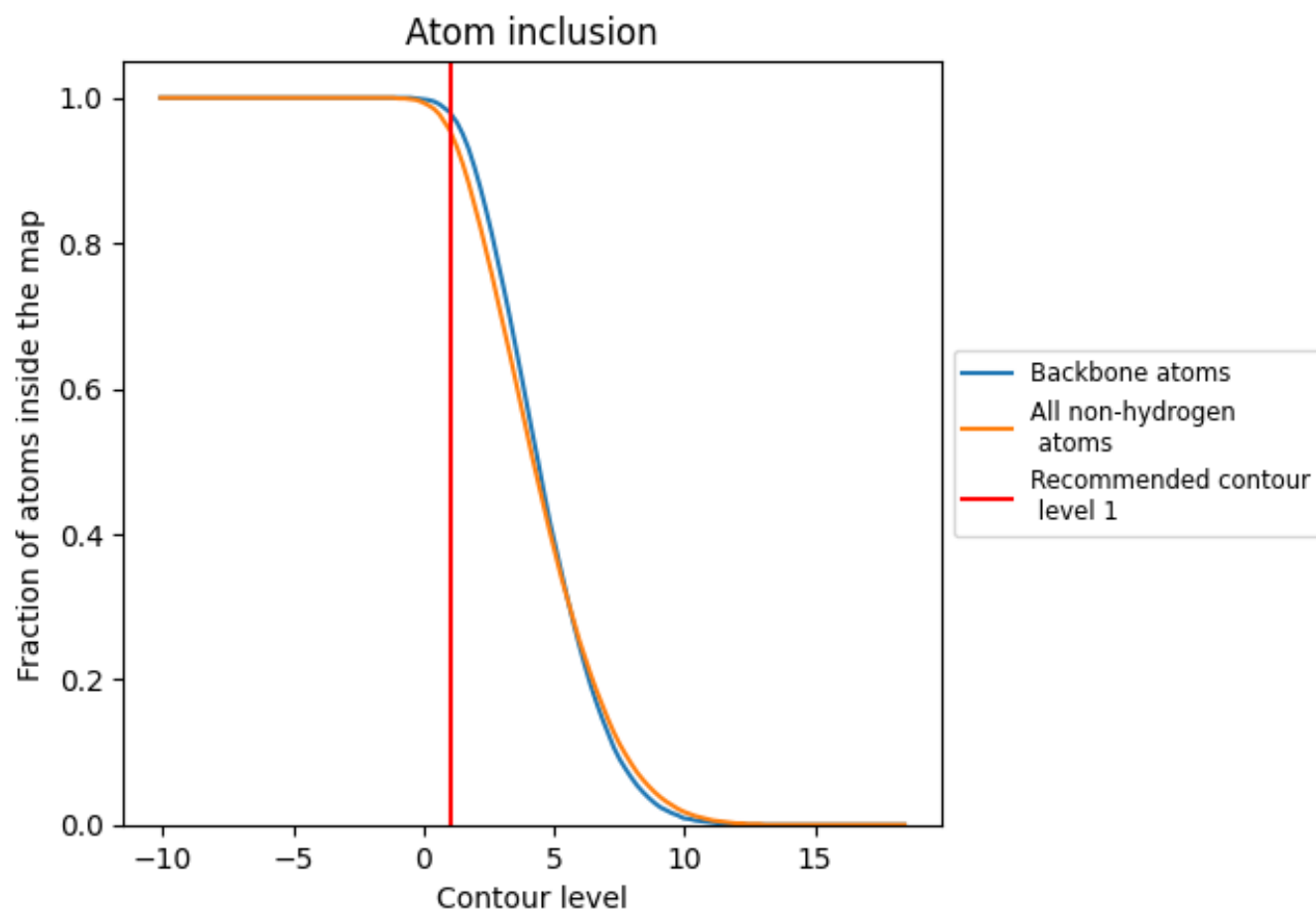


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% 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) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9550	 0.3440
1	 0.9810	 0.3690
2	 0.9810	 0.3220
3	 0.9780	 0.3250
4	 0.8990	 0.2650
5	 0.9690	 0.2720
6	 0.8140	 0.1420
7	 0.9640	 0.1980
8	 0.9450	 0.1980
B	 0.9440	 0.4080
C	 0.8010	 0.3280
D	 0.9320	 0.4600
E	 0.9210	 0.4520
F	 0.8250	 0.3660
G	 0.8770	 0.3100
H	 0.8650	 0.3350
I	 0.8190	 0.2570
J	 0.9230	 0.3780
K	 0.9470	 0.3620
L	 0.9350	 0.3110
M	 0.9180	 0.3820
N	 0.8890	 0.2990
O	 0.7900	 0.3020
P	 0.9410	 0.3800
Q	 0.9480	 0.3940
R	 0.9300	 0.2810
S	 0.8480	 0.3030
T	 0.9490	 0.3710
U	 0.9150	 0.3260
V	 0.9370	 0.3680
W	 0.9280	 0.3380
X	 0.9530	 0.3170
Y	 0.9060	 0.2760
Z	 0.8630	 0.3000
a	 0.8500	 0.1600



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Chain	Atom inclusion	Q-score
b	 0.9490	 0.4490
c	 0.9450	 0.4370
d	 0.9430	 0.3850
e	 0.9290	 0.2730
f	 0.9500	 0.3040
g	 0.7560	 0.2610
h	 0.7120	 0.1250
i	 0.7930	 0.1400
j	 0.9270	 0.4190
k	 0.9400	 0.4320
l	 0.9360	 0.4140
m	 0.9090	 0.4100
n	 0.9460	 0.4280
o	 0.9320	 0.3320
p	 0.9540	 0.4180
q	 0.9280	 0.4130
r	 0.9620	 0.4040
s	 0.9230	 0.4280
t	 0.9210	 0.3940
u	 0.9380	 0.3790
v	 0.9470	 0.3790
w	 0.9190	 0.4310
x	 0.9330	 0.4270
y	 0.9260	 0.3340
z	 0.9380	 0.3950