



wwPDB EM Validation Summary Report ⓘ

Mar 29, 2026 – 07:03 AM UTC

PDB ID : 6WD3 / pdb_00006wd3
EMDB ID : EMD-21622
Title : Cryo-EM of elongating ribosome with EF-Tu*GTP elucidates tRNA proof-reading (Cognate Structure II-B1)
Authors : Loveland, A.B.; Demo, G.; Korostelev, A.A.
Deposited on : 2020-03-31
Resolution : 3.60 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

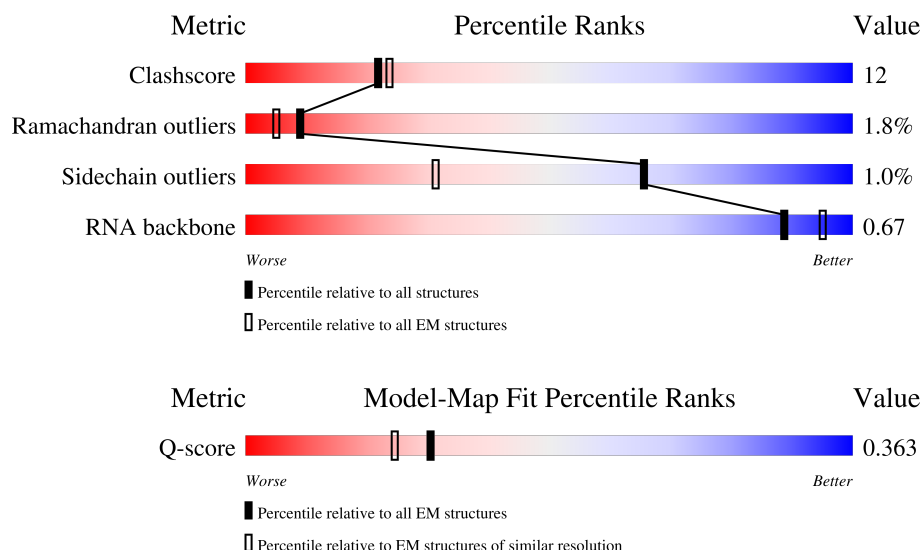
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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.



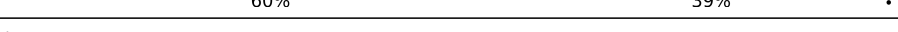
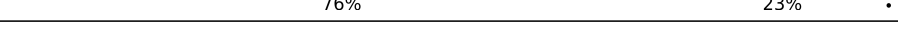
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	
5	f	176	
6	g	149	
7	h	131	
8	i	141	
9	j	142	
10	k	122	
11	l	143	
12	m	136	
13	n	120	
14	o	116	
15	p	114	
16	q	117	
17	r	103	
18	s	110	
19	t	93	
20	u	102	
21	v	94	
22	w	75	
23	x	77	
24	y	63	
25	z	58	
26	B	56	
27	C	50	
28	D	46	

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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	46% 48% 7%
55	5	77	65% 30% 5%
55	6	77	61% 35%
56	4	18	6% 50% 44% 6%
57	7	76	46% 43% 11%
58	8	400	54% 40%

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 153211 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	variant	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		

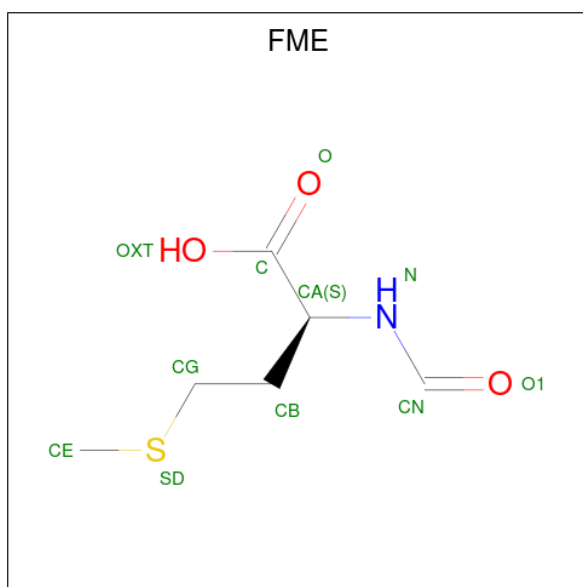
- Molecule 58 is a protein called Elongation factor Tu.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	8	383	Total	C	N	O	S	0	0
			2961	1876	507	565	13		

There are 7 discrepancies between the modelled and reference sequences:

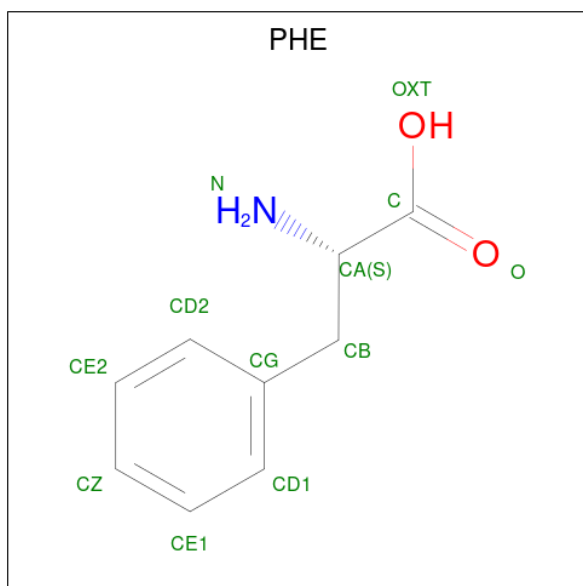
Chain	Residue	Modelled	Actual	Comment	Reference
8	395	SER	-	expression tag	UNP E2QFJ4
8	396	HIS	-	expression tag	UNP E2QFJ4
8	397	HIS	-	expression tag	UNP E2QFJ4
8	398	HIS	-	expression tag	UNP E2QFJ4
8	399	HIS	-	expression tag	UNP E2QFJ4
8	400	HIS	-	expression tag	UNP E2QFJ4
8	401	HIS	-	expression tag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

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



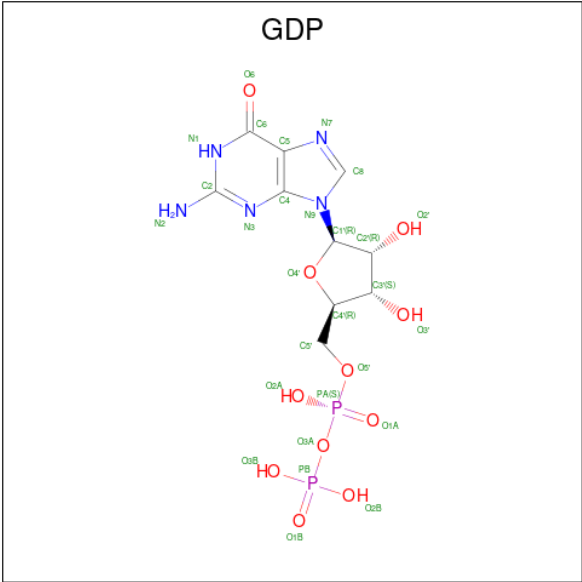
Mol	Chain	Residues	Atoms					AltConf
59	5	1	Total	C	N	O	S	0
			10	6	1	2	1	

- 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: $C_{10}H_{15}N_5O_{11}P_2$).

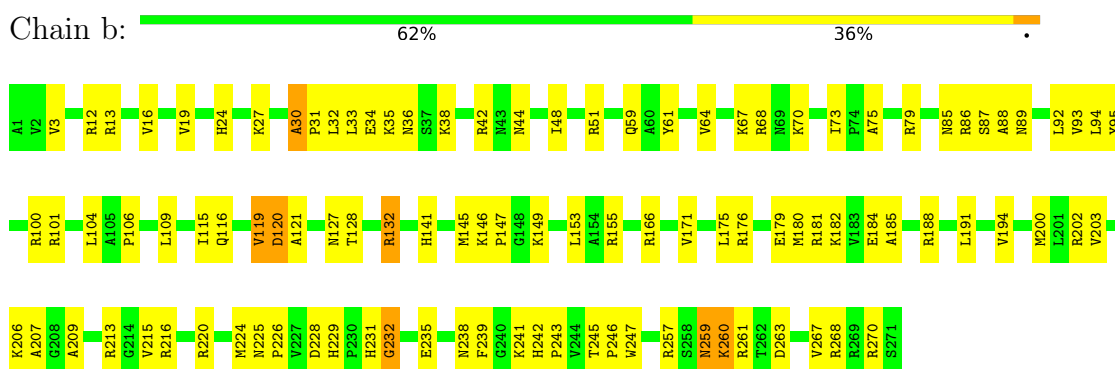


Mol	Chain	Residues	Atoms					AltConf
61	8	1	Total	C	N	O	P	0
			28	10	5	11	2	

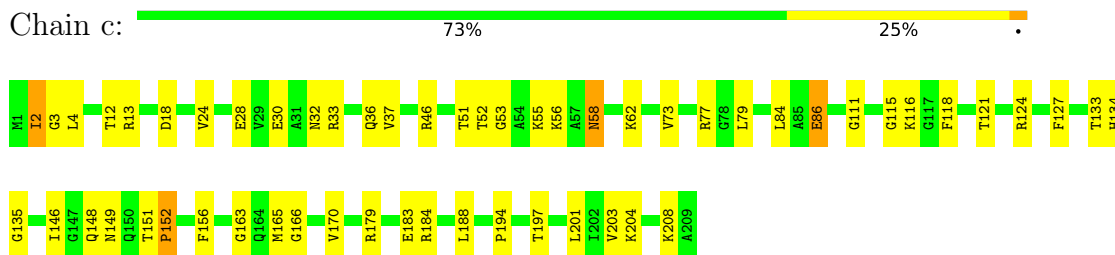
3 Residue-property plots

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.

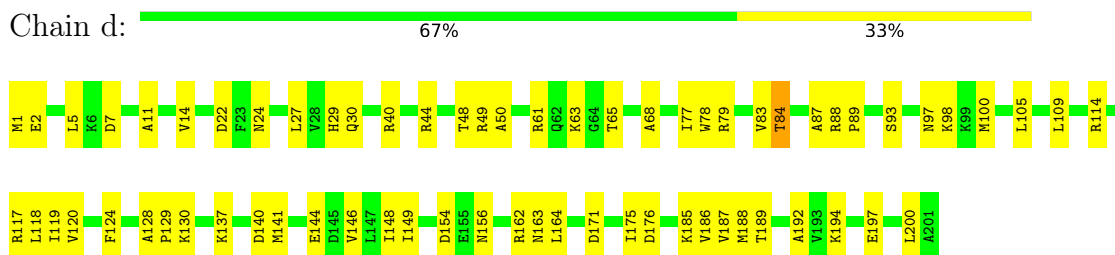
- Molecule 1: 50S ribosomal protein L2



- Molecule 2: 50S ribosomal protein L3

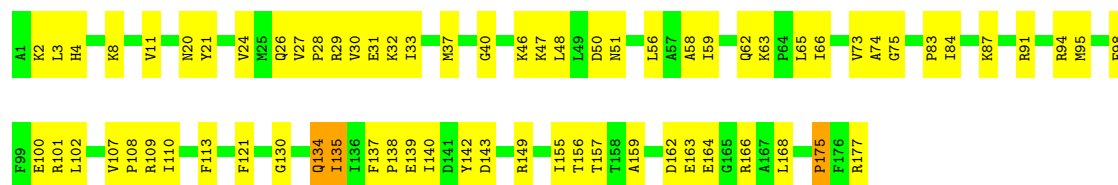


- Molecule 3: 50S ribosomal protein L4



- Molecule 4: 50S ribosomal protein L5





• Molecule 5: 50S ribosomal protein L6



• Molecule 6: 50S ribosomal protein L9



• Molecule 7: 50S ribosomal protein L10



• Molecule 8: 50S ribosomal protein L11



- Molecule 14: 50S ribosomal protein L18

Chain o:  71% 27%



- Molecule 15: 50S ribosomal protein L19

Chain p:  70% 29%



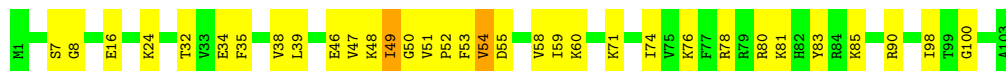
- Molecule 16: 50S ribosomal protein L20

Chain q:  83% 16%



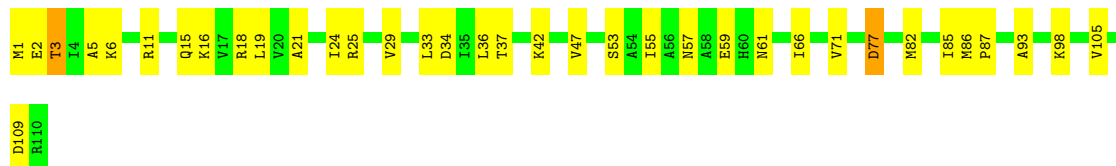
- Molecule 17: 50S ribosomal protein L21

Chain r:  68% 30%



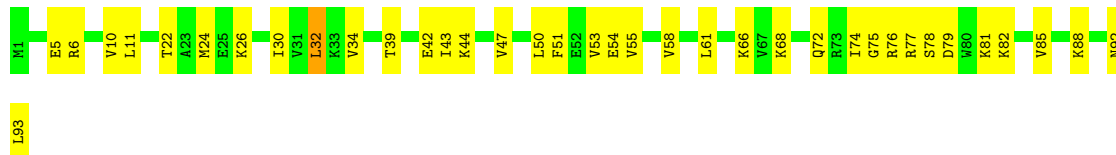
- Molecule 18: 50S ribosomal protein L22

Chain s:  67% 31%

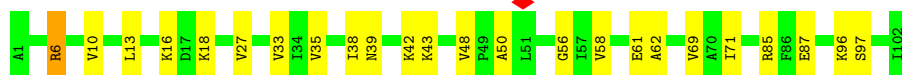
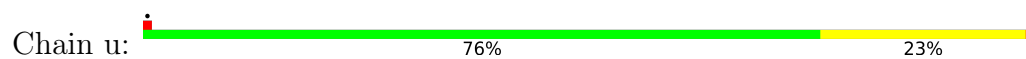


- Molecule 19: 50S ribosomal protein L23

Chain t:  60% 39%



- Molecule 20: 50S ribosomal protein L24



- Molecule 21: 50S ribosomal protein L25



- Molecule 22: 50S ribosomal protein L27



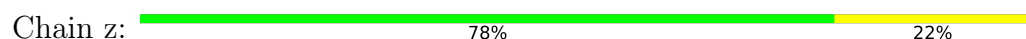
- Molecule 23: 50S ribosomal protein L28



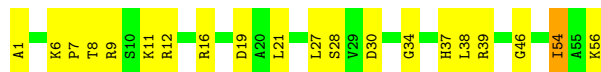
- Molecule 24: 50S ribosomal protein L29



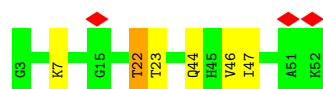
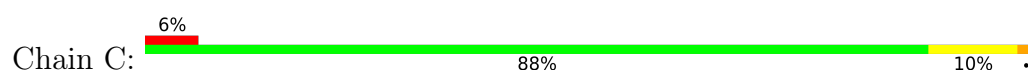
- Molecule 25: 50S ribosomal protein L30



- Molecule 26: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L33



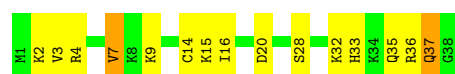
- Molecule 28: 50S ribosomal protein L34



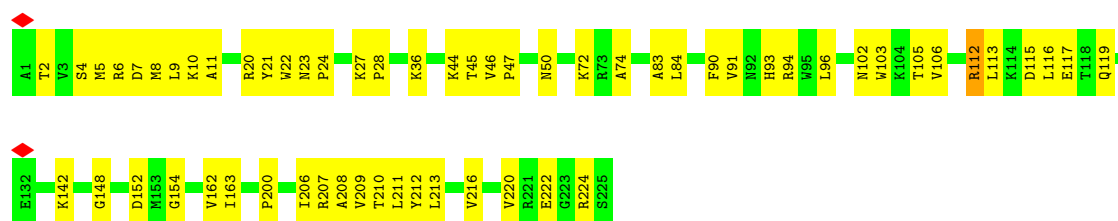
- Molecule 29: 50S ribosomal protein L35



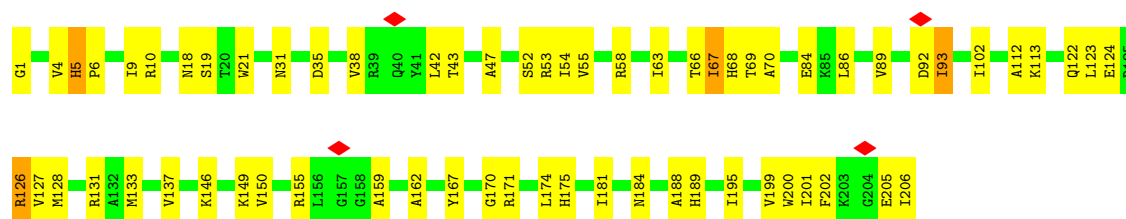
- Molecule 30: 50S ribosomal protein L36



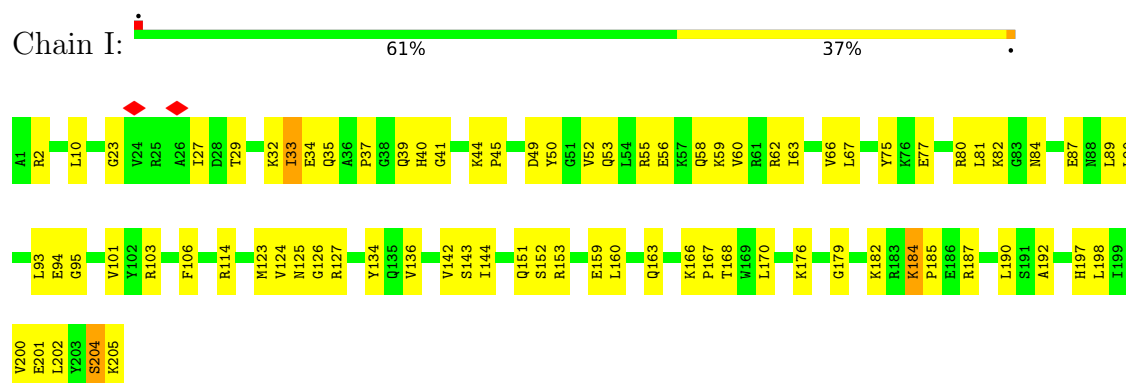
- Molecule 31: 30S ribosomal protein S2



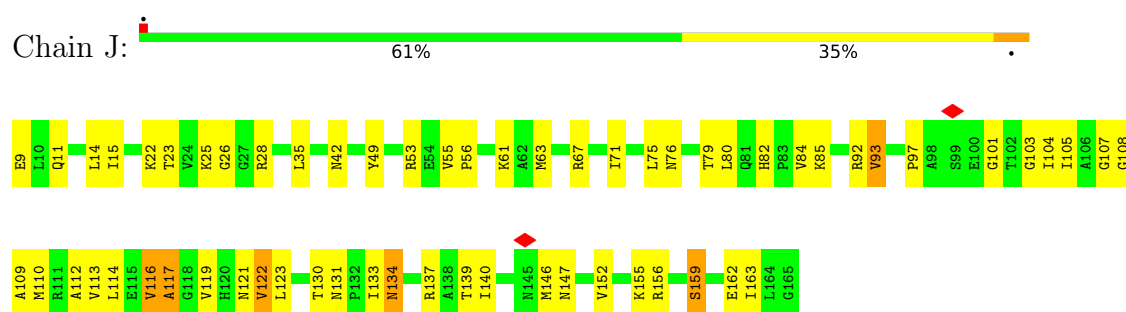
- Molecule 32: 30S ribosomal protein S3



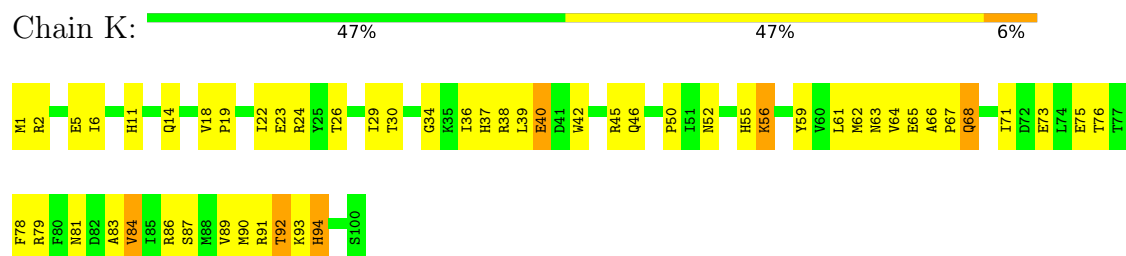
- Molecule 33: 30S ribosomal protein S4



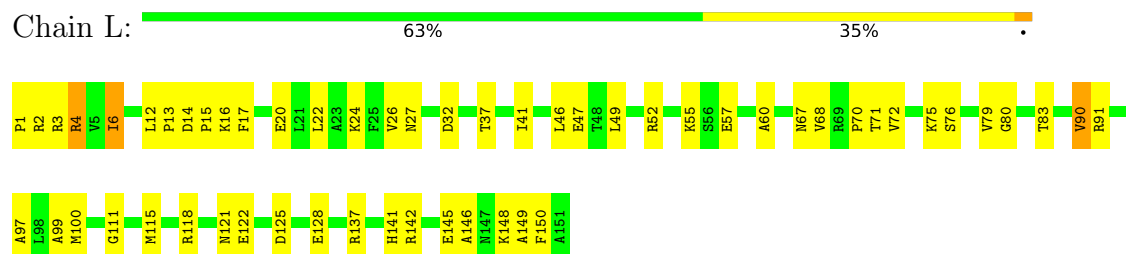
- Molecule 34: 30S ribosomal protein S5



- Molecule 35: 30S ribosomal protein S6

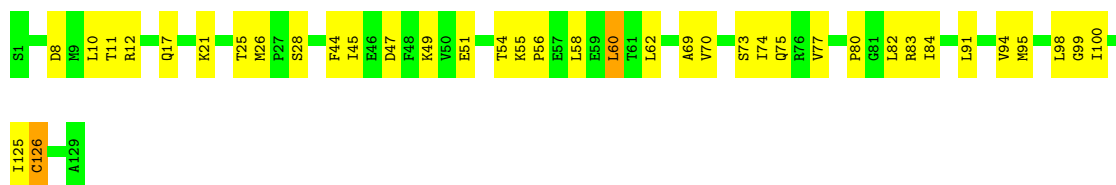


- Molecule 36: 30S ribosomal protein S7

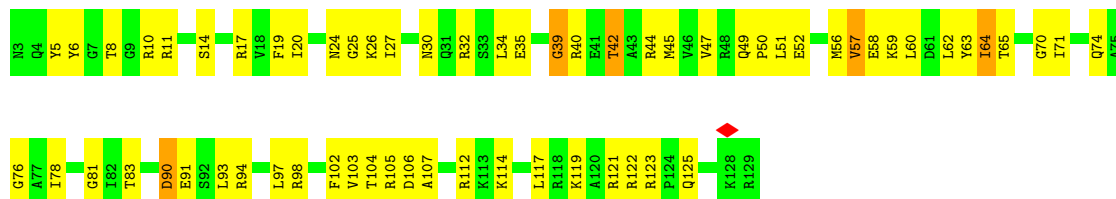


- Molecule 37: 30S ribosomal protein S8

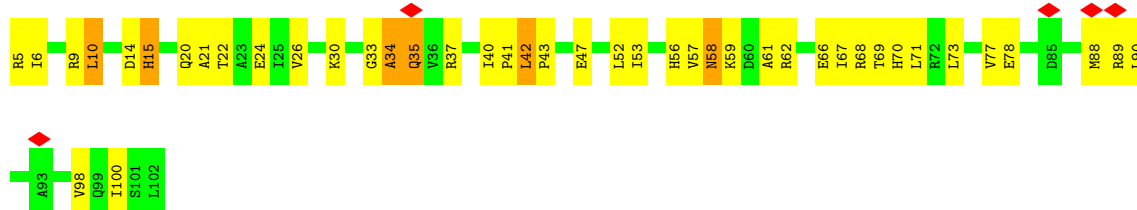




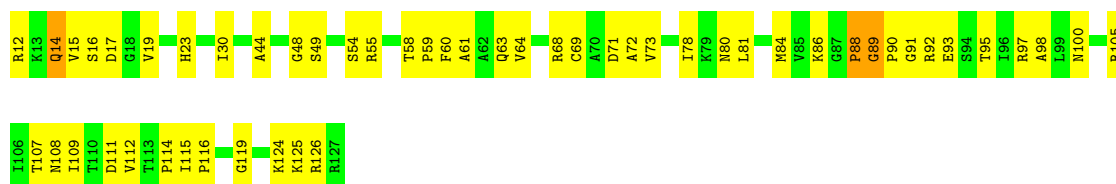
- Molecule 38: 30S ribosomal protein S9



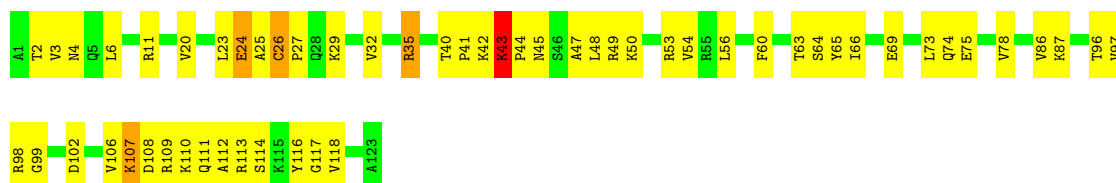
- Molecule 39: 30S ribosomal protein S10



- Molecule 40: 30S ribosomal protein S11

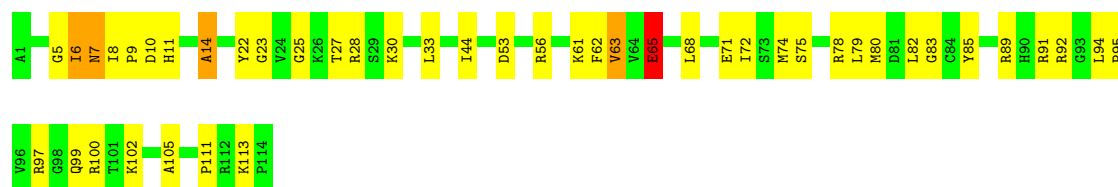


- Molecule 41: 30S ribosomal protein S12



- Molecule 42: 30S ribosomal protein S13

Chain R:  61% 35%



- Molecule 43: 30S ribosomal protein S14

Chain S:  49% 48%



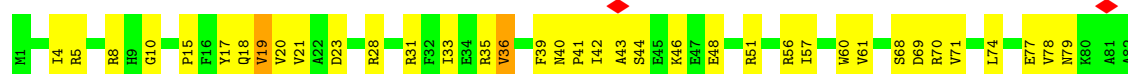
- Molecule 44: 30S ribosomal protein S15

Chain T:  78% 20%

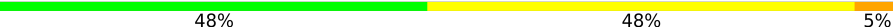


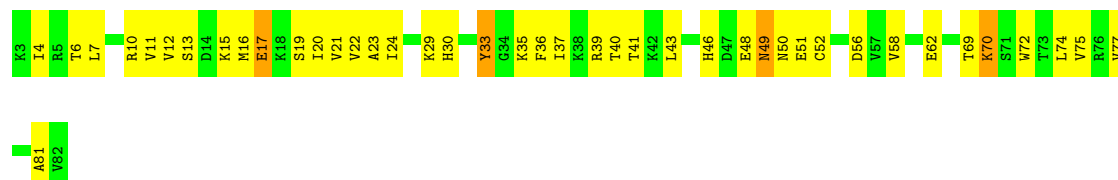
- Molecule 45: 30S ribosomal protein S16

Chain U:  55% 43%



- Molecule 46: 30S ribosomal protein S17

Chain V:  48% 48% 5%



- Molecule 47: 30S ribosomal protein S18

Chain W:  71% 28%





- Molecule 48: 30S ribosomal protein S19

Chain X: 58% 42%



- Molecule 49: 30S ribosomal protein S20

Chain Y: 61% 36%



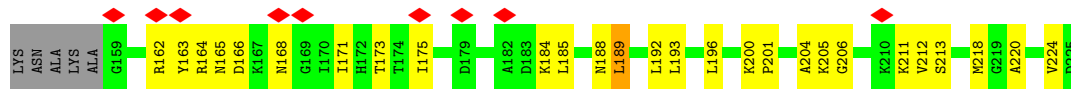
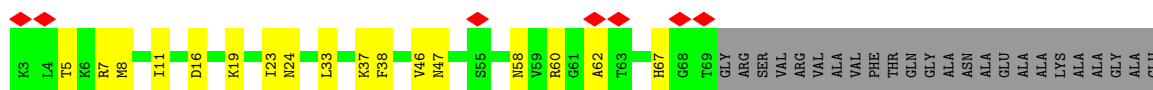
- Molecule 50: 30S ribosomal protein S21

Chain Z: 58% 35%



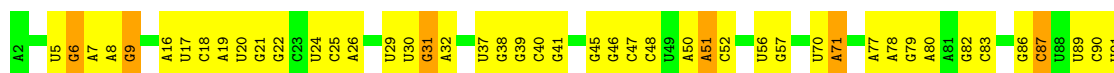
- Molecule 51: 50S ribosomal protein L1

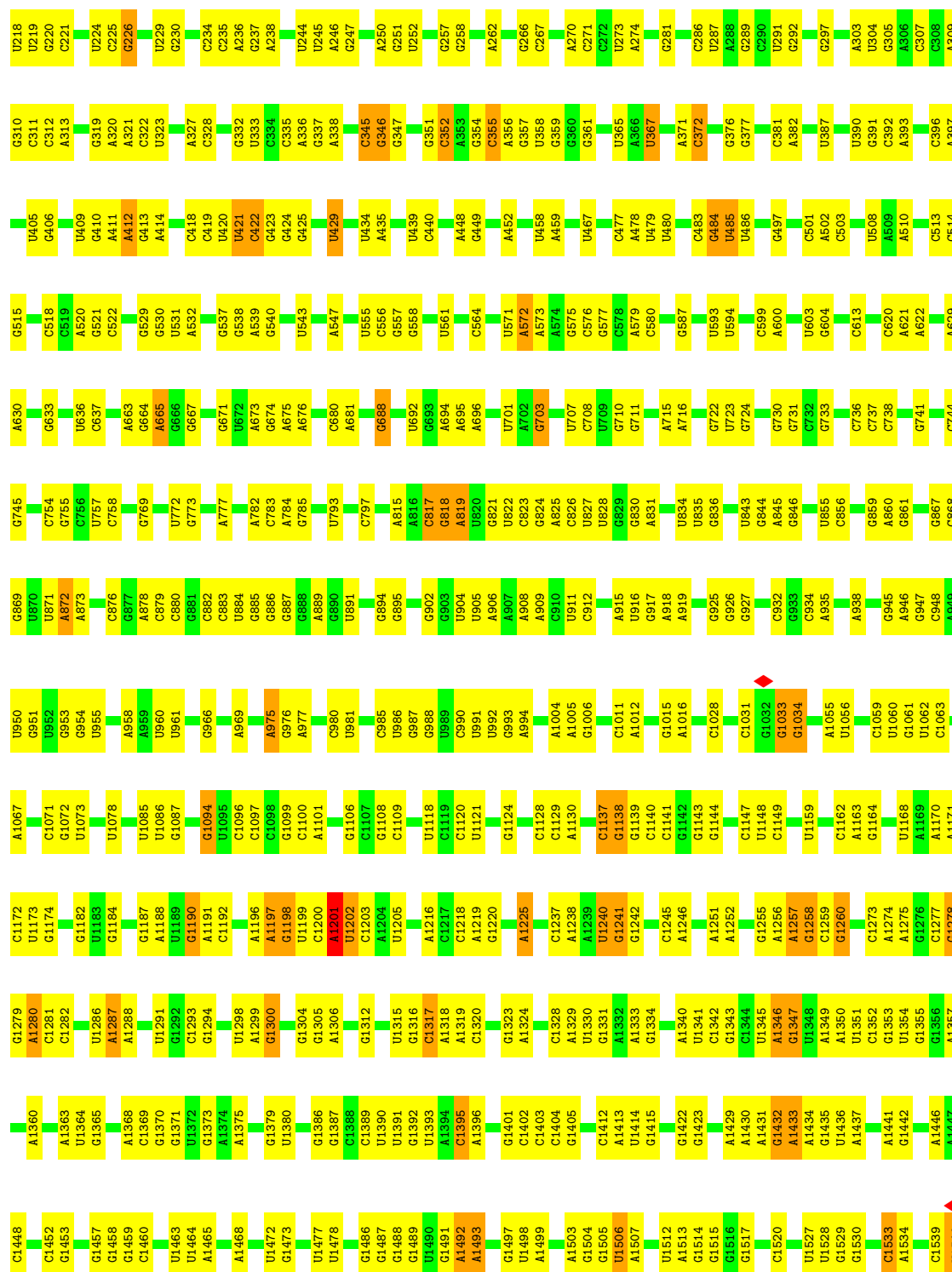
Chain a: 7% 40% 19% 40%



- Molecule 52: 16S ribosomal RNA

Chain 3: 58% 38%

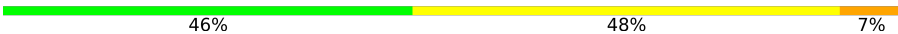


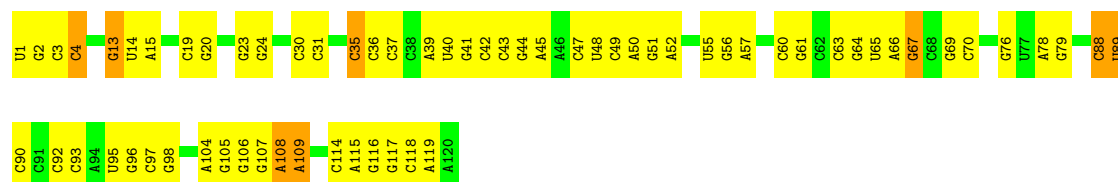




U2833	G2641	G2553	G2458	G2371	A2298	C2208	A2117	G2040	U1956	A1853	U1758	A1665	G1567
G2834	G2642	U2554	C2462	A2376	U2299	G2209	U2118	U2041	C1957	A1854	A1759	G1666	G1568
U2836	G2643	G2557	C2463	A2377	U2302	U2210	G2119	C2043	G1958	U1855	C1760	A1667	A1569
A2837	C2646	C2558	C2466	A2378	G2303	A2211	G2120	G2043	G1959	G1857	C1764	A1668	A1570
C2841	U2647	U2562	C2467	A2381	G2304	U2213	U2122	G2047	U1963	A1858	A1773	G1674	A1571
G2842	G2648	U2563	A2468	G2382	U2305	U2220	G2123	G2048	G1964	G1859	A1774	C1675	G1572
G2843	C2652	A2564	A2469	G2383	A2309	G2221	G2127	G2049	G1965	G1860	C1774	A1676	G1573
G2844	U2653	A2565	G2470	U2385	U2312	G2223	C2129	A2052	C1967	G1861	U1775	C1685	C1574
U2845	A2654	A2566	A2471	C2386	C2313	G2224	U2130	A2054	U1970	A1871	G1776	U1685	U1576
G2846	G2655	G2567	G2472	G2389	G2314	A2225	G2132	C2055	A1971	G1872	A1779	C1686	U1577
U2848	U2656	G2572	C2475	U2390	G2315	G2226	G2133	G2056	G1972	C1874	U1782	U1688	U1578
A2850	G2660	A2577	U2476	A2391	A2317	U2233	A2134	A2060	A1978	A1875	U1783	A1689	G1581
C2853	G2661	G2578	U2477	A2392	G2318	G2234	U2139	A2062	U1979	G1873	U1784	A1690	U1584
G2854	A2662	C2579	A2478	U2393	G2319	G2238	G2141	C2063	G1980	C1874	A1785	C1585	C1585
C2855	G2663	U2580	C2483	C2394	G2323	G2239	A2142	G2064	G1983	G1888	A1786	A1698	U1594
A2856	A2665	G2581	G2484	U2398	U2324	U2240	G2147	C2065	A1987	A1889	G1792	G1699	C1595
G2859	G2666	U2582	G2485	G2399	G2325	A2241	C2155	C2066	G1988	A1900	C1793	A1701	A1596
A2860	C2667	G2583	U2489	U2402	C2326	G2242	G2156	G2067	G1989	G1891	C1794	A1597	A1597
G2862	G2671	U2584	G2490	A2406	A2327	U2243	G2157	U2068	G1990	A1899	C1795	G1702	A1598
C2863	U2672	U2585	C2498	A2407	A2328	U2244	G2157	A2070	G1991	A1901	U1796	G1703	G1601
G2864	A2679	A2589	C2498	A2407	U2329	U2245	G2157	A2071	U1992	G1905	G1797	A1705	U1602
U2861	U2680	C2590	G2502	G2415	G2330	G2246	G2162	A2072	G1993	G1906	U1798	C1706	A1603
G2862	C2682	G2591	A2503	C2416	G2331	U2249	A2163	C2072	U1994	G1907	C1800	A1605	C1605
C2863	A2683	U2592	U2504	C2417	U2334	U2249	C2164	U2074	G1996	C1908	U1801	C1606	C1606
G2864	U2684	A2602	G2505	U2419	U2334	G2250	A2171	C2078	C1997	C1909	G1807	C1607	C1607
U2865	G2685	G2603	G2508	C2420	A2340	U2257	A2172	U2079	A1998	G1910	A1808	A1616	A1608
G2866	U2686	U2605	C2512	U2423	G2342	C2258	C2174	A2080	G1999	U1911	A1809	U1716	C1611
U2869	U2689	C2606	U2514	A2425	U2344	U2262	G2176	G2083	C2008	A1912	A1810	G1718	C1612
C2870	U2690	U2609	U2514	A2426	G2345	U2267	C2177	C2084	A2009	A1913	G1811	U1720	G1613
G2871	U2691	C2610	C2515	A2427	A2346	A2266	C2177	U2086	U2011	A1918	U1812	G1721	G1614
U2872	C2692	U2613	A2518	G2428	C2347	A2267	U2180	U2087	G2012	A1919	C1816	U1725	C1615
A2873	U2693	A2614	U2519	G2429	U2348	A2268	U2181	A2088	A2019	C1920	G1817	C1726	A1616
C2874	U2694	C2619	C2520	A2430	G2349	G2277	U2182	U2088	G1929	G1930	A1818	C1727	U1629
G2875	U2695	U2617	C2521	U2431	G2351	A2278	A2183	A2088	U1931	G1931	A1821	C1728	U1729
U2876	U2696	G2618	G2521	A2432	G2351	A2278	A2183	A2088	U1932	A1932	C1822	C1730	U1636
A2877	U2697	C2619	A2530	A2435	G2354	A2281	U2185	A2088	G2023	G1933	G1823	U1736	A1637
C2878	U2698	U2620	U2533	U2441	A2358	G2282	G2190	C2096	C2023	G1934	G1824	C1639	C1639
G2879	U2699	G2623	A2534	G2442	C2359	A2284	A2191	A2101	G2026	U1935	U1825	G1737	G1645
U2880	U2700	G2624	U2534	C2443	G2360	C2285	U2192	C2103	U2028	A1936	G1826	G1738	C1646
C2881	C2704	C2628	U2537	G2444	G2361	A2286	G2193	C2104	G2029	A1937	U1827	U1744	U1647
U2882	A2705	U2629	C2538	G2447	C2362	A2288	U2194	U2105	A2030	A1938	G1828	A1745	U1648
G2883	U2706	U2632	U2539	A2448	G2363	U2291	C2196	G2107	G2032	U1943	A1829	A1746	U1648
U2884	U2707	G2633	G2546	U2449	C2364	U2292	U2197	U2107	A2033	U1944	G1830	U1747	A1652
C2885	G2708	G2633	U2546	A2450	G2365	U2293	A2198	G2110	G2034	G1832	C1833	G1753	G1653
U2886	U2709	C2636	U2547	A2451	A2366	G2294	U2199	U2111	U2035	C1947	U1834	A1754	U1657
C2887	C2710	G2637	A2548	C2452	G2367	G2295	G2204	G2112	C2036	G1948	U1837	A1755	C1658
U2888	A2711	U2638	U2548	A2452	A2368	U2296	U2203	A2114	G2037	G1954	C1837	G1756	A1664
G2889	A2712	G2638	U2552	U2457	G2370	A2297	G2204	U2114	U2039	U1955		A1757	

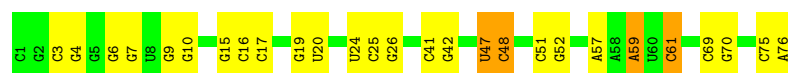
- Molecule 54: 5S ribosomal RNA

Chain 2: 



- Molecule 55: tRNA^{fMet}

Chain 5: 



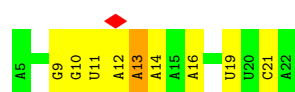
- Molecule 55: tRNA^{fMet}

Chain 6: 



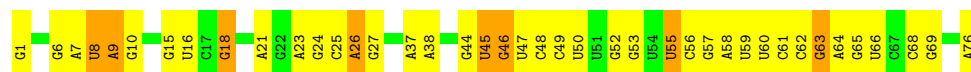
- Molecule 56: mRNA

Chain 4: 



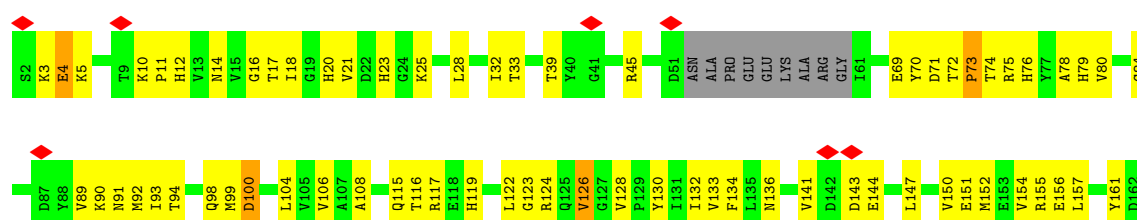
- Molecule 57: tRNA^{Phe}

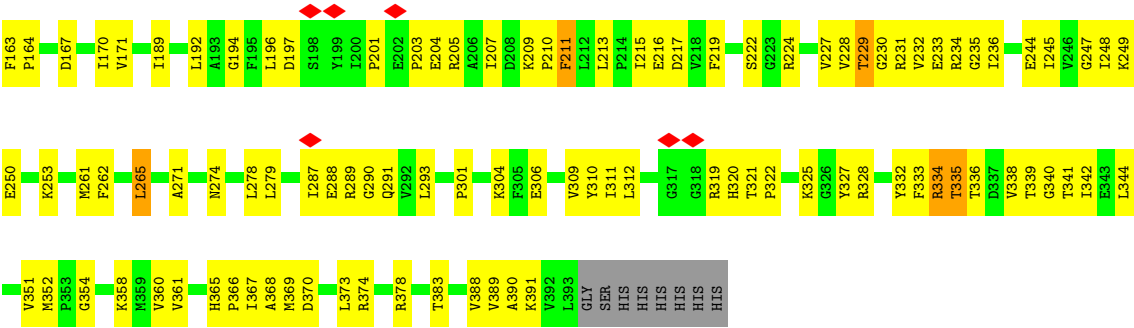
Chain 7: 



- 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	7401	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	18.877	Depositor
Minimum map value	-10.681	Depositor
Average map value	0.115	Depositor
Map value standard deviation	0.882	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	0.98	12/2852 (0.4%)
2	c	0.29	0/1586	0.89	2/2134 (0.1%)
3	d	0.29	0/1571	0.85	3/2113 (0.1%)
4	e	0.30	0/1435	0.88	3/1926 (0.2%)
5	f	0.30	0/1343	0.93	5/1816 (0.3%)
6	g	0.31	0/1122	0.90	2/1515 (0.1%)
7	h	0.34	0/1002	1.05	7/1350 (0.5%)
8	i	0.36	0/1046	0.97	6/1410 (0.4%)
9	j	0.30	0/1152	0.85	1/1551 (0.1%)
10	k	0.29	0/948	0.97	3/1268 (0.2%)
11	l	0.30	0/1054	1.05	10/1403 (0.7%)
12	m	0.29	0/1093	0.87	3/1460 (0.2%)
13	n	0.29	0/974	0.95	5/1301 (0.4%)
14	o	0.29	0/902	0.87	2/1209 (0.2%)
15	p	0.29	0/929	0.84	4/1242 (0.3%)
16	q	0.28	0/960	0.96	4/1278 (0.3%)
17	r	0.29	0/829	0.88	3/1107 (0.3%)
18	s	0.29	0/864	0.95	1/1156 (0.1%)
19	t	0.28	0/745	0.83	0/994
20	u	0.29	0/788	0.88	1/1051 (0.1%)
21	v	0.28	0/766	0.83	0/1025
22	w	0.27	0/582	0.86	1/769 (0.1%)
23	x	0.28	0/635	0.85	1/848 (0.1%)
24	y	0.29	0/510	0.90	3/677 (0.4%)
25	z	0.30	0/453	0.91	1/605 (0.2%)
26	B	0.29	0/450	0.82	1/599 (0.2%)
27	C	0.32	0/417	0.80	0/554
28	D	0.32	0/380	0.89	1/498 (0.2%)
29	E	0.30	0/513	1.00	3/676 (0.4%)
30	F	0.33	0/303	0.99	2/397 (0.5%)
31	G	0.29	0/1788	0.90	5/2408 (0.2%)
32	H	0.32	0/1652	0.93	5/2225 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	I	0.30	0/1665	0.94	8/2227 (0.4%)
34	J	0.34	0/1170	0.99	6/1573 (0.4%)
35	K	0.31	0/836	1.00	7/1128 (0.6%)
36	L	0.29	0/1196	0.96	5/1602 (0.3%)
37	M	0.29	0/989	0.97	5/1326 (0.4%)
38	N	0.29	0/1034	0.89	2/1375 (0.1%)
39	O	0.32	0/797	0.90	2/1077 (0.2%)
40	P	0.33	0/886	0.92	1/1195 (0.1%)
41	Q	0.32	0/969	1.03	9/1300 (0.7%)
42	R	0.32	0/893	0.93	2/1193 (0.2%)
43	S	0.30	0/817	0.92	5/1088 (0.5%)
44	T	0.28	0/722	0.89	5/964 (0.5%)
45	U	0.30	0/659	0.87	2/884 (0.2%)
46	V	0.29	0/658	0.98	3/881 (0.3%)
47	W	0.31	0/545	0.93	2/731 (0.3%)
48	X	0.31	0/653	0.93	1/877 (0.1%)
49	Y	0.29	0/671	0.97	4/888 (0.5%)
50	Z	0.33	0/551	0.97	3/728 (0.4%)
51	a	0.32	0/1034	0.82	2/1387 (0.1%)
52	3	0.41	0/36963	0.47	2/57662 (0.0%)
53	1	0.40	0/69796	0.48	3/108888 (0.0%)
54	2	0.41	0/2872	0.47	0/4479
55	5	0.41	0/1832	0.46	0/2855
55	6	0.42	0/1832	0.48	0/2855
56	4	0.41	0/436	0.47	0/679
57	7	0.40	0/1809	0.48	0/2819
58	8	0.32	0/3015	0.90	8/4079 (0.2%)
All	All	0.38	0/166214	0.63	187/248157 (0.1%)

There are no bond length outliers.

The worst 5 of 187 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	V	75	VAL	N-CA-C	-10.67	103.19	111.62
40	P	73	VAL	N-CA-C	-10.56	103.06	113.20
34	J	117	ALA	N-CA-C	-10.27	100.16	112.89
17	r	50	GLY	N-CA-C	-9.67	100.79	112.49
1	b	87	SER	N-CA-C	-9.62	102.34	114.56

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	78	0
2	c	1565	0	1616	41	0
3	d	1552	0	1619	53	0
4	e	1411	0	1447	56	0
5	f	1323	0	1374	30	0
6	g	1111	0	1148	35	0
7	h	989	0	1025	60	0
8	i	1032	0	1088	45	0
9	j	1129	0	1162	31	0
10	k	939	0	1012	38	0
11	l	1045	0	1117	37	0
12	m	1074	0	1157	41	0
13	n	961	0	1000	22	0
14	o	892	0	923	20	0
15	p	917	0	965	34	0
16	q	947	0	1022	20	0
17	r	816	0	839	24	0
18	s	857	0	922	26	0
19	t	739	0	807	25	0
20	u	780	0	834	18	0
21	v	753	0	780	14	0
22	w	575	0	592	21	0
23	x	625	0	655	23	0
24	y	509	0	543	15	0
25	z	449	0	491	9	0
26	B	444	0	461	16	0
27	C	410	0	440	4	0
28	D	377	0	418	16	0
29	E	504	0	574	20	0
30	F	302	0	343	12	0
31	G	1757	0	1787	41	0
32	H	1625	0	1699	50	0
33	I	1643	0	1710	57	0
34	J	1157	0	1199	48	0
35	K	818	0	808	39	0
36	L	1182	0	1240	44	0
37	M	979	0	1034	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	N	1022	0	1070	48	0
39	O	787	0	828	38	0
40	P	870	0	878	39	0
41	Q	955	0	1019	46	0
42	R	884	0	944	34	0
43	S	805	0	847	42	0
44	T	714	0	737	15	0
45	U	649	0	666	32	0
46	V	649	0	691	33	0
47	W	536	0	552	12	0
48	X	638	0	665	28	0
49	Y	665	0	714	30	0
50	Z	545	0	579	34	0
51	a	1027	0	1092	37	0
52	3	33012	0	16618	542	0
53	1	62317	0	31346	962	0
54	2	2568	0	1303	66	0
55	5	1640	0	836	21	0
55	6	1640	0	837	23	0
56	4	388	0	196	10	0
57	7	1619	0	821	39	0
58	8	2961	0	2978	117	0
59	5	10	0	10	3	0
60	7	11	0	8	3	0
61	8	28	0	12	0	0
All	All	153211	0	104255	2988	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 12.

The worst 5 of 2988 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)
50:Z:44:ARG:HE	52:3:722:G:H5'	1.16	1.08
53:1:1906:G:H2'	53:1:1907:G:H5''	1.39	1.03
58:8:16:GLY:HA3	58:8:80:VAL:HG22	1.42	1.01
35:K:2:ARG:HG3	35:K:92:THR:HG22	1.40	1.00
20:u:16:LYS:HG3	53:1:329:G:H1	1.24	1.00

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%)	224 (83%)	41 (15%)	4 (2%)	8	37
2	c	207/209 (99%)	185 (89%)	20 (10%)	2 (1%)	12	45
3	d	199/201 (99%)	178 (89%)	18 (9%)	3 (2%)	8	37
4	e	175/177 (99%)	147 (84%)	25 (14%)	3 (2%)	7	35
5	f	174/176 (99%)	156 (90%)	16 (9%)	2 (1%)	11	43
6	g	147/149 (99%)	123 (84%)	20 (14%)	4 (3%)	4	27
7	h	129/131 (98%)	92 (71%)	33 (26%)	4 (3%)	3	25
8	i	139/141 (99%)	119 (86%)	14 (10%)	6 (4%)	2	18
9	j	140/142 (99%)	125 (89%)	14 (10%)	1 (1%)	18	51
10	k	120/122 (98%)	100 (83%)	18 (15%)	2 (2%)	7	35
11	l	141/143 (99%)	117 (83%)	21 (15%)	3 (2%)	5	31
12	m	134/136 (98%)	117 (87%)	15 (11%)	2 (2%)	8	37
13	n	118/120 (98%)	99 (84%)	19 (16%)	0	100	100
14	o	114/116 (98%)	104 (91%)	7 (6%)	3 (3%)	4	27
15	p	112/114 (98%)	93 (83%)	19 (17%)	0	100	100
16	q	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
17	r	101/103 (98%)	85 (84%)	14 (14%)	2 (2%)	6	32
18	s	108/110 (98%)	96 (89%)	11 (10%)	1 (1%)	14	46
19	t	91/93 (98%)	79 (87%)	11 (12%)	1 (1%)	11	43
20	u	100/102 (98%)	84 (84%)	14 (14%)	2 (2%)	6	32
21	v	92/94 (98%)	83 (90%)	9 (10%)	0	100	100
22	w	73/75 (97%)	65 (89%)	8 (11%)	0	100	100
23	x	75/77 (97%)	69 (92%)	5 (7%)	1 (1%)	9	39
24	y	61/63 (97%)	55 (90%)	5 (8%)	1 (2%)	7	36
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%)	47 (87%)	7 (13%)	0	100	100
27	C	48/50 (96%)	42 (88%)	6 (12%)	0	100	100
28	D	44/46 (96%)	37 (84%)	7 (16%)	0	100	100
29	E	62/64 (97%)	55 (89%)	6 (10%)	1 (2%)	7	36
30	F	36/38 (95%)	28 (78%)	7 (19%)	1 (3%)	4	26
31	G	223/225 (99%)	203 (91%)	18 (8%)	2 (1%)	14	46
32	H	204/206 (99%)	192 (94%)	11 (5%)	1 (0%)	24	57
33	I	203/205 (99%)	181 (89%)	21 (10%)	1 (0%)	24	57
34	J	155/157 (99%)	130 (84%)	21 (14%)	4 (3%)	4	27
35	K	98/100 (98%)	81 (83%)	13 (13%)	4 (4%)	2	19
36	L	149/151 (99%)	128 (86%)	19 (13%)	2 (1%)	9	39
37	M	127/129 (98%)	113 (89%)	13 (10%)	1 (1%)	16	49
38	N	125/127 (98%)	102 (82%)	17 (14%)	6 (5%)	2	16
39	O	96/98 (98%)	72 (75%)	15 (16%)	9 (9%)	0	6
40	P	114/116 (98%)	94 (82%)	16 (14%)	4 (4%)	3	23
41	Q	121/123 (98%)	94 (78%)	21 (17%)	6 (5%)	1	16
42	R	112/114 (98%)	95 (85%)	12 (11%)	5 (4%)	2	17
43	S	98/100 (98%)	80 (82%)	18 (18%)	0	100	100
44	T	86/88 (98%)	79 (92%)	7 (8%)	0	100	100
45	U	80/82 (98%)	67 (84%)	12 (15%)	1 (1%)	9	39
46	V	78/80 (98%)	60 (77%)	14 (18%)	4 (5%)	1	15
47	W	63/65 (97%)	57 (90%)	5 (8%)	1 (2%)	7	36
48	X	77/79 (98%)	62 (80%)	14 (18%)	1 (1%)	9	39
49	Y	83/85 (98%)	76 (92%)	7 (8%)	0	100	100
50	Z	63/65 (97%)	44 (70%)	14 (22%)	5 (8%)	1	8
51	a	130/223 (58%)	125 (96%)	5 (4%)	0	100	100
58	8	379/400 (95%)	333 (88%)	41 (11%)	5 (1%)	9	39
All	All	6298/6512 (97%)	5433 (86%)	754 (12%)	111 (2%)	9	34

5 of 111 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	b	232	GLY

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Mol	Chain	Res	Type
2	c	86	GLU
3	d	83	VAL
5	f	45	ALA
5	f	174	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	b	216/216 (100%)	214 (99%)	2 (1%)	70	76
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%)	146 (99%)	2 (1%)	59	71
5	f	137/137 (100%)	136 (99%)	1 (1%)	76	78
6	g	114/114 (100%)	113 (99%)	1 (1%)	70	76
7	h	100/100 (100%)	96 (96%)	4 (4%)	28	54
8	i	109/109 (100%)	109 (100%)	0	100	100
9	j	116/116 (100%)	116 (100%)	0	100	100
10	k	103/103 (100%)	101 (98%)	2 (2%)	50	67
11	l	102/102 (100%)	99 (97%)	3 (3%)	37	60
12	m	109/109 (100%)	109 (100%)	0	100	100
13	n	100/100 (100%)	99 (99%)	1 (1%)	68	75
14	o	86/86 (100%)	85 (99%)	1 (1%)	63	73
15	p	99/99 (100%)	99 (100%)	0	100	100
16	q	89/89 (100%)	89 (100%)	0	100	100
17	r	84/84 (100%)	83 (99%)	1 (1%)	63	73
18	s	93/93 (100%)	91 (98%)	2 (2%)	45	65
19	t	80/80 (100%)	79 (99%)	1 (1%)	61	72
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%)	76 (97%)	2 (3%)	40	62
22	w	57/57 (100%)	56 (98%)	1 (2%)	51	68
23	x	67/67 (100%)	67 (100%)	0	100	100
24	y	55/55 (100%)	54 (98%)	1 (2%)	51	68
25	z	48/48 (100%)	48 (100%)	0	100	100
26	B	47/47 (100%)	47 (100%)	0	100	100
27	C	45/45 (100%)	44 (98%)	1 (2%)	45	65
28	D	38/38 (100%)	37 (97%)	1 (3%)	40	62
29	E	51/51 (100%)	49 (96%)	2 (4%)	28	54
30	F	34/34 (100%)	34 (100%)	0	100	100
31	G	186/186 (100%)	186 (100%)	0	100	100
32	H	170/170 (100%)	167 (98%)	3 (2%)	51	68
33	I	172/172 (100%)	172 (100%)	0	100	100
34	J	119/119 (100%)	117 (98%)	2 (2%)	53	69
35	K	87/87 (100%)	86 (99%)	1 (1%)	65	74
36	L	124/124 (100%)	124 (100%)	0	100	100
37	M	104/104 (100%)	103 (99%)	1 (1%)	68	75
38	N	105/105 (100%)	104 (99%)	1 (1%)	68	75
39	O	86/86 (100%)	84 (98%)	2 (2%)	44	64
40	P	89/89 (100%)	89 (100%)	0	100	100
41	Q	103/103 (100%)	101 (98%)	2 (2%)	50	67
42	R	92/92 (100%)	91 (99%)	1 (1%)	65	74
43	S	83/83 (100%)	83 (100%)	0	100	100
44	T	76/76 (100%)	76 (100%)	0	100	100
45	U	65/65 (100%)	62 (95%)	3 (5%)	24	51
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%)	69 (99%)	1 (1%)	59	71
49	Y	65/65 (100%)	64 (98%)	1 (2%)	57	70
50	Z	55/55 (100%)	55 (100%)	0	100	100
51	a	110/174 (63%)	109 (99%)	1 (1%)	70	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
58	8	318/332 (96%)	318 (100%)	0	100	100
All	All	5226/5304 (98%)	5176 (99%)	50 (1%)	65	75

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
28	D	44	VAL
34	J	159	SER
51	a	189	LEU
29	E	6	VAL
32	H	93	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 108 such sidechains are listed below:

Mol	Chain	Res	Type
23	x	16	ASN
31	G	176	ASN
46	V	30	HIS
24	y	39	GLN
27	C	25	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
52	3	1538/1539 (99%)	139 (9%)	4 (0%)
53	1	2902/2903 (99%)	327 (11%)	12 (0%)
54	2	119/120 (99%)	9 (7%)	1 (0%)
55	5	76/77 (98%)	7 (9%)	0
55	6	76/77 (98%)	6 (7%)	1 (1%)
56	4	17/18 (94%)	3 (17%)	0
57	7	75/76 (98%)	14 (18%)	0
All	All	4803/4810 (99%)	505 (10%)	18 (0%)

5 of 505 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
52	3	6	G
52	3	7	A
52	3	9	G

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Mol	Chain	Res	Type
52	3	22	G
52	3	31	G

5 of 18 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
53	1	2326	C
55	6	17(A)	U
54	2	88	C
53	1	1020	A
53	1	2296	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
61	GDP	8	501	-	29,30,30	1.28	3 (10%)	45,47,47	2.24	17 (37%)
59	FME	5	101	55	8,9,10	0.48	0	8,9,11	0.86	0
60	PHE	7	101	57	10,11,12	0.70	0	8,13,15	0.25	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
61	GDP	8	501	-	-	2/16/32/32	0/3/3/3
59	FME	5	101	55	-	1/7/9/11	-
60	PHE	7	101	57	-	0/5/6/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	8	501	GDP	PB-O1B	2.97	1.59	1.50
61	8	501	GDP	PA-O3A	2.91	1.62	1.59
61	8	501	GDP	PB-O2B	2.35	1.63	1.54

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	8	501	GDP	C2-N3-C4	5.55	121.86	112.30
61	8	501	GDP	C5-C4-N3	-5.34	119.89	128.39
61	8	501	GDP	O2B-PB-O1B	-4.47	93.41	110.83
61	8	501	GDP	O3B-PB-O1B	4.29	127.56	110.83
61	8	501	GDP	N9-C4-N3	4.02	133.99	125.95

There are no chirality outliers.

All (3) 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

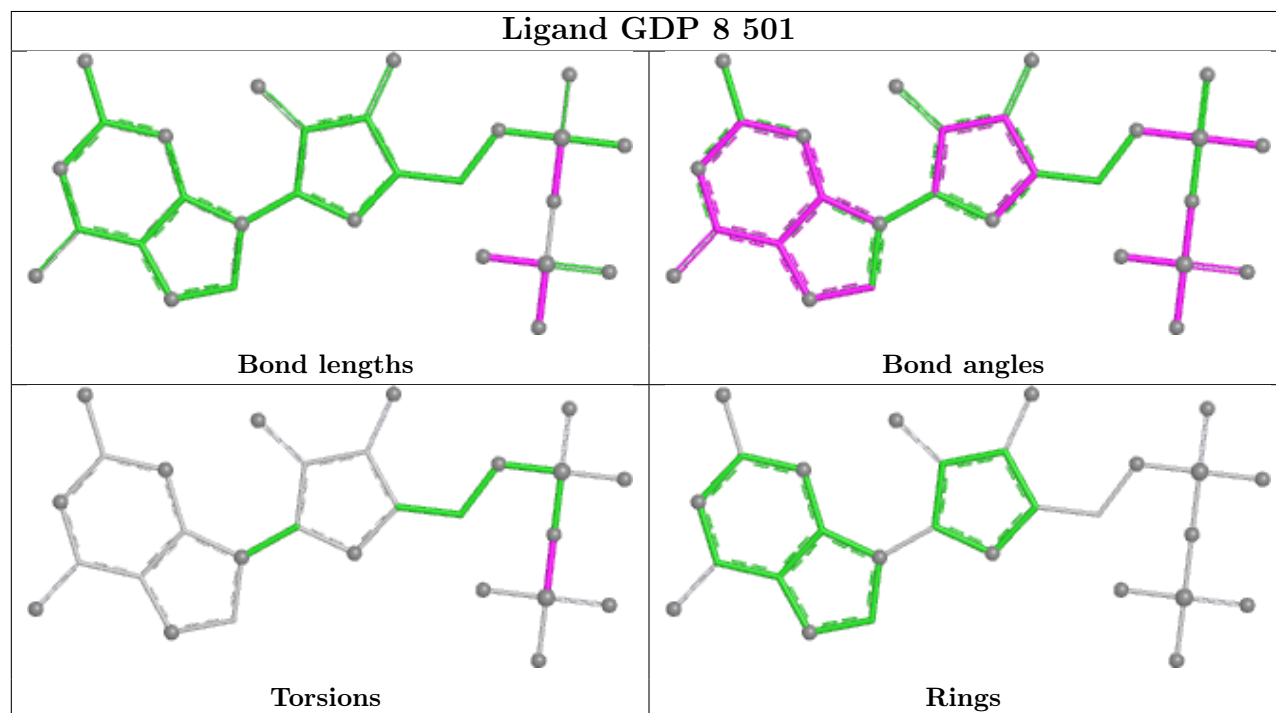
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	5	101	FME	3	0
60	7	101	PHE	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

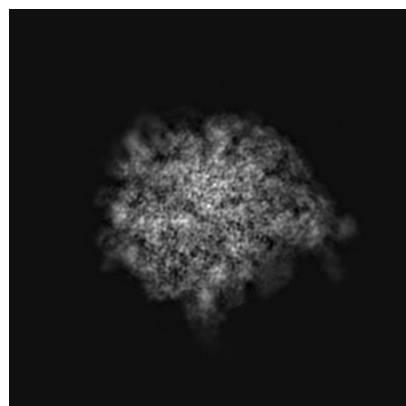
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21622. These allow visual inspection of the internal detail of the map and identification of artifacts.

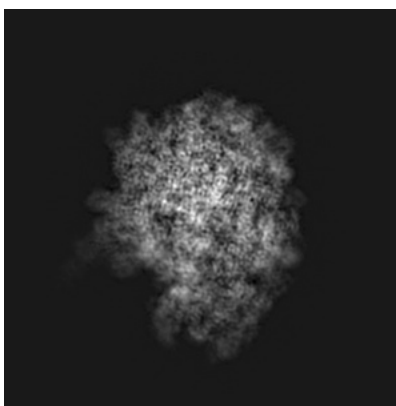
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

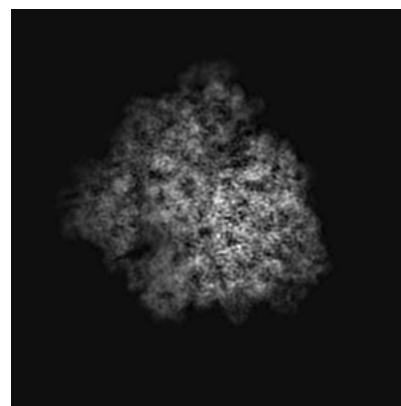
6.1.1 Primary map



X

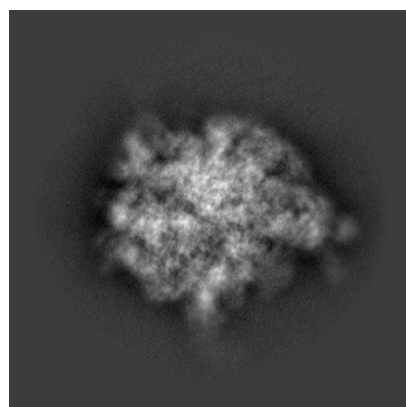


Y

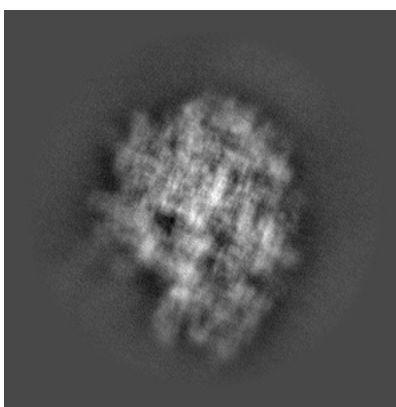


Z

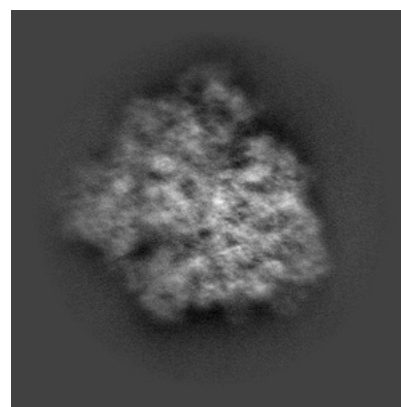
6.1.2 Raw map



X



Y

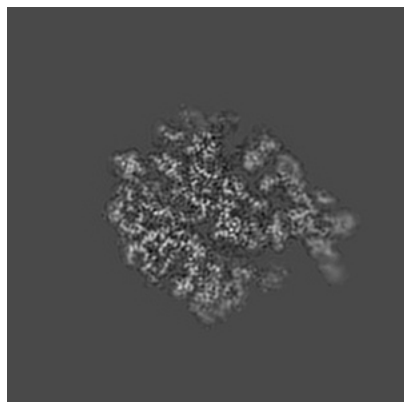


Z

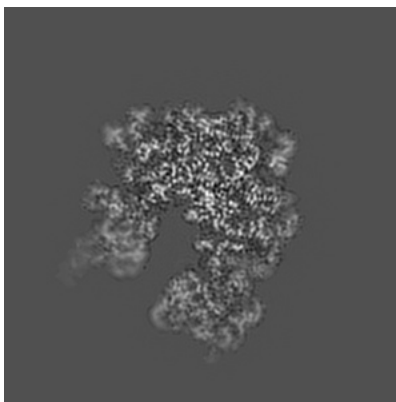
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

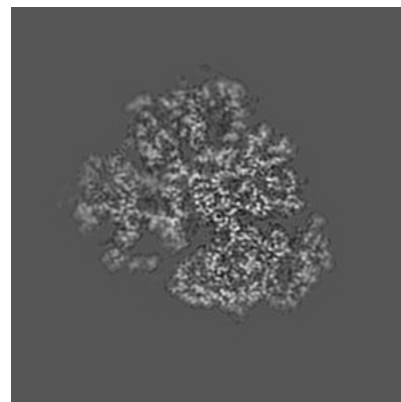
6.2.1 Primary map



X Index: 144

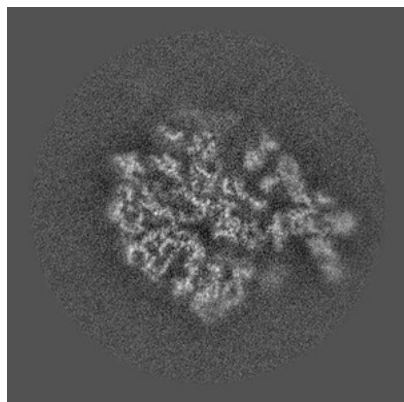


Y Index: 144

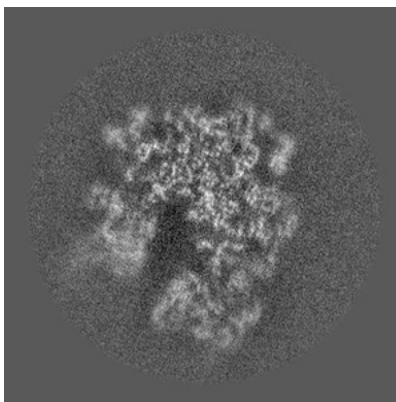


Z Index: 144

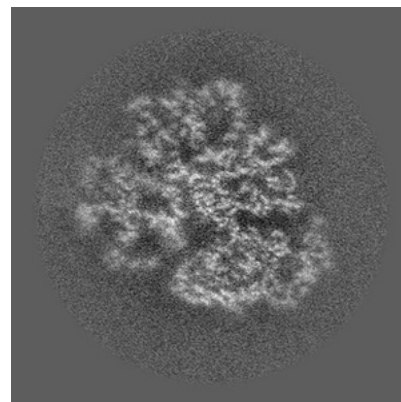
6.2.2 Raw map



X Index: 144



Y Index: 144

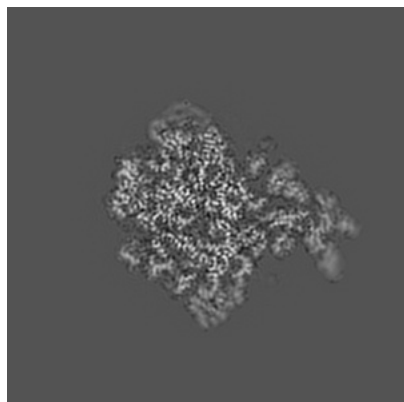


Z Index: 144

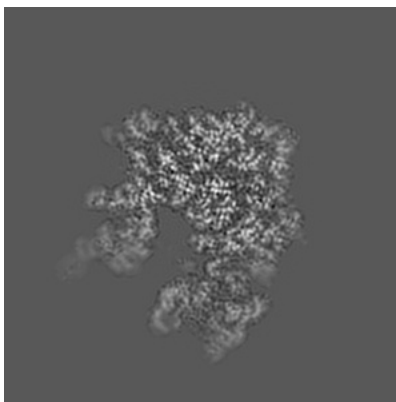
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

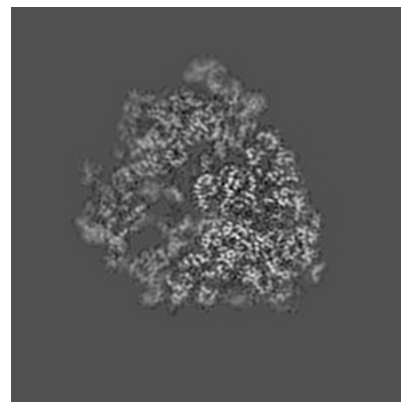
6.3.1 Primary map



X Index: 149

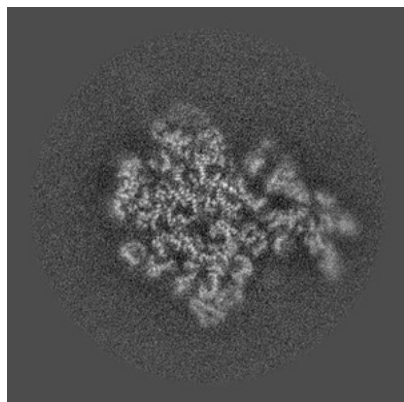


Y Index: 148

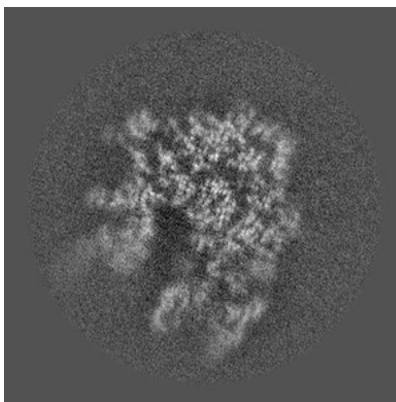


Z Index: 135

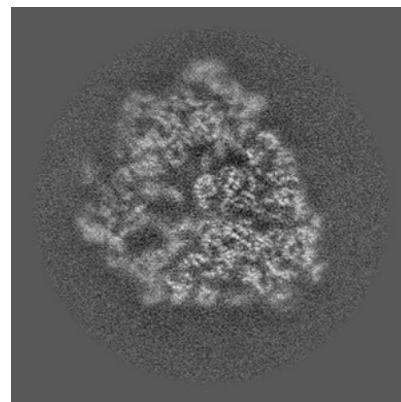
6.3.2 Raw map



X Index: 148



Y Index: 148

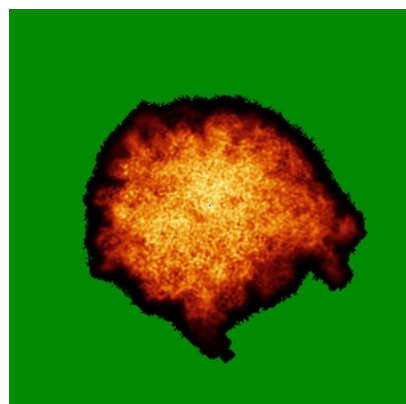


Z Index: 135

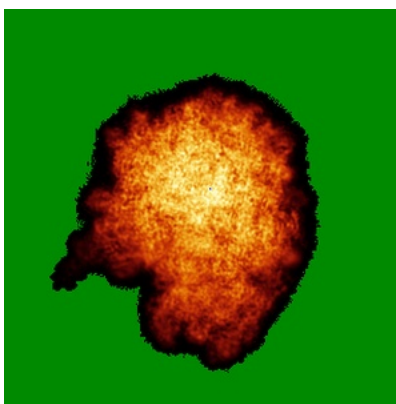
The images above show the largest variance slices of the map in three orthogonal directions.

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

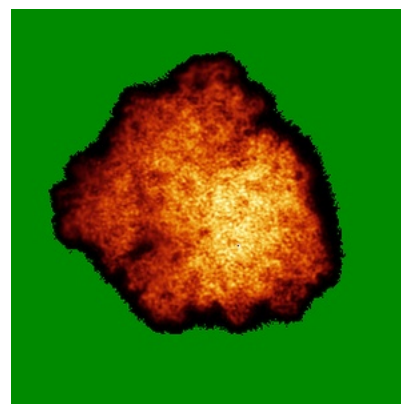
6.4.1 Primary map



X

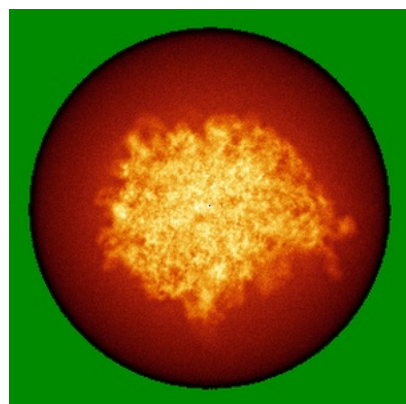


Y

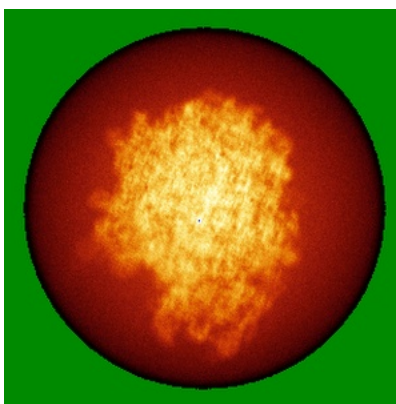


Z

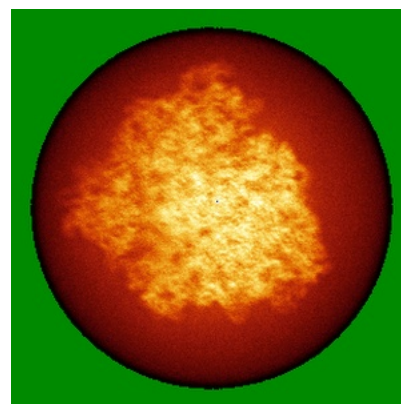
6.4.2 Raw map



X



Y



Z

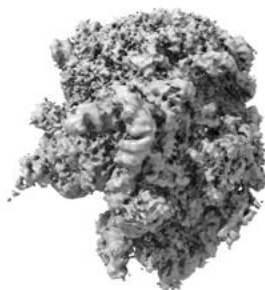
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



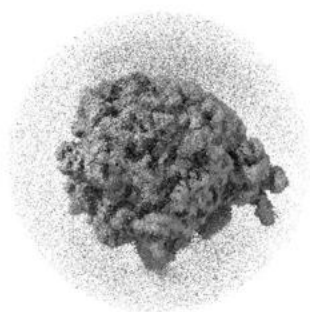
Y



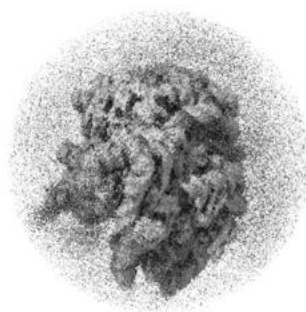
Z

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.

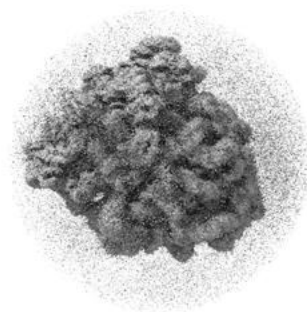
6.5.2 Raw map



X



Y



Z

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

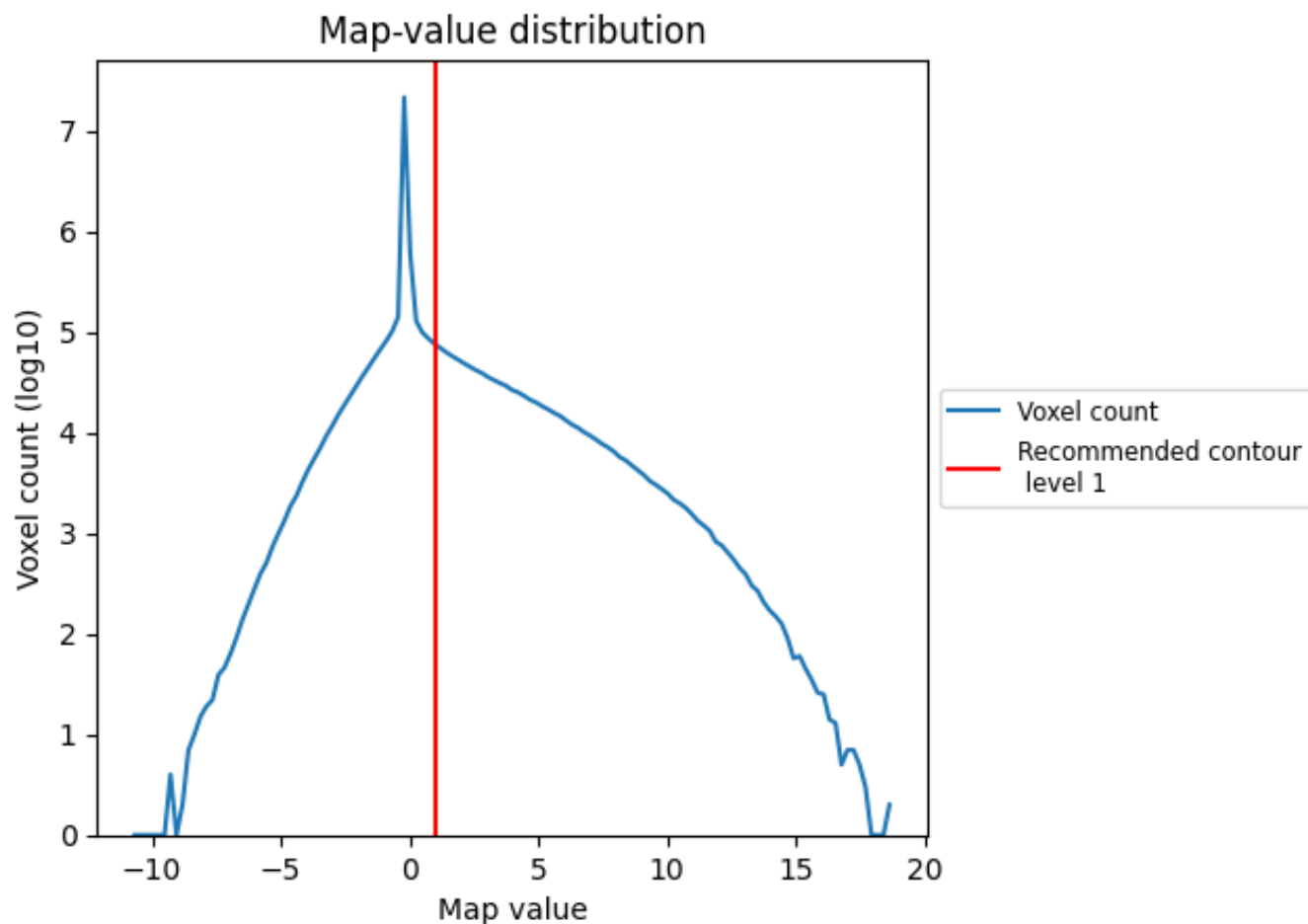
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

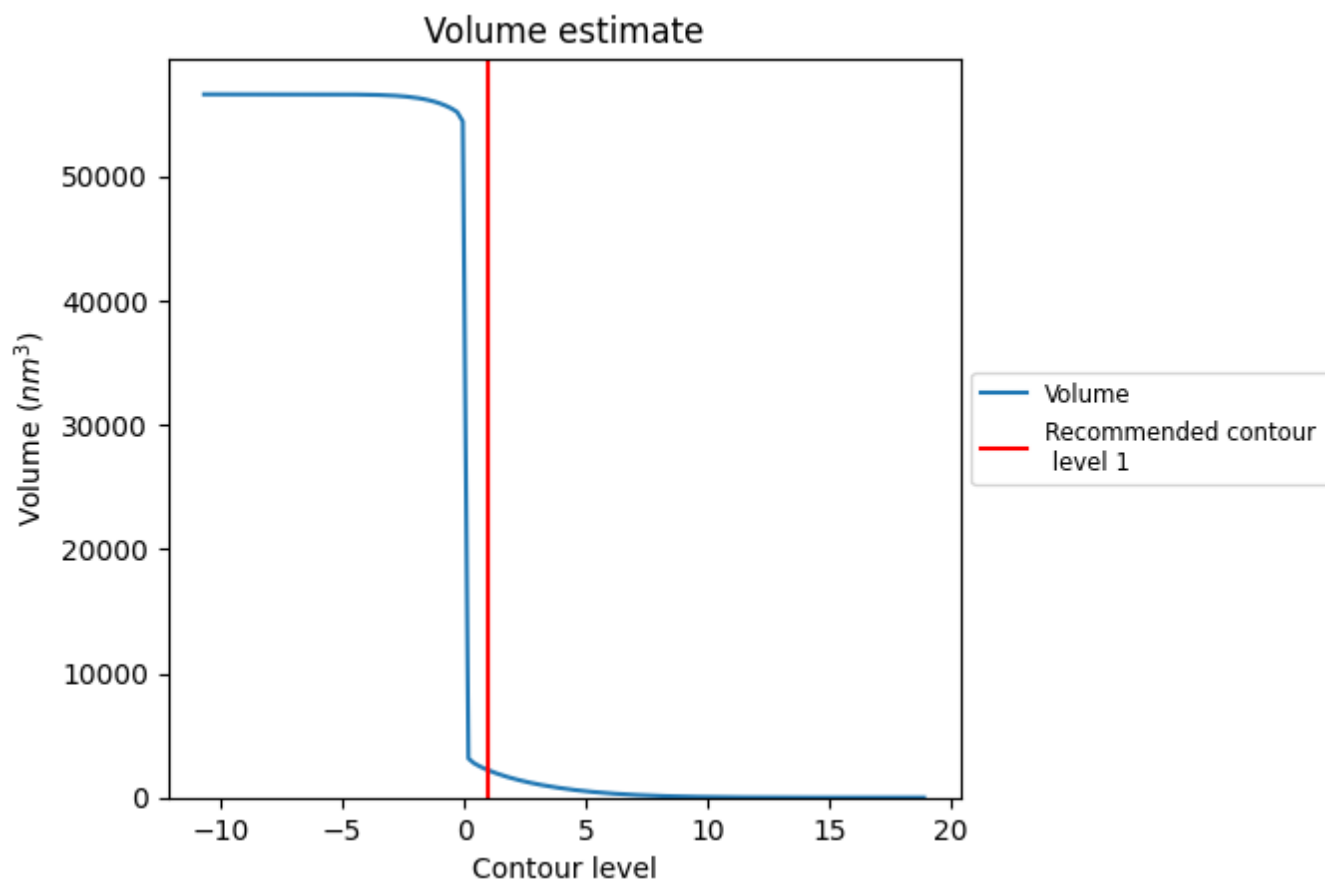
This section contains the results of statistical analysis of the map.

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.

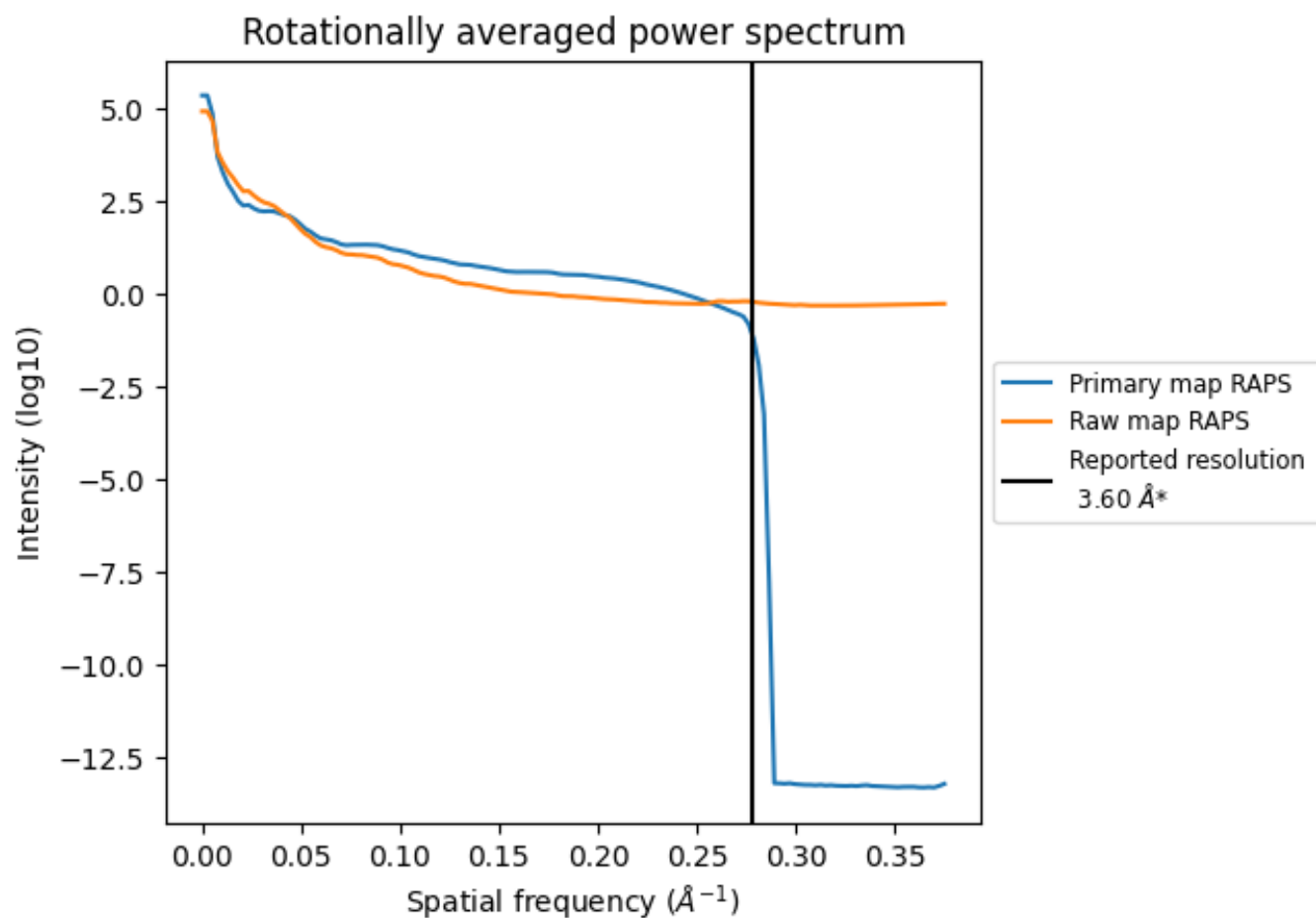
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2191 nm³; this corresponds to an approximate mass of 1979 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 ⓘ

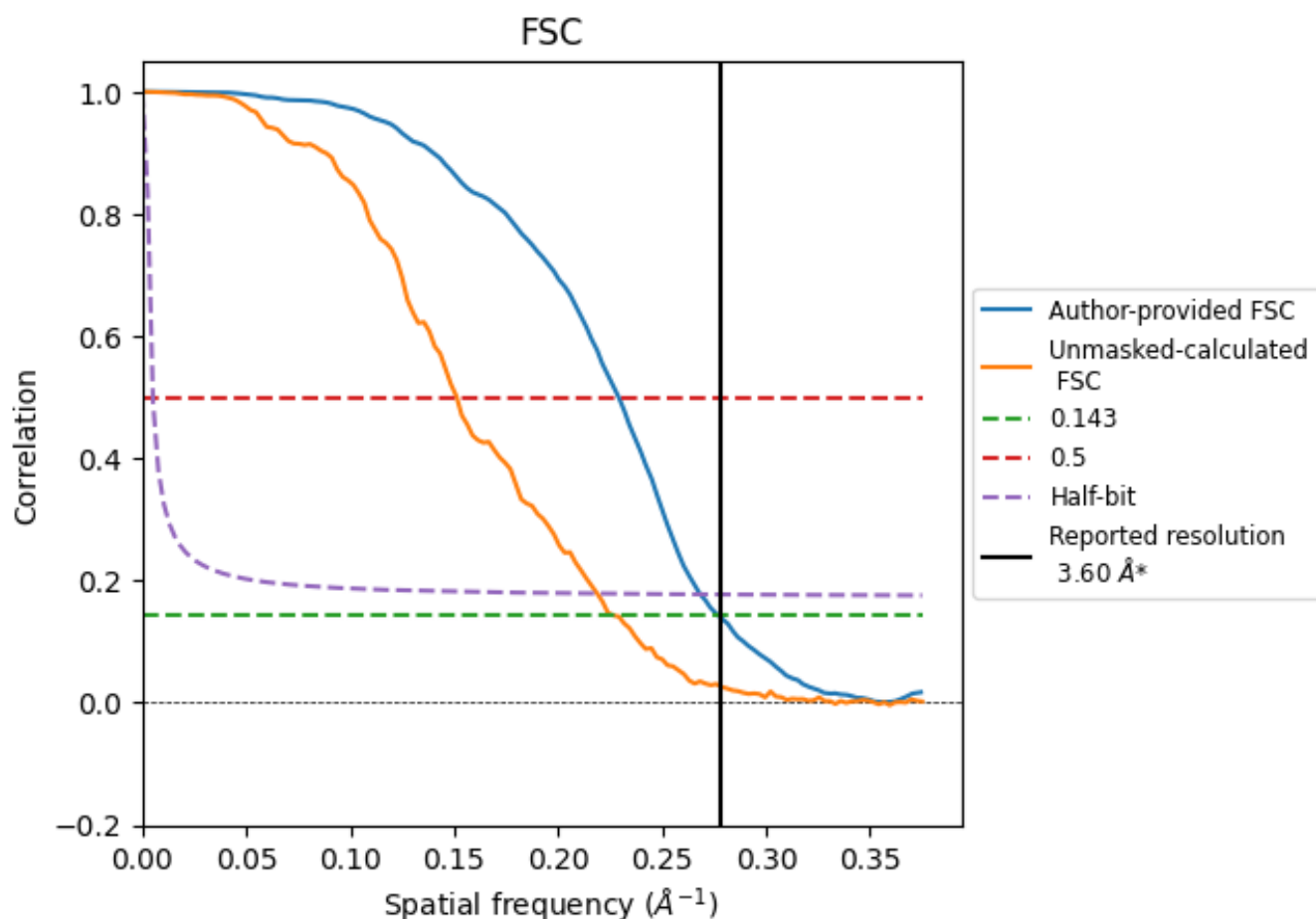


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 $0.278 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

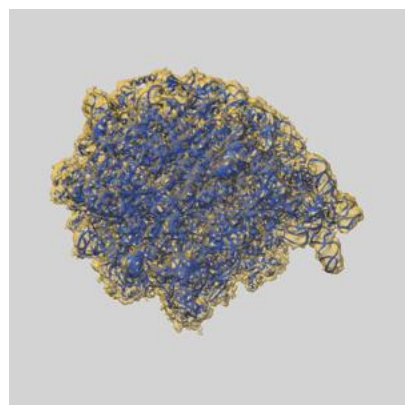
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.61	4.36	3.73
Unmasked-calculated*	4.42	6.61	4.57

*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 4.42 differs from the reported value 3.6 by more than 10 %

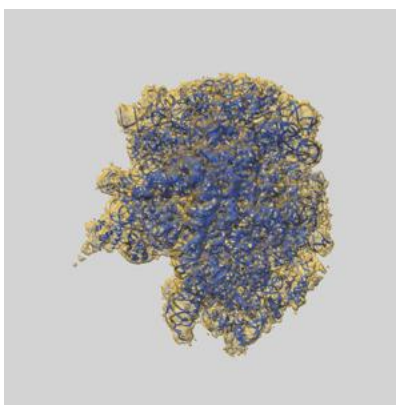
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21622 and PDB model 6WD3. Per-residue inclusion information can be found in section [3](#) on page [17](#).

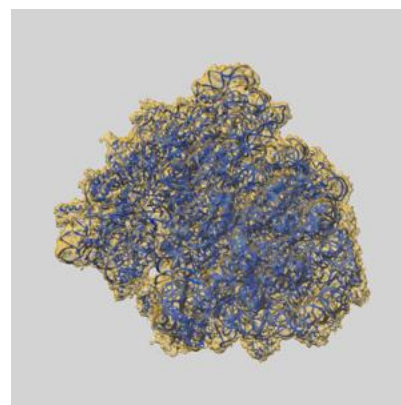
9.1 Map-model overlay [i](#)



X



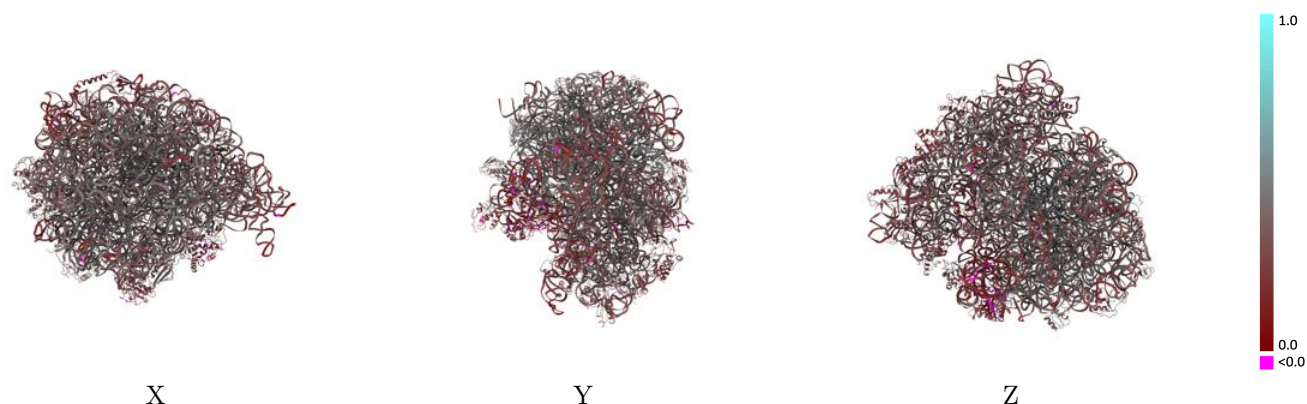
Y



Z

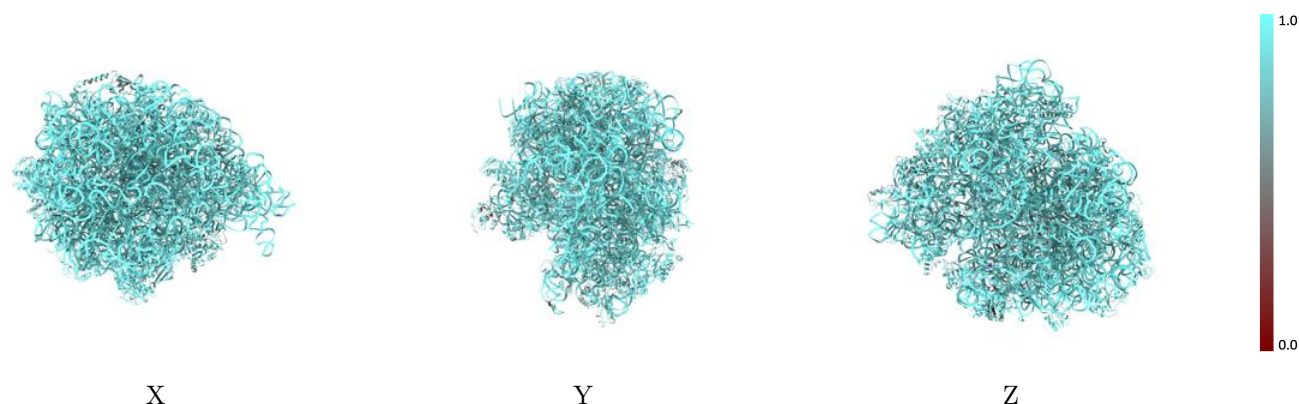
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



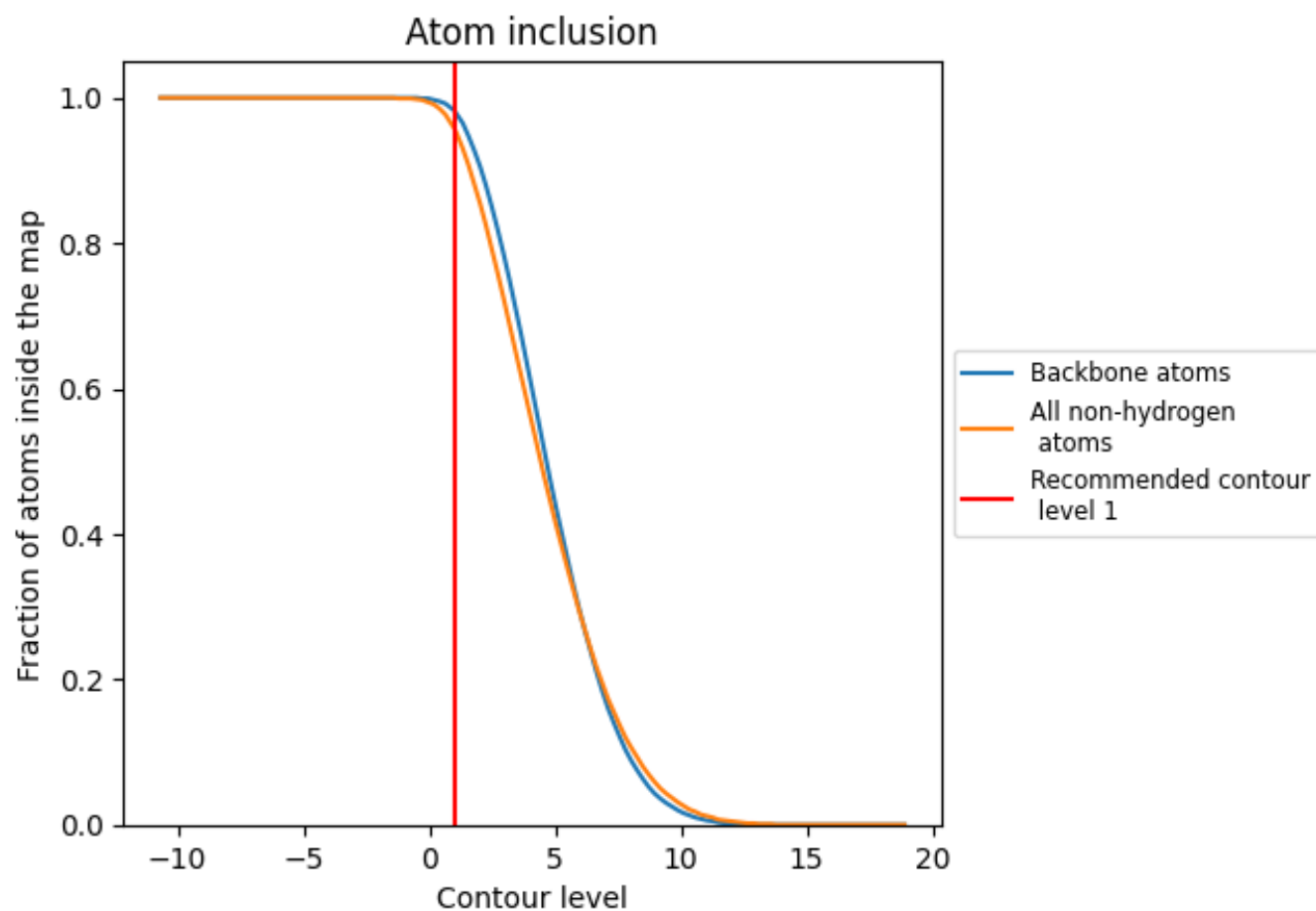
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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).

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	 0.9570	 0.3630
1	 0.9840	 0.3850
2	 0.9880	 0.3360
3	 0.9800	 0.3470
4	 0.8350	 0.2100
5	 0.9680	 0.3190
6	 0.8110	 0.1460
7	 0.9320	 0.1770
8	 0.8990	 0.2070
B	 0.9440	 0.4370
C	 0.8480	 0.3910
D	 0.9240	 0.4510
E	 0.9670	 0.4760
F	 0.9010	 0.4220
G	 0.9000	 0.3150
H	 0.8140	 0.3500
I	 0.8820	 0.3080
J	 0.9370	 0.4040
K	 0.9510	 0.3740
L	 0.9370	 0.3380
M	 0.9280	 0.4100
N	 0.8790	 0.3320
O	 0.7820	 0.3150
P	 0.9480	 0.3810
Q	 0.9110	 0.4120
R	 0.9430	 0.3320
S	 0.8370	 0.3270
T	 0.9610	 0.3860
U	 0.9030	 0.3690
V	 0.9230	 0.3630
W	 0.9240	 0.3720
X	 0.9680	 0.3250
Y	 0.8980	 0.3390
Z	 0.8730	 0.2940
a	 0.7970	 0.1520



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Chain	Atom inclusion	Q-score
b	 0.9590	 0.4600
c	 0.9560	 0.4610
d	 0.9520	 0.4080
e	 0.9480	 0.3330
f	 0.9490	 0.3340
g	 0.7740	 0.2590
h	 0.7580	 0.1650
i	 0.8240	 0.1870
j	 0.9540	 0.4500
k	 0.9220	 0.4480
l	 0.9500	 0.4270
m	 0.9460	 0.4490
n	 0.9440	 0.4420
o	 0.9530	 0.3510
p	 0.9490	 0.4470
q	 0.9540	 0.4400
r	 0.9620	 0.4170
s	 0.9410	 0.4460
t	 0.9410	 0.4210
u	 0.9410	 0.3990
v	 0.9510	 0.4050
w	 0.9500	 0.4640
x	 0.9630	 0.4480
y	 0.9300	 0.3440
z	 0.9430	 0.4170