



wwPDB EM Validation Summary Report ⓘ

Jun 21, 2026 – 10:58 am BST

PDB ID : 8AYE / pdb_00008aye
EMDB ID : EMD-15712
Title : E. coli 70S ribosome bound to thermorubin and fMet-tRNA
Authors : Sanyal, S.; Parajuli, N.P.; Emmerich, A.G.
Deposited on : 2022-09-02
Resolution : 1.96 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:

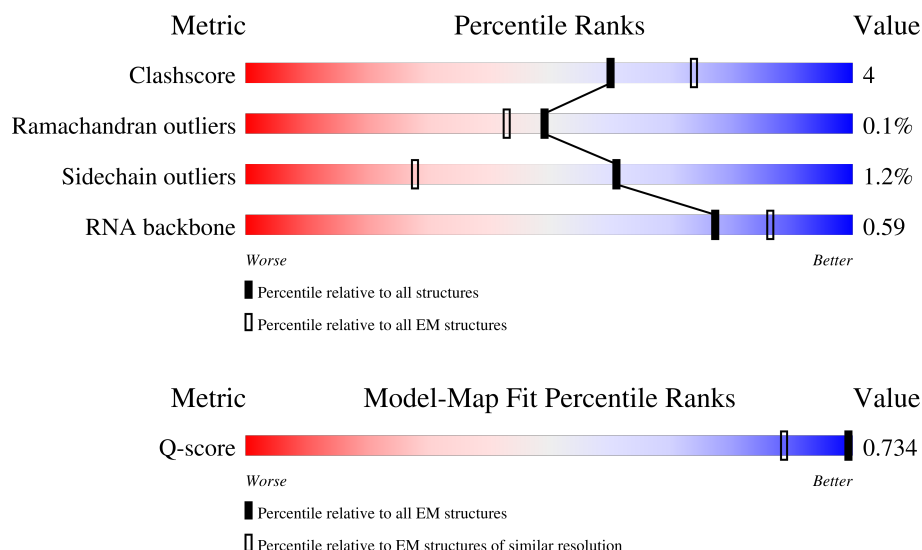
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD 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 1.96 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.



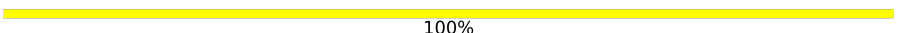
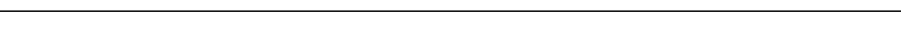
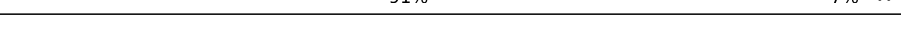
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	1340 (1.46 - 2.46)

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	0	55	
2	1	46	
3	2	65	

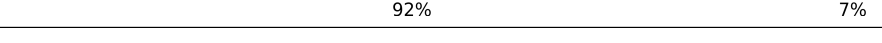
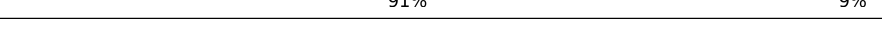
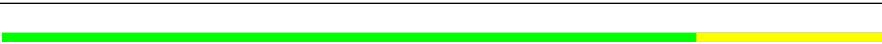
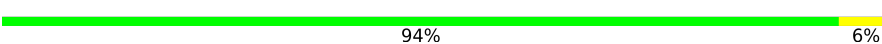
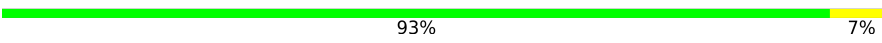
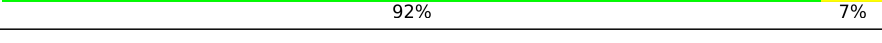
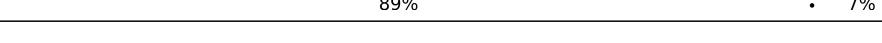
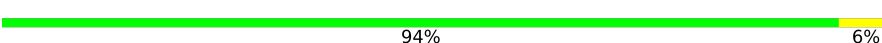
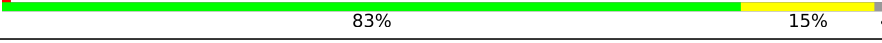
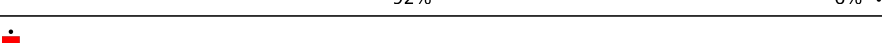
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Mol	Chain	Length	Quality of chain
4	3	38	
5	4	70	
6	5	2	
7	A	1542	
8	B	241	
9	C	233	
10	D	206	
11	E	167	
12	F	135	
13	G	179	
14	H	130	
15	I	130	
16	J	103	
17	K	129	
18	L	124	
19	M	118	
20	N	101	
21	O	89	
22	P	82	
23	Q	84	
24	R	75	
25	S	92	
26	T	87	
27	U	71	
28	X	6	

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Mol	Chain	Length	Quality of chain
29	Z	76	
30	a	2903	
31	b	120	
32	c	273	
33	d	209	
34	e	201	
35	f	179	
36	g	177	
37	h	149	
38	i	142	
39	j	123	
40	k	144	
41	l	136	
42	m	127	
43	n	117	
44	o	115	
45	p	118	
46	q	103	
47	r	110	
48	s	100	
49	t	104	
50	u	94	
51	v	85	
52	w	78	
53	x	63	

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Mol	Chain	Length	Quality of chain
54	y	59	 86%10%••
55	z	57	 79%19%•

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 140205 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 L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 2 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 3 is a protein called 50S ribosomal protein L35.

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

- Molecule 4 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 5 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 6 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	2	Total	C	N	O	P	0	0
			42	19	8	13	2		

- Molecule 7 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	1519	Total	C	N	O	P	0	0
			32612	14552	5986	10555	1519		

- Molecule 8 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 9 is a protein called 30S ribosomal protein S3.

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

- Molecule 10 is a protein called 30S ribosomal protein S4.

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

- Molecule 11 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 12 is a protein called 30S ribosomal protein S6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	103	Total	C	N	O	S	0	0
			839	530	151	151	7		

- Molecule 13 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

- Molecule 14 is a protein called 30S ribosomal protein S8.

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

- Molecule 15 is a protein called 30S ribosomal protein S9.

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

- Molecule 16 is a protein called 30S ribosomal protein S10.

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

- Molecule 17 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	ASP	ASN	conflict	UNP P0A7R9

- Molecule 18 is a protein called 30S ribosomal protein S12.

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

- Molecule 19 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 20 is a protein called 30S ribosomal protein S14.

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

- Molecule 21 is a protein called 30S ribosomal protein S15.

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

- Molecule 22 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 23 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 24 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	66	Total	C	N	O	S	0	0
			544	345	102	96	1		

- Molecule 25 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 26 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 27 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 28 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	6	Total	C	N	O	P	0	0
			131	59	27	39	6		

- Molecule 29 is a RNA chain called P-site tRNA-fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	76	Total	C	N	O	P	0	0
			1623	723	294	530	76		

- Molecule 30 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	2753	Total	C	N	O	P	0	0
			59129	26383	10897	19096	2753		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	2163	G	A	conflict	GB 937521852

- Molecule 31 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 32 is a protein called 50S ribosomal protein L2.

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

- Molecule 33 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 34 is a protein called 50S ribosomal protein L4.

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

- Molecule 35 is a protein called 50S ribosomal protein L5.

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

- Molecule 36 is a protein called 50S ribosomal protein L6.

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

- Molecule 37 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h	41	Total	C	N	O	S	0	0
			303	194	54	54	1		

- Molecule 38 is a protein called 50S ribosomal protein L13.

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

- Molecule 39 is a protein called 50S ribosomal protein L14.

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

- Molecule 40 is a protein called 50S ribosomal protein L15.

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

- Molecule 41 is a protein called 50S ribosomal protein L16.

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

- Molecule 42 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 43 is a protein called 50S ribosomal protein L18.

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

- Molecule 44 is a protein called 50S ribosomal protein L19.

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

- Molecule 45 is a protein called 50S ribosomal protein L20.

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

- Molecule 46 is a protein called 50S ribosomal protein L21.

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

- Molecule 47 is a protein called 50S ribosomal protein L22.

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

- Molecule 48 is a protein called 50S ribosomal protein L23.

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

- Molecule 49 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	t	102	Total	C	N	O	S	0	0
			779	492	146	141			

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

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

- Molecule 51 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	v	78	Total	C	N	O	S	0	0
			586	362	116	107	1		

- Molecule 52 is a protein called 50S ribosomal protein L28.

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

- Molecule 53 is a protein called 50S ribosomal protein L29.

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

- Molecule 54 is a protein called 50S ribosomal protein L30.

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

- Molecule 55 is a protein called 50S ribosomal protein L32.

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

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
56	3	1	Total	Zn	0
			1	1	
56	4	1	Total	Zn	0
			1	1	

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

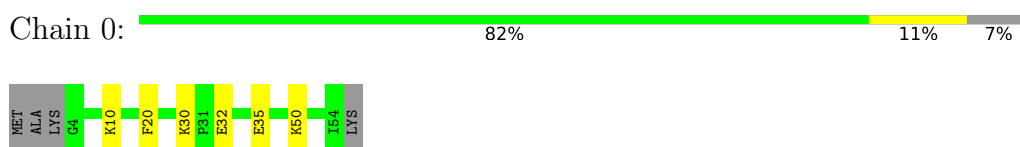
Mol	Chain	Residues	Atoms		AltConf
57	A	89	Total	Mg	0
			89	89	
57	E	1	Total	Mg	0
			1	1	
57	N	1	Total	Mg	0
			1	1	
57	Q	1	Total	Mg	0
			1	1	
57	a	207	Total	Mg	0
			207	207	
57	b	5	Total	Mg	0
			5	5	
57	d	1	Total	Mg	0
			1	1	
57	k	1	Total	Mg	0
			1	1	
57	p	1	Total	Mg	0
			1	1	
57	z	1	Total	Mg	0
			1	1	

- Molecule 58 is Thermorubin (CCD ID: T8B) (formula: C₃₂H₂₄O₁₂) (labeled as "Ligand of Interest" by depositor).

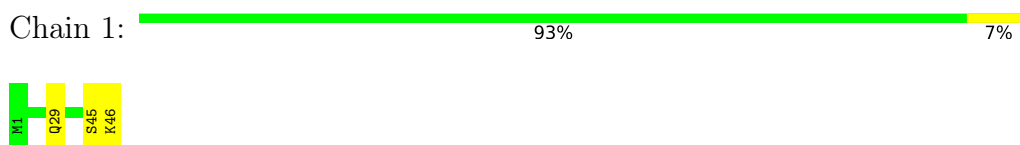
3 Residue-property plots [i](#)

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

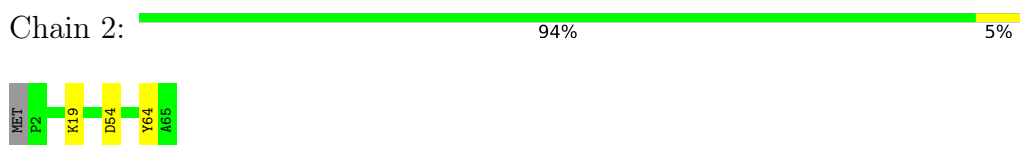
- Molecule 1: 50S ribosomal protein L33



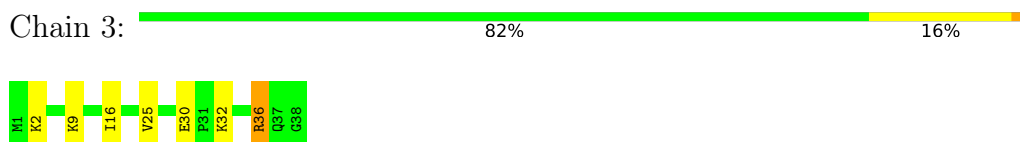
- Molecule 2: 50S ribosomal protein L34



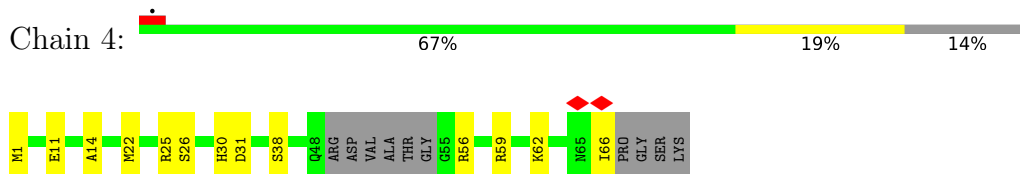
- Molecule 3: 50S ribosomal protein L35



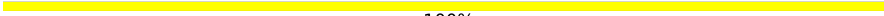
- Molecule 4: 50S ribosomal protein L36



- Molecule 5: 50S ribosomal protein L31



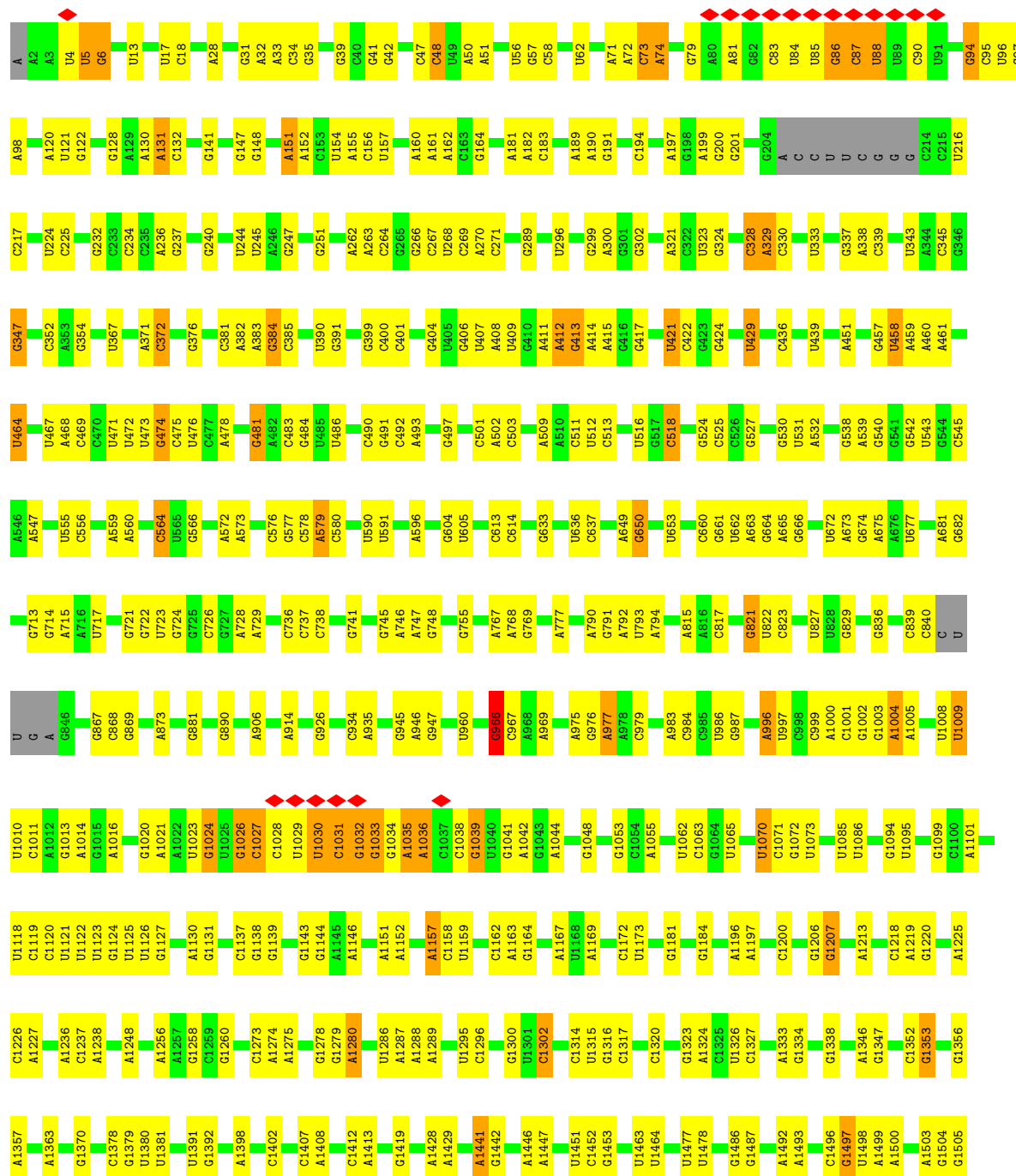
- Molecule 6: E-site tRNA

Chain 5:  100%

C75
A76

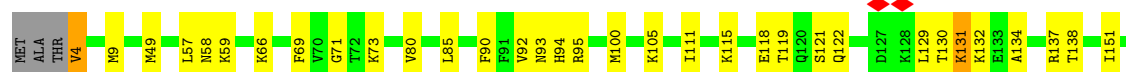
• Molecule 7: 16S rRNA

Chain A:  67% 28% . .

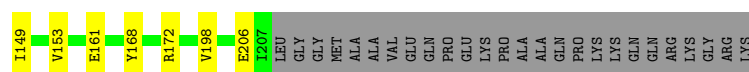




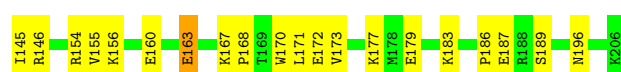
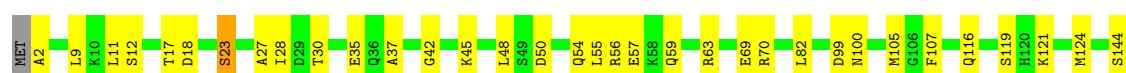
• Molecule 8: 30S ribosomal protein S2



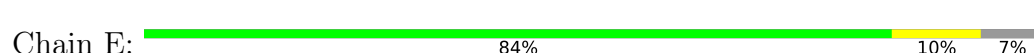
• Molecule 9: 30S ribosomal protein S3



• Molecule 10: 30S ribosomal protein S4



• Molecule 11: 30S ribosomal protein S5



• Molecule 12: 30S ribosomal protein S6, fully modified isoform



GLU
THR
ALA
ASP
ASP
GLU
GLU
GLU
GLU

- Molecule 13: 30S ribosomal protein S7

Chain G:  71% 14% 15%

MET PHE SER HIS GLN ALA GLY ALA SER SER LYS GLN PRO ALA LEU TYR LEU ASN
F2 R3 R4 R5 V6 L22 F26 K36 E40 E48 Q52 E60 A61 F62 E63 L66 R70 P71 R96 N97 M101 D113 L120 S125 E129 V135 R138 E139 D140 V141 H142 K149 Y154 ARG TRP LEU SER LEU ARG SER

- Molecule 14: 30S ribosomal protein S8

Chain H:  92% 8%

MET S2 Q18 M27 K50 L63 K64 Y65 F66 Q67 V71 M96 A130

- Molecule 15: 30S ribosomal protein S9

Chain I:  82% 16%

MET ALA GLU N4 Q5 Y6 K13 R41 V47 L52 E53 L54 V55 D56 M57 V58 L63 R80 E89 Y90 D91 L94 L98 E112 V116 A121 R130

- Molecule 16: 30S ribosomal protein S10

Chain J:  6% 69% 24% 5%

MET GLN ASN GLN R5 I6 R7 L10 H15 VAL T22 T25 T28 A34 Q35 V36 R37 I40 T44 L52 V57 R62 E66 H70 L71 D75 I76 V77 E78 P79 T80 E81 K82 D85 R89 L90 D91 S101 L102 GLY

- Molecule 17: 30S ribosomal protein S11

Chain K:  73% 16% 9%

MET ALA LYS ALA PRO THR ARG ALA ARG LYS ARG VAL R13 V16 S17 D18 T35 A41 L42 S50 G51 F52 R53 F61 R69 Y77 G78 I79 E83 V84 R85 V86 K87 M109 V113 T114 P115 I116 I117 H118 D119 V129

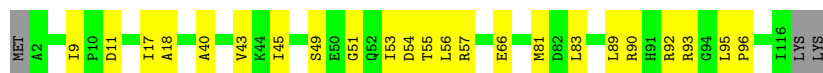
- Molecule 18: 30S ribosomal protein S12

Chain L:  91% 7% 2%

MET R2 R9 K10 K15 R54 E62 R110 K111 R114 V119 K120 R121 A124

- Molecule 19: 30S ribosomal protein S13

Chain M:  78% 19%



- Molecule 20: 30S ribosomal protein S14

Chain N:  86% 13%



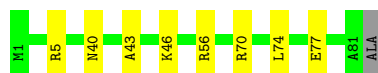
- Molecule 21: 30S ribosomal protein S15

Chain O:  87% 12%



- Molecule 22: 30S ribosomal protein S16

Chain P:  89% 10%



- Molecule 23: 30S ribosomal protein S17

Chain Q:  82% 10% 6%



- Molecule 24: 30S ribosomal protein S18

Chain R:  75% 11% 12%



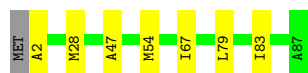
- Molecule 25: 30S ribosomal protein S19

Chain S:  83% 9% 9%



- Molecule 26: 30S ribosomal protein S20

Chain T:  91% 8%



- Molecule 27: 30S ribosomal protein S21

Chain U:  85% 14%



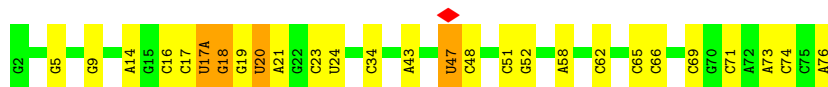
- Molecule 28: mRNA

Chain X:  100%

There are no outlier residues recorded for this chain.

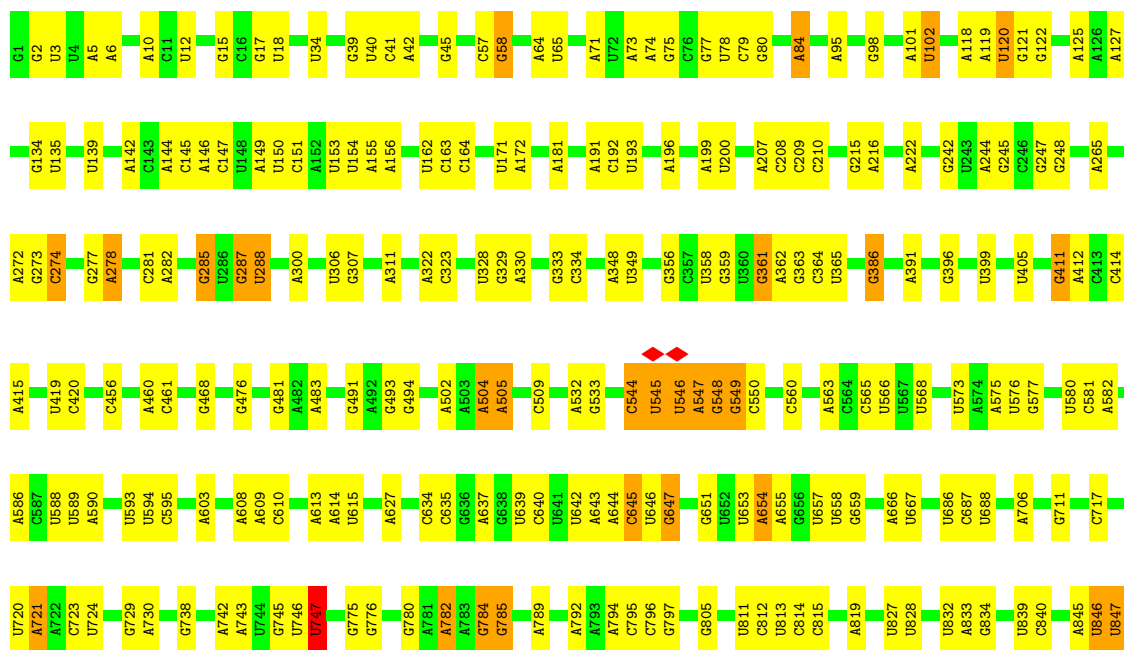
- Molecule 29: P-site tRNA-fMet

Chain Z:  64% 30% 5%

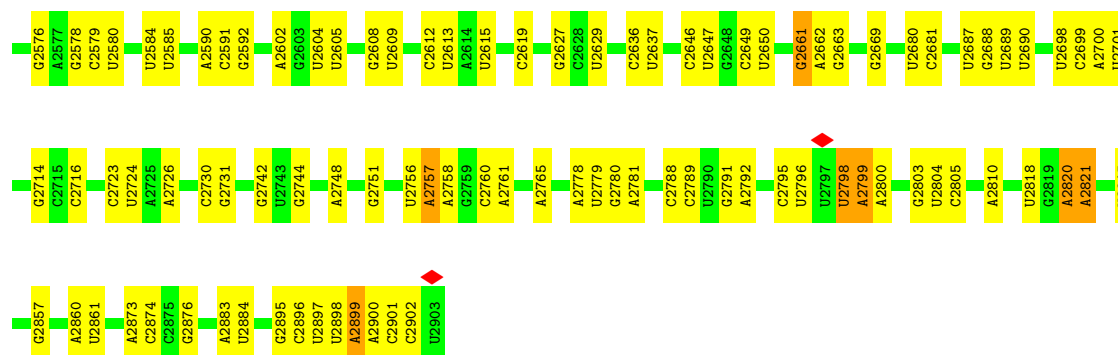


- Molecule 30: 23S rRNA

Chain a:  68% 24% 5%

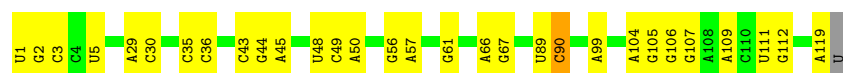


C2462	A2335	G2223	C	A2071	U1939	U1796	G1649	U1487	G1361	G1149	G	C848
C2463	A2336	G2224	A	C2072	U1946	G1797	C1656	C1493	G1362	C1150	A	A849
G2464	G2345	A2225	G	C2073	C1947	C1800	C1657	A1494	A1365	G1168	A	U850
A2469	A2346	G2228	U	U2074	A1801	A1800	A1668	A1495	A1366	A1169	C	C851
G2470	C2347	U2229	C	U2075	U1955	A1805	A1669	A1496	C1370	C1170	A	U852
U2473	G2361	U2233	C	U2086	G1962	A1808	G1674	U1497	G1371	G1171	G	C853
A2476	A2369	G2234	A	G2087	C1965	A1808	G1681	U1506	A1383	C1172	C	G856
U2477	G2373	G2239	G	U2092	A1966	C1816	G1682	C1507	C1386	U	C	G857
A2478	G2374	G2239	G	A2097	C1967	A1966	U1683	A1508	A1387	A	U	G858
G2481	C2380	U2243	G	U2098	U1970	U1820	U1714	A1509	G1380	U	A	U860
G2488	A2381	U2244	C		A1971	A1829	G1715	G1513	A1383	G1177	A	G861
U2491	G2382	G2250	C		G1972	G1835	A1717	U1515	C1386	C1178	U	G862
C2496	G2383	G2251	G		U1991	C1838	G1718	A1534	A1387	U	A	A863
A2497	U2384	G2251	C		G1992	C1838	G1719	U1535	U1405	C1178	A	U871
C2498	C2385	A2288	C		U1993	G1842	U1720	C1536	U1406	C1179	G	C873
C2499	G2393	A2273	U		C1999	C1843	G1721	G1537	U1406	U	A	G874
G2502	G2395	A2274	G			A1847	C1726	U1542	G1410	G1187	A	C875
A2503	U2402	G2277	A			A1848	C1727	G1543	U1411	A1189	A	C876
U2504	U2403	C2283	A			A1853	G1728	A1544	G1416	U	A	A877
C2505	C2403	G2283	U			U2017	U1729	A1545	G1416	U	A	A878
U2506	A2406	G2286	C			A1858	G1731	G1546	A1419	U	A	G879
C2512	G2287	A2287	C			C1868	G1732	C1547	A1427	C1200	U	G880
A2513	U2291	U2291	C				G1733	A1548	C1428	U	A	G881
U2514	U2292	G2292	C			A1871	G1738	U1563	G1429	G1225	C	G882
C2515	G2293	G2293	C			A1872	U1746	C1564	G1430	G1226	U	G883
U2518	C2422	G2294	U			G1873	A1744	C1565	A1434	G1227	C	U884
U2519	U2423	G2294	U			C1874	A1745	A1566	G1435	A1253	A	U885
C2520	C2424	A2298	A			G1875	A1746	A1569	U1442	U	U	C886
G2529	G2429	U2299	A			U1898	U1747	A1578	U1443	G1266	U	A886
U2537	A2430	G2300	U			C1902	C1748	U1578	G1444	A1264	A	U887
C2538	U2431	G2304	G			G1906	A1762	A1583	G1452	U	A	C888
A2432	A2432	U2305	U			G1907	G1763	U1584	A1453	C1270	U	C889
A2435	G2308	G2308	U			U1911	C1764	C1585	G1459	G1271	C	C890
U2548	U2312	U2312	G			C1914	A1773	A1590	A1469	A1272	A	G891
U2552	A2322	A2322	A			U1915	U1778	A1591	A1470	U	G	U895
G2557	G2325	G2325	G			A1916	U1782	C1595	A1476	G1300	A	A896
C2558	C2326	A2327	U			U1917	A1783	U1594	U1476	A1301	U	C897
U2448	A2327	A2328	G			G1929	A1784	C1607	G1478	G1338	A	U899
U2449	G2204	U2329	U			G1930	A1786	A1608	U1352	U	G	A909
A2566	U2329	G2330	G			U1931	U1790	A1618	A1353	U	U	A910
G2567	G2330	G2331	G			A1932	C1790	G1622	A1482	A1354	U	C911
U2457	C2332	U2333	A			G1933	A1791	U1618	G1483	G1355	U	U912
G2570	A2333	U2334	C			A1937	A1794	G1647	U1484	G1356	C	U913
C2573	G2218		C			A1938	C1795	U1648	U1486	A1142	A	G914
												G930
												U931
												U932
												A933
												U934



• Molecule 31: 5S rRNA

Chain b: 74% 24% ..



• Molecule 32: 50S ribosomal protein L2

Chain c: 92% 7% .



• Molecule 33: 50S ribosomal protein L3

Chain d: 91% 9%



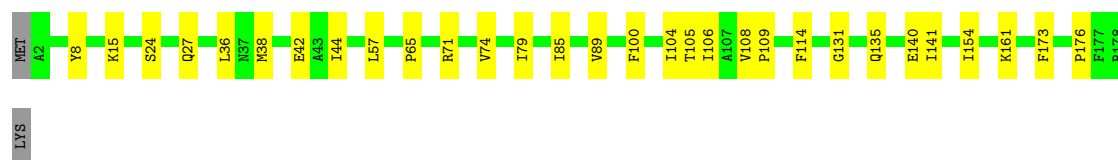
• Molecule 34: 50S ribosomal protein L4

Chain e: 90% 9%



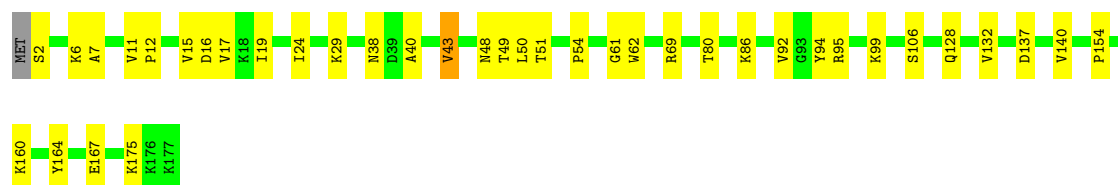
• Molecule 35: 50S ribosomal protein L5

Chain f: 82% 17% .



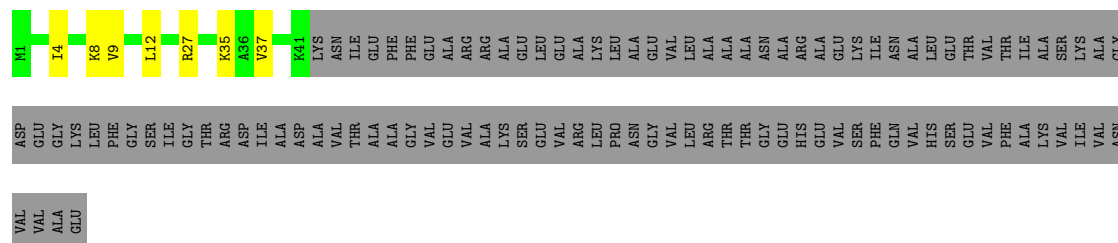
• Molecule 36: 50S ribosomal protein L6

Chain g:  78% 21% ..

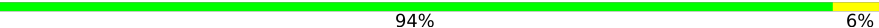


- Molecule 37: 50S ribosomal protein L9

Chain h:  23% 5% 72%

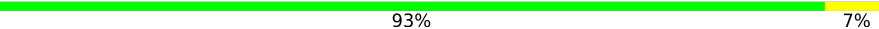


- Molecule 38: 50S ribosomal protein L13

Chain i:  94% 6%



- Molecule 39: 50S ribosomal protein L14

Chain j:  93% 7%



- Molecule 40: 50S ribosomal protein L15

Chain k:  87% 13%



- Molecule 41: 50S ribosomal protein L16

Chain l:  92% 7% .



- Molecule 42: 50S ribosomal protein L17

Chain m:  89% 7%



- Molecule 43: 50S ribosomal protein L18

Chain n:  85% 14%



- Molecule 44: 50S ribosomal protein L19

Chain o:  91% 8%



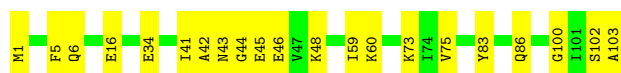
- Molecule 45: 50S ribosomal protein L20

Chain p:  93% 6%



- Molecule 46: 50S ribosomal protein L21

Chain q:  80% 20%



- Molecule 47: 50S ribosomal protein L22

Chain r:  94% 6%

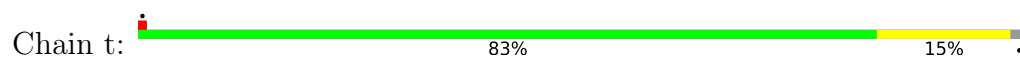


- Molecule 48: 50S ribosomal protein L23

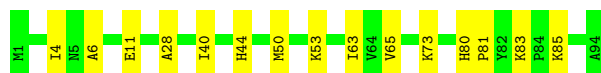
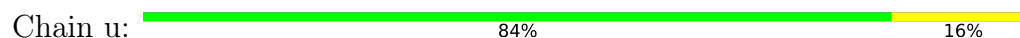
Chain s:  85% 8% 7%



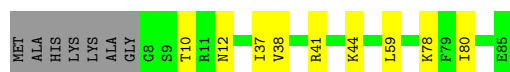
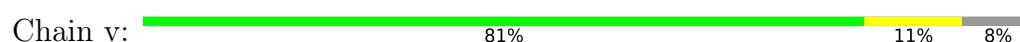
- Molecule 49: 50S ribosomal protein L24



- Molecule 50: 50S ribosomal protein L25



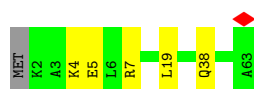
- Molecule 51: 50S ribosomal protein L27



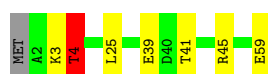
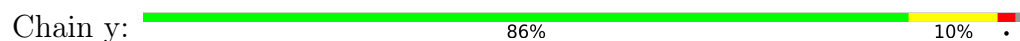
- Molecule 52: 50S ribosomal protein L28



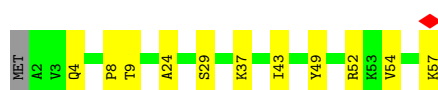
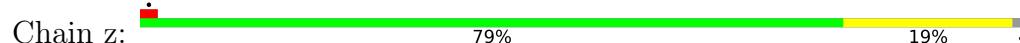
- Molecule 53: 50S ribosomal protein L29



- Molecule 54: 50S ribosomal protein L30



- Molecule 55: 50S ribosomal protein L32



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1088035	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30.745	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.598	Depositor
Minimum map value	-1.927	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.125	Depositor
Recommended contour level	0.21	Depositor
Map size ($\text{\AA}$)	426.496, 426.496, 426.496	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.833, 0.833, 0.833	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2MG, 1MG, MEQ, OMC, 6MZ, OMG, 5MU, MG, 5MC, OMU, MA6, 4OC, G7M, T8B, PSU, 2MA, ZN, UR3

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.33	0/424	0.46	0/565
2	1	0.34	0/380	0.51	0/498
3	2	0.34	0/513	0.44	0/676
4	3	0.33	0/303	0.39	0/397
5	4	0.22	0/488	0.44	0/649
6	5	0.26	0/46	0.24	0/69
7	A	0.38	0/36236	0.43	0/56520
8	B	0.28	0/1784	0.49	0/2403
9	C	0.28	0/1651	0.45	0/2225
10	D	0.26	0/1665	0.45	0/2227
11	E	0.32	0/1165	0.50	0/1568
12	F	0.35	1/858 (0.1%)	0.62	3/1160 (0.3%)
13	G	0.26	0/1219	0.46	0/1635
14	H	0.31	0/989	0.48	0/1326
15	I	0.30	0/1034	0.44	0/1375
16	J	0.31	0/796	0.49	0/1077
17	K	0.28	0/893	0.55	2/1205 (0.2%)
18	L	0.30	0/969	0.48	0/1300
19	M	0.27	0/900	0.44	1/1204 (0.1%)
20	N	0.28	0/817	0.39	0/1088
21	O	0.26	0/722	0.41	0/964
22	P	0.29	0/653	0.50	0/877
23	Q	0.31	0/650	0.47	0/871
24	R	0.29	0/553	0.51	0/742
25	S	0.24	0/685	0.44	0/922
26	T	0.28	0/676	0.43	0/895
27	U	0.27	0/597	0.47	0/792
28	X	0.35	0/147	0.41	0/227
29	Z	0.31	0/1813	0.43	0/2825
30	a	0.46	1/65696 (0.0%)	0.48	0/102485
31	b	0.36	0/2850	0.37	0/4444

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	c	0.36	0/2121	0.49	0/2852
33	d	0.33	0/1576	0.47	0/2119
34	e	0.30	0/1571	0.46	0/2113
35	f	0.27	0/1434	0.44	0/1926
36	g	0.27	0/1343	0.46	0/1816
37	h	0.26	0/306	0.57	0/413
38	i	0.32	0/1152	0.46	0/1551
39	j	0.37	0/955	0.53	0/1279
40	k	0.31	0/1062	0.45	0/1413
41	l	0.33	0/1092	0.51	1/1457 (0.1%)
42	m	0.36	0/958	0.52	0/1281
43	n	0.28	0/902	0.46	0/1209
44	o	0.33	0/929	0.47	0/1242
45	p	0.33	0/960	0.47	0/1278
46	q	0.31	0/829	0.45	0/1107
47	r	0.34	0/864	0.46	0/1156
48	s	0.29	0/744	0.46	0/994
49	t	0.29	0/787	0.48	0/1051
50	u	0.30	0/766	0.43	0/1025
51	v	0.33	0/593	0.46	0/785
52	w	0.31	0/635	0.42	0/848
53	x	0.25	0/502	0.36	0/667
54	y	0.33	0/453	0.51	0/605
55	z	0.33	0/450	0.43	0/599
All	All	0.40	2/151156 (0.0%)	0.46	7/225997 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
52	w	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	2449	U	C5-C6	7.93	1.50	1.34
12	F	101	PRO	CG-CD	-6.43	1.28	1.50

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	F	101	PRO	N-CD-CG	-10.47	87.50	103.20
17	K	118	HIS	CA-C-N	6.98	134.87	121.54
17	K	118	HIS	C-N-CA	6.98	134.87	121.54
41	l	81	ARG	N-CA-C	-6.49	102.14	110.19
12	F	101	PRO	CA-N-CD	-6.01	103.59	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
52	w	16	ASN	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	417	0	451	6	0
2	1	377	0	418	3	0
3	2	504	0	572	3	0
4	3	302	0	340	5	0
5	4	480	0	478	9	0
6	5	42	0	23	1	0
7	A	32612	0	16432	257	0
8	B	1753	0	1780	28	0
9	C	1624	0	1696	23	0
10	D	1643	0	1707	32	0
11	E	1152	0	1196	9	0
12	F	839	0	833	16	0
13	G	1203	0	1254	19	0
14	H	979	0	1031	6	0
15	I	1022	0	1070	16	0
16	J	786	0	828	17	0
17	K	877	0	885	13	0
18	L	955	0	1016	6	0
19	M	891	0	952	15	0
20	N	805	0	844	10	0
21	O	714	0	734	6	0
22	P	643	0	661	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	Q	641	0	682	10	0
24	R	544	0	565	10	0
25	S	668	0	693	4	0
26	T	670	0	719	6	0
27	U	589	0	629	7	0
28	X	131	0	66	0	0
29	Z	1623	0	825	7	0
30	a	59129	0	29761	369	0
31	b	2549	0	1291	16	0
32	c	2082	0	2154	12	0
33	d	1566	0	1618	11	0
34	e	1552	0	1619	15	0
35	f	1410	0	1444	20	0
36	g	1323	0	1371	23	0
37	h	303	0	327	4	0
38	i	1129	0	1162	5	0
39	j	946	0	1023	5	0
40	k	1053	0	1129	12	0
41	l	1074	0	1156	10	0
42	m	945	0	989	3	0
43	n	892	0	923	9	0
44	o	917	0	962	7	0
45	p	947	0	1019	5	0
46	q	816	0	839	11	0
47	r	857	0	922	5	0
48	s	738	0	807	4	0
49	t	779	0	831	9	0
50	u	753	0	780	9	0
51	v	586	0	596	8	0
52	w	625	0	652	3	0
53	x	501	0	531	6	0
54	y	449	0	488	4	0
55	z	444	0	458	7	0
56	3	1	0	0	0	0
56	4	1	0	0	0	0
57	A	89	0	0	0	0
57	E	1	0	0	0	0
57	N	1	0	0	0	0
57	Q	1	0	0	0	0
57	a	207	0	0	0	0
57	b	5	0	0	0	0
57	d	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	k	1	0	0	0	0
57	p	1	0	0	0	0
57	z	1	0	0	0	0
58	A	44	0	20	1	0
All	All	140205	0	94252	1036	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 4.

The worst 5 of 1036 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)
30:a:747:5MU:C5	30:a:747:5MU:C4	1.78	1.62
30:a:1939:5MU:C4	30:a:1939:5MU:C5	1.78	1.62
12:F:37:HIS:HB3	12:F:97:THR:HG22	1.53	0.91
7:A:1028:C:N4	7:A:1033:G:O6	2.06	0.89
30:a:2796:U:H3	30:a:2799:A:H61	1.16	0.88

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	49/55 (89%)	49 (100%)	0	0	100	100
2	1	44/46 (96%)	44 (100%)	0	0	100	100
3	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
5	4	56/70 (80%)	52 (93%)	4 (7%)	0	100	100
8	B	222/241 (92%)	216 (97%)	5 (2%)	1 (0%)	24	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	C	204/233 (88%)	195 (96%)	9 (4%)	0	100	100
10	D	203/206 (98%)	201 (99%)	2 (1%)	0	100	100
11	E	154/167 (92%)	152 (99%)	2 (1%)	0	100	100
12	F	101/135 (75%)	100 (99%)	1 (1%)	0	100	100
13	G	151/179 (84%)	143 (95%)	8 (5%)	0	100	100
14	H	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
15	I	125/130 (96%)	121 (97%)	4 (3%)	0	100	100
16	J	96/103 (93%)	92 (96%)	3 (3%)	1 (1%)	12	5
17	K	115/129 (89%)	109 (95%)	5 (4%)	1 (1%)	14	6
18	L	121/124 (98%)	116 (96%)	5 (4%)	0	100	100
19	M	113/118 (96%)	111 (98%)	2 (2%)	0	100	100
20	N	98/101 (97%)	98 (100%)	0	0	100	100
21	O	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
22	P	79/82 (96%)	71 (90%)	7 (9%)	1 (1%)	9	3
23	Q	77/84 (92%)	75 (97%)	2 (3%)	0	100	100
24	R	64/75 (85%)	61 (95%)	2 (3%)	1 (2%)	7	2
25	S	82/92 (89%)	82 (100%)	0	0	100	100
26	T	84/87 (97%)	84 (100%)	0	0	100	100
27	U	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
32	c	269/273 (98%)	262 (97%)	7 (3%)	0	100	100
33	d	206/209 (99%)	199 (97%)	7 (3%)	0	100	100
34	e	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
35	f	175/179 (98%)	169 (97%)	6 (3%)	0	100	100
36	g	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
37	h	39/149 (26%)	36 (92%)	3 (8%)	0	100	100
38	i	140/142 (99%)	140 (100%)	0	0	100	100
39	j	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
40	k	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
41	l	132/136 (97%)	126 (96%)	6 (4%)	0	100	100
42	m	116/127 (91%)	111 (96%)	5 (4%)	0	100	100
43	n	114/117 (97%)	112 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	o	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
45	p	115/118 (98%)	115 (100%)	0	0	100	100
46	q	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
47	r	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
48	s	91/100 (91%)	89 (98%)	2 (2%)	0	100	100
49	t	100/104 (96%)	90 (90%)	10 (10%)	0	100	100
50	u	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
51	v	76/85 (89%)	74 (97%)	2 (3%)	0	100	100
52	w	75/78 (96%)	75 (100%)	0	0	100	100
53	x	60/63 (95%)	60 (100%)	0	0	100	100
54	y	56/59 (95%)	54 (96%)	1 (2%)	1 (2%)	6	1
55	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
All	All	5484/5913 (93%)	5333 (97%)	145 (3%)	6 (0%)	49	41

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
24	R	10	PHE
16	J	57	VAL
17	K	119	ASP
22	P	46	LYS
54	y	4	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	46/49 (94%)	46 (100%)	0	100	100
2	1	38/38 (100%)	38 (100%)	0	100	100
3	2	51/52 (98%)	51 (100%)	0	100	100
4	3	34/34 (100%)	33 (97%)	1 (3%)	37	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	4	55/62 (89%)	54 (98%)	1 (2%)	51	47
8	B	186/199 (94%)	184 (99%)	2 (1%)	65	64
9	C	170/190 (90%)	167 (98%)	3 (2%)	51	47
10	D	172/173 (99%)	166 (96%)	6 (4%)	32	22
11	E	119/126 (94%)	119 (100%)	0	100	100
12	F	90/116 (78%)	88 (98%)	2 (2%)	45	40
13	G	126/147 (86%)	122 (97%)	4 (3%)	34	25
14	H	104/105 (99%)	103 (99%)	1 (1%)	68	67
15	I	105/107 (98%)	105 (100%)	0	100	100
16	J	86/90 (96%)	84 (98%)	2 (2%)	44	38
17	K	90/99 (91%)	88 (98%)	2 (2%)	45	40
18	L	103/104 (99%)	101 (98%)	2 (2%)	50	45
19	M	93/96 (97%)	93 (100%)	0	100	100
20	N	83/84 (99%)	83 (100%)	0	100	100
21	O	76/77 (99%)	73 (96%)	3 (4%)	28	18
22	P	65/65 (100%)	65 (100%)	0	100	100
23	Q	73/78 (94%)	70 (96%)	3 (4%)	27	17
24	R	57/65 (88%)	55 (96%)	2 (4%)	32	22
25	S	72/79 (91%)	71 (99%)	1 (1%)	59	56
26	T	65/66 (98%)	65 (100%)	0	100	100
27	U	60/61 (98%)	59 (98%)	1 (2%)	53	49
32	c	216/218 (99%)	214 (99%)	2 (1%)	70	70
33	d	163/163 (100%)	162 (99%)	1 (1%)	78	79
34	e	165/165 (100%)	164 (99%)	1 (1%)	78	79
35	f	148/150 (99%)	146 (99%)	2 (1%)	59	56
36	g	137/138 (99%)	132 (96%)	5 (4%)	31	21
37	h	32/114 (28%)	31 (97%)	1 (3%)	35	26
38	i	116/116 (100%)	115 (99%)	1 (1%)	70	70
39	j	104/104 (100%)	103 (99%)	1 (1%)	68	67
40	k	103/103 (100%)	102 (99%)	1 (1%)	68	67
41	l	109/109 (100%)	109 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	m	98/103 (95%)	98 (100%)	0	100	100
43	n	86/87 (99%)	85 (99%)	1 (1%)	63	61
44	o	99/100 (99%)	99 (100%)	0	100	100
45	p	89/90 (99%)	89 (100%)	0	100	100
46	q	84/84 (100%)	82 (98%)	2 (2%)	43	36
47	r	93/93 (100%)	93 (100%)	0	100	100
48	s	80/84 (95%)	80 (100%)	0	100	100
49	t	83/85 (98%)	83 (100%)	0	100	100
50	u	78/78 (100%)	77 (99%)	1 (1%)	61	58
51	v	58/63 (92%)	58 (100%)	0	100	100
52	w	67/68 (98%)	67 (100%)	0	100	100
53	x	54/55 (98%)	54 (100%)	0	100	100
54	y	48/49 (98%)	47 (98%)	1 (2%)	47	41
55	z	47/48 (98%)	46 (98%)	1 (2%)	47	41
All	All	4576/4829 (95%)	4519 (99%)	57 (1%)	61	61

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	O	80	GLN
54	y	4	THR
27	U	4	ILE
50	u	11	GLU
39	j	76	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
35	f	5	HIS
39	j	3	GLN
35	f	21	ASN
37	h	2	GLN
41	l	60	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	X	5/6 (83%)	0	0
29	Z	75/76 (98%)	20 (26%)	0
30	a	2749/2903 (94%)	311 (11%)	0
31	b	118/120 (98%)	12 (10%)	0
6	5	1/2 (50%)	1 (100%)	0
7	A	1516/1542 (98%)	186 (12%)	6 (0%)
All	All	4464/4649 (96%)	530 (11%)	6 (0%)

5 of 530 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	5	76	A
7	A	4	U
7	A	5	U
7	A	6	G
7	A	13	U

5 of 6 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	A	1026	G
7	A	1035	A
7	A	1492	A
7	A	199	A
7	A	5	U

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
30	PSU	a	2605	30	18,21,22	1.14	1 (5%)	22,30,33	1.74	4 (18%)
7	2MG	A	1207	7	23,26,27	3.00	7 (30%)	32,38,41	2.49	11 (34%)
7	5MC	A	967	7	18,22,23	3.61	7 (38%)	26,32,35	1.05	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	2MG	A	1516	7	23,26,27	2.88	7 (30%)	32,38,41	2.41	11 (34%)
30	PSU	a	2604	30	18,21,22	1.10	1 (5%)	22,30,33	1.80	4 (18%)
30	PSU	a	1911	30	18,21,22	1.14	1 (5%)	22,30,33	1.88	4 (18%)
30	PSU	a	2457	30	18,21,22	1.15	1 (5%)	22,30,33	1.90	4 (18%)
7	G7M	A	527	7	23,26,27	2.55	9 (39%)	35,39,42	1.94	10 (28%)
30	1MG	a	745	30	22,26,27	2.70	6 (27%)	33,39,42	2.19	9 (27%)
30	OMG	a	2251	29,30	23,26,27	2.31	9 (39%)	33,38,41	1.96	13 (39%)
33	MEQ	d	150	33	8,9,10	0.83	0	5,10,12	0.98	0
30	G7M	a	2069	30	23,26,27	2.55	9 (39%)	35,39,42	1.67	8 (22%)
7	UR3	A	1498	57,7	19,22,23	2.76	8 (42%)	26,32,35	1.47	1 (3%)
30	2MA	a	2503	57,30	22,25,26	3.45	9 (40%)	33,37,40	2.71	10 (30%)
30	PSU	a	2580	30	18,21,22	1.14	2 (11%)	22,30,33	1.80	5 (22%)
30	OMC	a	2498	57,30	19,22,23	2.89	8 (42%)	26,31,34	0.96	1 (3%)
30	5MU	a	1939	30	19,22,23	7.11	8 (42%)	28,32,35	3.45	8 (28%)
7	5MC	A	1407	7	18,22,23	3.48	7 (38%)	26,32,35	1.18	3 (11%)
30	OMU	a	2552	30	19,22,23	2.94	8 (42%)	26,31,34	1.72	4 (15%)
7	2MG	A	966	7	23,26,27	2.89	7 (30%)	32,38,41	2.43	12 (37%)
7	4OC	A	1402	7	20,23,24	2.92	8 (40%)	26,32,35	1.19	2 (7%)
30	5MU	a	747	30	19,22,23	7.18	8 (42%)	28,32,35	3.41	8 (28%)
30	2MG	a	1835	30	23,26,27	2.81	7 (30%)	32,38,41	2.50	13 (40%)
7	MA6	A	1518	7	23,26,27	1.63	5 (21%)	34,38,41	3.31	13 (38%)
30	6MZ	a	1618	30	22,25,26	2.94	5 (22%)	30,36,39	2.51	11 (36%)
30	6MZ	a	2030	30	22,25,26	2.78	5 (22%)	30,36,39	2.66	11 (36%)
7	PSU	A	516	7	18,21,22	1.20	1 (5%)	22,30,33	1.79	5 (22%)
30	2MG	a	2445	30	23,26,27	3.03	8 (34%)	32,38,41	2.57	11 (34%)
30	PSU	a	2504	30	18,21,22	1.14	1 (5%)	22,30,33	1.89	2 (9%)
30	5MC	a	1962	30	18,22,23	3.47	7 (38%)	26,32,35	1.05	1 (3%)
30	PSU	a	746	57,30	18,21,22	1.23	1 (5%)	22,30,33	1.67	4 (18%)
30	PSU	a	955	30	18,21,22	1.20	1 (5%)	22,30,33	2.04	3 (13%)
7	MA6	A	1519	7	23,26,27	1.63	6 (26%)	34,38,41	3.53	13 (38%)
30	PSU	a	1917	30	18,21,22	1.06	1 (5%)	22,30,33	1.70	3 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	PSU	a	2605	30	-	0/7/25/26	0/2/2/2
7	2MG	A	1207	7	-	0/9/27/28	0/3/3/3
7	5MC	A	967	7	-	0/7/25/26	0/2/2/2
7	2MG	A	1516	7	-	0/9/27/28	0/3/3/3
30	PSU	a	2604	30	-	0/7/25/26	0/2/2/2
30	PSU	a	1911	30	-	1/7/25/26	0/2/2/2
30	PSU	a	2457	30	-	0/7/25/26	0/2/2/2
7	G7M	A	527	7	-	0/7/25/26	0/3/3/3
30	1MG	a	745	30	-	0/7/25/26	0/3/3/3
30	OMG	a	2251	29,30	-	1/9/27/28	0/3/3/3
33	MEQ	d	150	33	-	2/8/9/11	-
30	G7M	a	2069	30	-	2/7/25/26	0/3/3/3
7	UR3	A	1498	57,7	-	0/7/25/26	0/2/2/2
30	2MA	a	2503	57,30	-	2/7/25/26	0/3/3/3
30	PSU	a	2580	30	-	0/7/25/26	0/2/2/2
30	OMC	a	2498	57,30	-	0/9/27/28	0/2/2/2
30	5MU	a	1939	30	-	0/7/25/26	0/2/2/2
7	5MC	A	1407	7	-	0/7/25/26	0/2/2/2
30	OMU	a	2552	30	-	1/9/27/28	0/2/2/2
7	2MG	A	966	7	-	0/9/27/28	0/3/3/3
7	4OC	A	1402	7	-	0/9/29/30	0/2/2/2
30	5MU	a	747	30	-	1/7/25/26	0/2/2/2
30	2MG	a	1835	30	-	0/9/27/28	0/3/3/3
7	MA6	A	1518	7	-	0/11/29/30	0/3/3/3
30	6MZ	a	1618	30	-	0/9/27/28	0/3/3/3
30	6MZ	a	2030	30	-	2/9/27/28	0/3/3/3
7	PSU	A	516	7	-	0/7/25/26	0/2/2/2
30	2MG	a	2445	30	-	0/9/27/28	0/3/3/3
30	PSU	a	2504	30	-	0/7/25/26	0/2/2/2
30	5MC	a	1962	30	-	0/7/25/26	0/2/2/2
30	PSU	a	746	57,30	-	3/7/25/26	0/2/2/2
30	PSU	a	955	30	-	0/7/25/26	0/2/2/2
7	MA6	A	1519	7	-	2/11/29/30	0/3/3/3
30	PSU	a	1917	30	-	0/7/25/26	0/2/2/2

The worst 5 of 179 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	747	5MU	C4-C5	20.47	1.78	1.44
30	a	1939	5MU	C4-C5	20.34	1.78	1.44
30	a	747	5MU	C6-N1	15.03	1.63	1.38
30	a	1939	5MU	C6-N1	14.78	1.63	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	1618	6MZ	C6-N6	12.37	1.47	1.34

The worst 5 of 224 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1519	MA6	N1-C6-N6	-13.75	102.05	117.08
7	A	1518	MA6	N1-C6-N6	-11.92	104.05	117.08
30	a	1939	5MU	C5-C4-N3	10.68	124.43	115.31
30	a	747	5MU	C5-C4-N3	9.36	123.30	115.31
30	a	1939	5MU	C5-C6-N1	-9.07	114.01	123.34

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	a	746	PSU	C2'-C1'-C5-C4
30	a	746	PSU	O4'-C1'-C5-C6
30	a	2030	6MZ	O4'-C4'-C5'-O5'
30	a	2030	6MZ	C3'-C4'-C5'-O5'
33	d	150	MEQ	NE2-CD-CG-CB

There are no ring outliers.

9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1207	2MG	1	0
30	a	2251	OMG	1	0
33	d	150	MEQ	2	0
30	a	2503	2MA	1	0
30	a	1939	5MU	1	0
30	a	2552	OMU	1	0
7	A	966	2MG	1	0
30	a	747	5MU	3	0
30	a	2030	6MZ	2	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 311 ligands modelled in this entry, 310 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	T8B	A	1689	57	48,48,48	0.80	2 (4%)	63,71,71	1.07	2 (3%)

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
58	T8B	A	1689	57	-	2/26/26/26	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	A	1689	T8B	C10-C11	3.91	1.38	1.34
58	A	1689	T8B	O1-C1	-2.19	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	A	1689	T8B	C21-C23-C24	-5.27	118.89	125.03
58	A	1689	T8B	O7-C16-C15	-2.61	116.08	121.29

There are no chirality outliers.

All (2) torsion outliers are listed below:

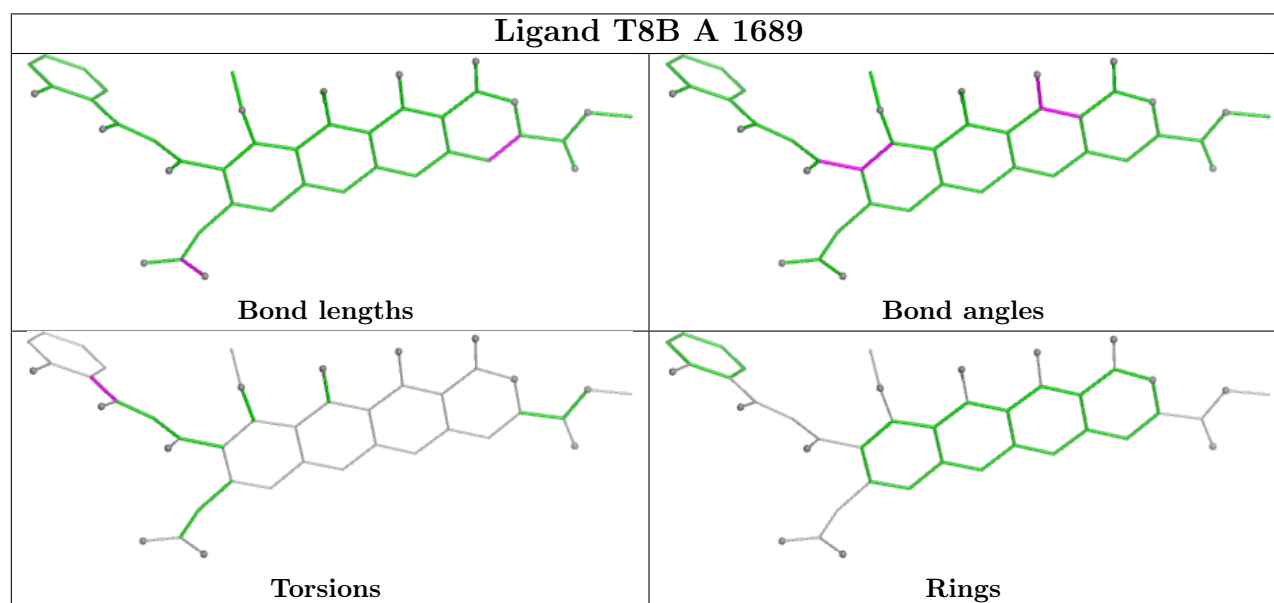
Mol	Chain	Res	Type	Atoms
58	A	1689	T8B	O11-C26-C27-C32
58	A	1689	T8B	C25-C26-C27-C28

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	A	1689	T8B	1	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
41	1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	81:ARG	C	82:MET	N	2.56

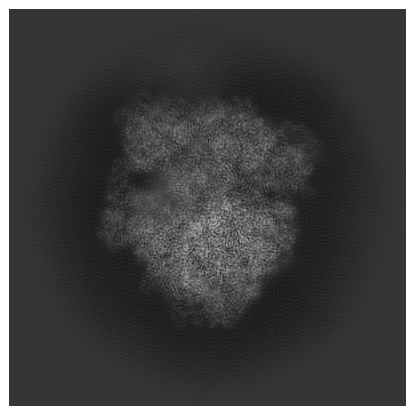
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15712. These allow visual inspection of the internal detail of the map and identification of artifacts.

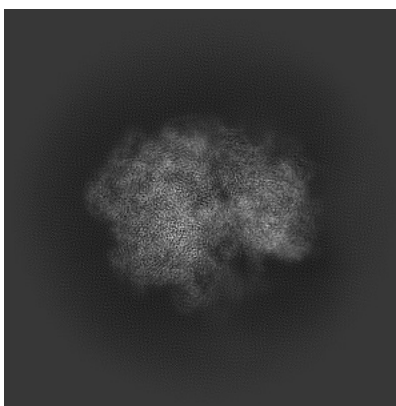
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

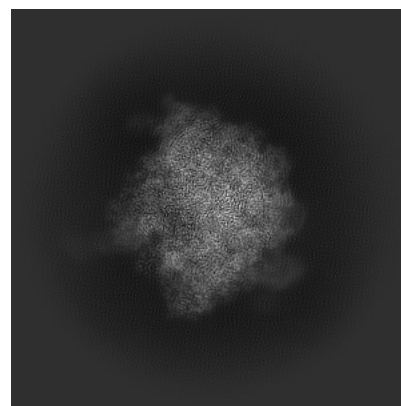
6.1.1 Primary map



X

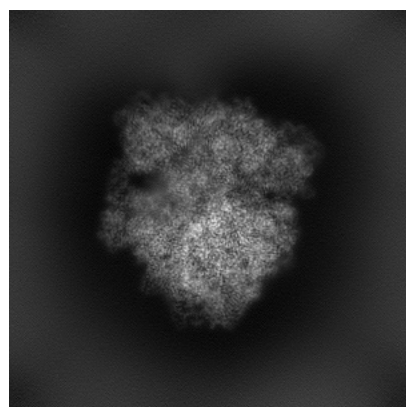


Y

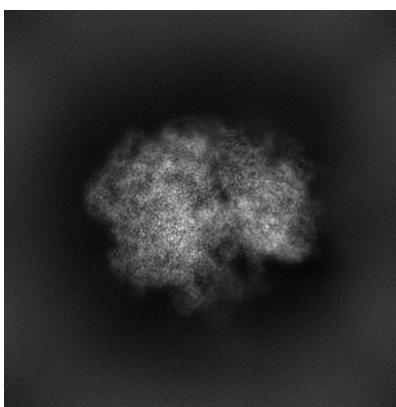


Z

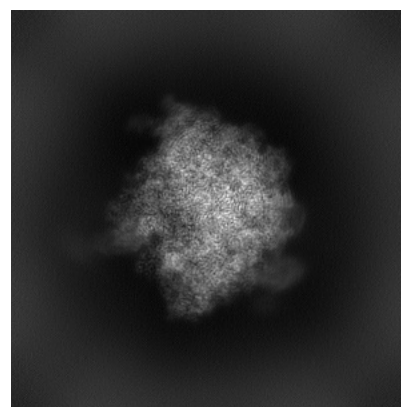
6.1.2 Raw map



X



Y

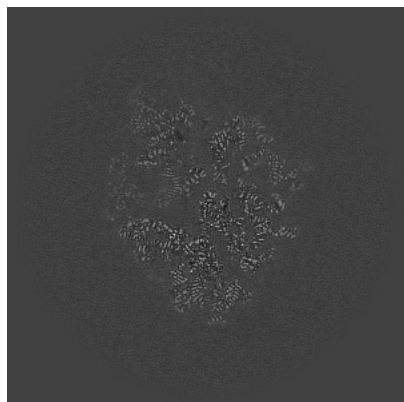


Z

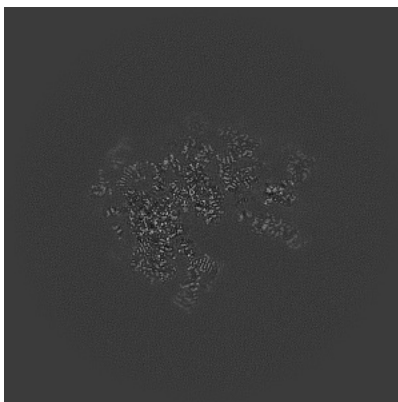
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

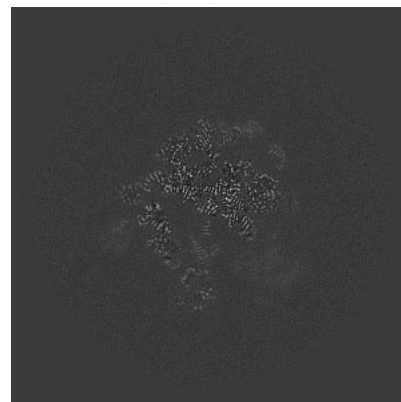
6.2.1 Primary map



X Index: 256

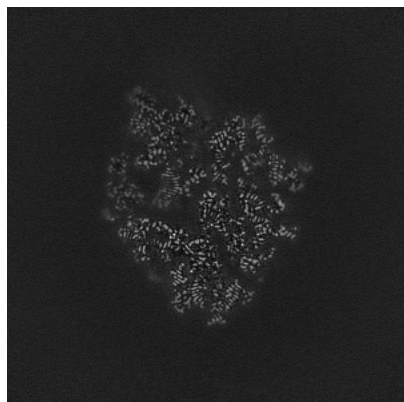


Y Index: 256

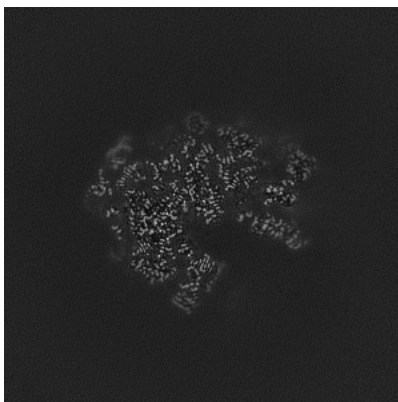


Z Index: 256

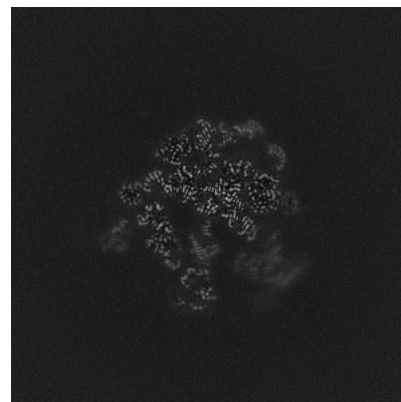
6.2.2 Raw map



X Index: 256



Y Index: 256

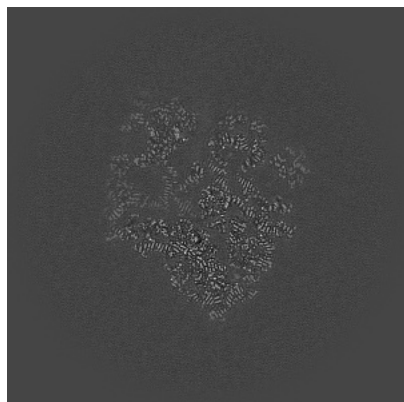


Z Index: 256

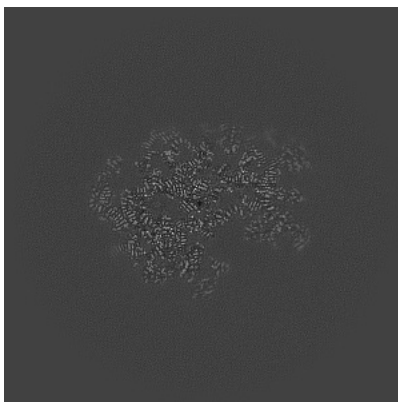
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

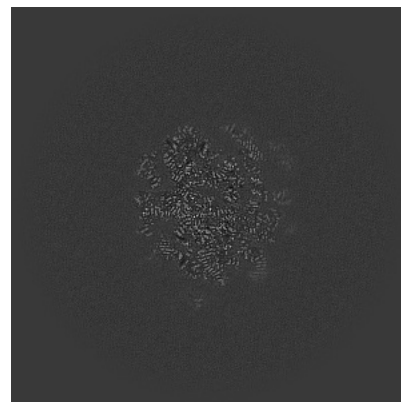
6.3.1 Primary map



X Index: 250

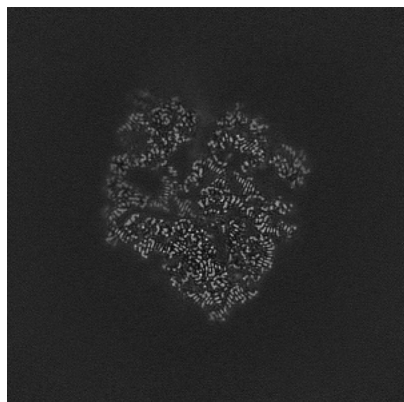


Y Index: 270

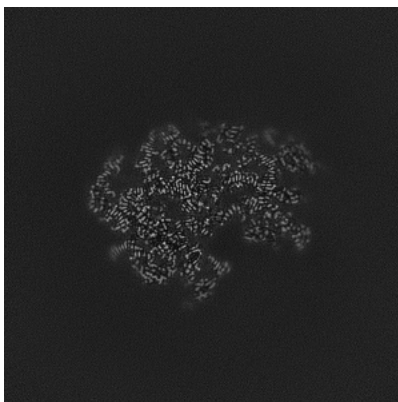


Z Index: 205

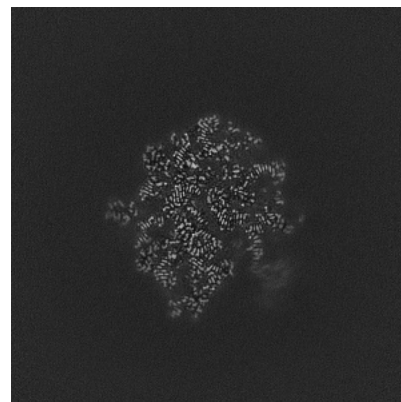
6.3.2 Raw map



X Index: 249



Y Index: 268

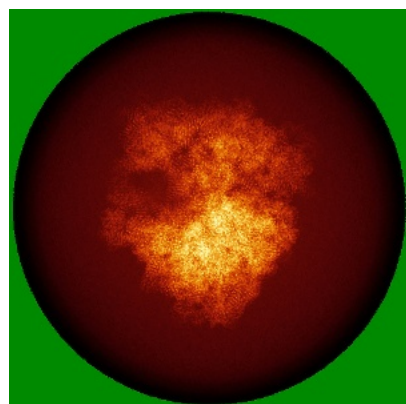


Z Index: 228

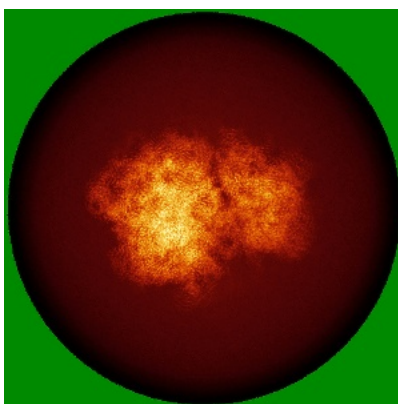
The images above show the largest variance slices of the map in three orthogonal directions.

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

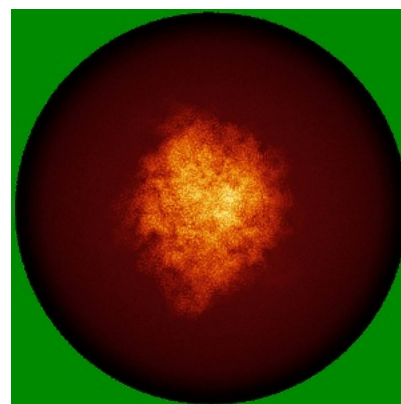
6.4.1 Primary map



X

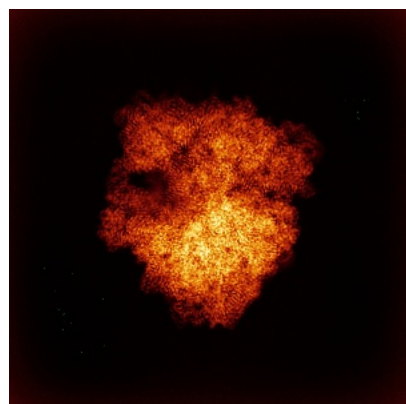


Y

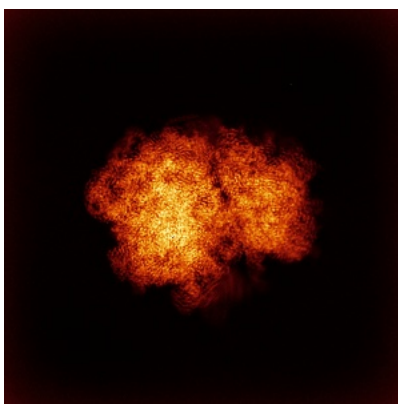


Z

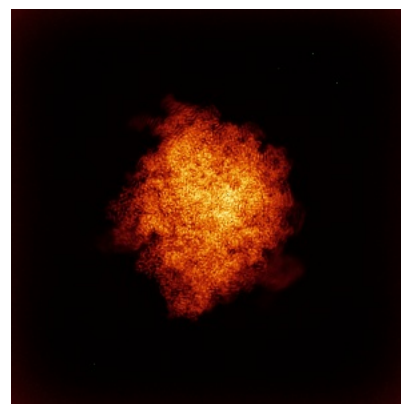
6.4.2 Raw map



X



Y

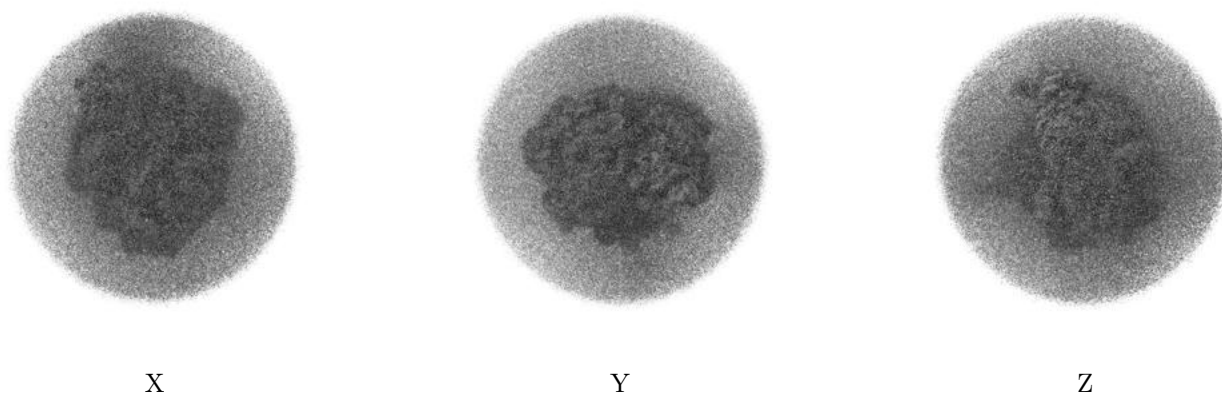


Z

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

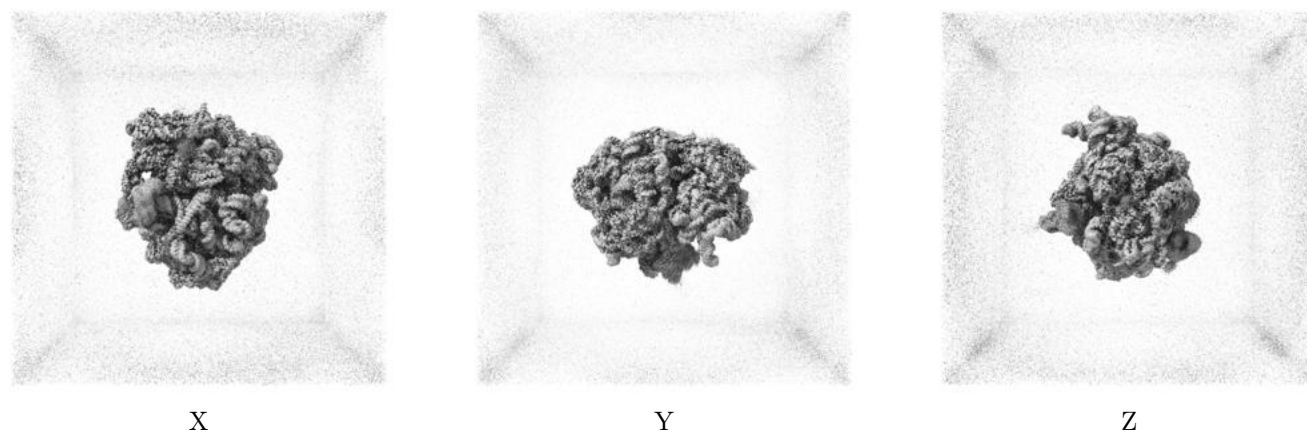
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.21. 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.

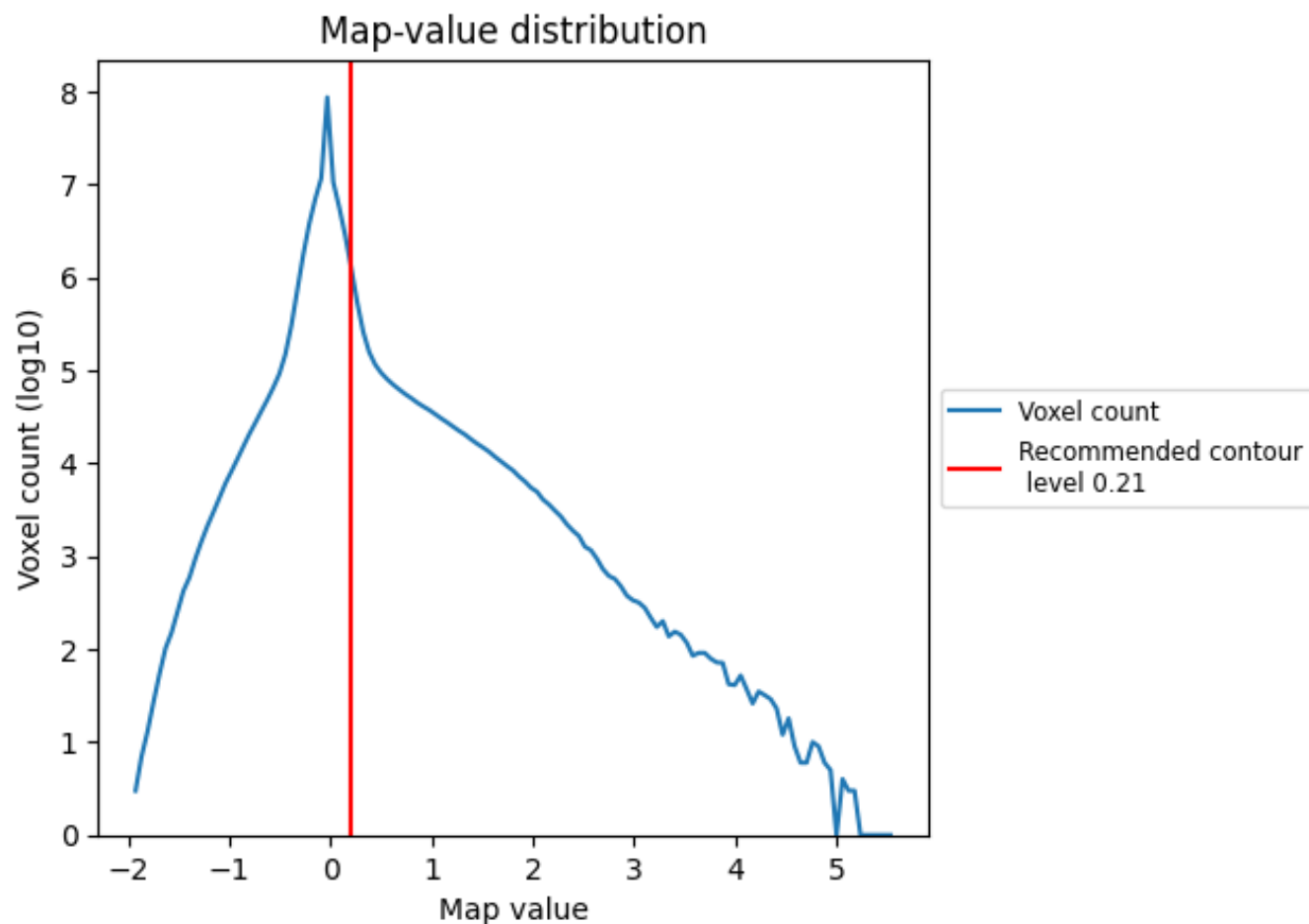
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

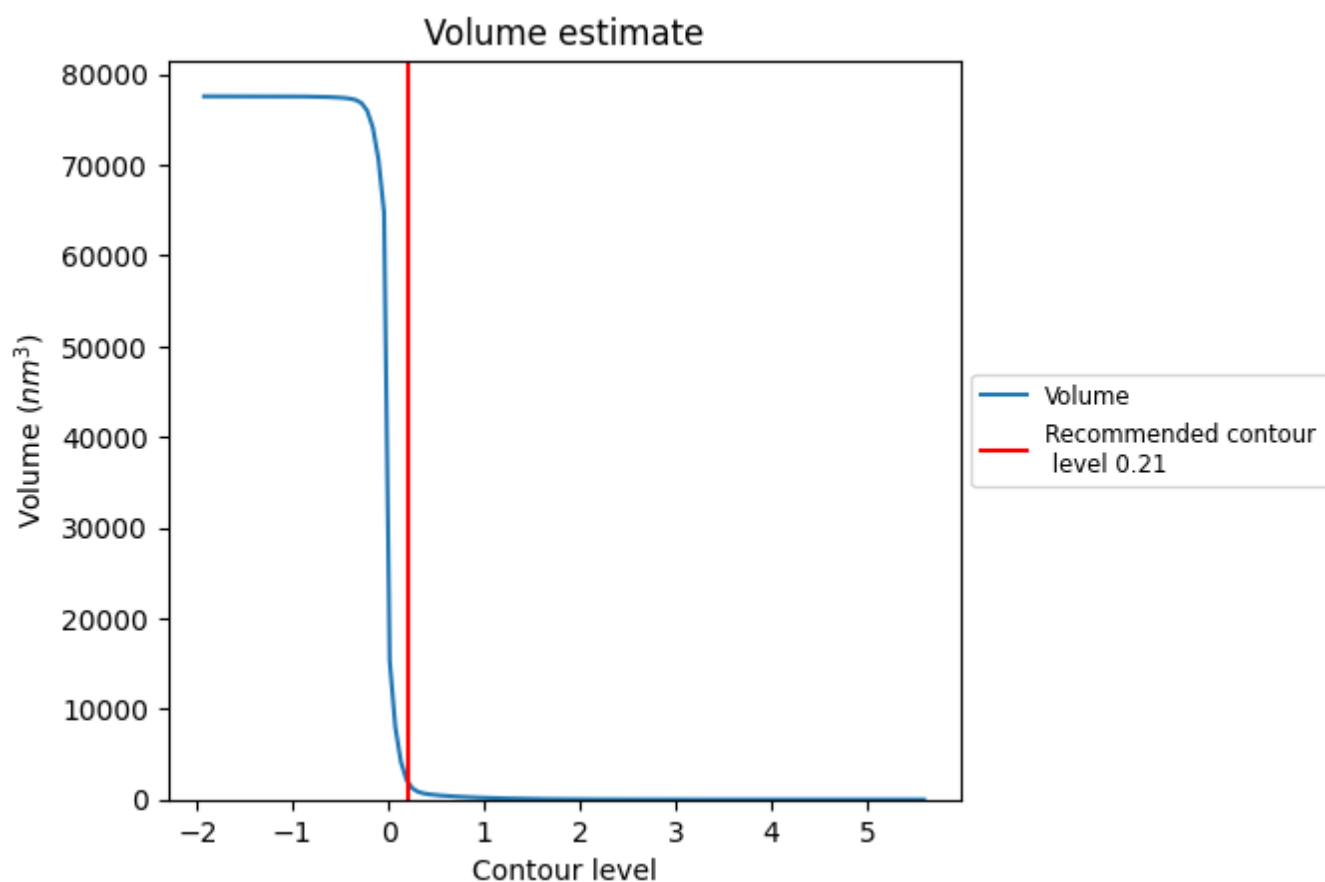
This section contains the results of statistical analysis of the map.

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.

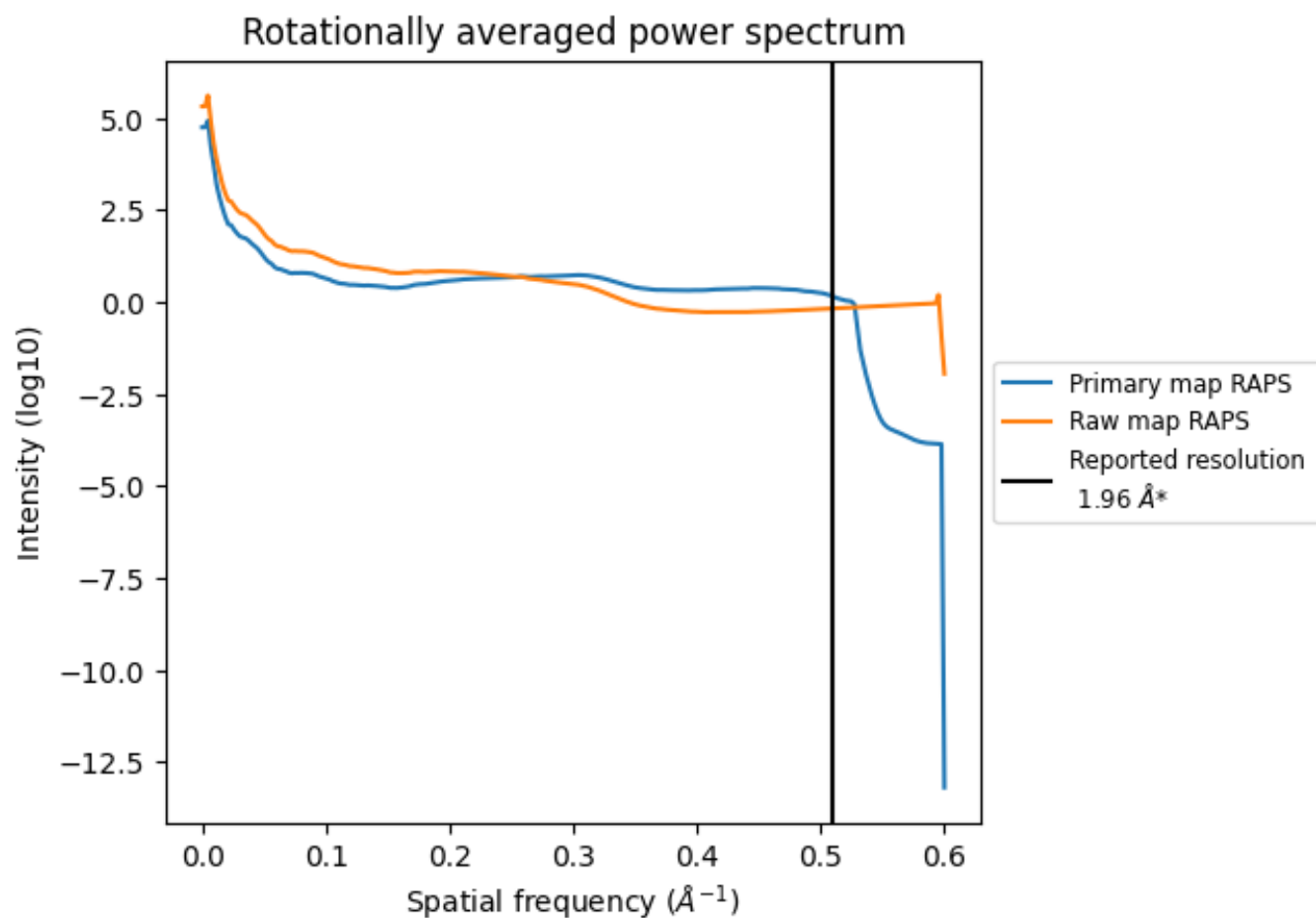
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1845 nm³; this corresponds to an approximate mass of 1666 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 ⓘ

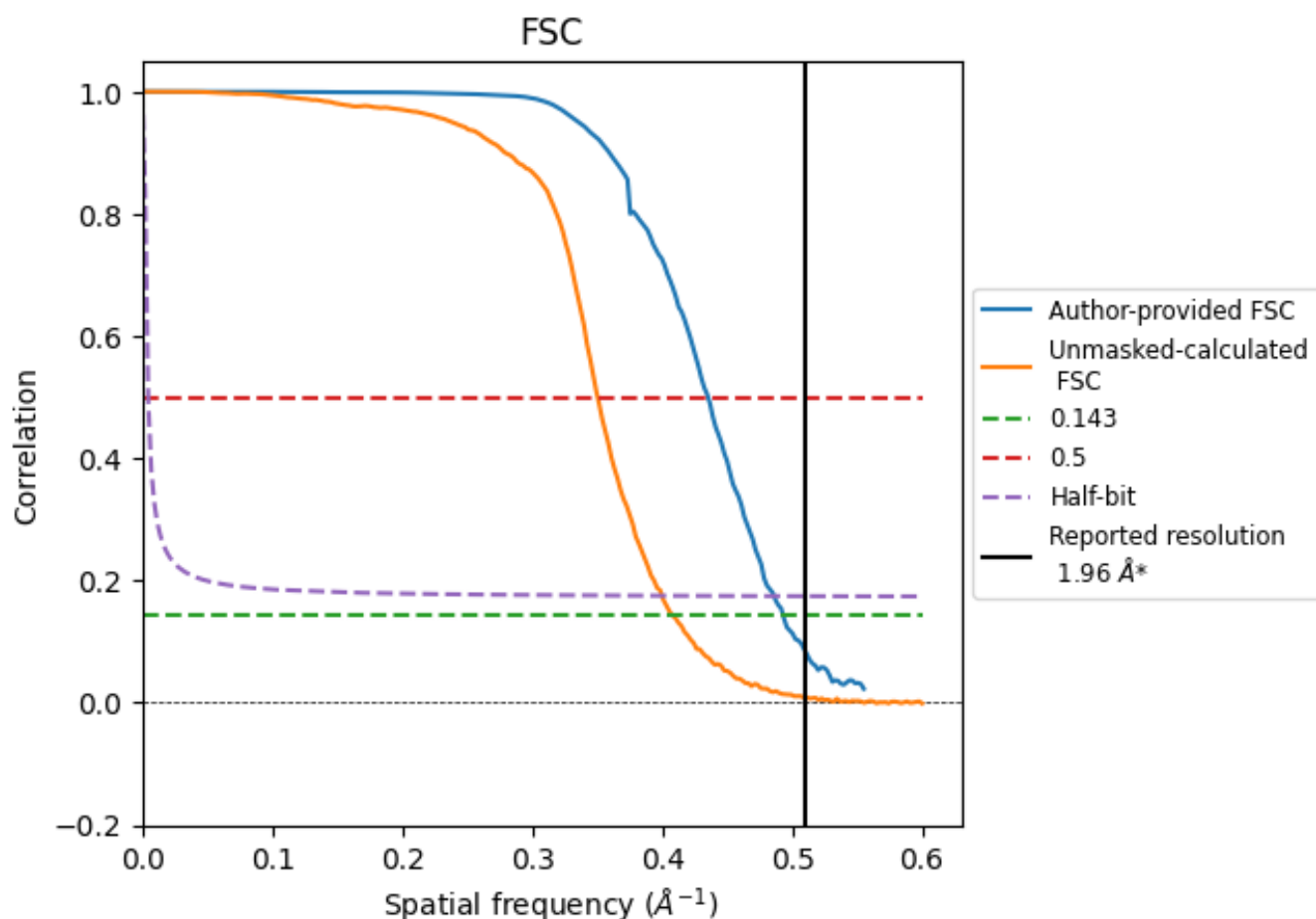


*Reported resolution corresponds to spatial frequency of 0.510 Å⁻¹

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 0.510 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

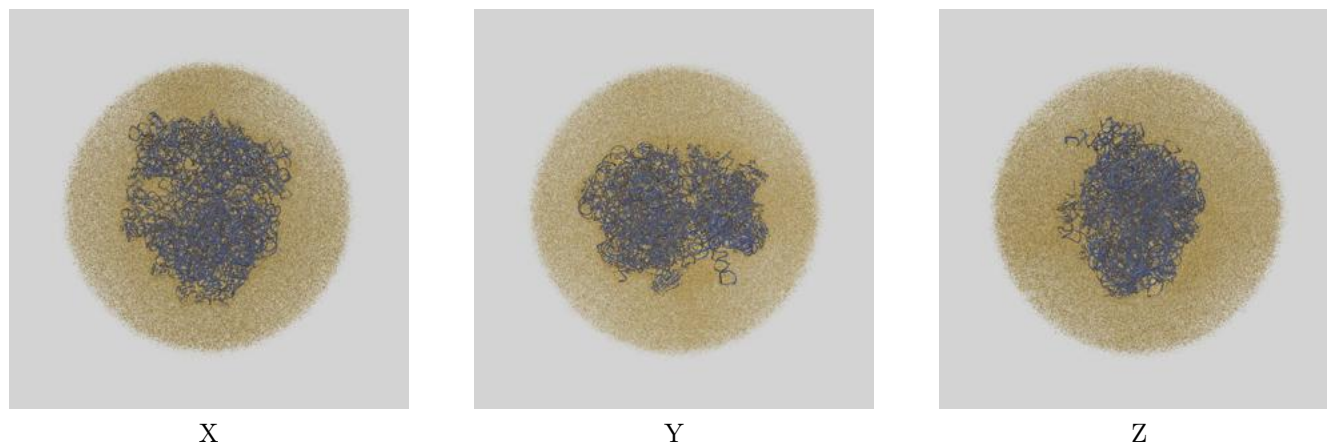
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.96	-	-
Author-provided FSC curve	2.03	2.30	2.06
Unmasked-calculated*	2.45	2.85	2.50

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.45 differs from the reported value 1.96 by more than 10 %

9 Map-model fit [i](#)

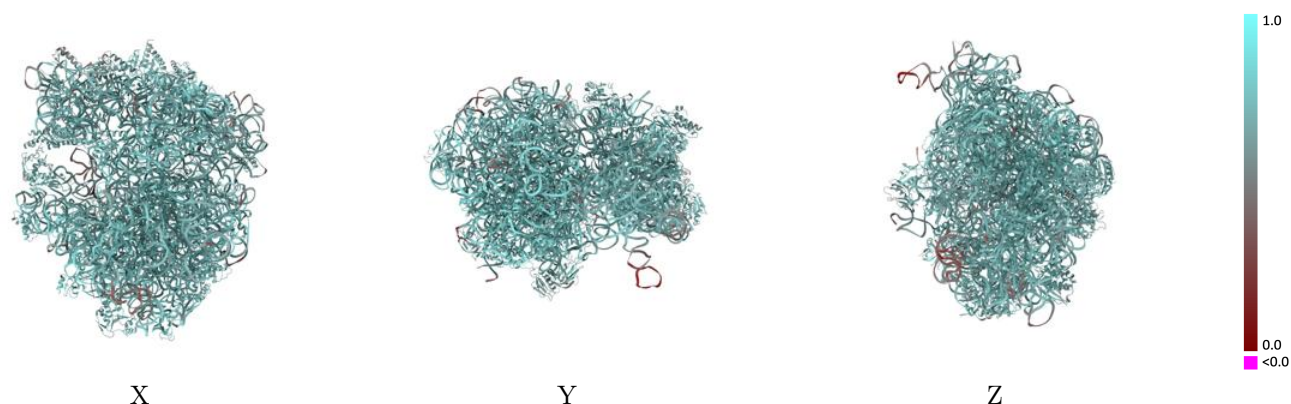
This section contains information regarding the fit between EMDB map EMD-15712 and PDB model 8AYE. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



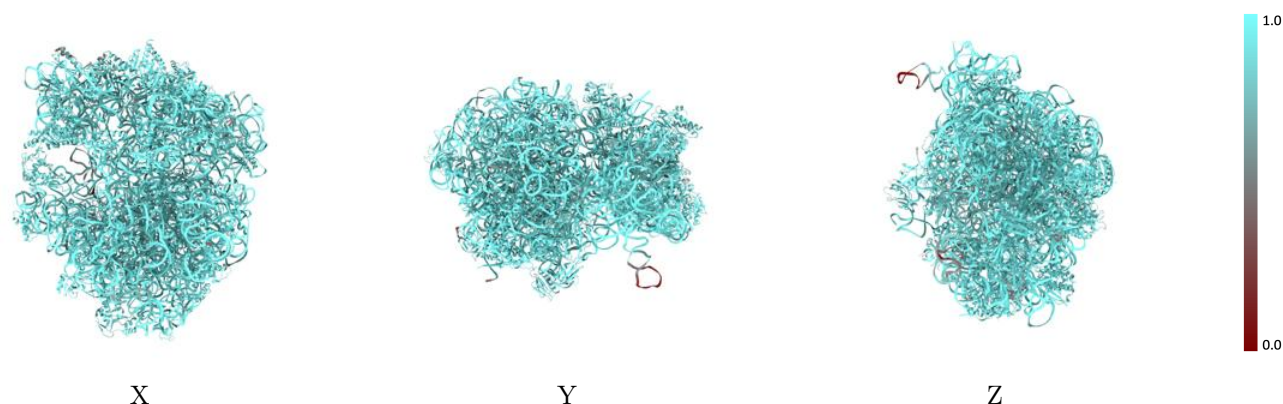
The images above show the 3D surface view of the map at the recommended contour level 0.21 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



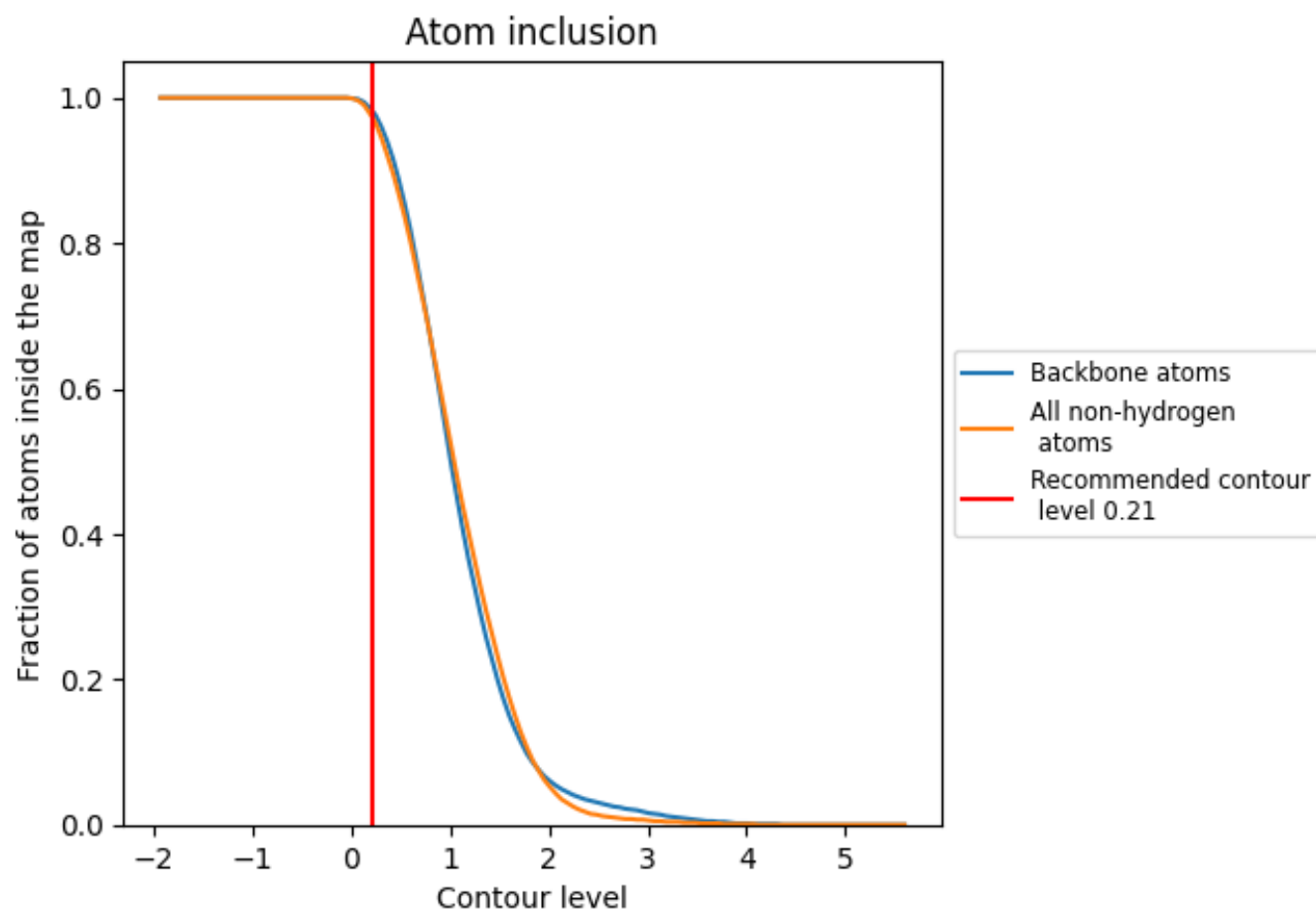
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.21).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.21) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9740	 0.7340
0	 0.9830	 0.7670
1	 0.9920	 0.8020
2	 1.0000	 0.8050
3	 0.9930	 0.7800
4	 0.8390	 0.6080
5	 0.7860	 0.6560
A	 0.9710	 0.7100
B	 0.9240	 0.6760
C	 0.9610	 0.7160
D	 0.9570	 0.7160
E	 0.9800	 0.7650
F	 0.9490	 0.6870
G	 0.9420	 0.6930
H	 0.9770	 0.7630
I	 0.9500	 0.6980
J	 0.8400	 0.6310
K	 0.9660	 0.7280
L	 0.9760	 0.7520
M	 0.9640	 0.7110
N	 0.9690	 0.7190
O	 0.9770	 0.7490
P	 0.9570	 0.7210
Q	 0.9550	 0.7000
R	 0.9500	 0.7160
S	 0.9290	 0.6770
T	 0.9740	 0.7370
U	 0.8710	 0.6500
X	 0.9620	 0.7100
Z	 0.9360	 0.6540
a	 0.9850	 0.7480
b	 0.9840	 0.7100
c	 0.9950	 0.7970
d	 0.9850	 0.7890
e	 0.9630	 0.7510



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Chain	Atom inclusion	Q-score
f	 0.9590	 0.6970
g	 0.9290	 0.6630
h	 0.9400	 0.6800
i	 0.9890	 0.7860
j	 0.9920	 0.7910
k	 0.9820	 0.7750
l	 0.9910	 0.7800
m	 1.0000	 0.8040
n	 0.9690	 0.7320
o	 0.9820	 0.7780
p	 0.9980	 0.8040
q	 0.9770	 0.7670
r	 0.9840	 0.7870
s	 0.9630	 0.7490
t	 0.9640	 0.7200
u	 0.9630	 0.7330
v	 0.9830	 0.7820
w	 0.9920	 0.7810
x	 0.9410	 0.7130
y	 0.9790	 0.7810
z	 0.9770	 0.7820