



wwPDB EM Validation Summary Report ⓘ

Dec 11, 2022 – 05:23 pm GMT

PDB ID : 6SWC
EMDB ID : EMD-10322
Title : IC2B model of cryo-EM structure of a full archaeal ribosomal translation initiation complex devoid of aIF1 in *P. abyssi*
Authors : Coureux, P.-D.; Mechulam, Y.; Schmitt, E.
Deposited on : 2019-09-20
Resolution : 3.30 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.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

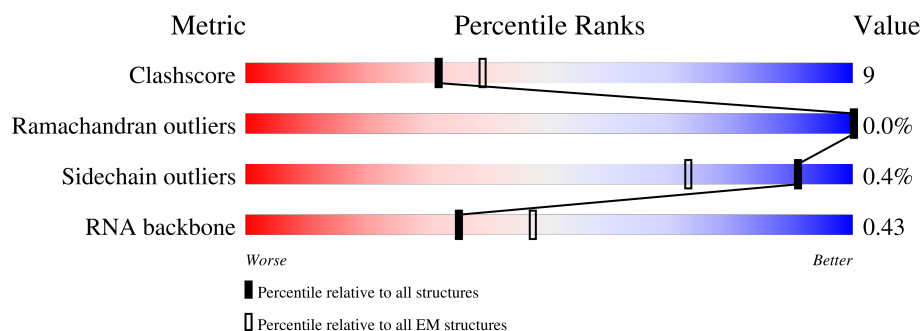
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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




























Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	2	1497	63% 29% 8%
2	A	199	73% 22% 6%
3	B	202	80% 17% .
4	C	63	78% 19% .
5	D	180	86% 11% . .
6	E	243	79% 20%
7	F	236	80% 17% .




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Mol	Chain	Length	Quality of chain
8	G	125	
9	H	215	
10	I	130	
11	J	127	
12	K	135	
13	L	102	
14	M	137	
15	N	147	
16	O	148	
17	P	56	
18	Q	158	
19	R	113	
20	S	67	
21	T	132	
22	U	150	
23	V	99	
24	W	65	
25	X	71	
26	Y	51	
27	Z	210	
28	0	36	
29	3	123	
30	5	20	
31	4	76	
32	6	113	

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Mol	Chain	Length	Quality of chain
33	7	415	
34	8	139	
35	9	266	

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 70744 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1497	Total	C	N	O	P	0	0
			32291	14394	5959	10441	1497		

- Molecule 2 is a protein called 30S ribosomal protein S3Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	188	Total	C	N	O	S	0	0
			1533	995	268	266	4		

- Molecule 3 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	196	Total	C	N	O	S	0	0
			1571	1017	269	281	4		

- Molecule 4 is a protein called Zn-ribbon RNA-binding protein involved in translation.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	61	Total	C	N	O	S	0	0
			482	304	85	85	8		

- Molecule 5 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	175	Total	C	N	O	S	0	0
			1470	924	284	258	4		

- Molecule 6 is a protein called 30S ribosomal protein S4e.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	242	Total	C	N	O	S	0	0
			1983	1281	358	339	5		

- Molecule 7 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	229	Total	C	N	O	S	0	0
			1808	1147	334	320	7		

- Molecule 8 is a protein called 30S ribosomal protein S6e.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	124	Total	C	N	O	S	0	0
			977	621	178	176	2		

- Molecule 9 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	213	Total	C	N	O	S	0	0
			1720	1092	322	299	7		

- Molecule 10 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	129	Total	C	N	O	S	0	0
			1034	668	184	180	2		

- Molecule 11 is a protein called 30S ribosomal protein S8e.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	126	Total	C	N	O	S	0	0
			996	617	206	173			

- Molecule 12 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	134	Total	C	N	O	S	0	0
			1065	668	206	188	3		

- Molecule 13 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	101	Total	C	N	O	S	0	0
			817	507	158	148	4		

- Molecule 14 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	128	Total	C	N	O	S	0	0
			964	597	192	173	2		

- Molecule 15 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	146	Total	C	N	O	S	0	0
			1148	727	224	194	3		

- Molecule 16 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	143	Total	C	N	O	S	0	0
			1151	721	229	196	5		

- Molecule 17 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	55	Total	C	N	O	S	0	0
			455	288	95	67	5		

- Molecule 18 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	152	Total	C	N	O	S	0	0
			1262	804	240	214	4		

- Molecule 19 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	109	Total	C	N	O	S	0	0
			900	572	174	151	3		

- Molecule 20 is a protein called 30S ribosomal protein S17e.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	66	Total	C	N	O	S	0	0
			558	355	106	96	1		

- Molecule 21 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	130	Total	C	N	O	S	0	0
			1057	675	201	174	7		

- Molecule 22 is a protein called 30S ribosomal protein S19e.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	149	Total	C	N	O		0	0
			1223	790	221	212			

- Molecule 23 is a protein called 30S ribosomal protein S24e.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	94	Total	C	N	O	S	0	0
			790	516	125	146	3		

- Molecule 24 is a protein called 30S ribosomal protein S27e.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	63	Total	C	N	O	S	0	0
			481	303	93	80	5		

- Molecule 25 is a protein called 30S ribosomal protein S28e.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	X	67	Total	C	N	O	0	0
			536	327	111	98		

- Molecule 26 is a protein called 30S ribosomal protein S27ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	50	Total	C	N	O	S	0	0
			408	262	77	63	6		

- Molecule 27 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	197	Total	C	N	O	S	0	0
			1550	989	286	271	4		

- Molecule 28 is a protein called 30S ribosomal protein aL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	0	36	Total	C	N	O	S	0	0
			343	218	84	39	2		

- Molecule 29 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	3	123	Total	C	N	O	S	0	0
			941	599	157	181	4		

- Molecule 30 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	5	20	Total	C	N	O	P	0	0
			430	192	78	140	20		

- Molecule 31 is a RNA chain called initiator Met-tRNA fMet from E. coli (A1U72 variant).

Mol	Chain	Residues	Atoms						AltConf	Trace
31	4	76	Total	C	N	O	P	S	0	0
			1622	724	291	530	76	1		

- Molecule 32 is a protein called Translation initiation factor 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	6	95	Total	C	N	O	S	0	0
			777	496	148	130	3		

- Molecule 33 is a protein called Translation initiation factor 2 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	7	414	Total	C	N	O	S	0	0
			3213	2058	548	595	12		

- Molecule 34 is a protein called Translation initiation factor 2 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	8	129	Total	C	N	O	S	0	0
			1033	659	172	192	10		

- Molecule 35 is a protein called Translation initiation factor 2 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	9	254	Total	C	N	O	S	0	0
			2033	1301	346	384	2		

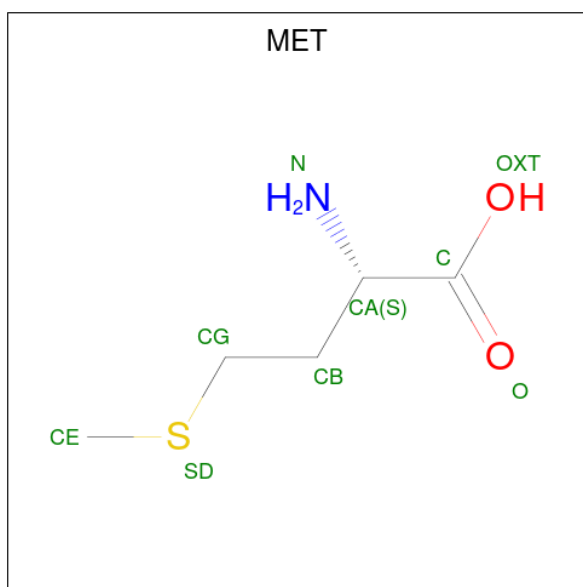
- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
36	2	30	Total	Mg	0
			30	30	
36	5	2	Total	Mg	0
			2	2	
36	4	1	Total	Mg	0
			1	1	
36	7	1	Total	Mg	0
			1	1	

- Molecule 37 is ZINC ION (three-letter code: ZN) (formula: Zn).

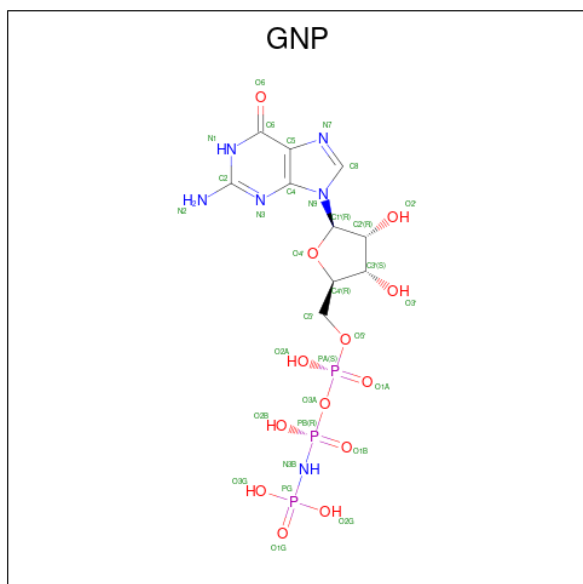
Mol	Chain	Residues	Atoms		AltConf
37	C	2	Total	Zn	0
			2	2	
37	F	1	Total	Zn	0
			1	1	
37	P	1	Total	Zn	0
			1	1	
37	R	1	Total	Zn	0
			1	1	
37	W	1	Total	Zn	0
			1	1	

- Molecule 38 is METHIONINE (three-letter code: MET) (formula: C₅H₁₁NO₂S).



Mol	Chain	Residues	Atoms					AltConf
38	4	1	Total	C	N	O	S	0
			8	5	1	1	1	

- Molecule 39 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
39	7	1	Total	C	N	O	P	0
			32	10	6	13	3	

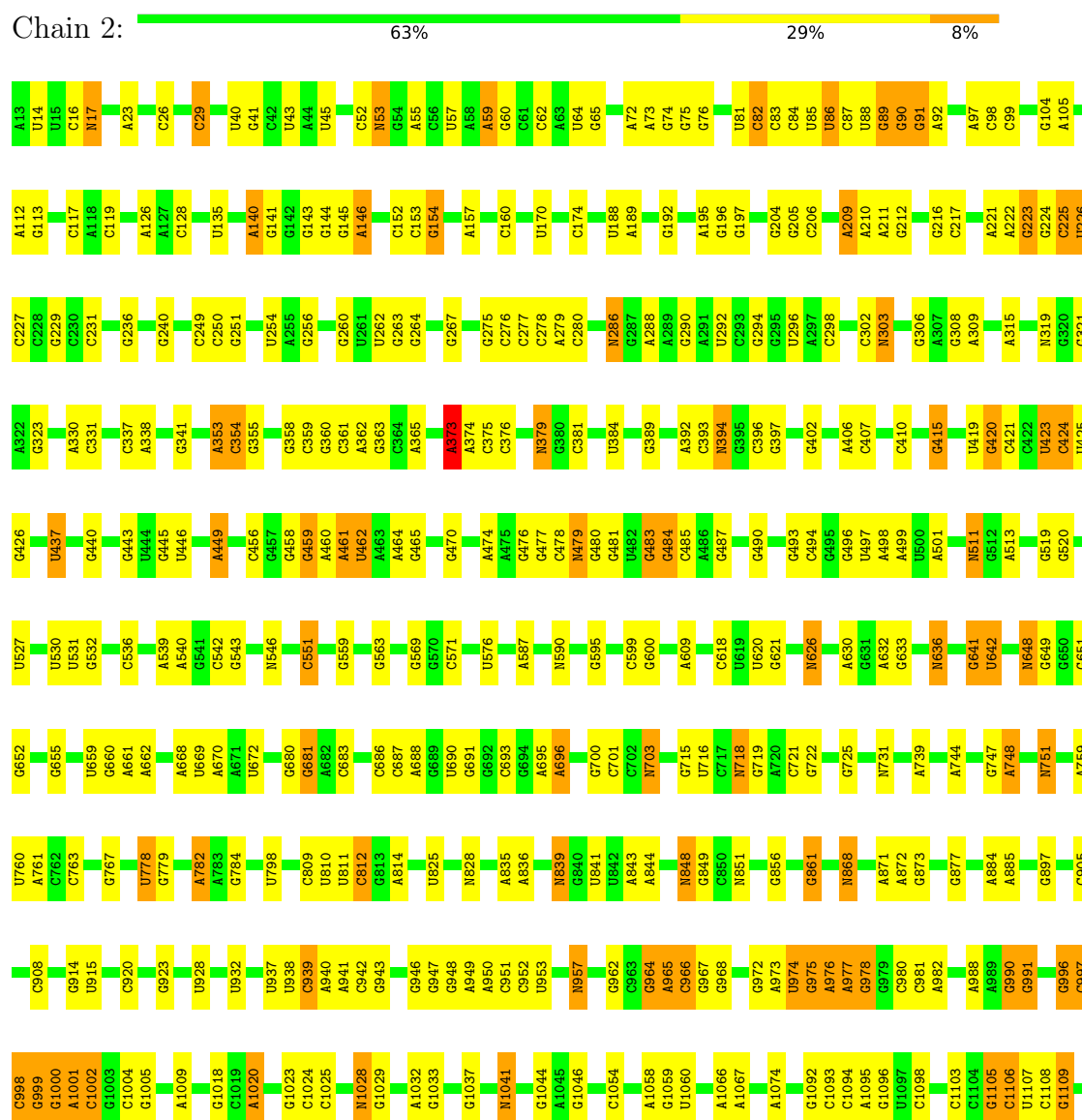
- Molecule 40 is water.

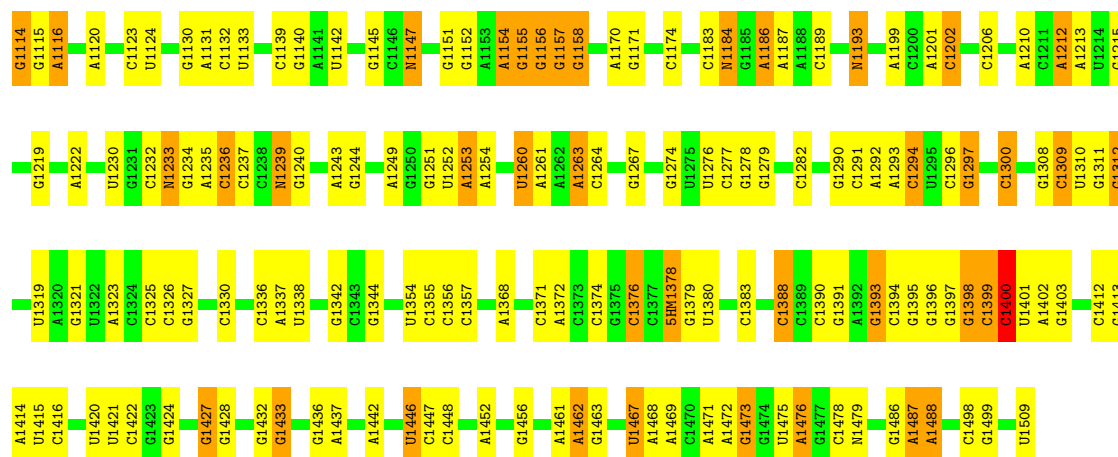
Mol	Chain	Residues	Atoms		AltConf
40	2	39	Total 39	O 39	0
40	K	1	Total 1	O 1	0
40	Q	1	Total 1	O 1	0
40	U	1	Total 1	O 1	0

3 Residue-property plots

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

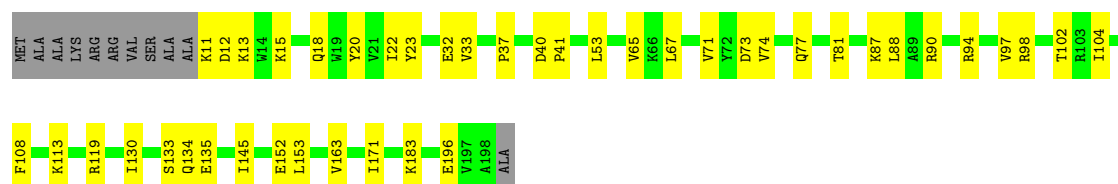
• Molecule 1: 16S ribosomal rRNA





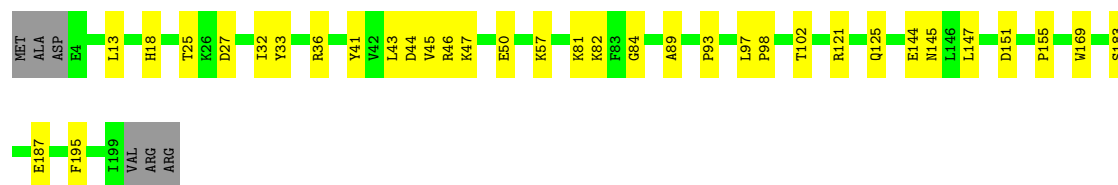
• Molecule 2: 30S ribosomal protein S3Ae

Chain A: 73% 22% 6%



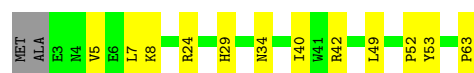
• Molecule 3: 30S ribosomal protein S2

Chain B: 80% 17% .



• Molecule 4: Zn-ribbon RNA-binding protein involved in translation

Chain C: 78% 19% .




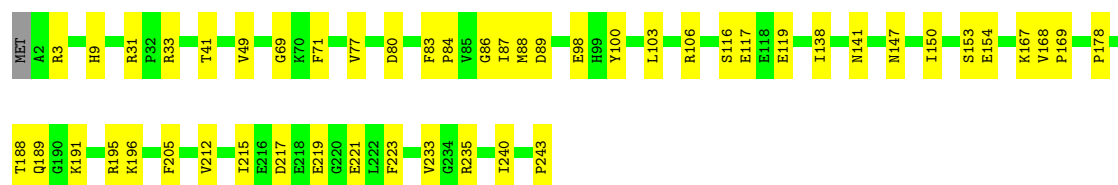
• Molecule 5: 30S ribosomal protein S4

Chain D: 86% 11% . .




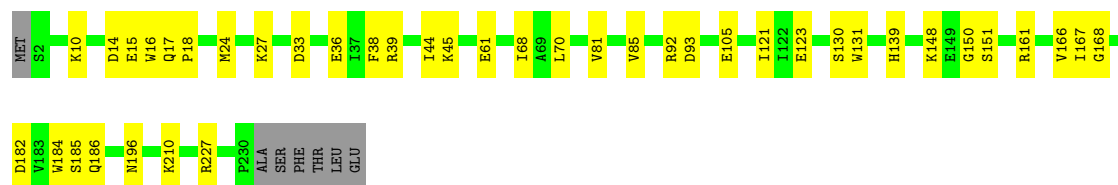
• Molecule 6: 30S ribosomal protein S4e

Chain E:  79% 20%



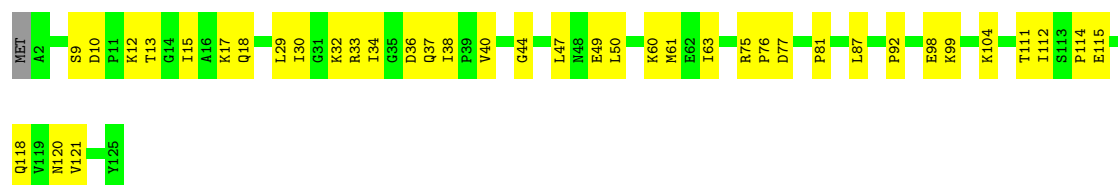
- Molecule 7: 30S ribosomal protein S5

Chain F:  80% 17%




- Molecule 8: 30S ribosomal protein S6e

Chain G:  68% 31%



- Molecule 9: 30S ribosomal protein S7

Chain H:  79% 20%



- Molecule 10: 30S ribosomal protein S8

Chain I:  76% 23%



- Molecule 11: 30S ribosomal protein S8e

Chain J:  79% 20%



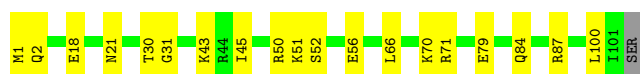
- Molecule 12: 30S ribosomal protein S9

Chain K: 81% 19%



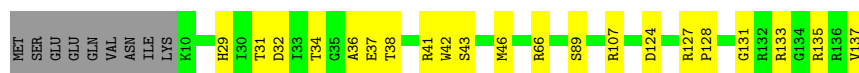
- Molecule 13: 30S ribosomal protein S10

Chain L: 80% 19%



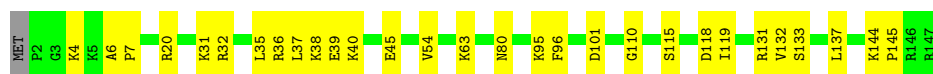
- Molecule 14: 30S ribosomal protein S11

Chain M: 78% 15% 7%



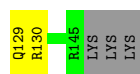
- Molecule 15: 30S ribosomal protein S12

Chain N: 80% 20%



- Molecule 16: 30S ribosomal protein S13

Chain O: 73% 24%



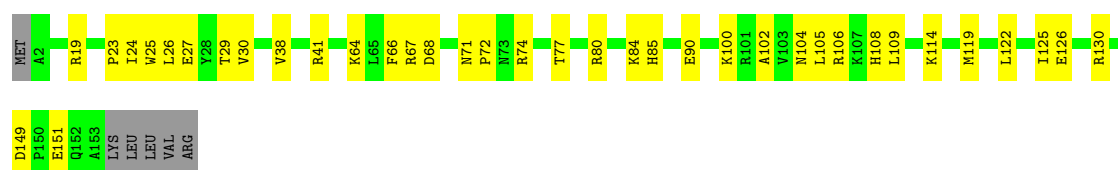
- Molecule 17: 30S ribosomal protein S14 type Z

Chain P: 82% 16%




- Molecule 18: 30S ribosomal protein S15

Chain Q:  73% 23% .



- Molecule 19: 30S ribosomal protein S17

Chain R:  80% 16% . .



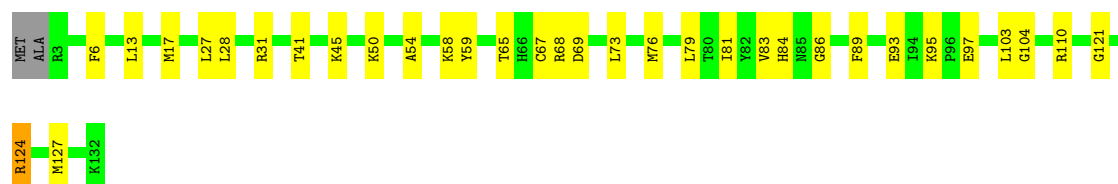
- Molecule 20: 30S ribosomal protein S17e

Chain S:  72% 27% .




- Molecule 21: 30S ribosomal protein S19

Chain T:  73% 24% . .



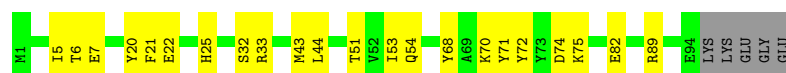
- Molecule 22: 30S ribosomal protein S19e

Chain U:  83% 16% .



- Molecule 23: 30S ribosomal protein S24e

Chain V:  73% 22% 5%



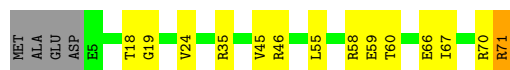
- Molecule 24: 30S ribosomal protein S27e

Chain W:  62% 35% .



- Molecule 25: 30S ribosomal protein S28e

Chain X: 75% 18% 6%



- Molecule 26: 30S ribosomal protein S27ae

Chain Y: 61% 31% 6%



- Molecule 27: 30S ribosomal protein S3

Chain Z: 78% 16% 6%



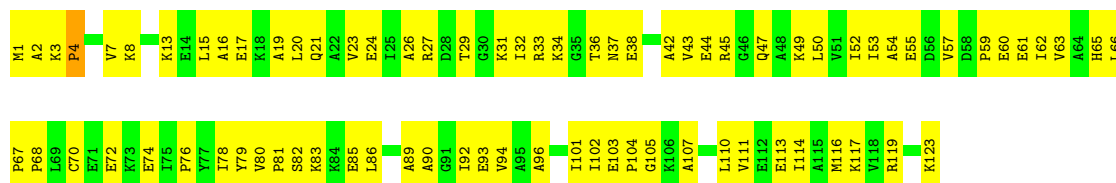
- Molecule 28: 30S ribosomal protein aL41

Chain 0: 75% 25%



- Molecule 29: 50S ribosomal protein L7Ae

Chain 3: 37% 63%




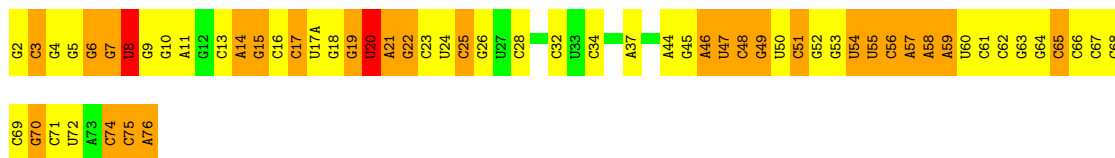
- Molecule 30: mRNA

Chain 5: 60% 30% 10%



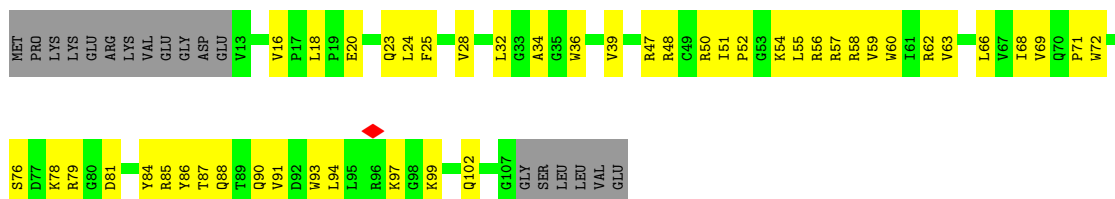
- Molecule 31: initiator Met-tRNA fMet from *E. coli* (A1U72 variant)

Chain 4: 



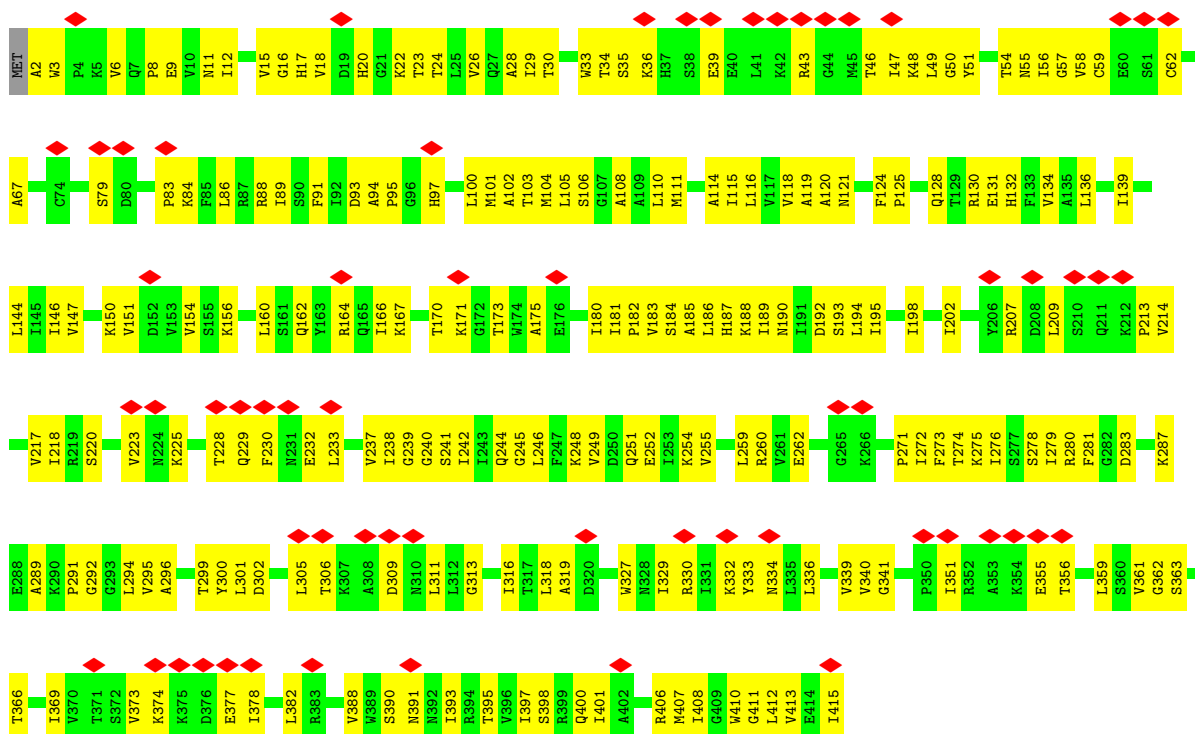
- Molecule 32: Translation initiation factor 1A

Chain 6: 



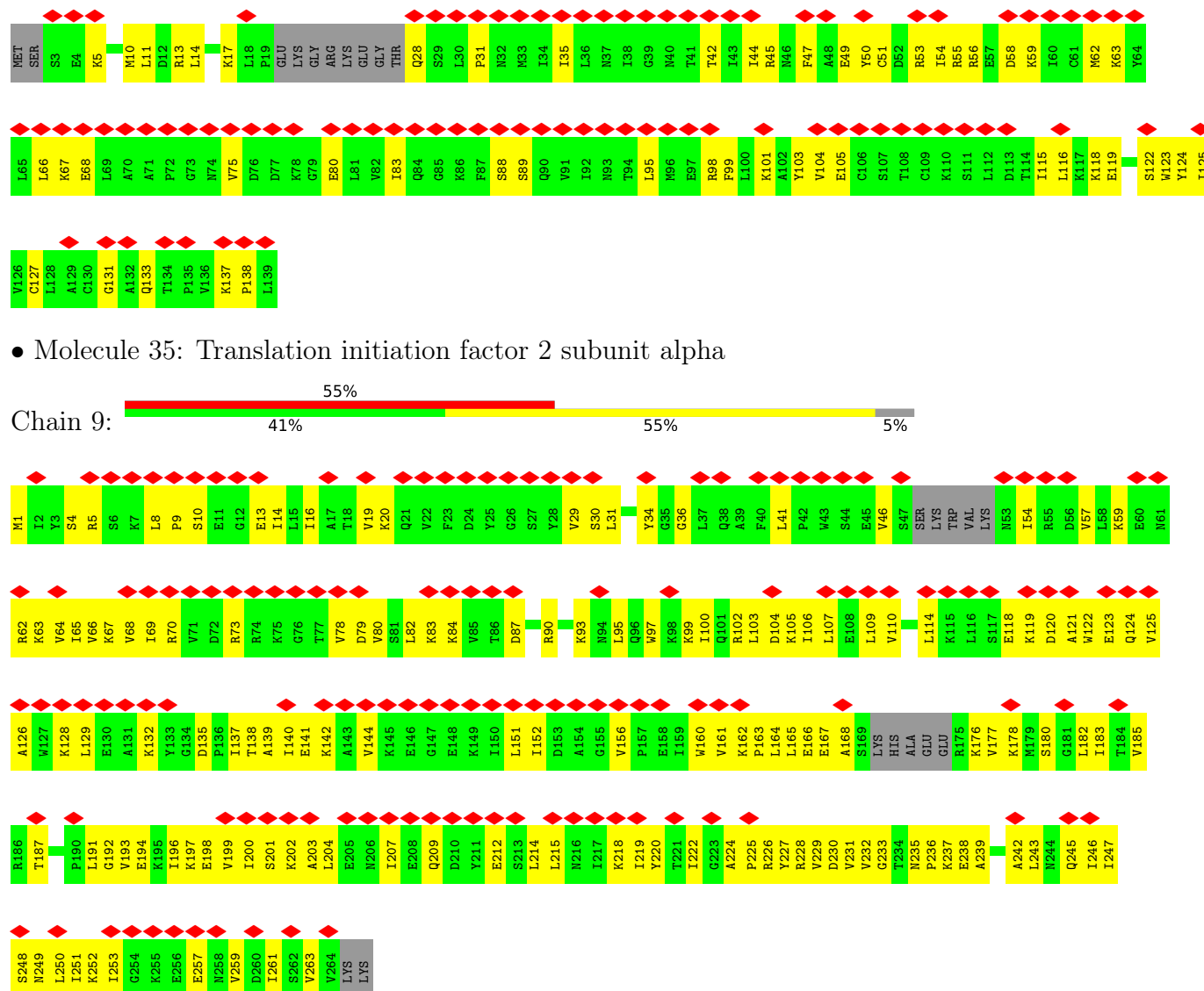
- Molecule 33: Translation initiation factor 2 subunit gamma

Chain 7: 



- Molecule 34: Translation initiation factor 2 subunit beta

Chain 8: 



- Molecule 35: Translation initiation factor 2 subunit alpha

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	142000	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 ($e^-/\text{\AA}^2$)	2	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	0.065	Depositor
Minimum map value	-0.017	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.003	Depositor
Map size (Å)	379.32, 379.32, 379.32	wwPDB
Map dimensions	348, 348, 348	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 6MZ, GNP, 4AC, B8H, PSU, MA6, H2U, A2M, MG, ZN, OMC, LHH, 4SU, 5HM, UR3, 5MC, 5MU

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	2	1.21	7/35019 (0.0%)	1.02	41/54586 (0.1%)
2	A	0.51	0/1559	0.52	0/2090
3	B	0.49	0/1602	0.53	0/2165
4	C	0.53	0/496	0.57	0/673
5	D	0.49	0/1494	0.50	0/2003
6	E	0.57	0/2032	0.54	0/2742
7	F	0.56	0/1838	0.56	0/2478
8	G	0.37	0/993	0.50	0/1329
9	H	0.48	0/1757	0.53	0/2359
10	I	0.58	0/1055	0.57	0/1415
11	J	0.45	0/1005	0.53	0/1339
12	K	0.49	0/1081	0.54	0/1449
13	L	0.42	0/825	0.49	0/1107
14	M	0.47	0/982	0.54	0/1322
15	N	0.53	0/1165	0.56	0/1547
16	O	0.47	0/1170	0.54	0/1573
17	P	0.59	0/465	0.58	0/613
18	Q	0.49	0/1290	0.52	0/1734
19	R	0.54	0/923	0.54	0/1247
20	S	0.43	0/565	0.50	1/747 (0.1%)
21	T	0.48	0/1077	0.53	0/1439
22	U	0.57	0/1253	0.53	0/1689
23	V	0.52	0/808	0.52	0/1086
24	W	0.37	0/488	0.51	0/659
25	X	0.45	0/538	0.58	0/719
26	Y	0.30	0/420	0.51	0/559
27	Z	0.46	0/1572	0.55	0/2110
28	0	0.57	0/349	0.58	0/451
29	3	0.31	0/953	0.55	0/1284
30	5	0.80	0/481	0.96	0/748
31	4	0.69	0/1699	1.08	1/2648 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	6	0.32	0/793	0.48	0/1072
33	7	0.29	0/3272	0.55	2/4430 (0.0%)
34	8	0.26	0/1046	0.52	0/1402
35	9	0.28	0/2058	0.52	0/2770
All	All	0.90	7/74123 (0.0%)	0.83	45/107584 (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
26	Y	0	1
35	9	0	1
All	All	0	2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1046	G	C5-C4	-5.24	1.34	1.38
1	2	540	A	N9-C4	-5.15	1.34	1.37
1	2	1263	A	N9-C4	-5.08	1.34	1.37
1	2	1326	C	N1-C6	-5.08	1.34	1.37
1	2	1323	A	N7-C5	-5.07	1.36	1.39

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	7	2	ALA	C-N-CA	7.39	140.17	121.70
1	2	721	C	C2-N1-C1'	6.88	126.37	118.80
31	4	56	C	C2-N1-C1'	6.59	126.05	118.80
1	2	1388	C	C2-N1-C1'	6.34	125.78	118.80
1	2	437	U	N1-C2-O2	6.26	127.18	122.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
35	9	167	GLU	Peptide
26	Y	8	TYR	Peptide

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	2	32291	0	16317	236	0
2	A	1533	0	1627	32	0
3	B	1571	0	1630	23	0
4	C	482	0	462	11	0
5	D	1470	0	1542	15	0
6	E	1983	0	2060	33	0
7	F	1808	0	1879	29	0
8	G	977	0	1037	27	0
9	H	1720	0	1775	33	0
10	I	1034	0	1069	21	0
11	J	996	0	1076	17	0
12	K	1065	0	1121	18	0
13	L	817	0	871	16	0
14	M	964	0	994	15	0
15	N	1148	0	1248	22	0
16	O	1151	0	1191	23	0
17	P	455	0	475	7	0
18	Q	1262	0	1331	27	0
19	R	900	0	922	18	0
20	S	558	0	595	12	0
21	T	1057	0	1131	25	0
22	U	1223	0	1263	19	0
23	V	790	0	806	15	0
24	W	481	0	512	16	0
25	X	536	0	571	12	0
26	Y	408	0	413	13	0
27	Z	1550	0	1637	22	0
28	0	343	0	407	6	0
29	3	941	0	994	68	0
30	5	430	0	215	3	0
31	4	1622	0	830	64	0
32	6	777	0	806	42	0
33	7	3213	0	3331	196	0
34	8	1033	0	1074	45	0
35	9	2033	0	2145	118	0
36	2	30	0	0	0	0
36	4	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	5	2	0	0	0	0
36	7	1	0	0	0	0
37	C	2	0	0	0	0
37	F	1	0	0	0	0
37	P	1	0	0	0	0
37	R	1	0	0	0	0
37	W	1	0	0	0	0
38	4	8	0	8	4	0
39	7	32	0	13	1	0
40	2	39	0	0	7	0
40	K	1	0	0	0	0
40	Q	1	0	0	0	0
40	U	1	0	0	0	0
All	All	70744	0	55378	1185	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 9.

The worst 5 of 1185 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)
33:7:241:SER:OG	33:7:294:LEU:HD23	1.32	1.24
33:7:51:TYR:CD1	33:7:294:LEU:HD12	1.79	1.17
21:T:124:ARG:HH21	21:T:124:ARG:HB3	1.13	1.14
19:R:16:CYS:SG	19:R:24:HIS:CE1	2.42	1.12
33:7:51:TYR:CE1	33:7:294:LEU:HG	1.87	1.10

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	
2	A	186/199 (94%)	158 (85%)	28 (15%)	0	100	100
3	B	194/202 (96%)	175 (90%)	19 (10%)	0	100	100
4	C	59/63 (94%)	51 (86%)	8 (14%)	0	100	100
5	D	173/180 (96%)	158 (91%)	15 (9%)	0	100	100
6	E	240/243 (99%)	206 (86%)	34 (14%)	0	100	100
7	F	227/236 (96%)	197 (87%)	30 (13%)	0	100	100
8	G	122/125 (98%)	95 (78%)	27 (22%)	0	100	100
9	H	211/215 (98%)	182 (86%)	29 (14%)	0	100	100
10	I	127/130 (98%)	114 (90%)	13 (10%)	0	100	100
11	J	124/127 (98%)	107 (86%)	17 (14%)	0	100	100
12	K	132/135 (98%)	116 (88%)	16 (12%)	0	100	100
13	L	99/102 (97%)	87 (88%)	12 (12%)	0	100	100
14	M	126/137 (92%)	109 (86%)	17 (14%)	0	100	100
15	N	144/147 (98%)	120 (83%)	24 (17%)	0	100	100
16	O	141/148 (95%)	125 (89%)	16 (11%)	0	100	100
17	P	53/56 (95%)	46 (87%)	7 (13%)	0	100	100
18	Q	150/158 (95%)	134 (89%)	16 (11%)	0	100	100
19	R	107/113 (95%)	91 (85%)	16 (15%)	0	100	100
20	S	64/67 (96%)	57 (89%)	7 (11%)	0	100	100
21	T	128/132 (97%)	109 (85%)	19 (15%)	0	100	100
22	U	147/150 (98%)	133 (90%)	14 (10%)	0	100	100
23	V	92/99 (93%)	82 (89%)	10 (11%)	0	100	100
24	W	61/65 (94%)	52 (85%)	9 (15%)	0	100	100
25	X	65/71 (92%)	45 (69%)	20 (31%)	0	100	100
26	Y	48/51 (94%)	30 (62%)	18 (38%)	0	100	100
27	Z	195/210 (93%)	163 (84%)	32 (16%)	0	100	100
28	0	34/36 (94%)	29 (85%)	5 (15%)	0	100	100
29	3	121/123 (98%)	93 (77%)	27 (22%)	1 (1%)	19	51
32	6	93/113 (82%)	77 (83%)	16 (17%)	0	100	100
33	7	412/415 (99%)	377 (92%)	35 (8%)	0	100	100
34	8	125/139 (90%)	114 (91%)	11 (9%)	0	100	100
35	9	248/266 (93%)	218 (88%)	30 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	4448/4653 (96%)	3850 (87%)	597 (13%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
29	3	4	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	161/167 (96%)	161 (100%)	0	100	100
3	B	168/173 (97%)	168 (100%)	0	100	100
4	C	54/55 (98%)	54 (100%)	0	100	100
5	D	158/160 (99%)	157 (99%)	1 (1%)	86	91
6	E	213/214 (100%)	213 (100%)	0	100	100
7	F	192/198 (97%)	192 (100%)	0	100	100
8	G	107/108 (99%)	107 (100%)	0	100	100
9	H	183/184 (100%)	181 (99%)	2 (1%)	73	85
10	I	106/107 (99%)	106 (100%)	0	100	100
11	J	102/103 (99%)	102 (100%)	0	100	100
12	K	110/111 (99%)	109 (99%)	1 (1%)	78	87
13	L	90/91 (99%)	90 (100%)	0	100	100
14	M	95/104 (91%)	95 (100%)	0	100	100
15	N	120/121 (99%)	118 (98%)	2 (2%)	60	78
16	O	119/123 (97%)	119 (100%)	0	100	100
17	P	45/46 (98%)	45 (100%)	0	100	100
18	Q	137/143 (96%)	135 (98%)	2 (2%)	65	81
19	R	98/102 (96%)	96 (98%)	2 (2%)	55	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	S	60/61 (98%)	60 (100%)	0	100	100
21	T	113/114 (99%)	112 (99%)	1 (1%)	78	87
22	U	126/127 (99%)	126 (100%)	0	100	100
23	V	86/90 (96%)	86 (100%)	0	100	100
24	W	54/56 (96%)	54 (100%)	0	100	100
25	X	57/60 (95%)	56 (98%)	1 (2%)	59	78
26	Y	41/42 (98%)	38 (93%)	3 (7%)	14	41
27	Z	156/168 (93%)	156 (100%)	0	100	100
28	0	34/34 (100%)	34 (100%)	0	100	100
29	3	99/99 (100%)	99 (100%)	0	100	100
32	6	83/99 (84%)	83 (100%)	0	100	100
33	7	356/357 (100%)	356 (100%)	0	100	100
34	8	118/126 (94%)	118 (100%)	0	100	100
35	9	227/239 (95%)	226 (100%)	1 (0%)	91	95
All	All	3868/3982 (97%)	3852 (100%)	16 (0%)	91	95

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	Y	40	CYS
26	Y	37	ARG
19	R	8	ARG
26	Y	17	ARG
18	Q	130	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
27	Z	95	GLN
33	7	244	GLN
27	Z	148	GLN
33	7	148	GLN
33	7	400	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1458/1497 (97%)	322 (22%)	6 (0%)
30	5	19/20 (95%)	7 (36%)	0
31	4	75/76 (98%)	33 (44%)	1 (1%)
All	All	1552/1593 (97%)	362 (23%)	7 (0%)

5 of 362 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	14	U
1	2	16	C
1	2	23	A
1	2	29	C
1	2	40	U

5 of 7 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	599	C
1	2	952	C
31	4	74	C
1	2	998	C
1	2	461	A

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

48 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	$\# Z > 2$
1	4AC	2	851	1	21,24,25	1.16	1 (4%)	29,34,37	1.35	4 (13%)
31	4SU	4	8	31	18,21,22	1.84	5 (27%)	26,30,33	2.15	6 (23%)
1	4AC	2	1184	1	21,24,25	1.03	2 (9%)	29,34,37	1.26	4 (13%)
1	4AC	2	868	1	21,24,25	1.06	2 (9%)	29,34,37	1.25	4 (13%)
31	PSU	4	55	31	18,21,22	1.34	2 (11%)	22,30,33	2.00	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	OMC	4	32	31	19,22,23	0.97	2 (10%)	26,31,34	0.89	1 (3%)
1	6MZ	2	1469	1,36	18,25,26	0.85	1 (5%)	16,36,39	2.04	3 (18%)
31	5MU	4	54	31	19,22,23	1.43	5 (26%)	28,32,35	1.99	6 (21%)
1	B8H	2	938	1	19,22,23	0.91	2 (10%)	22,32,35	1.48	2 (9%)
1	4AC	2	1479	1	21,24,25	1.05	1 (4%)	29,34,37	1.22	2 (6%)
1	4AC	2	1233	1	21,24,25	1.08	2 (9%)	29,34,37	1.47	4 (13%)
1	4AC	2	648	1	21,24,25	1.04	2 (9%)	29,34,37	1.54	5 (17%)
1	4AC	2	1193	1	21,24,25	1.12	3 (14%)	29,34,37	2.15	7 (24%)
1	OMC	2	1376	1	19,22,23	0.99	2 (10%)	26,31,34	0.90	1 (3%)
1	MA6	2	1487	1	19,26,27	0.87	0	18,38,41	1.25	2 (11%)
1	4AC	2	957	1	21,24,25	1.16	2 (9%)	29,34,37	1.58	4 (13%)
1	4AC	2	731	1	21,24,25	1.02	2 (9%)	29,34,37	1.15	3 (10%)
1	4AC	2	479	1	21,24,25	1.05	2 (9%)	29,34,37	1.50	5 (17%)
1	4AC	2	17	1	21,24,25	1.07	3 (14%)	29,34,37	1.47	5 (17%)
1	4AC	2	546	1	21,24,25	1.03	2 (9%)	29,34,37	1.26	4 (13%)
1	4AC	2	1028	1	21,24,25	1.12	1 (4%)	29,34,37	1.37	4 (13%)
1	4AC	2	626	1	21,24,25	1.07	3 (14%)	29,34,37	1.38	4 (13%)
1	UR3	2	1467	1	19,22,23	0.99	2 (10%)	26,32,35	1.48	3 (11%)
1	4AC	2	839	1	21,24,25	1.06	2 (9%)	29,34,37	1.38	4 (13%)
1	4AC	2	511	1	21,24,25	1.02	2 (9%)	29,34,37	1.38	4 (13%)
1	4AC	2	394	1	21,24,25	0.98	1 (4%)	29,34,37	1.60	5 (17%)
1	4AC	2	590	1	21,24,25	1.02	2 (9%)	29,34,37	1.34	4 (13%)
1	4AC	2	379	1	21,24,25	1.04	2 (9%)	29,34,37	1.55	5 (17%)
1	4AC	2	848	1	21,24,25	1.15	3 (14%)	29,34,37	1.24	3 (10%)
1	4AC	2	718	1	21,24,25	0.99	2 (9%)	29,34,37	1.38	4 (13%)
1	4AC	2	828	1	21,24,25	1.03	2 (9%)	29,34,37	1.32	5 (17%)
1	4AC	2	1239	1	21,24,25	1.03	2 (9%)	29,34,37	1.48	3 (10%)
1	4AC	2	319	1	21,24,25	1.04	2 (9%)	29,34,37	1.32	4 (13%)
1	4AC	2	303	1	21,24,25	1.09	2 (9%)	29,34,37	1.40	4 (13%)
31	H2U	4	20	31	18,21,22	0.87	2 (11%)	21,30,33	1.72	2 (9%)
1	4AC	2	53	1	21,24,25	1.05	2 (9%)	29,34,37	1.34	4 (13%)
1	5MC	2	1202	1	18,22,23	0.97	1 (5%)	26,32,35	1.21	4 (15%)
1	4AC	2	286	1	21,24,25	1.08	1 (4%)	29,34,37	1.52	4 (13%)
1	4AC	2	1147	1	21,24,25	0.95	2 (9%)	29,34,37	1.32	4 (13%)
1	A2M	2	373	1	18,25,26	0.95	0	18,36,39	1.39	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	4AC	2	751	1	21,24,25	1.00	2 (9%)	29,34,37	1.25	4 (13%)
1	LHH	2	250	1	22,25,26	2.61	8 (36%)	29,35,38	1.41	7 (24%)
1	4AC	2	636	1	21,24,25	1.08	2 (9%)	29,34,37	1.64	4 (13%)
1	4AC	2	703	1	21,24,25	1.06	3 (14%)	29,34,37	1.53	5 (17%)
1	5MC	2	939	1	18,22,23	1.01	2 (11%)	26,32,35	1.30	4 (15%)
1	4AC	2	1041	1	21,24,25	1.03	2 (9%)	29,34,37	1.26	4 (13%)
1	MA6	2	1488	1	19,26,27	0.90	0	18,38,41	1.31	2 (11%)
1	5HM	2	1378	1	19,23,24	2.90	7 (36%)	25,33,36	0.79	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
1	4AC	2	851	1	-	0/11/29/30	0/2/2/2
31	4SU	4	8	31	-	4/7/25/26	0/2/2/2
1	4AC	2	1184	1	-	2/11/29/30	0/2/2/2
1	4AC	2	868	1	-	1/11/29/30	0/2/2/2
31	PSU	4	55	31	-	0/7/25/26	0/2/2/2
31	OMC	4	32	31	-	0/9/27/28	0/2/2/2
1	6MZ	2	1469	1,36	-	0/5/27/28	0/3/3/3
31	5MU	4	54	31	-	1/7/25/26	0/2/2/2
1	B8H	2	938	1	-	0/7/25/26	0/2/2/2
1	4AC	2	1479	1	-	0/11/29/30	0/2/2/2
1	4AC	2	1233	1	-	0/11/29/30	0/2/2/2
1	4AC	2	648	1	-	2/11/29/30	0/2/2/2
1	4AC	2	1193	1	-	0/11/29/30	0/2/2/2
1	OMC	2	1376	1	-	2/9/27/28	0/2/2/2
1	MA6	2	1487	1	-	0/7/29/30	0/3/3/3
1	4AC	2	957	1	-	2/11/29/30	0/2/2/2
1	4AC	2	731	1	-	0/11/29/30	0/2/2/2
1	4AC	2	479	1	-	0/11/29/30	0/2/2/2
1	4AC	2	17	1	-	2/11/29/30	0/2/2/2
1	4AC	2	546	1	-	2/11/29/30	0/2/2/2
1	4AC	2	1028	1	-	2/11/29/30	0/2/2/2
1	4AC	2	626	1	-	1/11/29/30	0/2/2/2
1	UR3	2	1467	1	-	2/7/25/26	0/2/2/2
1	4AC	2	839	1	-	2/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4AC	2	511	1	-	0/11/29/30	0/2/2/2
1	4AC	2	394	1	-	1/11/29/30	0/2/2/2
1	4AC	2	590	1	-	0/11/29/30	0/2/2/2
1	4AC	2	379	1	-	3/11/29/30	0/2/2/2
1	4AC	2	848	1	-	0/11/29/30	0/2/2/2
1	4AC	2	718	1	-	0/11/29/30	0/2/2/2
1	4AC	2	828	1	-	1/11/29/30	0/2/2/2
1	4AC	2	1239	1	-	2/11/29/30	0/2/2/2
1	4AC	2	319	1	-	0/11/29/30	0/2/2/2
1	4AC	2	303	1	-	1/11/29/30	0/2/2/2
31	H2U	4	20	31	-	6/7/38/39	0/2/2/2
1	4AC	2	53	1	-	0/11/29/30	0/2/2/2
1	5MC	2	1202	1	-	3/7/25/26	0/2/2/2
1	4AC	2	286	1	-	2/11/29/30	0/2/2/2
1	4AC	2	1147	1	-	1/11/29/30	0/2/2/2
1	A2M	2	373	1	-	2/5/27/28	0/3/3/3
1	4AC	2	751	1	-	0/11/29/30	0/2/2/2
1	LHH	2	250	1	-	1/13/31/32	0/2/2/2
1	4AC	2	636	1	-	2/11/29/30	0/2/2/2
1	4AC	2	703	1	-	0/11/29/30	0/2/2/2
1	5MC	2	939	1	-	2/7/25/26	0/2/2/2
1	4AC	2	1041	1	-	0/11/29/30	0/2/2/2
1	MA6	2	1488	1	-	0/7/29/30	0/3/3/3
1	5HM	2	1378	1	-	2/9/27/28	0/2/2/2

The worst 5 of 105 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	250	LHH	C4-N4	6.70	1.49	1.39
1	2	1378	5HM	C4-N3	6.12	1.44	1.34
1	2	250	LHH	C7-N4	6.07	1.48	1.37
1	2	1378	5HM	C2-N3	5.74	1.48	1.36
1	2	1378	5HM	C4-N4	5.44	1.48	1.34

The worst 5 of 183 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	4	20	H2U	C4-N3-C2	-6.66	120.27	125.79
1	2	1469	6MZ	C2-N1-C6	6.24	121.94	116.59
31	4	55	PSU	N1-C2-N3	6.22	122.18	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1193	4AC	O7-C7-N4	6.09	131.68	121.82
31	4	8	4SU	C4-N3-C2	-6.03	121.48	127.34

There are no chirality outliers.

5 of 54 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	250	LHH	C1'-C2'-O2'-C1
1	2	286	4AC	O4'-C4'-C5'-O5'
1	2	286	4AC	C3'-C4'-C5'-O5'
1	2	546	4AC	O4'-C4'-C5'-O5'
1	2	546	4AC	C3'-C4'-C5'-O5'

There are no ring outliers.

34 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	4	8	4SU	3	0
1	2	1184	4AC	2	0
1	2	868	4AC	1	0
31	4	55	PSU	2	0
31	4	54	5MU	1	0
1	2	1233	4AC	1	0
1	2	648	4AC	1	0
1	2	1193	4AC	2	0
1	2	1487	MA6	1	0
1	2	957	4AC	1	0
1	2	479	4AC	2	0
1	2	17	4AC	1	0
1	2	1028	4AC	1	0
1	2	626	4AC	1	0
1	2	1467	UR3	1	0
1	2	839	4AC	1	0
1	2	511	4AC	2	0
1	2	394	4AC	1	0
1	2	379	4AC	1	0
1	2	848	4AC	2	0
1	2	718	4AC	1	0
1	2	1239	4AC	3	0
1	2	303	4AC	1	0
31	4	20	H2U	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	53	4AC	1	0
1	2	286	4AC	3	0
1	2	1147	4AC	1	0
1	2	373	A2M	1	0
1	2	751	4AC	1	0
1	2	636	4AC	3	0
1	2	703	4AC	4	0
1	2	1041	4AC	1	0
1	2	1488	MA6	1	0
1	2	1378	5HM	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 40 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
38	MET	4	101	-	6,7,8	0.46	0	2,7,9	0.14	0
39	GNP	7	501	36	29,34,34	1.63	7 (24%)	33,54,54	2.15	6 (18%)

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
38	MET	4	101	-	-	2/5/6/8	-
39	GNP	7	501	36	-	6/14/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	7	501	GNP	PB-O3A	4.38	1.64	1.59
39	7	501	GNP	PG-N3B	3.13	1.71	1.63
39	7	501	GNP	C6-N1	3.10	1.38	1.33
39	7	501	GNP	PB-O1B	3.06	1.51	1.46
39	7	501	GNP	PG-O1G	2.56	1.50	1.46

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	7	501	GNP	C5-C6-N1	-8.44	111.89	123.43
39	7	501	GNP	C2-N1-C6	5.82	125.18	115.93
39	7	501	GNP	PB-O3A-PA	-2.93	122.28	132.62
39	7	501	GNP	N3-C2-N1	-2.79	123.50	127.22
39	7	501	GNP	C4-C5-C6	-2.61	118.31	120.80

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
39	7	501	GNP	PB-N3B-PG-O1G
39	7	501	GNP	PG-N3B-PB-O1B
39	7	501	GNP	C5'-O5'-PA-O1A
39	7	501	GNP	C5'-O5'-PA-O2A
38	4	101	MET	CA-CB-CG-SD

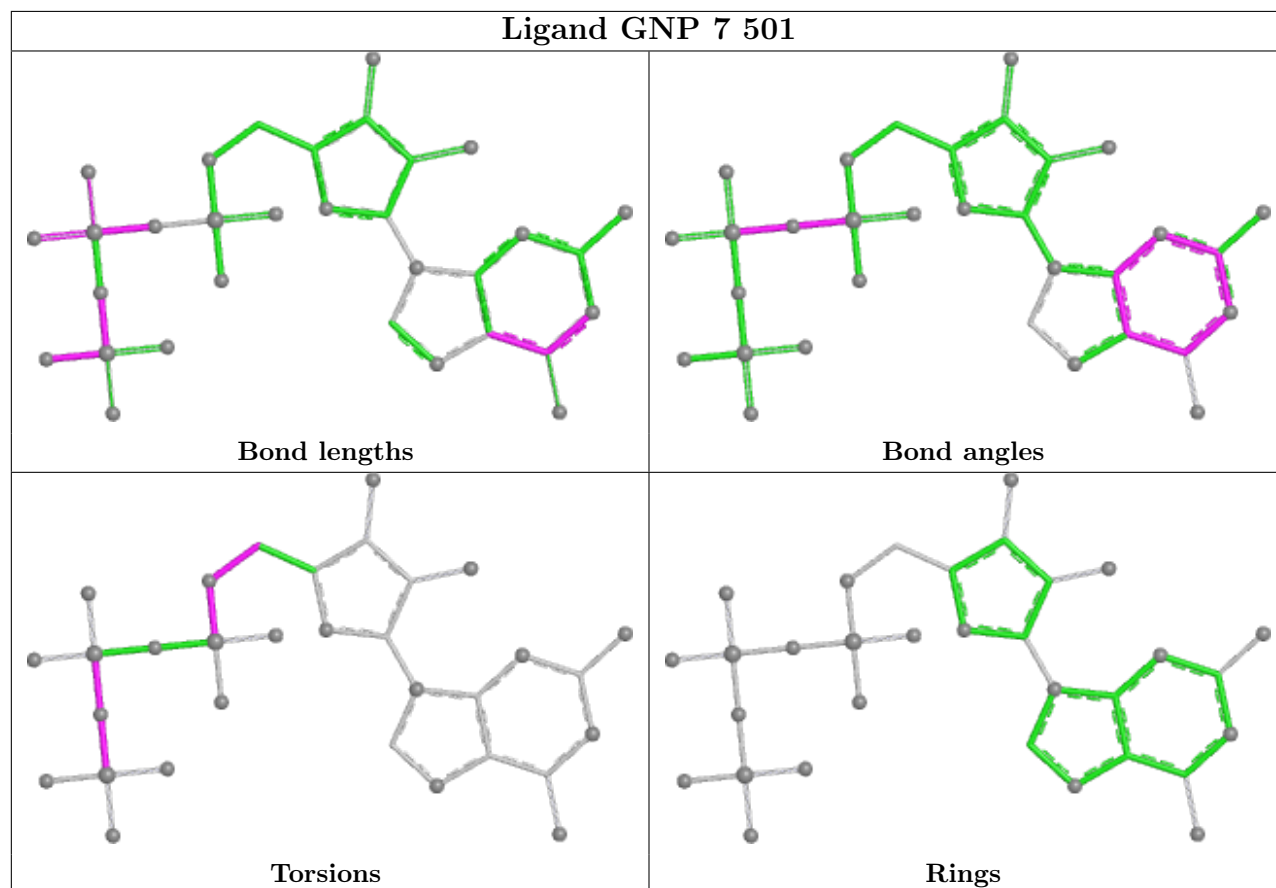
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	4	101	MET	4	0
39	7	501	GNP	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](#)

There are no chain breaks in this entry.

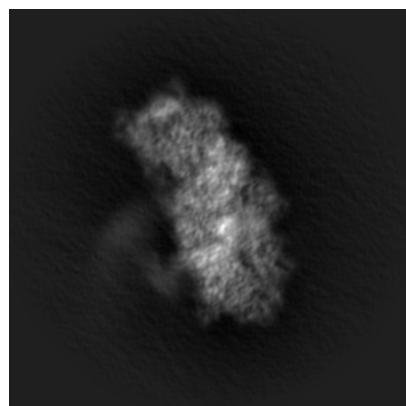
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10322. These allow visual inspection of the internal detail of the map and identification of artifacts.

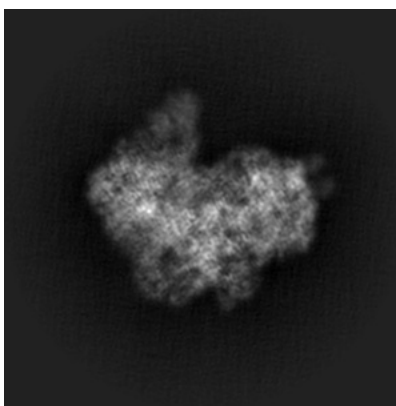
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

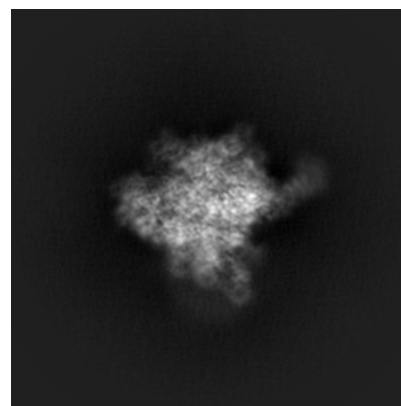
6.1.1 Primary map



X

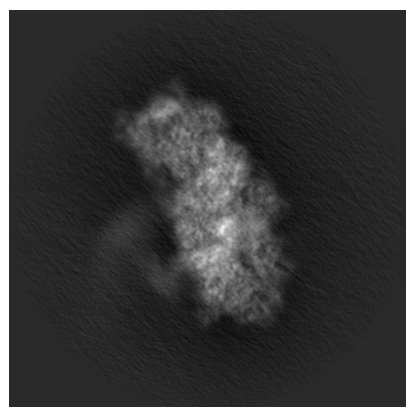


Y

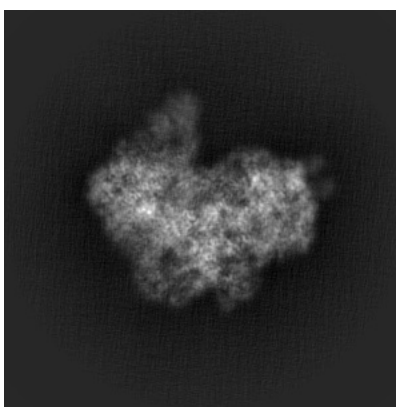


Z

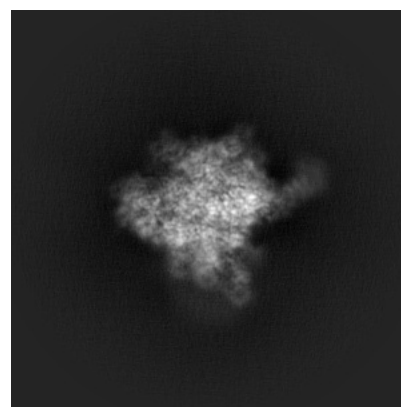
6.1.2 Raw map



X



Y

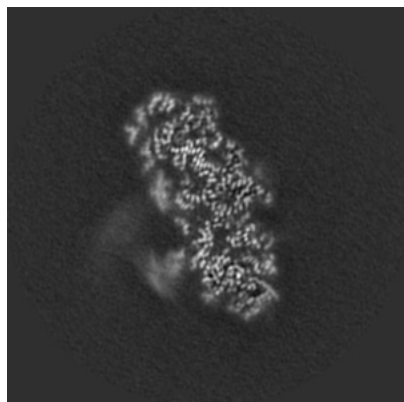


Z

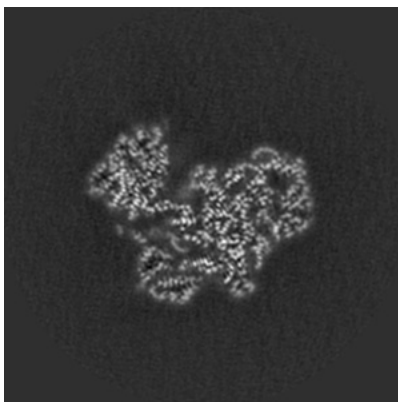
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

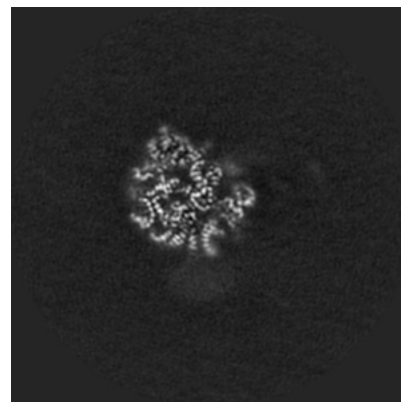
6.2.1 Primary map



X Index: 174

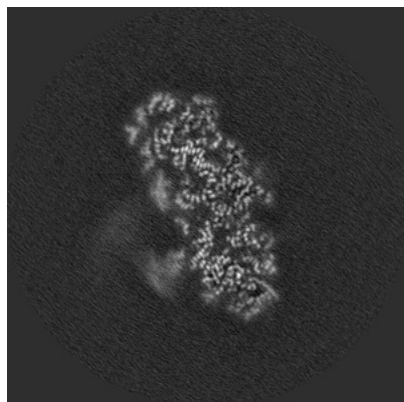


Y Index: 174

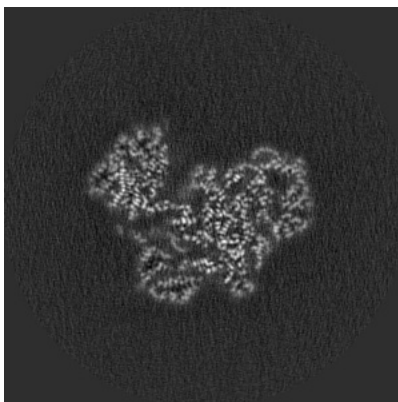


Z Index: 174

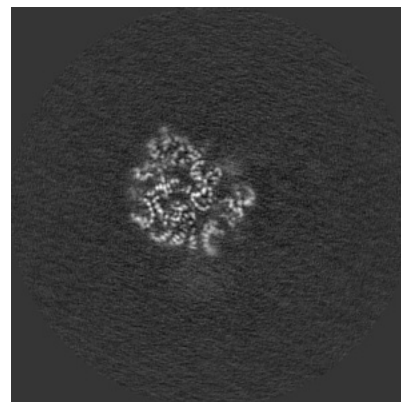
6.2.2 Raw map



X Index: 174



Y Index: 174

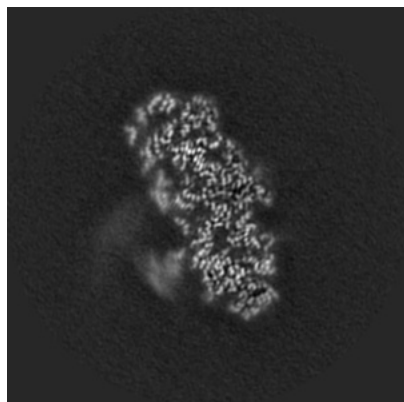


Z Index: 174

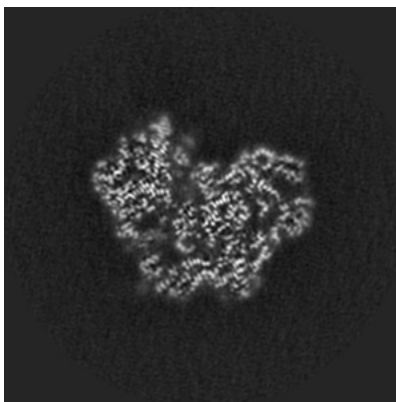
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

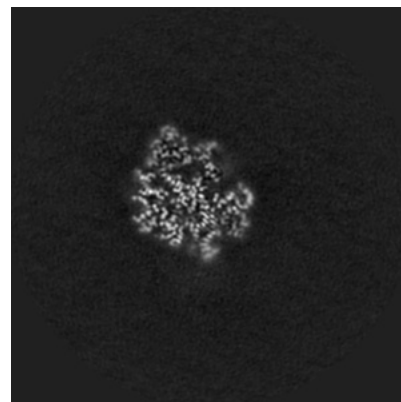
6.3.1 Primary map



X Index: 173

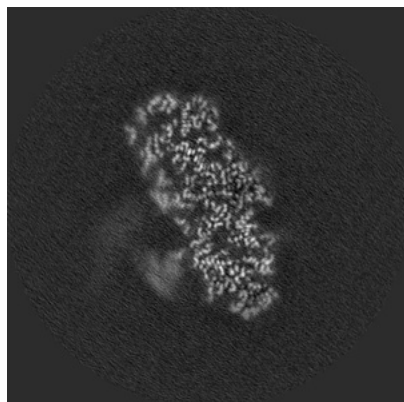


Y Index: 179

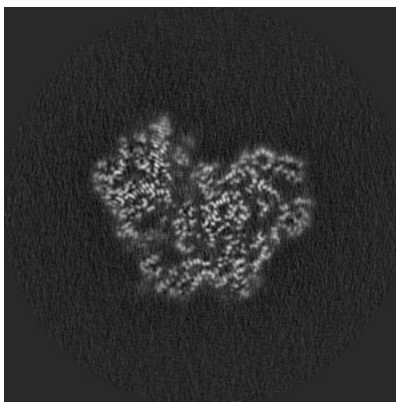


Z Index: 180

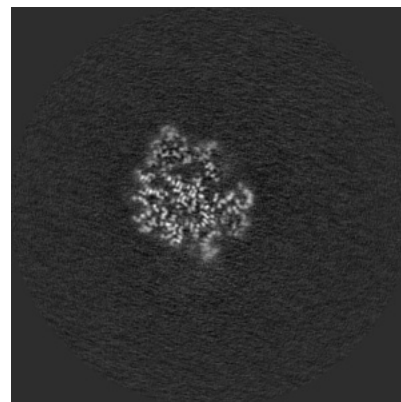
6.3.2 Raw map



X Index: 172



Y Index: 179

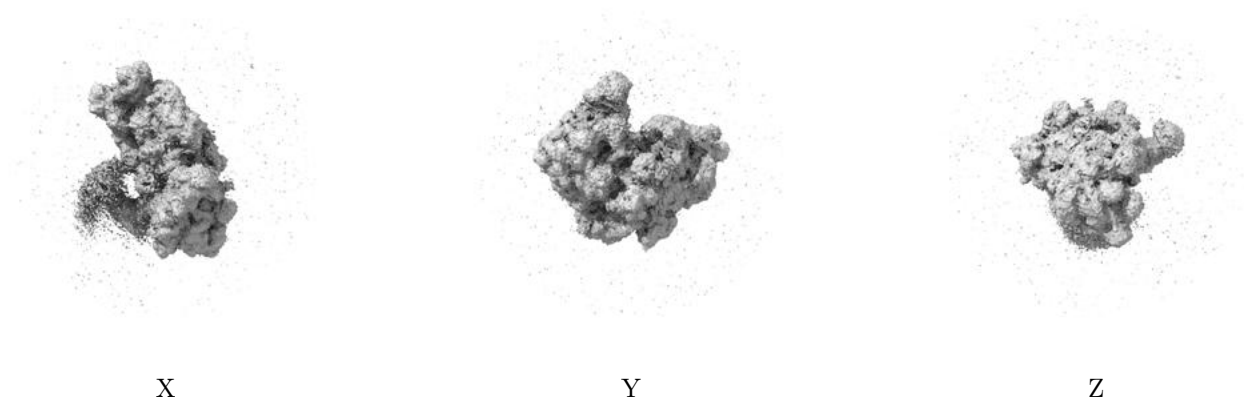


Z Index: 180

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

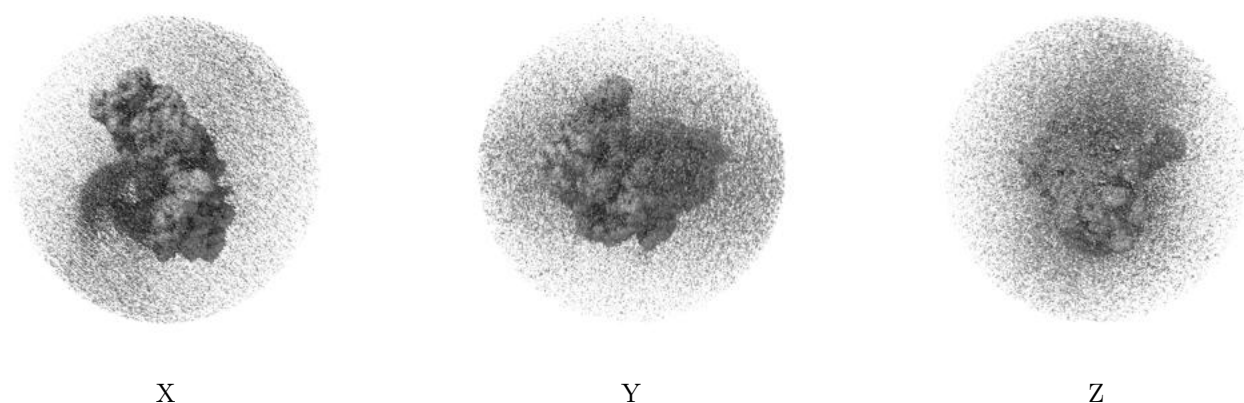
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.003. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

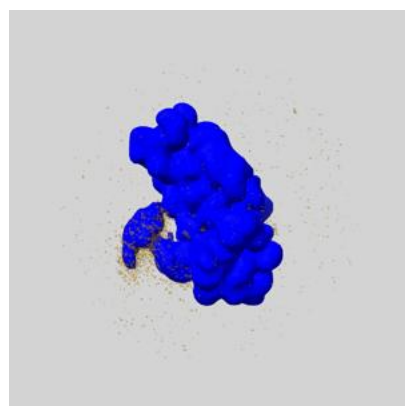
6.5 Mask visualisation [i](#)

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

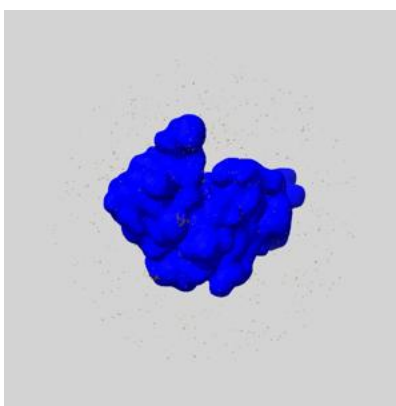
A mask typically either:

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

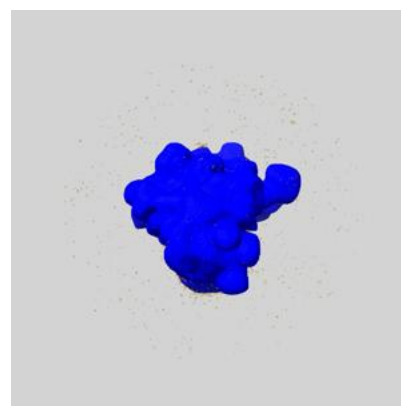
6.5.1 emd_10322_msk_1.map [i](#)



X



Y

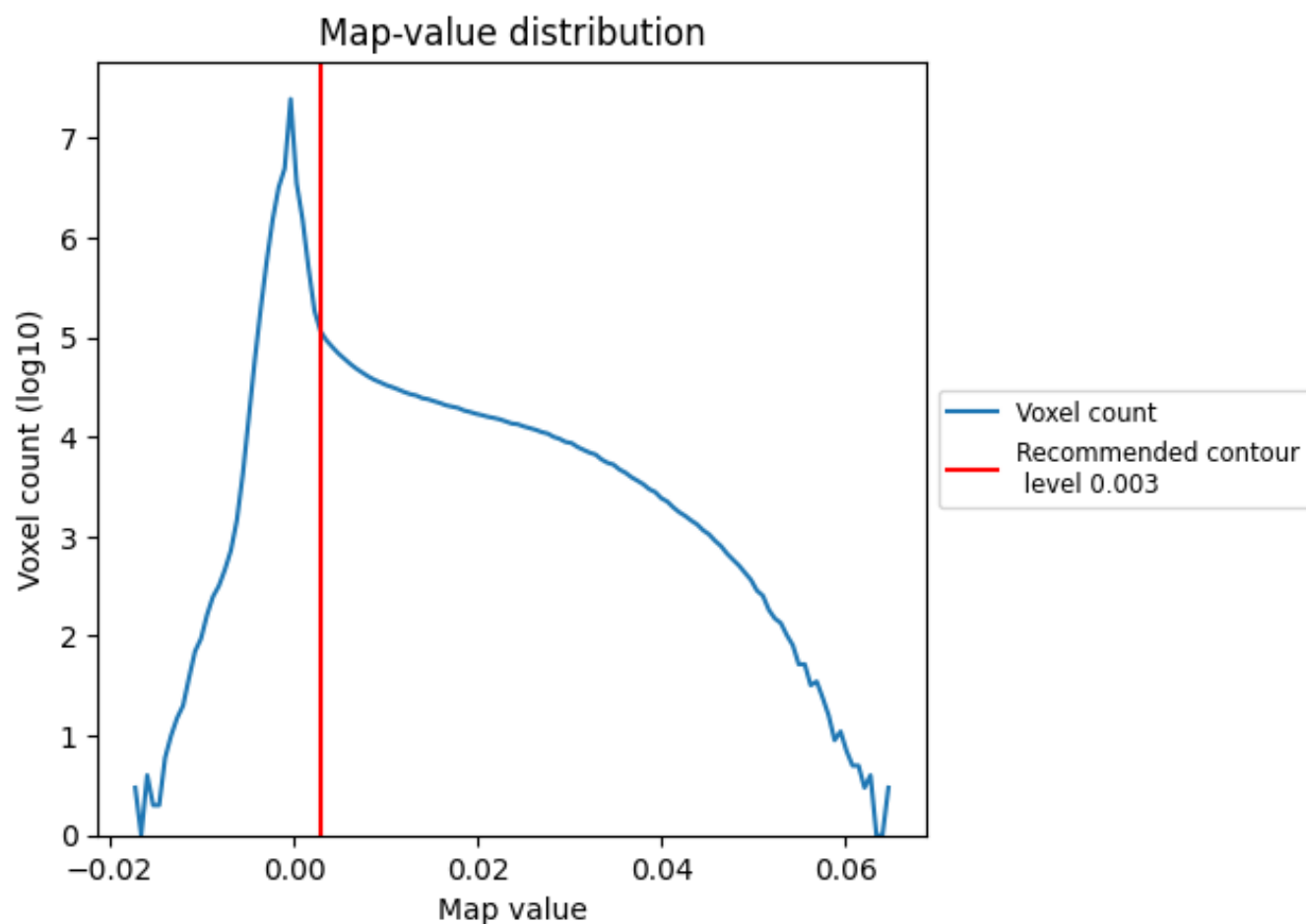


Z

7 Map analysis [i](#)

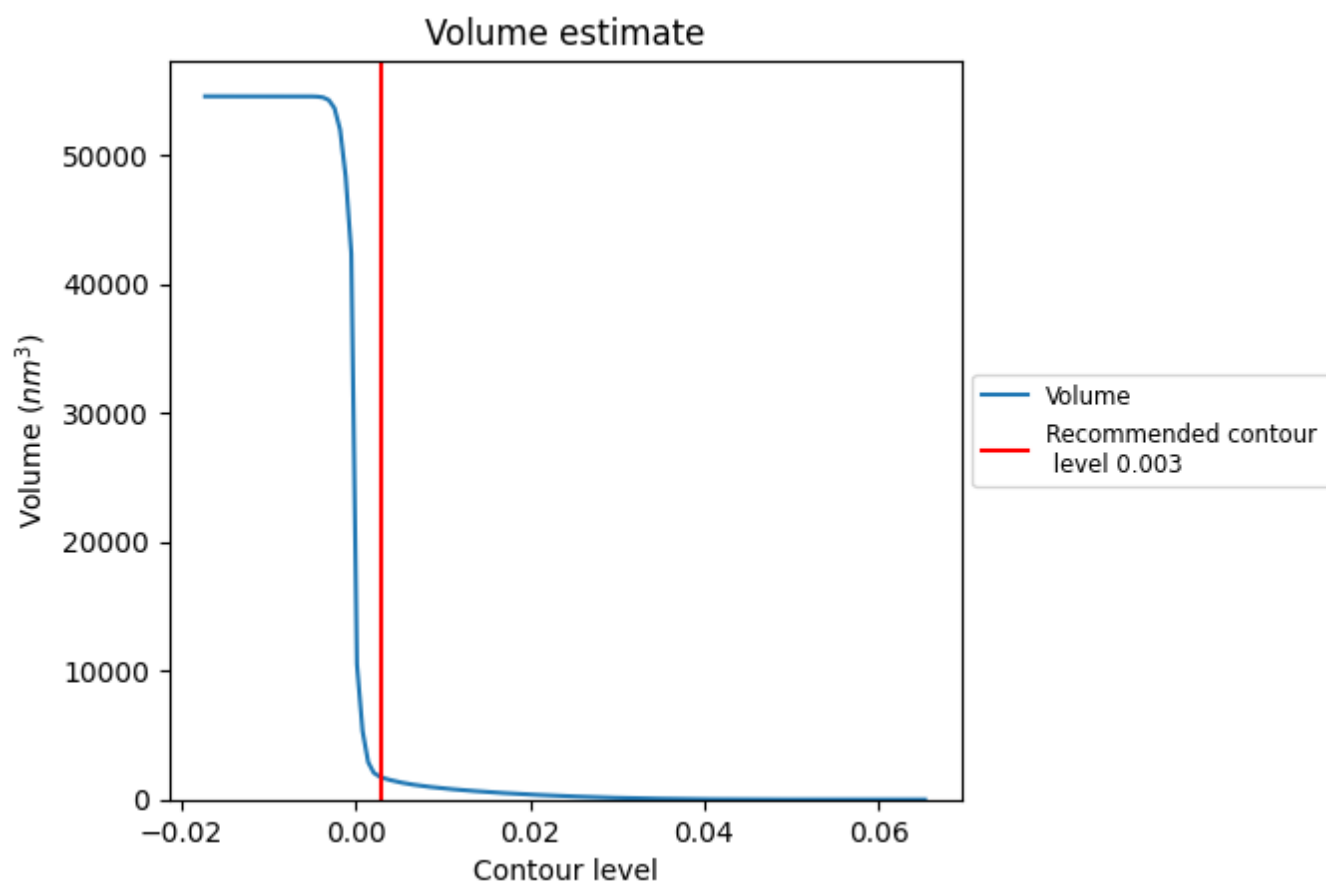
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

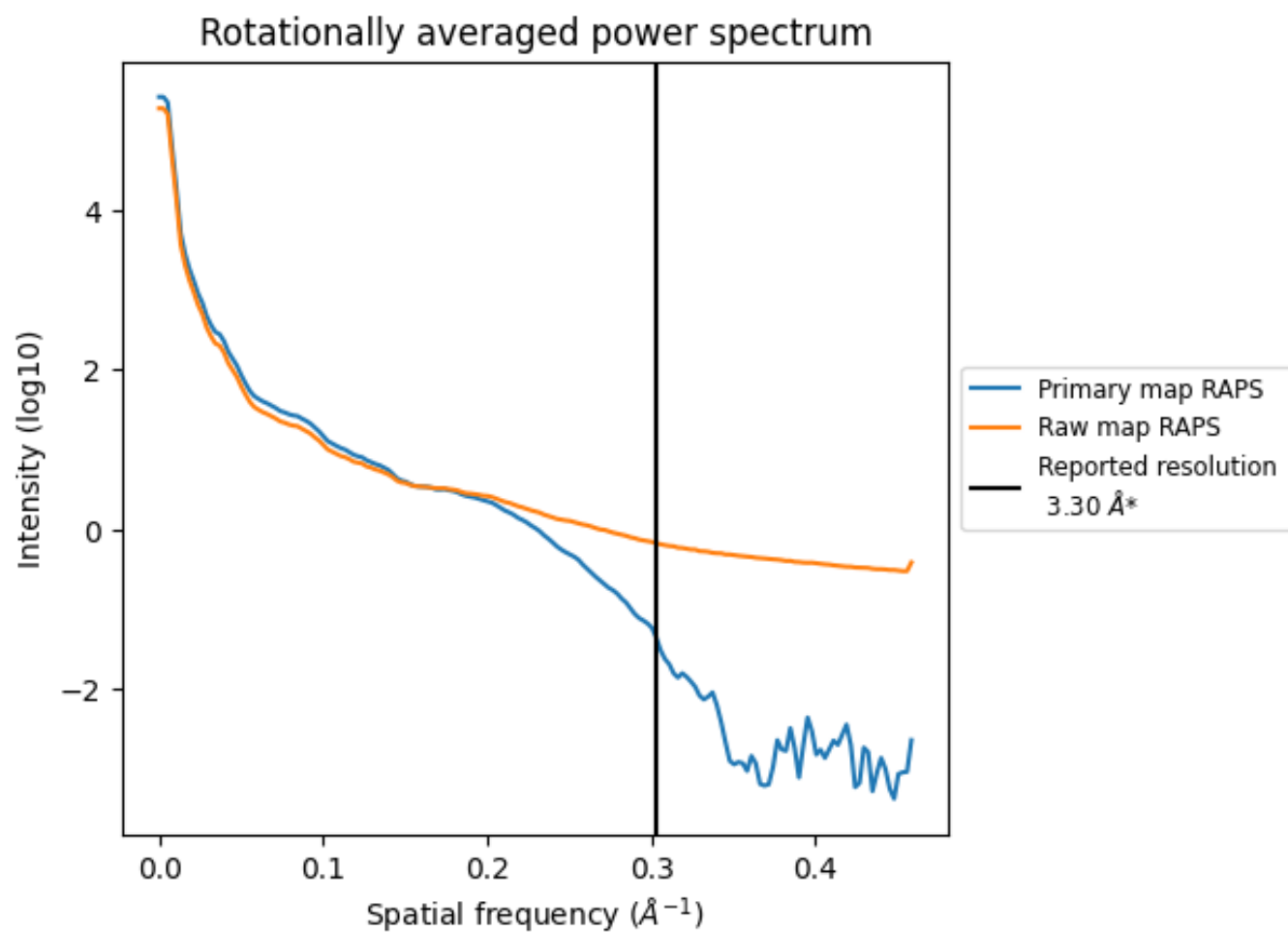
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1725 nm³; this corresponds to an approximate mass of 1559 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 ⓘ

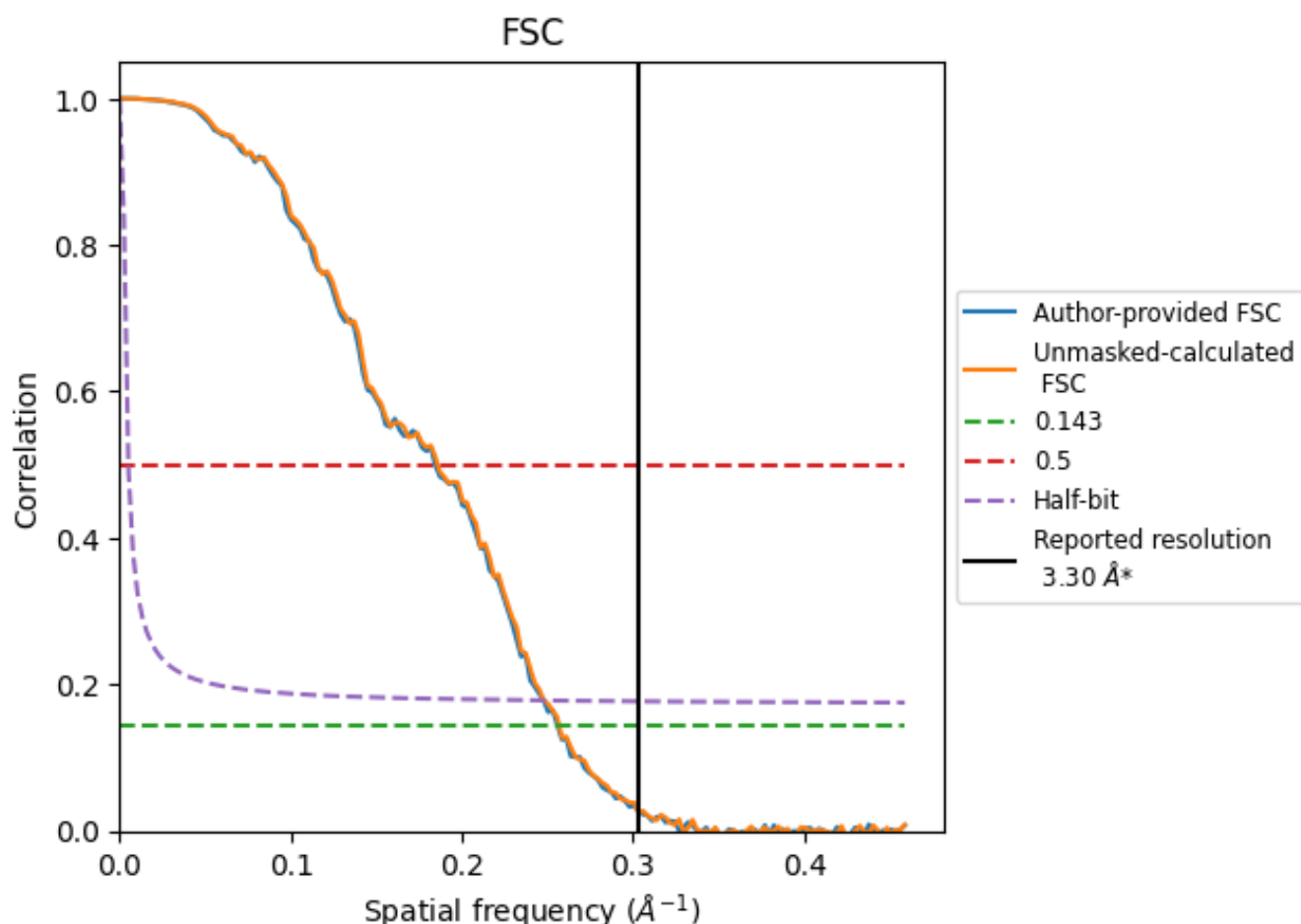


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.91	5.42	4.04
Unmasked-calculated*	3.89	5.38	4.03

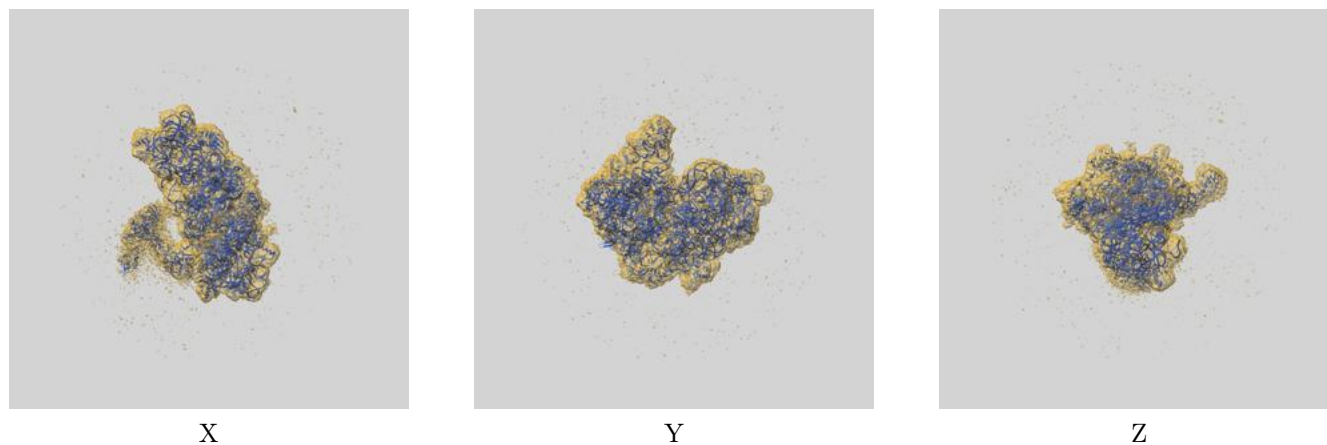
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.91 differs from the reported value 3.3 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.89 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

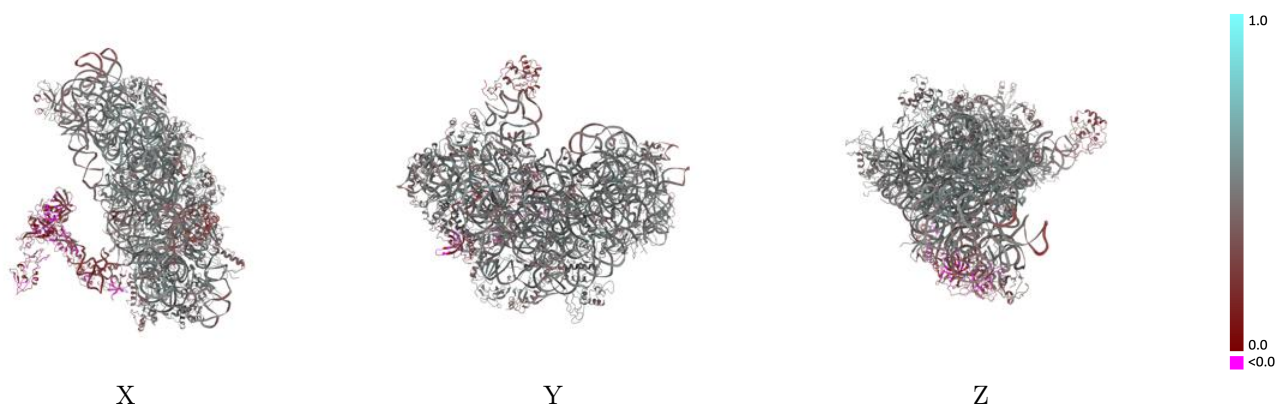
This section contains information regarding the fit between EMDB map EMD-10322 and PDB model 6SWC. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



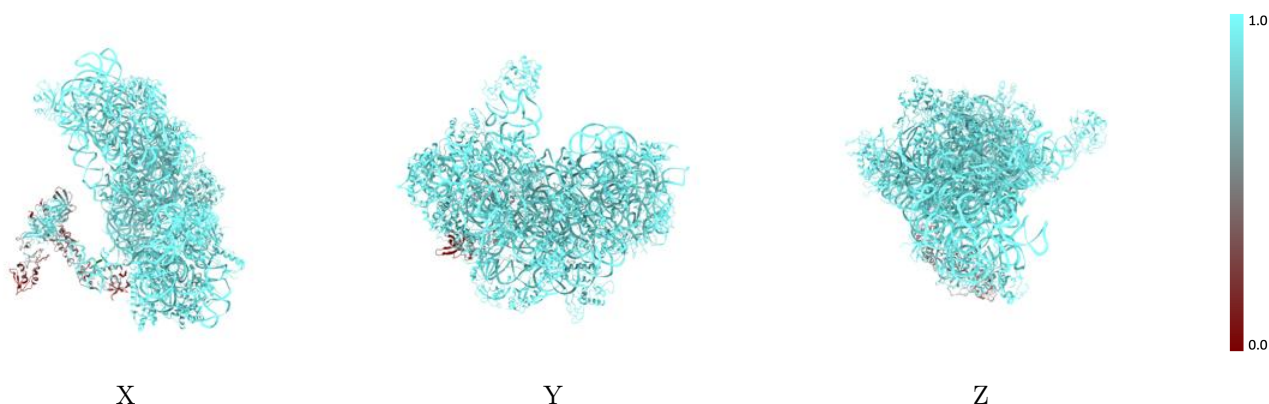
The images above show the 3D surface view of the map at the recommended contour level 0.003 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



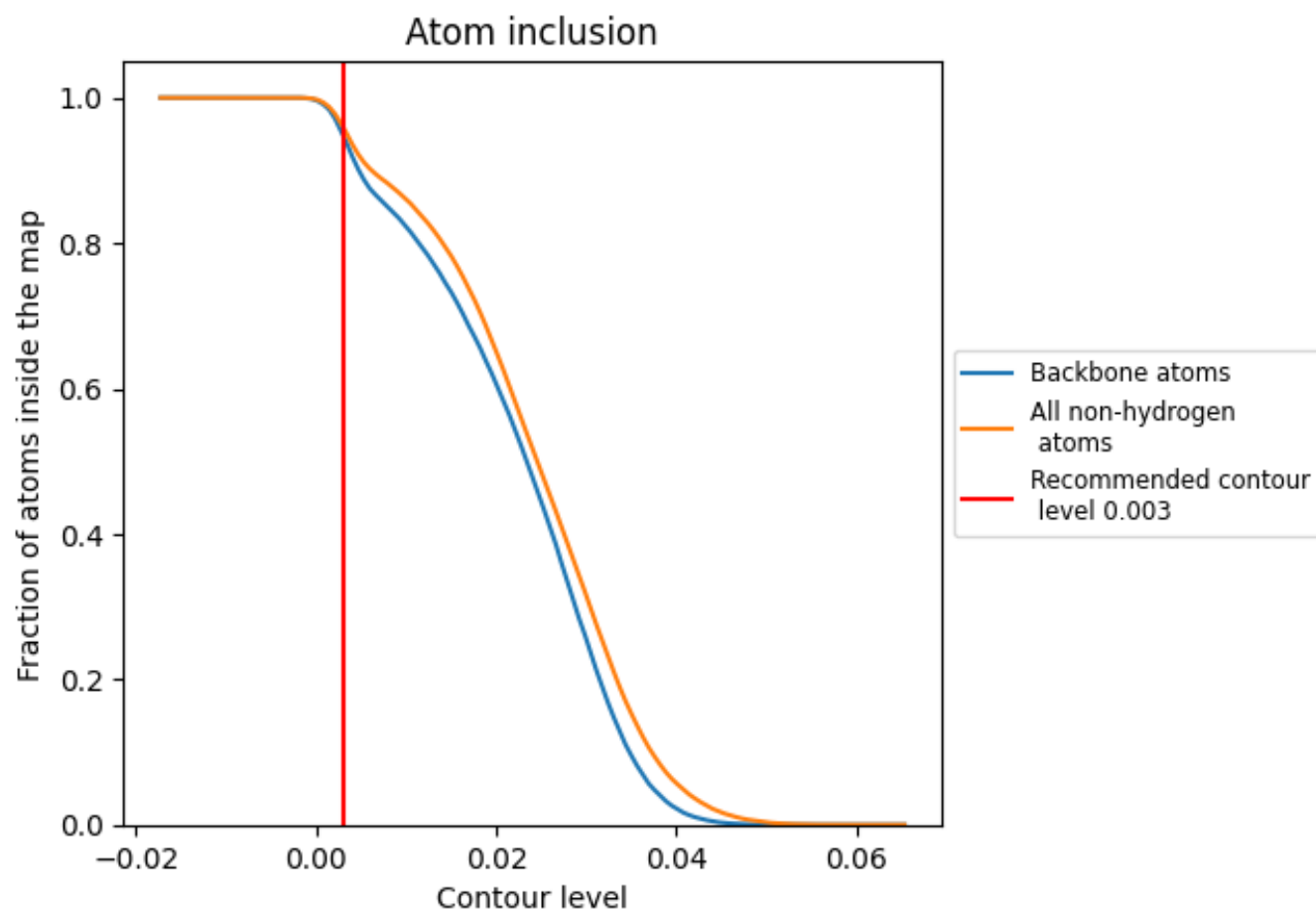
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.003).









































































9.4 Atom inclusion ⓘ



At the recommended contour level, 95% 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 (0.003) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9598	 0.4380
0	 1.0000	 0.5010
2	 1.0000	 0.4860
3	 0.9989	 0.2680
4	 0.9804	 0.2700
5	 1.0000	 0.4290
6	 0.9398	 0.2860
7	 0.7681	 0.1590
8	 0.3116	 0.1710
9	 0.3801	 0.1540
A	 0.9993	 0.4620
B	 0.9993	 0.4620
C	 0.9979	 0.4570
D	 0.9986	 0.4770
E	 1.0000	 0.4840
F	 0.9966	 0.4830
G	 1.0000	 0.4200
H	 0.9994	 0.4660
I	 0.9970	 0.4910
J	 1.0000	 0.4780
K	 0.9981	 0.4850
L	 0.9987	 0.4530
M	 1.0000	 0.4840
N	 1.0000	 0.4820
O	 1.0000	 0.4500
P	 1.0000	 0.4910
Q	 0.9992	 0.4660
R	 0.9977	 0.4900
S	 0.9908	 0.4300
T	 0.9990	 0.4600
U	 0.9949	 0.4730
V	 1.0000	 0.4570
W	 1.0000	 0.4700
X	 0.9980	 0.4620
Y	 1.0000	 0.2540
Z	 0.9980	 0.4460

