



wwPDB EM Validation Summary Report ⓘ

Aug 11, 2026 – 08:35 am BST

PDB ID : 9TI8 / pdb_00009ti8
EMDB ID : EMD-55947
Title : Staphylococcus aureus 50S ribosome in complex with RRF, EF-G and fusidic acid (50S-RRF-EF-G-FA)
Authors : Gonzalez-Lopez, A.; Selmer, M.
Deposited on : 2025-12-05
Resolution : 2.18 Å (reported)
Based on initial models : 9GHG, .

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:

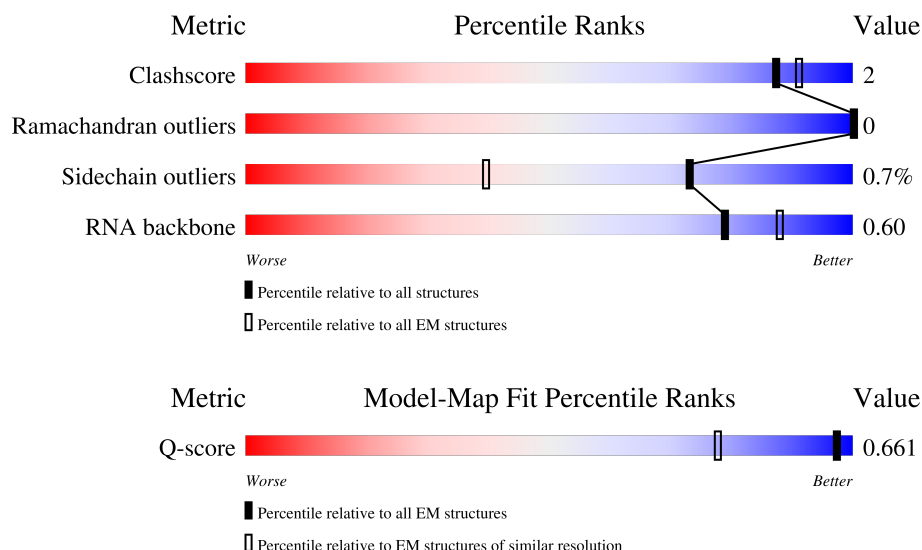
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 2.18 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	2701 (1.70 - 2.68)

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	1	62	
2	2	69	
3	3	59	

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Mol	Chain	Length	Quality of chain
4	4	84	 58% 49% 21% 30%
5	5	57	 89% 7%
6	6	49	 94%
7	7	45	 96%
8	8	66	 94% 5%
9	9	37	 100%
10	A	2923	 76% 18%
11	B	115	 78% 18%
12	C	186	 15% 89% 10%
13	E	693	 26% 84% 11% 5%
14	G	277	 94% 5%
15	H	220	 96%
16	I	207	 96%
17	J	179	 22% 80% 18%
18	K	178	 93% 6%
19	M	145	 94% 6%
20	N	122	 94% 6%
21	O	146	 97%
22	P	144	 85% 9% 6%
23	Q	122	 89% 9%
24	R	119	 98%
25	S	116	 5% 95%
26	T	118	 87% 12%
27	U	102	 100%
28	V	117	 91% 5%

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Mol	Chain	Length	Quality of chain
29	W	91	98%
30	X	105	7% 91% 6%
31	Y	217	41% 57%
32	Z	94	77% 19%

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 93901 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 L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	61	Total	C	N	O	S	0	0
			482	298	104	79	1		

- Molecule 2 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	65	Total	C	N	O	S	0	0
			535	329	100	105	1		

- Molecule 3 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	3	57	Total	C	N	O	0	0
			446	277	84	85		

- Molecule 4 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	59	Total	C	N	O	S	0	0
			485	310	76	96	3		

- Molecule 5 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	53	Total	C	N	O	S	0	0
			422	256	86	75	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	?	-	ARG	deletion	UNP Q2FZF1

- Molecule 6 is a protein called Large ribosomal subunit protein bL33A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	48	Total	C	N	O	S	0	0
			402	245	79	73	5		

- Molecule 7 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	44	Total	C	N	O	S	0	0
			373	228	90	54	1		

- Molecule 8 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	65	Total	C	N	O	S	0	0
			531	330	115	84	2		

- Molecule 9 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	37	Total	C	N	O	S	0	0
			297	186	60	46	5		

- Molecule 10 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	2808	Total	C	N	O	P	0	0
			60220	26892	11024	19496	2808		

- Molecule 11 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	113	Total	C	N	O	P	0	0
			2408	1076	431	788	113		

- Molecule 12 is a protein called Ribosome-recycling factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	185	Total	C	N	O	S	0	0
			1433	874	257	297	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP Q2FZ21
C	-1	HIS	-	expression tag	UNP Q2FZ21

- Molecule 13 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	661	Total	C	N	O	S	0	0
			5114	3207	854	1025	28		

- Molecule 14 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	273	Total	C	N	O	S	0	0
			2085	1297	413	370	5		

- Molecule 15 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	215	Total	C	N	O	S	0	0
			1628	1018	299	306	5		

- Molecule 16 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	205	Total	C	N	O	S	0	0
			1569	983	287	297	2		

- Molecule 17 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	177	Total	C	N	O	S	0	0
			1403	891	242	263	7		

- Molecule 18 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	177	Total	C	N	O	S	0	0
			1382	858	253	268	3		

- Molecule 19 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	145	Total	C	N	O	S	0	0
			1151	717	211	220	3		

- Molecule 20 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	122	Total	C	N	O	S	0	0
			920	572	174	170	4		

- Molecule 21 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	146	Total	C	N	O	S	0	0
			1099	680	215	203	1		

- Molecule 22 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	136	Total	C	N	O	S	0	0
			1089	698	206	181	4		

- Molecule 23 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	120	Total	C	N	O	S	0	0
			952	584	182	185	1		

- Molecule 24 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	119	Total	C	N	O	S	0	0
			922	574	174	173	1		

- Molecule 25 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	S	114	Total	C	N	O	0	0
			922	580	185	157		

- Molecule 26 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	117	Total	C	N	O	S	0	0
			953	599	191	159	4		

- Molecule 27 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	102	Total	C	N	O	S	0	0
			799	506	142	150	1		

- Molecule 28 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	111	Total	C	N	O	S	0	0
			853	532	163	155	3		

- Molecule 29 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	90	Total	C	N	O	S	0	0
			734	461	132	137	4		

- Molecule 30 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	X	102	Total	C	N	O	S	0	0
			787	497	144	144	2		

- Molecule 31 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Y	94	Total	C	N	O	S	0	0
			738	471	131	134	2		

- Molecule 32 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	Z	76	Total	C	N	O	0	0
			585	361	114	110		

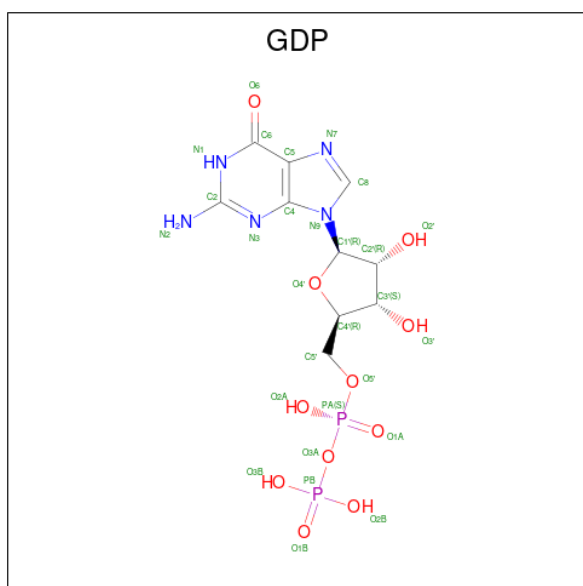
- Molecule 33 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
33	5	1	Total	Zn	0
			1	1	
33	9	1	Total	Zn	0
			1	1	

- Molecule 34 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

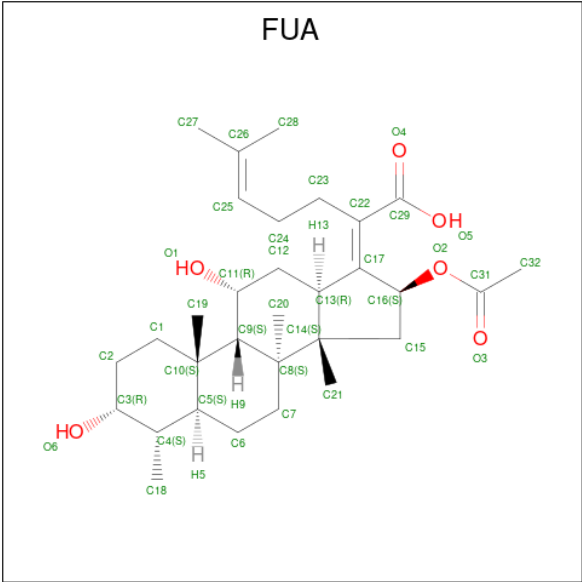
Mol	Chain	Residues	Atoms		AltConf
34	A	112	Total	Mg	0
			112	112	
34	E	1	Total	Mg	0
			1	1	
34	G	1	Total	Mg	0
			1	1	
34	H	1	Total	Mg	0
			1	1	

- Molecule 35 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

- Molecule 36 is FUSIDIC ACID (CCD ID: FUA) (formula: C₃₁H₄₈O₆) (labeled as "Ligand of Interest" by depositor).



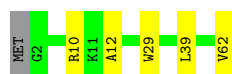
Mol	Chain	Residues	Atoms			AltConf
36	E	1	Total	C	O	0
			37	31	6	

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 L28

Chain 1: 

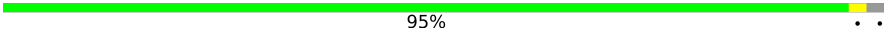


- Molecule 2: 50S ribosomal protein L29

Chain 2: 



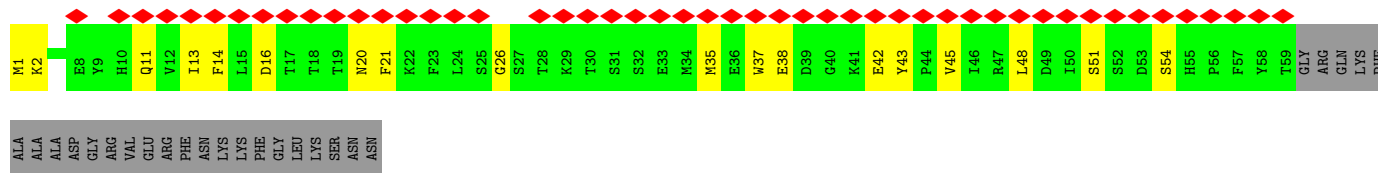
- Molecule 3: 50S ribosomal protein L30

Chain 3: 



- Molecule 4: 50S ribosomal protein L31 type B

Chain 4: 



- Molecule 5: Large ribosomal subunit protein bL32

Chain 5: 



- Molecule 6: Large ribosomal subunit protein bL33A

Chain 6: 94%



- Molecule 7: 50S ribosomal protein L34

Chain 7: 96%



- Molecule 8: 50S ribosomal protein L35

Chain 8: 94%



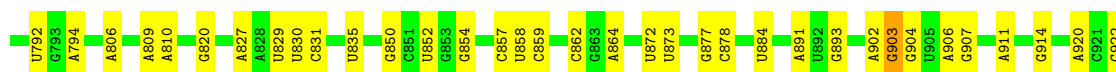
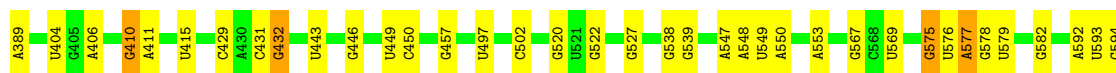
- Molecule 9: 50S ribosomal protein L36

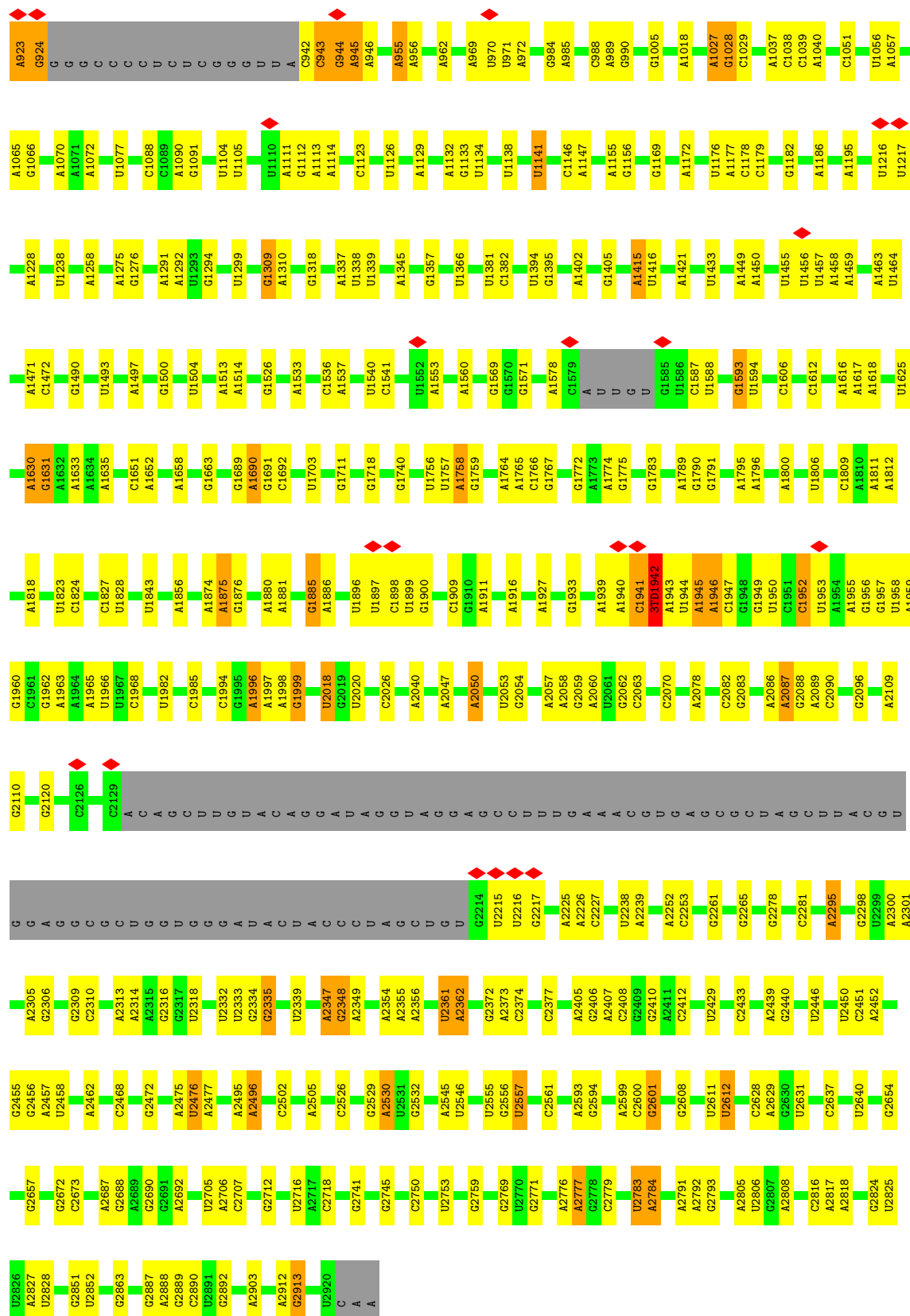
Chain 9: 100%

There are no outlier residues recorded for this chain.

- Molecule 10: 23S rRNA

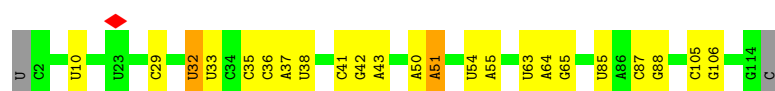
Chain A: 76%





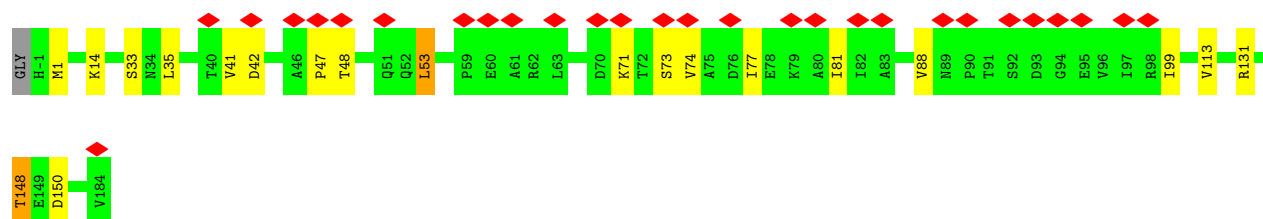
• Molecule 11: 5S rRNA

Chain B:  78% 18% ..



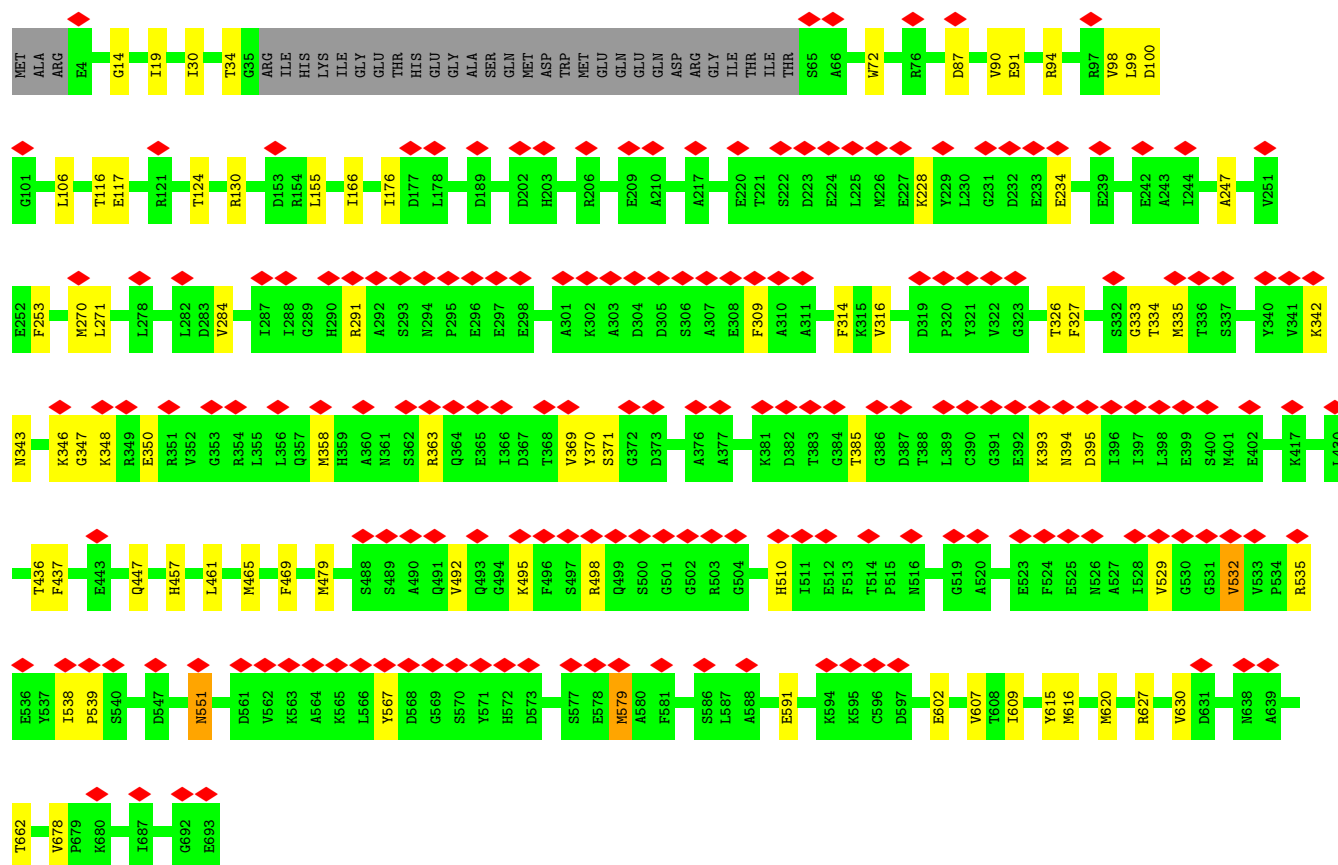
- Molecule 12: Ribosome-recycling factor

Chain C:  15% 89% 10% ..

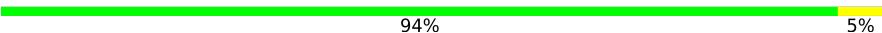


- Molecule 13: Elongation factor G

Chain E:  26% 84% 11% 5%



- Molecule 14: 50S ribosomal protein L2

Chain G:  94% 5% ..



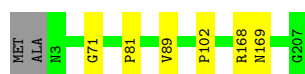
- Molecule 15: 50S ribosomal protein L3

Chain H: 96% ..



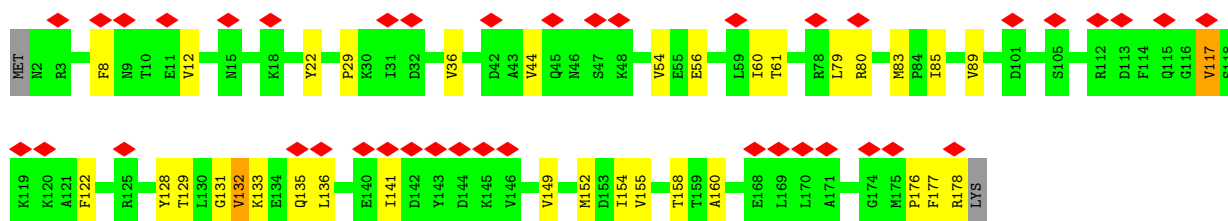
- Molecule 16: 50S ribosomal protein L4

Chain I: 96% ..



- Molecule 17: 50S ribosomal protein L5

Chain J: 22% 80% 18% ..



- Molecule 18: Large ribosomal subunit protein uL6

Chain K: 93% 6% ..



- Molecule 19: 50S ribosomal protein L13

Chain M: 94% 6%

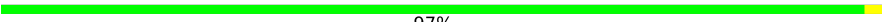


- Molecule 20: 50S ribosomal protein L14

Chain N: 94% 6%



- Molecule 21: 50S ribosomal protein L15

Chain O:  97% .



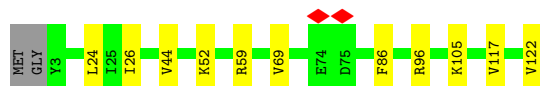
- Molecule 22: 50S ribosomal protein L16

Chain P:  85% 9% 6%



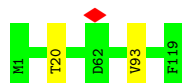
- Molecule 23: 50S ribosomal protein L17

Chain Q:  89% 9% .



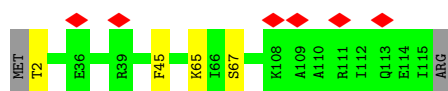
- Molecule 24: 50S ribosomal protein L18

Chain R:  98% .



- Molecule 25: 50S ribosomal protein L19

Chain S:  5% 95% . .



- Molecule 26: 50S ribosomal protein L20

Chain T:  87% 12% .



- Molecule 27: 50S ribosomal protein L21

Chain U:  100%

There are no outlier residues recorded for this chain.

- Molecule 28: 50S ribosomal protein L22

Chain V:  91% 5%



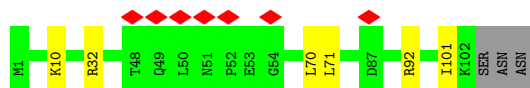
- Molecule 29: 50S ribosomal protein L23

Chain W:  98%



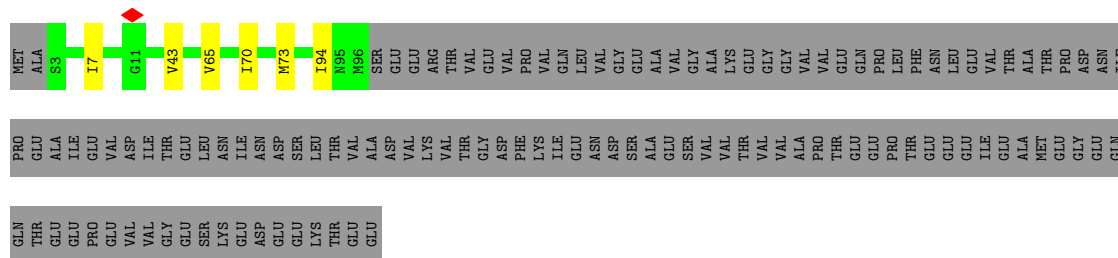
- Molecule 30: 50S ribosomal protein L24

Chain X:  7% 91% 6%



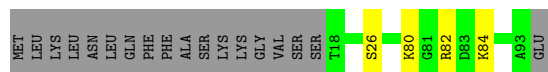
- Molecule 31: 50S ribosomal protein L25

Chain Y:  41% 57%



- Molecule 32: 50S ribosomal protein L27

Chain Z:  77% 19%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77333	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	165000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	43.009	Depositor
Minimum map value	-18.546	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.927	Depositor
Recommended contour level	2.4	Depositor
Map size (Å)	403.19998, 403.19998, 403.19998	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.672, 0.672, 0.672	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 2MG, 5MU, FUA, 2MA, GDP, G7M, OMG, 3TD, ZN, H2U, MG

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	1	0.47	0/488	0.82	0/649
2	2	0.45	0/536	1.05	0/713
3	3	0.48	0/448	0.94	0/601
4	4	0.51	0/499	0.91	0/674
5	5	0.51	0/429	0.86	0/571
6	6	0.46	0/407	0.86	0/545
7	7	0.50	0/377	0.94	0/491
8	8	0.49	0/536	0.90	0/701
9	9	0.52	0/300	0.86	0/393
10	A	0.53	1/67216 (0.0%)	0.81	23/104821 (0.0%)
11	B	0.55	0/2692	0.78	1/4193 (0.0%)
12	C	0.48	0/1442	1.05	0/1940
13	E	0.49	0/5204	0.96	0/7037
14	G	0.51	0/2120	0.87	0/2847
15	H	0.48	0/1652	0.88	0/2216
16	I	0.49	0/1592	0.93	0/2148
17	J	0.47	0/1421	0.96	0/1907
18	K	0.50	0/1400	0.92	0/1881
19	M	0.50	0/1173	0.87	0/1578
20	N	0.49	0/927	0.89	0/1243
21	O	0.50	0/1113	0.90	0/1482
22	P	0.49	0/1113	0.88	0/1493
23	Q	0.46	0/956	0.94	0/1277
24	R	0.49	0/931	0.95	0/1244
25	S	0.49	0/934	0.85	0/1249
26	T	0.47	0/965	0.99	0/1276
27	U	0.47	0/809	0.83	0/1080
28	V	0.49	0/861	0.90	0/1159
29	W	0.46	0/742	0.91	0/989
30	X	0.49	0/796	0.89	0/1063
31	Y	0.48	0/746	0.89	0/1000
32	Z	0.49	0/591	0.89	0/785

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
All	All	0.51	1/101416 (0.0%)	0.84	24/151246 (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
2	2	0	1
5	5	0	1
14	G	0	2
16	I	0	1
18	K	0	1
30	X	0	2
32	Z	0	1
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	2601	G7M	O3'-P	5.04	1.61	1.56

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1962	G	O3'-P-O5'	-8.14	91.78	104.00
10	A	2628	C	O3'-P-O5'	-7.07	93.39	104.00
10	A	2673	C	O3'-P-O5'	-6.90	93.64	104.00
10	A	1182	G	O3'-P-O5'	-6.54	94.19	104.00
10	A	2546	U	O3'-P-O5'	-6.18	94.73	104.00

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	52	ARG	Sidechain
5	5	6	ARG	Sidechain
14	G	13	ARG	Sidechain
14	G	177	ARG	Sidechain
16	I	168	ARG	Sidechain

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	1	482	0	523	3	0
2	2	535	0	566	3	0
3	3	446	0	486	0	0
4	4	485	0	458	11	0
5	5	422	0	426	0	0
6	6	402	0	413	2	0
7	7	373	0	420	1	0
8	8	531	0	599	2	0
9	9	297	0	339	0	0
10	A	60220	0	30287	158	0
11	B	2408	0	1218	5	0
12	C	1433	0	1464	14	0
13	E	5114	0	5010	46	0
14	G	2085	0	2192	7	0
15	H	1628	0	1667	4	0
16	I	1569	0	1614	4	0
17	J	1403	0	1457	19	0
18	K	1382	0	1415	7	0
19	M	1151	0	1145	6	0
20	N	920	0	981	4	0
21	O	1099	0	1142	3	0
22	P	1089	0	1155	7	0
23	Q	952	0	999	5	0
24	R	922	0	968	3	0
25	S	922	0	994	3	0
26	T	953	0	1027	10	0
27	U	799	0	836	0	0
28	V	853	0	914	3	0
29	W	734	0	767	1	0
30	X	787	0	853	2	0
31	Y	738	0	787	5	0
32	Z	585	0	597	2	0
33	5	1	0	0	0	0
33	9	1	0	0	0	0
34	A	112	0	0	0	0
34	E	1	0	0	0	0
34	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	H	1	0	0	0	0
35	E	28	0	12	0	0
36	E	37	0	47	5	0
All	All	93901	0	63778	307	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 2.

The worst 5 of 307 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)
31:Y:7:ILE:HD11	31:Y:65:VAL:HA	1.56	0.88
13:E:106:LEU:HD21	13:E:116:THR:HG21	1.72	0.72
10:A:1806:U:H5	10:A:1811:A:N7	1.89	0.70
20:N:88:ARG:HG2	20:N:94:ARG:HD2	1.75	0.69
4:4:16:ASP:HB3	4:4:21:PHE:HB3	1.76	0.68

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	59/62 (95%)	57 (97%)	2 (3%)	0	100	100
2	2	63/69 (91%)	63 (100%)	0	0	100	100
3	3	55/59 (93%)	53 (96%)	2 (4%)	0	100	100
4	4	57/84 (68%)	56 (98%)	1 (2%)	0	100	100
5	5	51/57 (90%)	49 (96%)	2 (4%)	0	100	100
6	6	46/49 (94%)	46 (100%)	0	0	100	100
7	7	42/45 (93%)	42 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	8	63/66 (96%)	63 (100%)	0	0	100	100
9	9	35/37 (95%)	35 (100%)	0	0	100	100
12	C	183/186 (98%)	181 (99%)	2 (1%)	0	100	100
13	E	657/693 (95%)	649 (99%)	8 (1%)	0	100	100
14	G	271/277 (98%)	267 (98%)	4 (2%)	0	100	100
15	H	213/220 (97%)	205 (96%)	8 (4%)	0	100	100
16	I	203/207 (98%)	200 (98%)	3 (2%)	0	100	100
17	J	175/179 (98%)	170 (97%)	5 (3%)	0	100	100
18	K	175/178 (98%)	172 (98%)	3 (2%)	0	100	100
19	M	143/145 (99%)	141 (99%)	2 (1%)	0	100	100
20	N	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
21	O	144/146 (99%)	138 (96%)	6 (4%)	0	100	100
22	P	134/144 (93%)	131 (98%)	3 (2%)	0	100	100
23	Q	118/122 (97%)	117 (99%)	1 (1%)	0	100	100
24	R	117/119 (98%)	114 (97%)	3 (3%)	0	100	100
25	S	112/116 (97%)	111 (99%)	1 (1%)	0	100	100
26	T	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
27	U	100/102 (98%)	100 (100%)	0	0	100	100
28	V	109/117 (93%)	108 (99%)	1 (1%)	0	100	100
29	W	88/91 (97%)	88 (100%)	0	0	100	100
30	X	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
31	Y	92/217 (42%)	92 (100%)	0	0	100	100
32	Z	74/94 (79%)	72 (97%)	2 (3%)	0	100	100
All	All	3914/4226 (93%)	3846 (98%)	68 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	1	51/52 (98%)	51 (100%)	0	100	100
2	2	59/62 (95%)	58 (98%)	1 (2%)	53	66
3	3	52/53 (98%)	51 (98%)	1 (2%)	50	63
4	4	56/75 (75%)	55 (98%)	1 (2%)	51	65
5	5	48/50 (96%)	47 (98%)	1 (2%)	47	59
6	6	46/47 (98%)	46 (100%)	0	100	100
7	7	39/40 (98%)	39 (100%)	0	100	100
8	8	56/57 (98%)	56 (100%)	0	100	100
9	9	35/35 (100%)	35 (100%)	0	100	100
12	C	162/162 (100%)	159 (98%)	3 (2%)	50	63
13	E	552/579 (95%)	544 (99%)	8 (1%)	59	72
14	G	220/224 (98%)	220 (100%)	0	100	100
15	H	173/177 (98%)	173 (100%)	0	100	100
16	I	168/169 (99%)	168 (100%)	0	100	100
17	J	156/158 (99%)	152 (97%)	4 (3%)	40	51
18	K	154/155 (99%)	154 (100%)	0	100	100
19	M	123/123 (100%)	123 (100%)	0	100	100
20	N	100/100 (100%)	100 (100%)	0	100	100
21	O	112/112 (100%)	112 (100%)	0	100	100
22	P	113/119 (95%)	112 (99%)	1 (1%)	70	81
23	Q	101/102 (99%)	100 (99%)	1 (1%)	68	79
24	R	95/95 (100%)	95 (100%)	0	100	100
25	S	100/102 (98%)	100 (100%)	0	100	100
26	T	97/98 (99%)	97 (100%)	0	100	100
27	U	86/86 (100%)	86 (100%)	0	100	100
28	V	90/94 (96%)	89 (99%)	1 (1%)	65	77
29	W	81/82 (99%)	81 (100%)	0	100	100
30	X	87/90 (97%)	87 (100%)	0	100	100
31	Y	83/190 (44%)	83 (100%)	0	100	100
32	Z	59/75 (79%)	59 (100%)	0	100	100
All	All	3354/3563 (94%)	3332 (99%)	22 (1%)	73	86

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	E	609	ILE
17	J	132	VAL
17	J	117	VAL
17	J	133	LYS
12	C	148	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
16	I	188	ASN
32	Z	20	ASN
18	K	99	GLN
28	V	40	ASN
18	K	38	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	2803/2923 (95%)	358 (12%)	55 (1%)
11	B	112/115 (97%)	14 (12%)	7 (6%)
All	All	2915/3038 (95%)	372 (12%)	62 (2%)

5 of 372 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	A	12	U
10	A	15	G
10	A	34	U
10	A	64	A
10	A	71	A

5 of 62 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	A	1593	G
11	B	32	U
10	A	1885	G
10	A	2887	G
11	B	64	A

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

9 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	$\# Z > 2$
10	3TD	A	1942	10	18,22,23	0.96	1 (5%)	22,32,35	0.82	0
10	2MA	A	2530	34,10	22,25,26	0.24	0	33,37,40	0.64	1 (3%)
10	2MG	A	2472	10	23,26,27	0.34	0	32,38,41	0.44	0
10	5MU	A	1966	10	19,22,23	0.32	0	28,32,35	0.38	0
10	H2U	A	2476	10	18,21,22	0.66	0	21,30,33	0.86	2 (9%)
10	OMG	A	2580	10	23,26,27	0.34	0	33,38,41	0.46	0
10	G7M	A	2601	34,10	23,26,27	0.70	1 (4%)	35,39,42	0.55	0
10	5MU	A	792	10	19,22,23	0.25	0	28,32,35	0.36	0
10	OMG	A	2278	10	23,26,27	0.32	0	33,38,41	0.52	1 (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
10	3TD	A	1942	10	-	2/7/25/26	0/2/2/2
10	2MA	A	2530	34,10	-	2/7/25/26	0/3/3/3
10	2MG	A	2472	10	-	0/9/27/28	0/3/3/3
10	5MU	A	1966	10	-	0/7/25/26	0/2/2/2
10	H2U	A	2476	10	-	0/7/38/39	0/2/2/2
10	OMG	A	2580	10	-	0/9/27/28	0/3/3/3
10	G7M	A	2601	34,10	-	0/7/25/26	0/3/3/3
10	5MU	A	792	10	-	0/7/25/26	0/2/2/2
10	OMG	A	2278	10	-	1/9/27/28	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1942	3TD	C6-C5	3.55	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	2601	G7M	C8-N7	2.46	1.37	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	2476	H2U	O2-C2-N1	-2.33	120.18	123.11
10	A	2476	H2U	N3-C2-N1	2.31	119.09	116.65
10	A	2278	OMG	O2'-C2'-C1'	2.25	113.47	109.08
10	A	2530	2MA	C5-C4-N3	-2.25	124.67	127.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	1942	3TD	O4'-C4'-C5'-O5'
10	A	2278	OMG	C1'-C2'-O2'-CM2
10	A	1942	3TD	C3'-C4'-C5'-O5'
10	A	2530	2MA	O4'-C4'-C5'-O5'
10	A	2530	2MA	C4'-C5'-O5'-P

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	1942	3TD	2	0
10	A	2530	2MA	1	0
10	A	2472	2MG	1	0
10	A	1966	5MU	1	0
10	A	2476	H2U	1	0
10	A	2601	G7M	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 119 ligands modelled in this entry, 117 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$
36	FUA	E	703	-	39,40,40	1.46	3 (7%)	49,64,64	1.09	4 (8%)
35	GDP	E	701	34	28,30,30	0.46	0	44,47,47	0.45	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
36	FUA	E	703	-	-	5/15/92/92	0/4/4/4
35	GDP	E	701	34	-	1/16/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	E	703	FUA	C29-C22	-7.92	1.36	1.47
36	E	703	FUA	O5-C29	-2.42	1.23	1.30
36	E	703	FUA	C9-C11	2.22	1.57	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	E	703	FUA	C16-O2-C31	2.60	121.01	117.06
36	E	703	FUA	C14-C8-C9	-2.30	104.90	109.40
36	E	703	FUA	C15-C14-C8	2.19	119.17	116.84
36	E	703	FUA	C6-C7-C8	2.04	116.35	112.84

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	E	703	FUA	C13-C17-C22-C29
36	E	703	FUA	C17-C22-C29-O5
36	E	703	FUA	C32-C31-O2-C16

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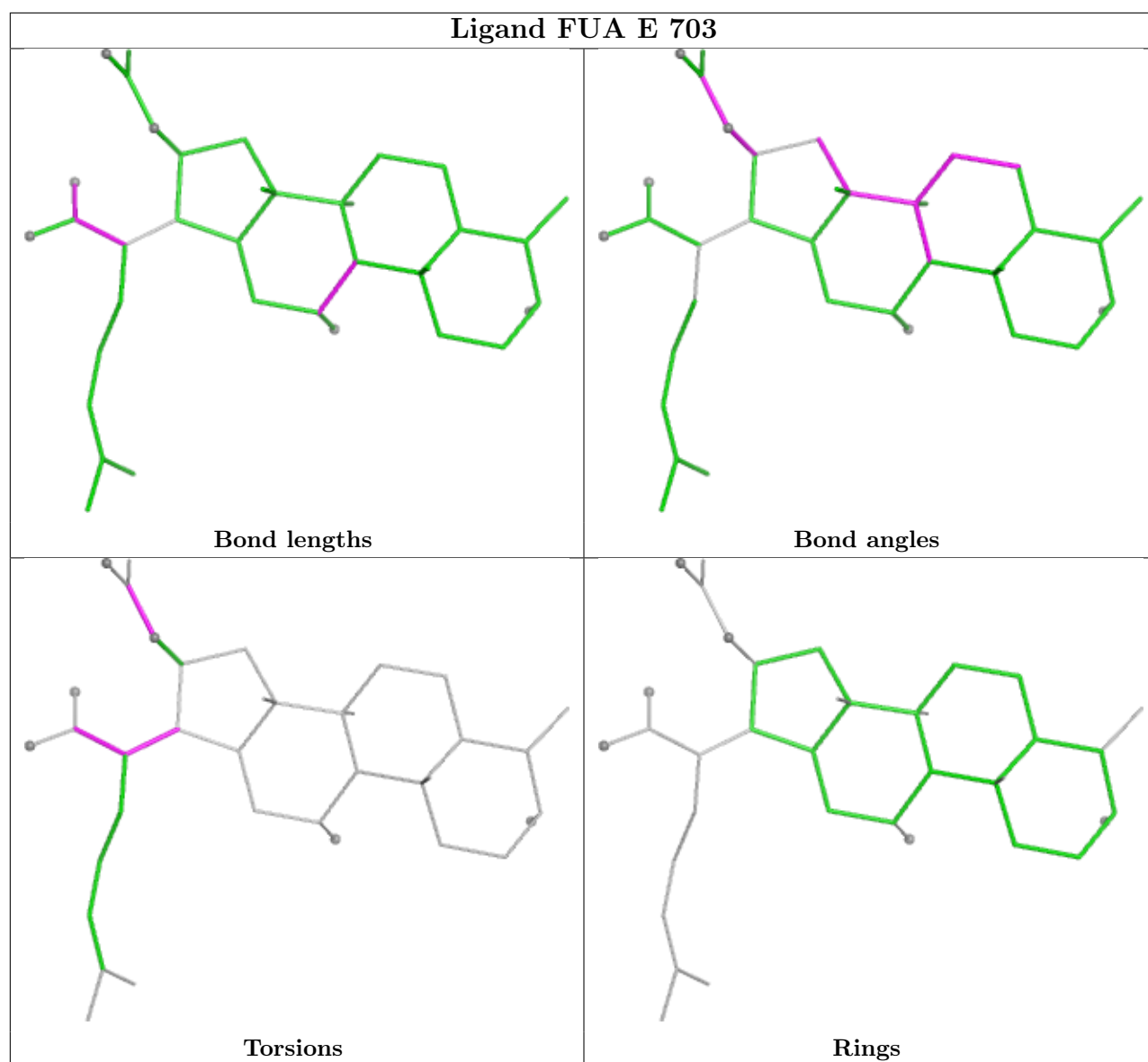
Mol	Chain	Res	Type	Atoms
36	E	703	FUA	O3-C31-O2-C16
35	E	701	GDP	O4'-C4'-C5'-O5'

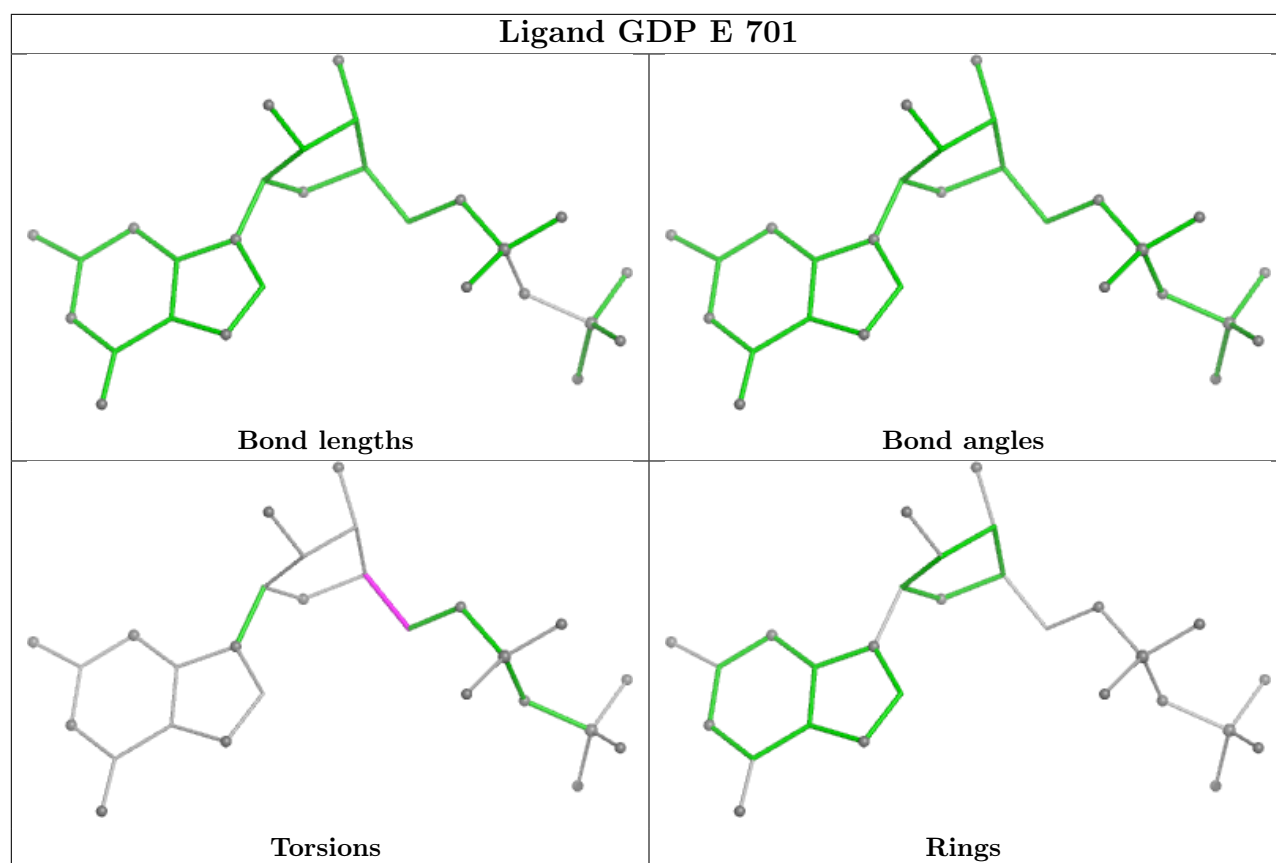
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	E	703	FUA	5	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.

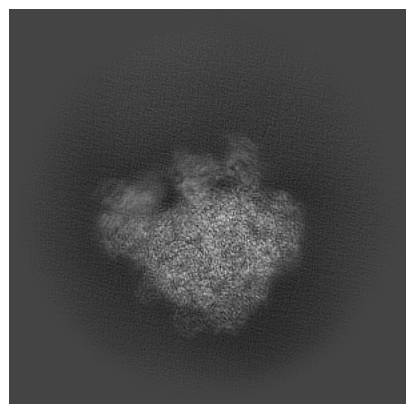
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55947. These allow visual inspection of the internal detail of the map and identification of artifacts.

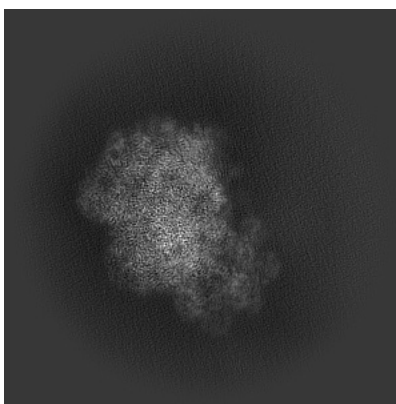
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

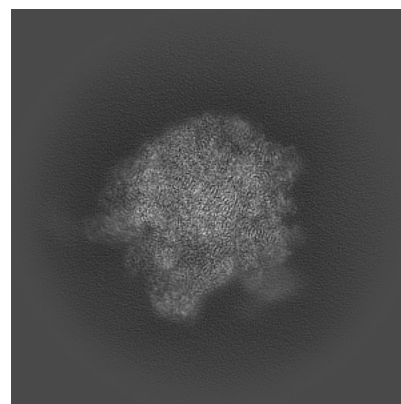
6.1.1 Primary map



X

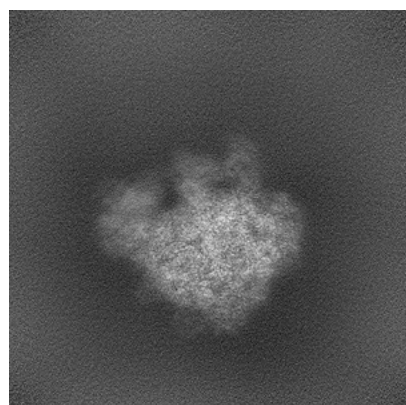


Y

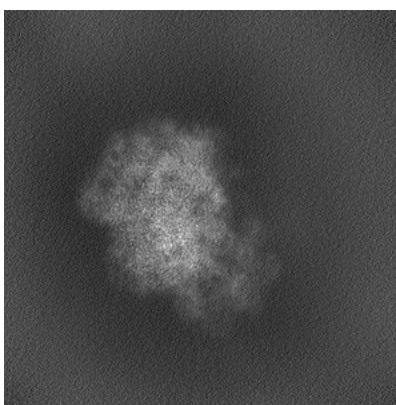


Z

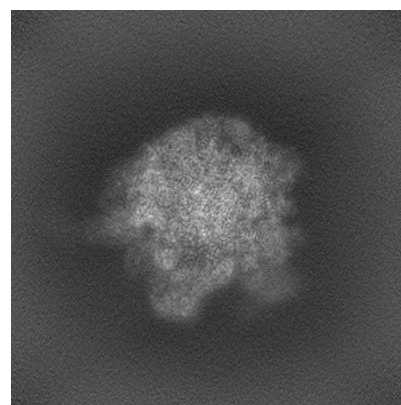
6.1.2 Raw map



X



Y

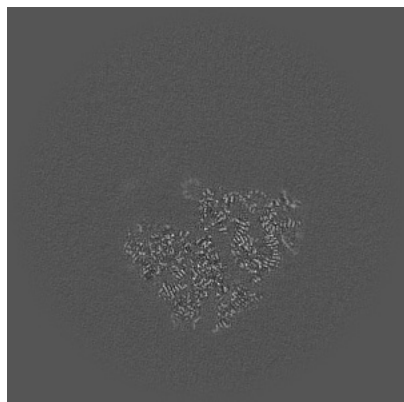


Z

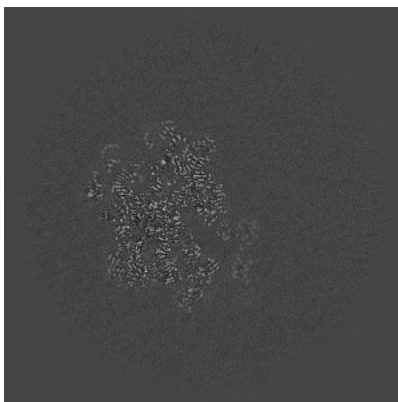
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

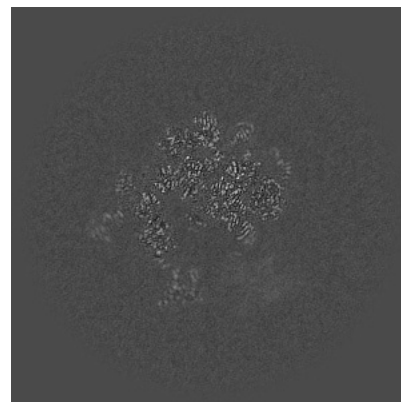
6.2.1 Primary map



X Index: 300

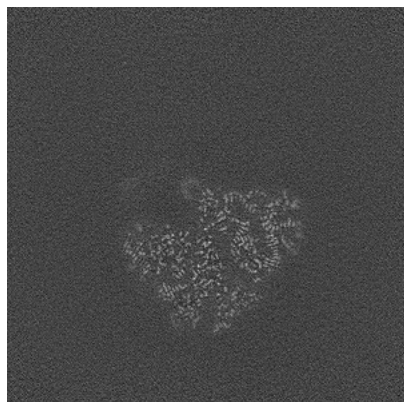


Y Index: 300

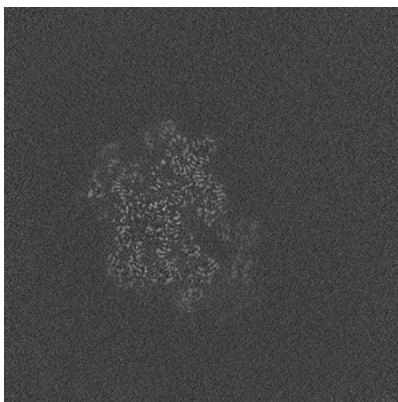


Z Index: 300

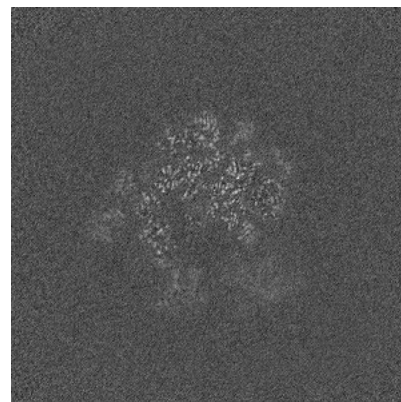
6.2.2 Raw map



X Index: 300



Y Index: 300

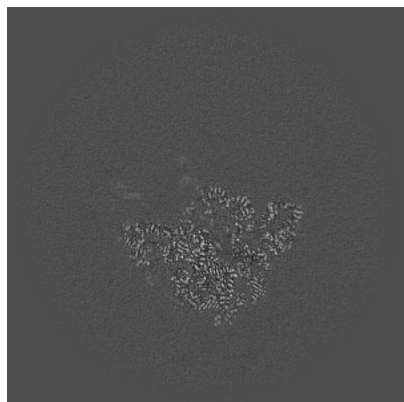


Z Index: 300

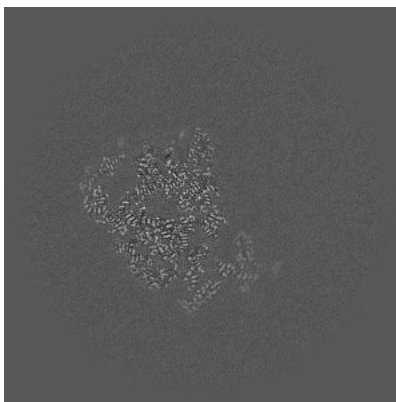
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

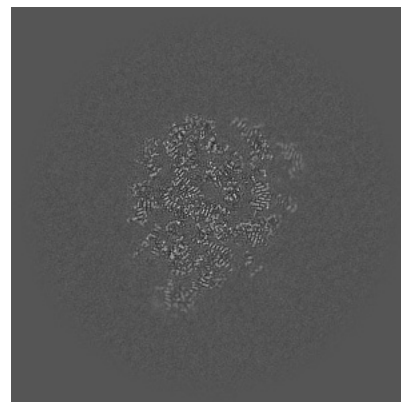
6.3.1 Primary map



X Index: 288

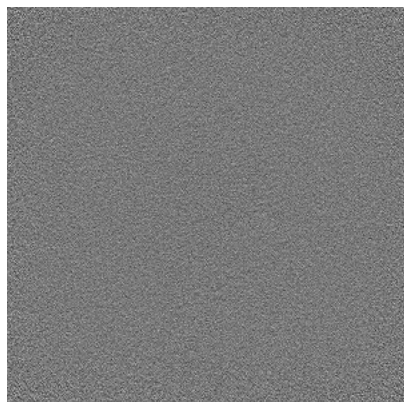


Y Index: 327

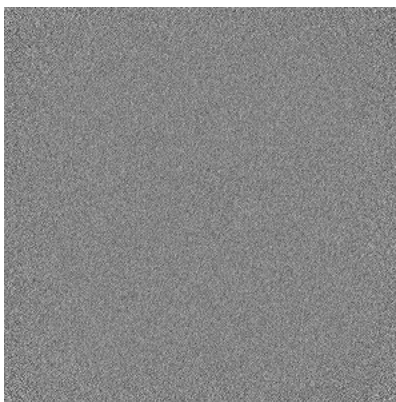


Z Index: 244

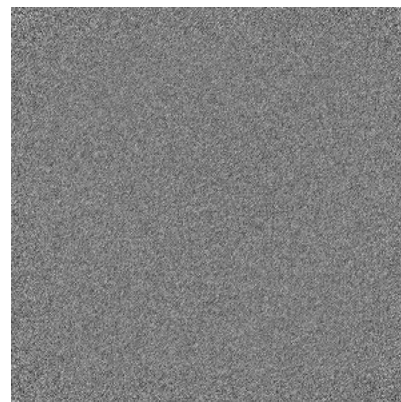
6.3.2 Raw map



X Index: 0



Y Index: 0

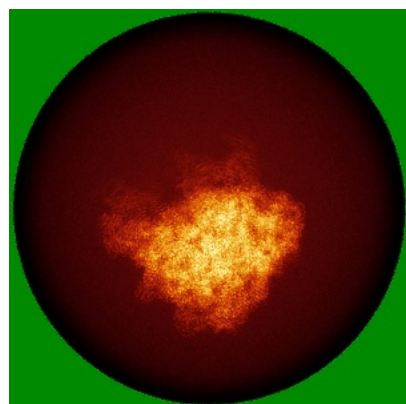


Z Index: 0

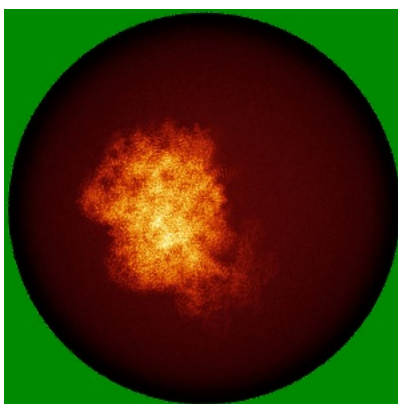
The images above show the largest variance slices of the map in three orthogonal directions.

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

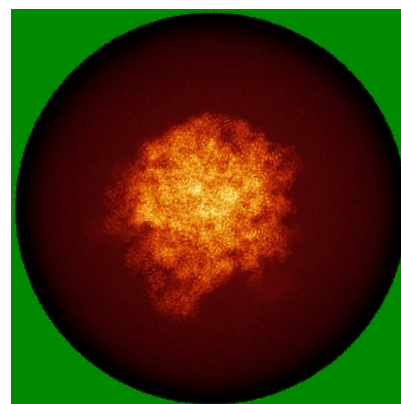
6.4.1 Primary map



X

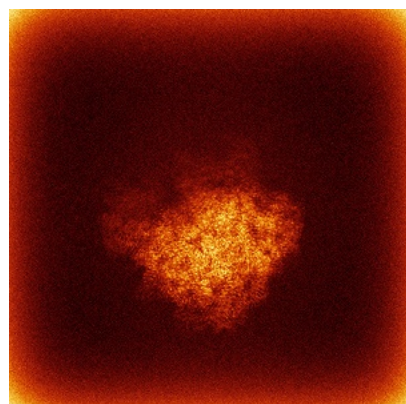


Y

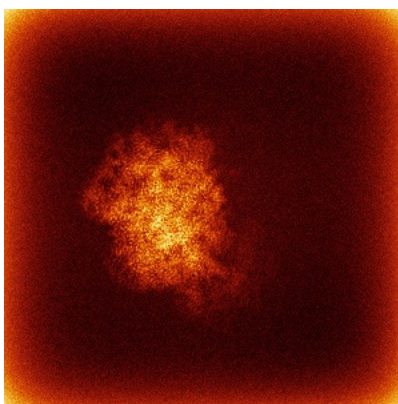


Z

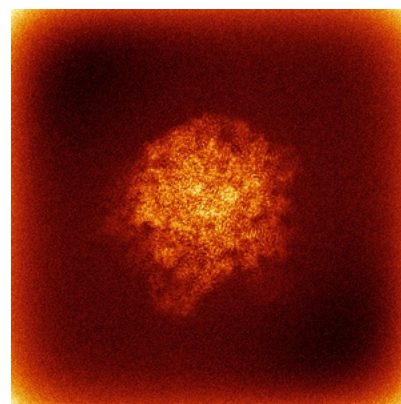
6.4.2 Raw map



X



Y

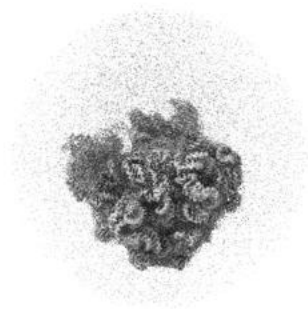


Z

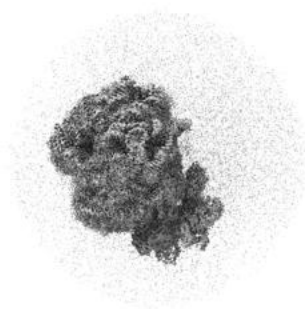
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

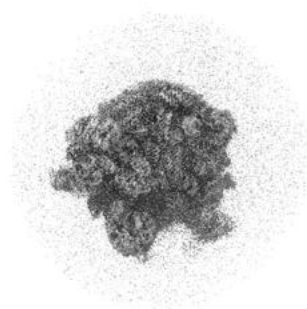
6.5.1 Primary map



X



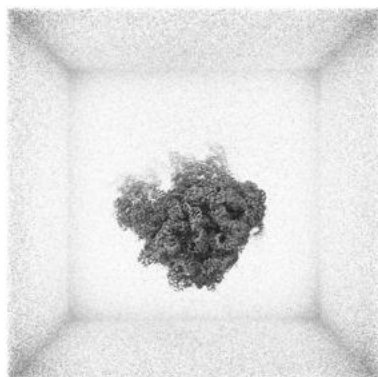
Y



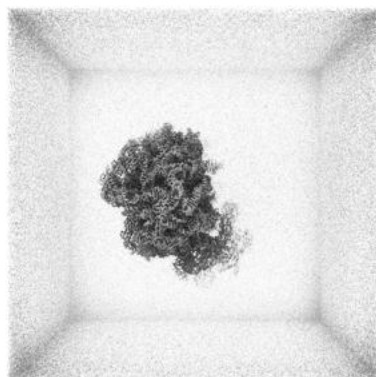
Z

The images above show the 3D surface view of the map at the recommended contour level 2.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

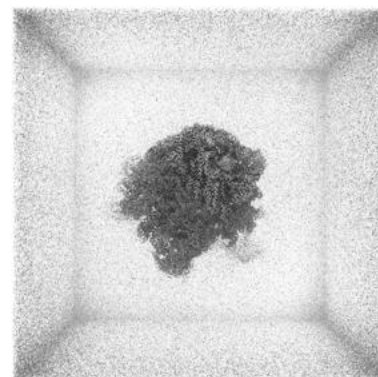
6.5.2 Raw map



X



Y



Z

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

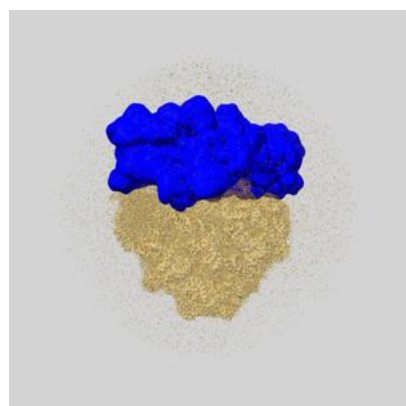
6.6 Mask visualisation [i](#)

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

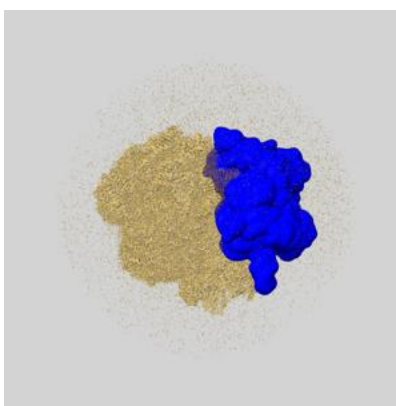
A mask typically either:

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

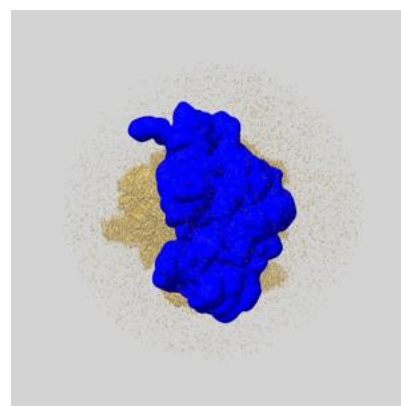
6.6.1 emd_55947_msk_1.map [i](#)



X

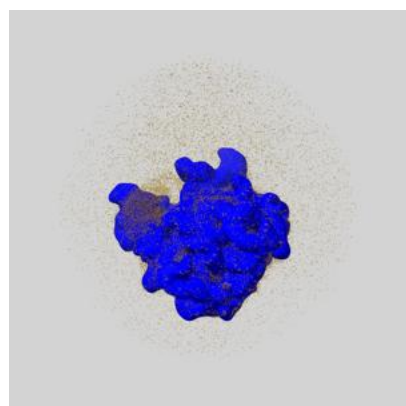


Y

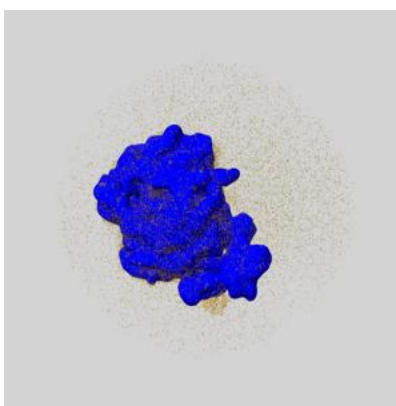


Z

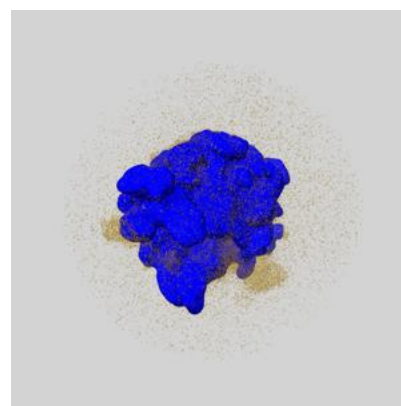
6.6.2 emd_55947_msk_2.map [i](#)



X

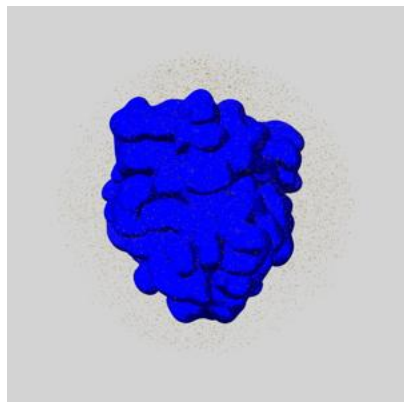


Y

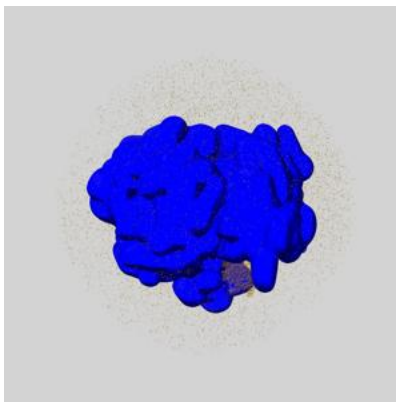


Z

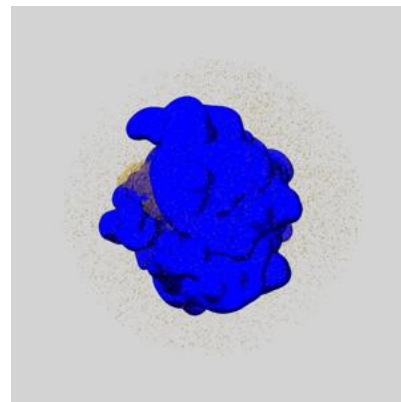
6.6.3 emd_55947_msk_3.map [i](#)



X

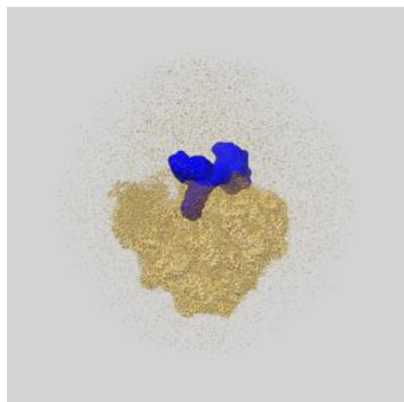


Y

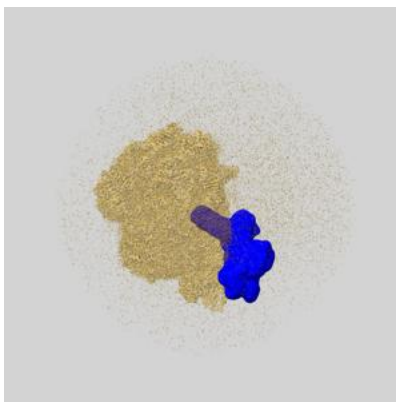


Z

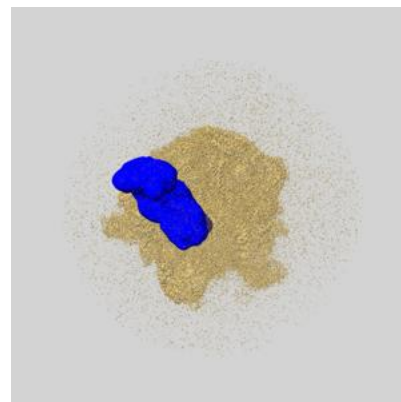
6.6.4 emd_55947_msk_4.map [i](#)



X



Y

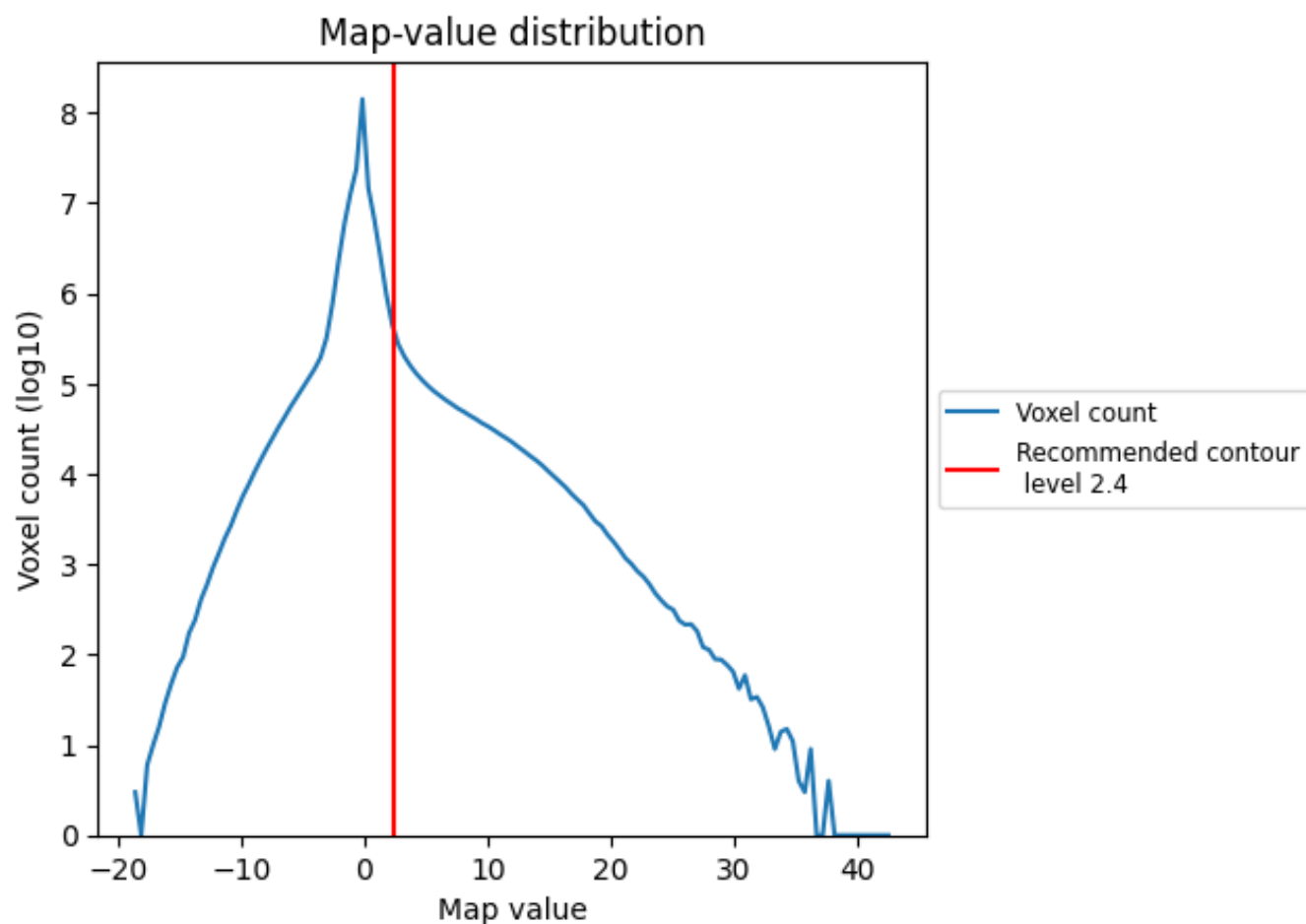


Z

7 Map analysis [i](#)

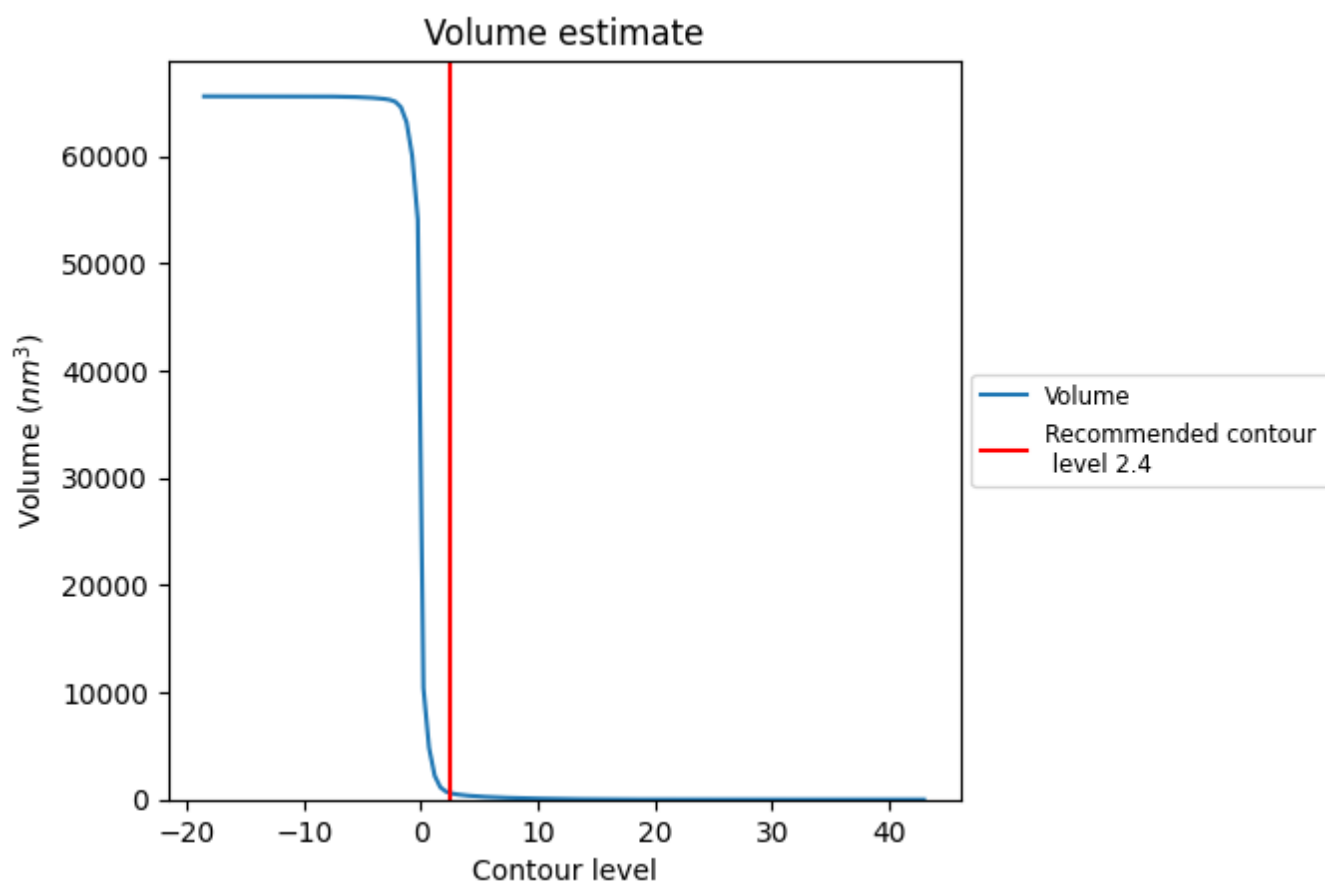
This section contains the results of statistical analysis of the map.

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.

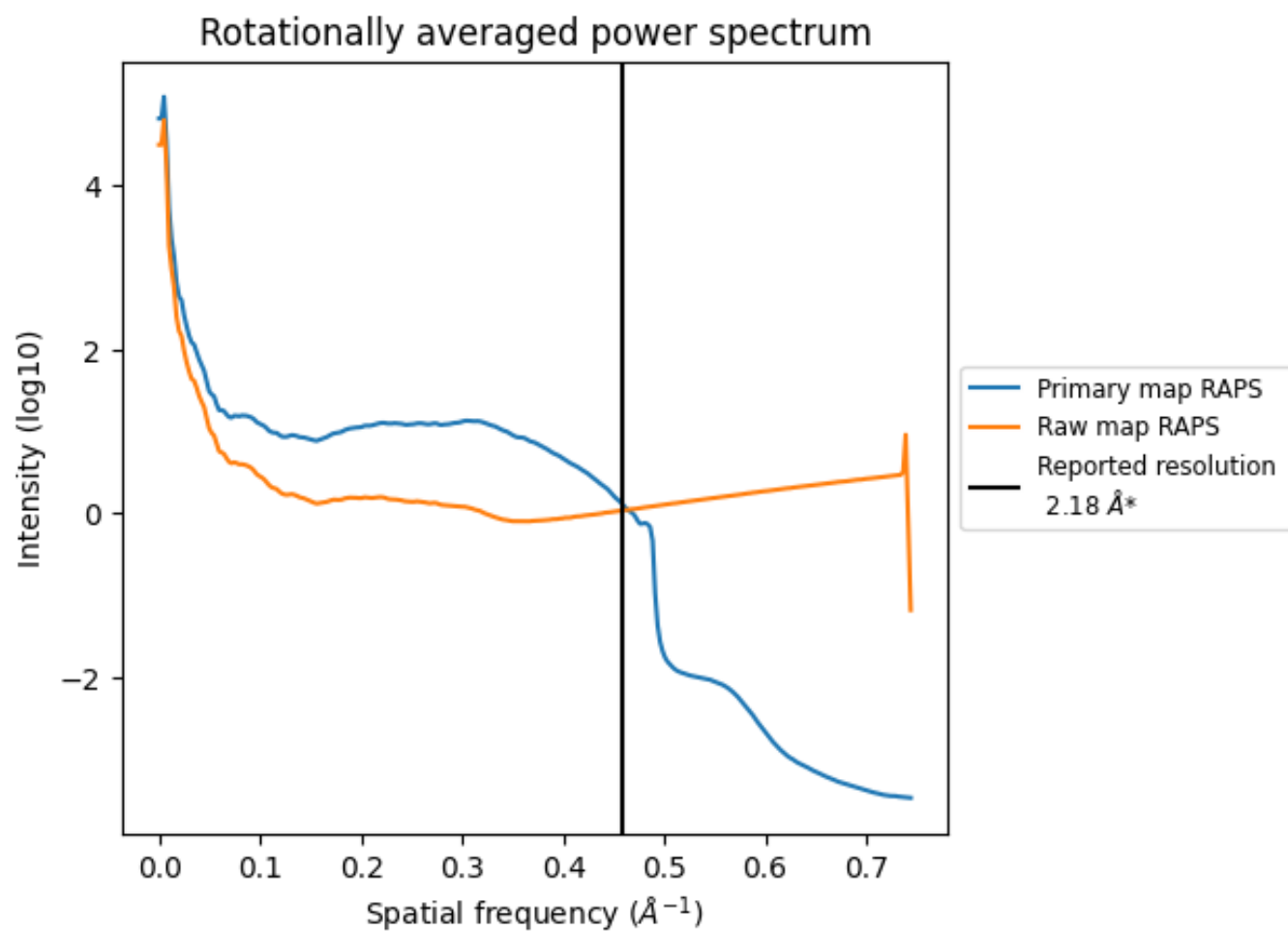
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 650 nm³; this corresponds to an approximate mass of 587 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 ⓘ

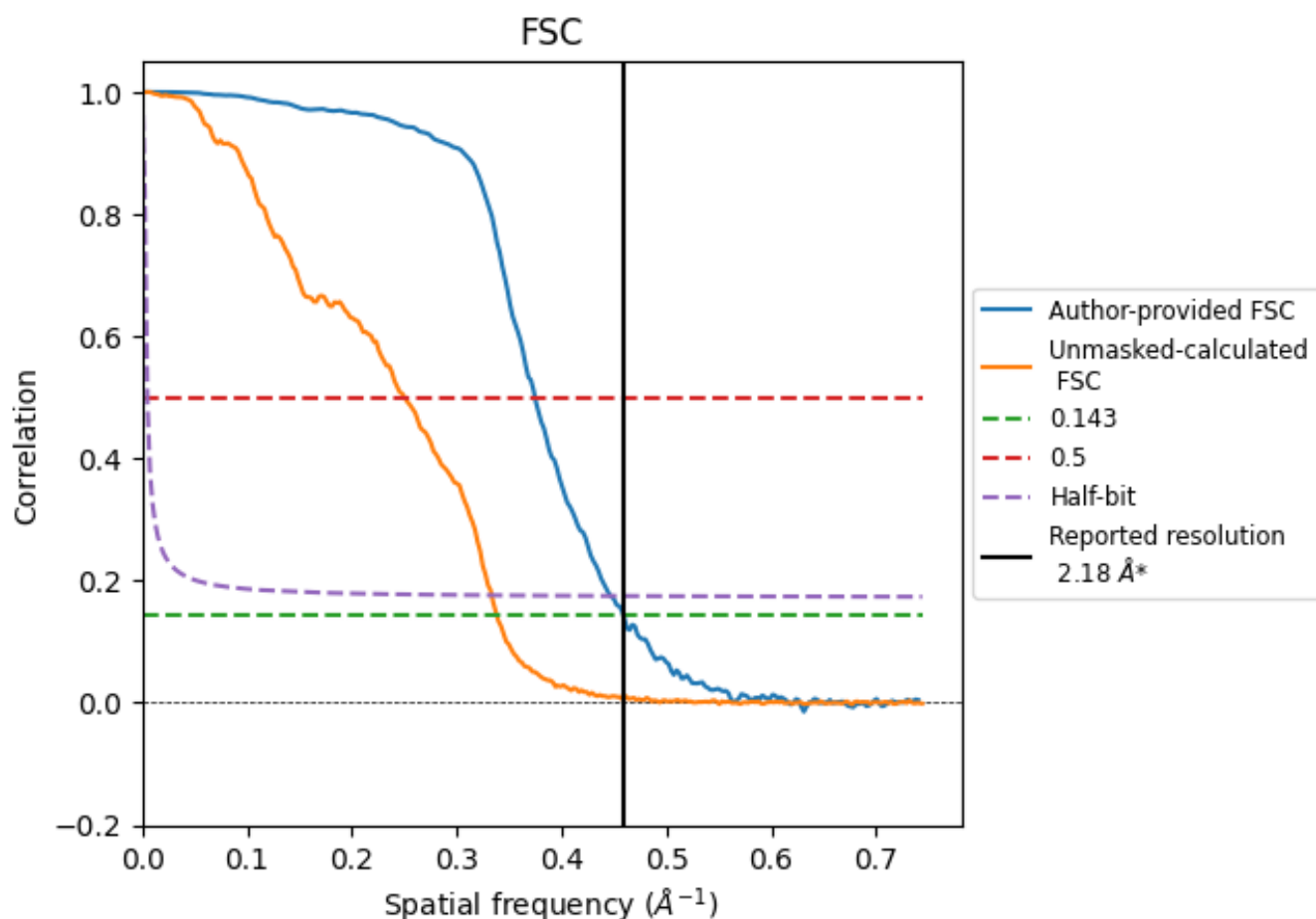


*Reported resolution corresponds to spatial frequency of 0.459 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.459 \text{ \AA}^{-1}$

8.2 Resolution estimates

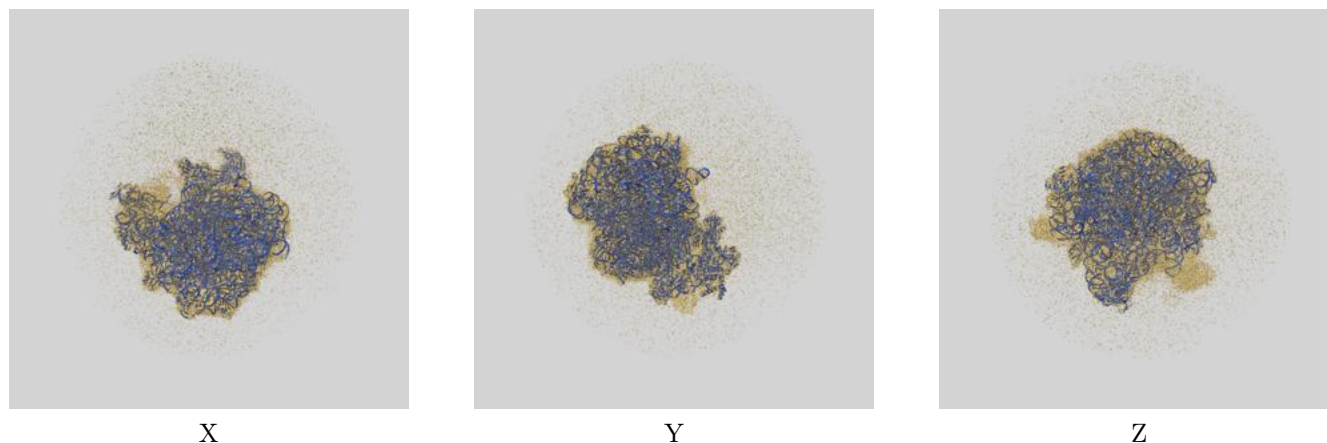
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.18	-	-
Author-provided FSC curve	2.18	2.67	2.24
Unmasked-calculated*	2.96	4.00	3.00

*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 2.96 differs from the reported value 2.18 by more than 10 %

9 Map-model fit [i](#)

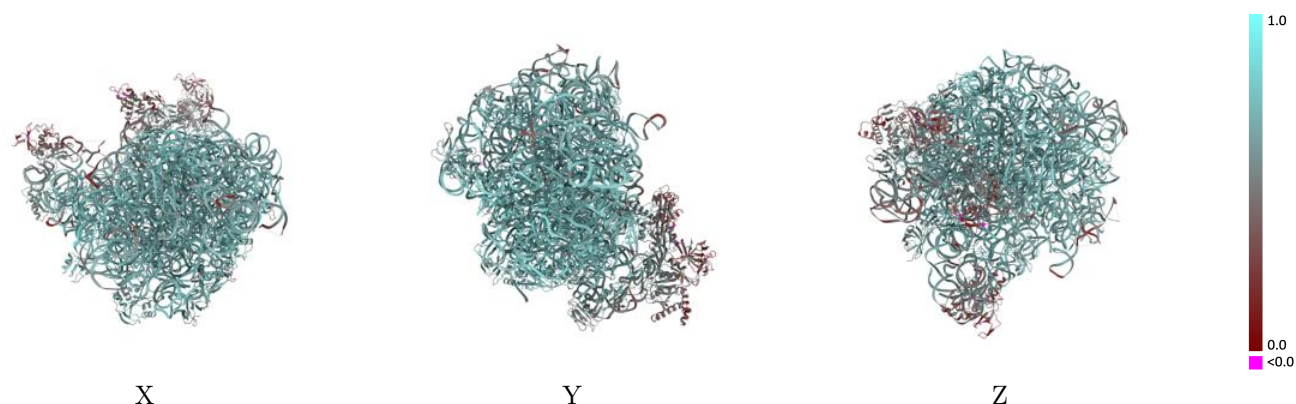
This section contains information regarding the fit between EMDB map EMD-55947 and PDB model 9TI8. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



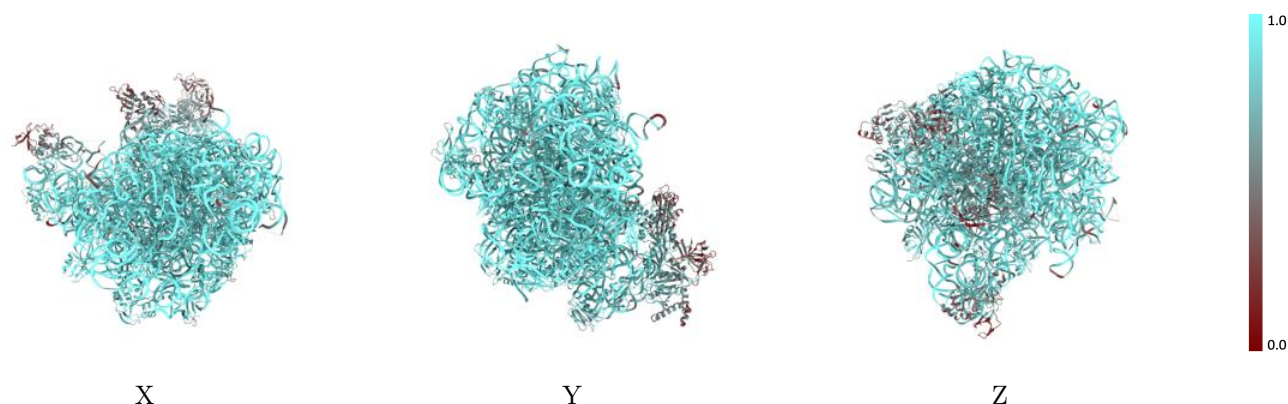
The images above show the 3D surface view of the map at the recommended contour level 2.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



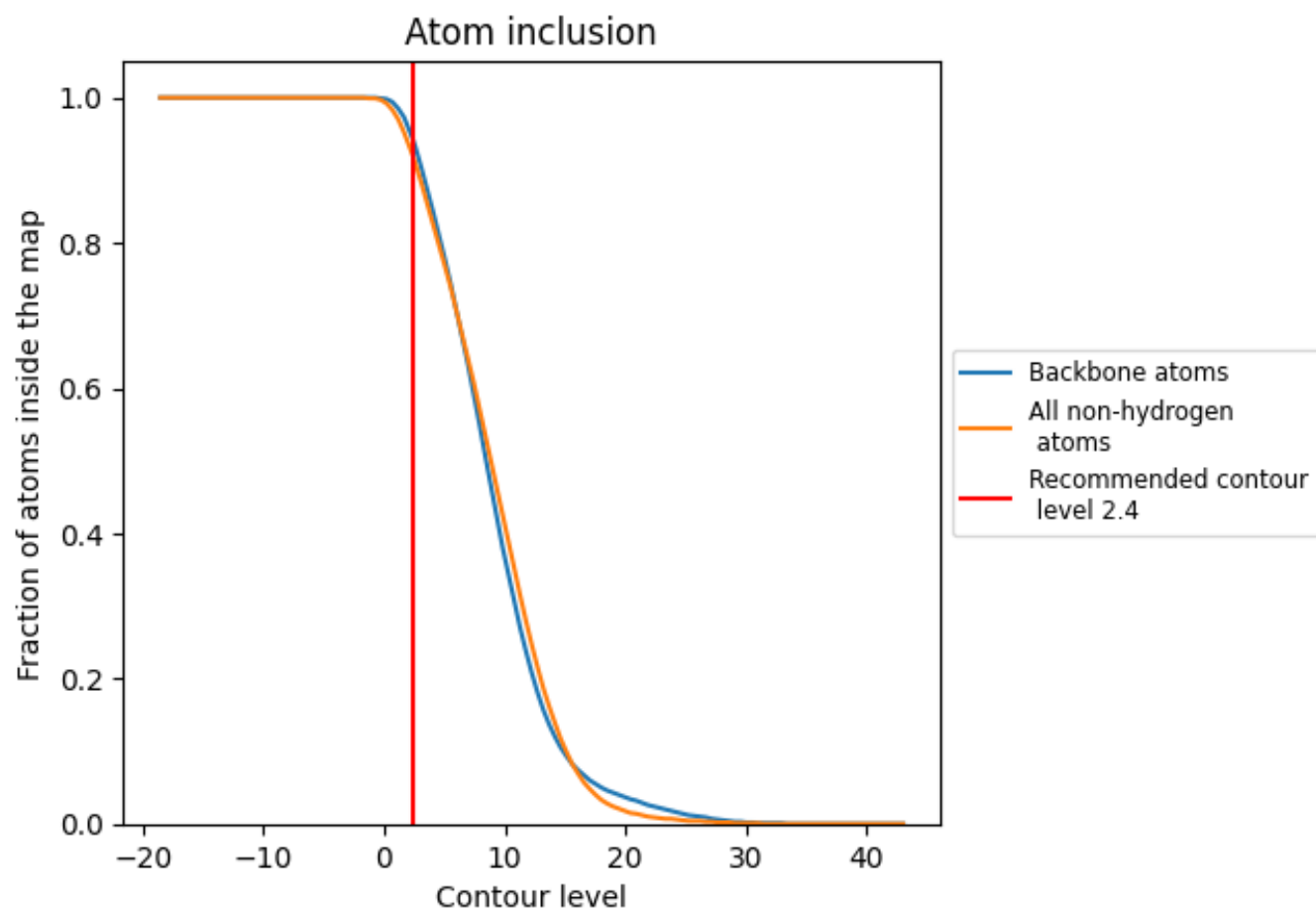
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 92% 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 (2.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9190	 0.6610
1	 0.9090	 0.6600
2	 0.8710	 0.6360
3	 0.9570	 0.7070
4	 0.2400	 0.2780
5	 0.9390	 0.7100
6	 0.8790	 0.6280
7	 0.9740	 0.7530
8	 0.9860	 0.7510
9	 0.9560	 0.6960
A	 0.9670	 0.6920
B	 0.9450	 0.6040
C	 0.6840	 0.5220
E	 0.5630	 0.4100
G	 0.9630	 0.7160
H	 0.9640	 0.7290
I	 0.9290	 0.6920
J	 0.5440	 0.3990
K	 0.7880	 0.5420
M	 0.9530	 0.7130
N	 0.9380	 0.6870
O	 0.9350	 0.6960
P	 0.9460	 0.6880
Q	 0.9490	 0.7120
R	 0.8340	 0.5650
S	 0.8830	 0.6540
T	 0.9690	 0.7320
U	 0.9400	 0.6920
V	 0.9420	 0.7230
W	 0.9050	 0.6730
X	 0.8050	 0.5730
Y	 0.8430	 0.5890
Z	 0.9540	 0.7020

