



Full wwPDB EM Validation Report ⓘ

Oct 13, 2024 – 11:20 am BST

PDB ID : 7QIX
EMDB ID : EMD-14002
Title : Specific features and methylation sites of a plant ribosome. 40S body ribosomal subunit.
Authors : Cottilli, P.; Itoh, Y.; Amunts, A.
Deposited on : 2021-12-16
Resolution : 2.53 Å(reported)

This is a Full wwPDB EM Validation 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.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

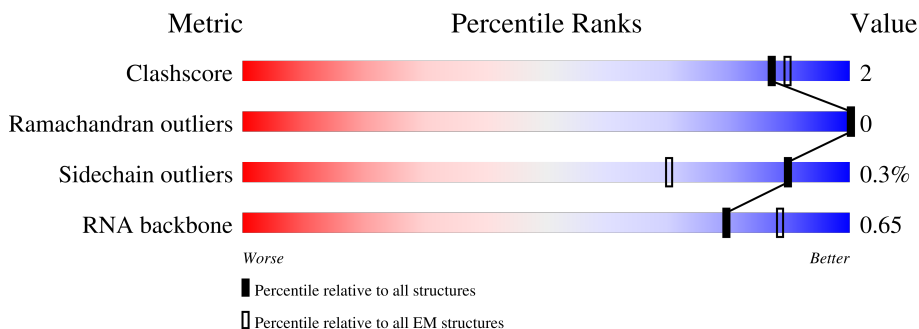
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.53 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	1807	
2	D	25	
3	E	296	
4	F	260	
5	G	264	
6	H	191	
7	I	220	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	J	159	
9	K	144	
10	L	82	
11	M	142	
12	N	127	
13	O	280	
14	P	249	
15	Q	197	
16	R	151	
17	S	150	
18	U	133	
19	V	86	
20	W	62	
21	T	130	
22	X	213	

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 84097 atoms, of which 36357 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 18S rRNA body.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	2	1110	Total	C	H	N	O	P	0	0
			35742	10635	11982	4285	7730	1110		

- Molecule 2 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	25	Total	C	H	N	O	S	0	0
			527	145	289	62	28	3		

- Molecule 3 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	E	202	Total	C	H	N	O	S	0	0
			3230	1024	1621	288	287	10		

- Molecule 4 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	F	215	Total	C	H	N	O	S	0	0
			3570	1112	1810	322	318	8		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	39	GLU	GLY	conflict	UNP A0A3Q7I881
F	141	ALA	GLY	conflict	UNP A0A3Q7I881
F	169	VAL	ARG	conflict	UNP A0A3Q7I881
F	173	ARG	VAL	conflict	UNP A0A3Q7I881
F	185	VAL	ALA	conflict	UNP A0A3Q7I881
F	205	PHE	TYR	conflict	UNP A0A3Q7I881

- Molecule 5 is a protein called 40S body ribosomal protein eS4.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	G	261	Total	C	H	N	O	S	0	0
			4264	1326	2180	389	361	8		

- Molecule 6 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	H	187	Total	C	H	N	O	S	0	0
			3103	962	1582	282	276	1		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	13	ALA	ASP	conflict	UNP A0A3Q7H0E8
H	19	HIS	PHE	conflict	UNP A0A3Q7H0E8
H	22	SER	THR	conflict	UNP A0A3Q7H0E8
H	24	GLY	ALA	conflict	UNP A0A3Q7H0E8

- Molecule 7 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	I	184	Total	C	H	N	O	S	0	0
			3032	929	1539	296	264	4		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	18	LYS	GLN	conflict	UNP A0A3Q7HJ03
I	20	SER	THR	conflict	UNP A0A3Q7HJ03
I	66	PHE	TYR	conflict	UNP A0A3Q7HJ03
I	159	ASN	LYS	conflict	UNP A0A3Q7HJ03
I	162	ALA	LYS	conflict	UNP A0A3Q7HJ03
I	165	LYS	THR	conflict	UNP A0A3Q7HJ03
I	175	ALA	SER	conflict	UNP A0A3Q7HJ03
I	180	LEU	TYR	conflict	UNP A0A3Q7HJ03

- Molecule 8 is a protein called Ribosomal_S17_N domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	J	147	Total	C	H	N	O	S	0	0
			2381	737	1217	224	198	5		

- Molecule 9 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	K	44	Total	C	H	N	O	S	0	0
			696	214	350	57	72	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	87	GLU	ASP	conflict	UNP P49215

- Molecule 10 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	L	82	Total	C	H	N	O	S	0	0
			1257	391	617	116	128	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	44	VAL	ARG	conflict	UNP A0A3Q7G7P4
L	68	MET	LEU	conflict	UNP A0A3Q7G7P4

- Molecule 11 is a protein called 40S body ribosomal protein uS12.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	M	141	Total	C	H	N	O	S	0	0
			2267	695	1167	215	187	3		

- Molecule 12 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	N	98	Total	C	H	N	O	S	0	0
			1628	495	831	164	130	8		

- Molecule 13 is a protein called S5 DRBM domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	O	220	Total	C	H	N	O	S	0	0
			3515	1104	1809	303	291	8		

- Molecule 14 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	P	237	Total	C	H	N	O	S	0	0
			3934	1187	2028	374	337	8		

- Molecule 15 is a protein called 40S body ribosomal protein uS4.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	Q	184	Total	C	H	N	O	S	0	0
			3130	965	1601	303	256	5		

- Molecule 16 is a protein called 30S ribosomal protein S15, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	R	150	Total	C	H	N	O	S	0	0
			2480	765	1285	224	204	2		

- Molecule 17 is a protein called Ribosomal protein S14.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	S	132	Total	C	H	N	O	S	0	0
			2031	612	1032	197	185	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	137	IAS	ASP	conflict	UNP Q38JI8

- Molecule 18 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	U	126	Total	C	H	N	O	S	0	0
			2136	654	1106	199	174	3		

- Molecule 19 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	V	68	Total	C	H	N	O	S	0	0
			1098	341	558	101	95	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	19	LYS	ARG	conflict	UNP A0A1U8DQX3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
V	76	ILE	THR	conflict	UNP A0A1U8DQX3

- Molecule 20 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	W	48	Total	C	H	N	O	S	0	0
			794	232	411	87	63	1		

- Molecule 21 is a protein called 40S ribosomal protein S15a-1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
21	T	129	Total	C	H	N	O	S	0	0
			2062	650	1047	182	179	4		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	20	ALA	ARG	conflict	UNP A0A1U7YEG5
T	23	ALA	ARG	conflict	UNP A0A1U7YEG5
T	26	GLU	MET	conflict	UNP A0A1U7YEG5
T	27	LEU	ILE	conflict	UNP A0A1U7YEG5
T	49	ASP	GLU	conflict	UNP A0A1U7YEG5
T	51	GLN	GLU	conflict	UNP A0A1U7YEG5
T	58	VAL	SER	conflict	UNP A0A1U7YEG5
T	84	ALA	LYS	conflict	UNP A0A1U7YEG5
T	85	THR	GLU	conflict	UNP A0A1U7YEG5

- Molecule 22 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	32	Total	C	H	N	O	0	0
			570	166	295	62	47		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	178	LYS	GLU	conflict	UNP A0A3Q7GQ29
X	179	LYS	GLU	conflict	UNP A0A3Q7GQ29

- Molecule 23 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
23	2	19	Total	K	0
			19	19	

- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
24	2	59	Total	Mg	0
			59	59	
24	P	1	Total	Mg	0
			1	1	

- Molecule 25 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
25	N	1	Total	Zn	0
			1	1	

- Molecule 26 is water.

Mol	Chain	Residues	Atoms		AltConf
26	2	462	Total	O	0
			462	462	
26	D	2	Total	O	0
			2	2	
26	F	3	Total	O	0
			3	3	
26	G	6	Total	O	0
			6	6	
26	I	5	Total	O	0
			5	5	
26	J	23	Total	O	0
			23	23	
26	L	2	Total	O	0
			2	2	
26	M	14	Total	O	0
			14	14	
26	N	14	Total	O	0
			14	14	
26	O	3	Total	O	0
			3	3	
26	P	3	Total	O	0
			3	3	

Continued on next page...

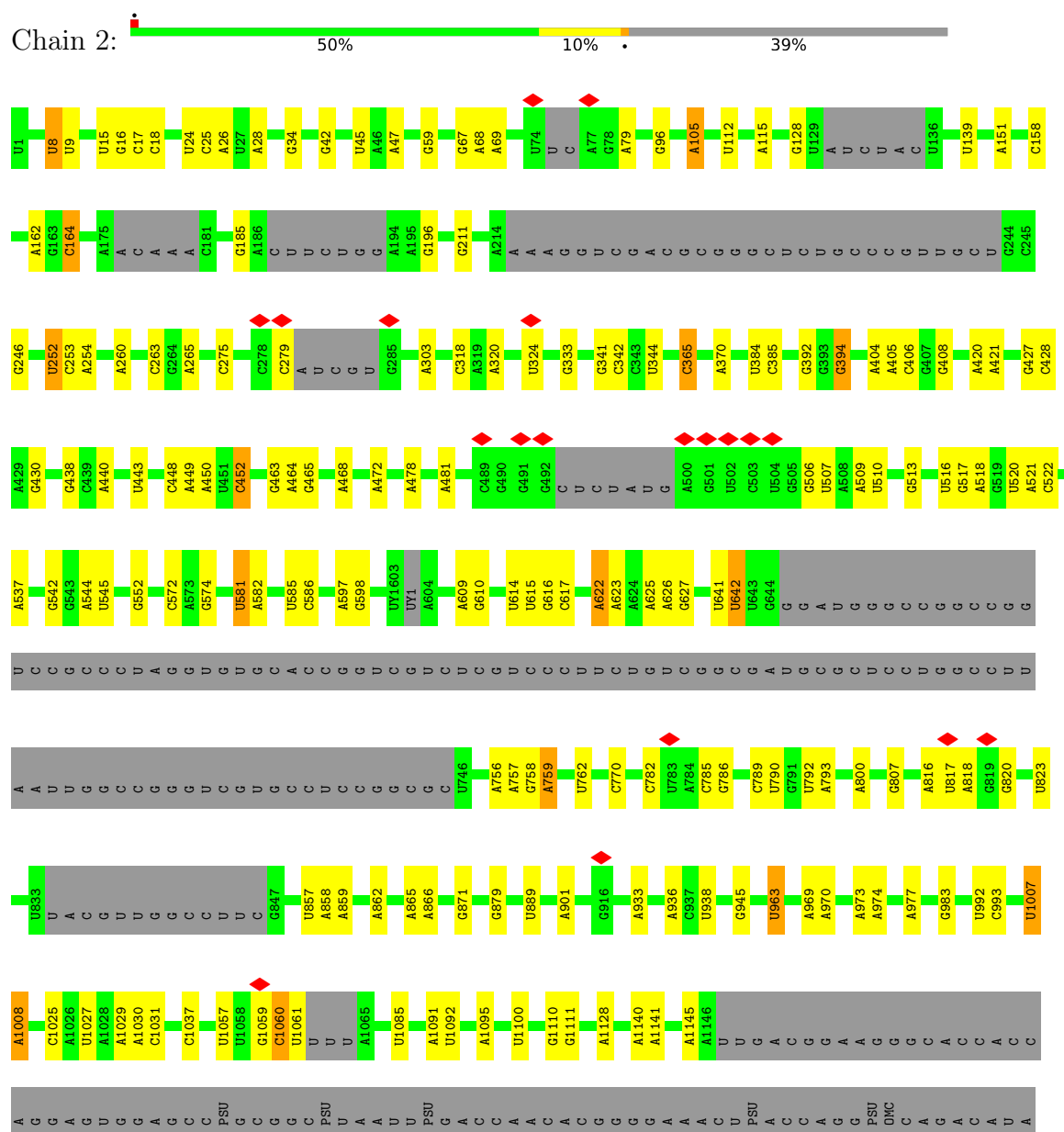
Continued from previous page...

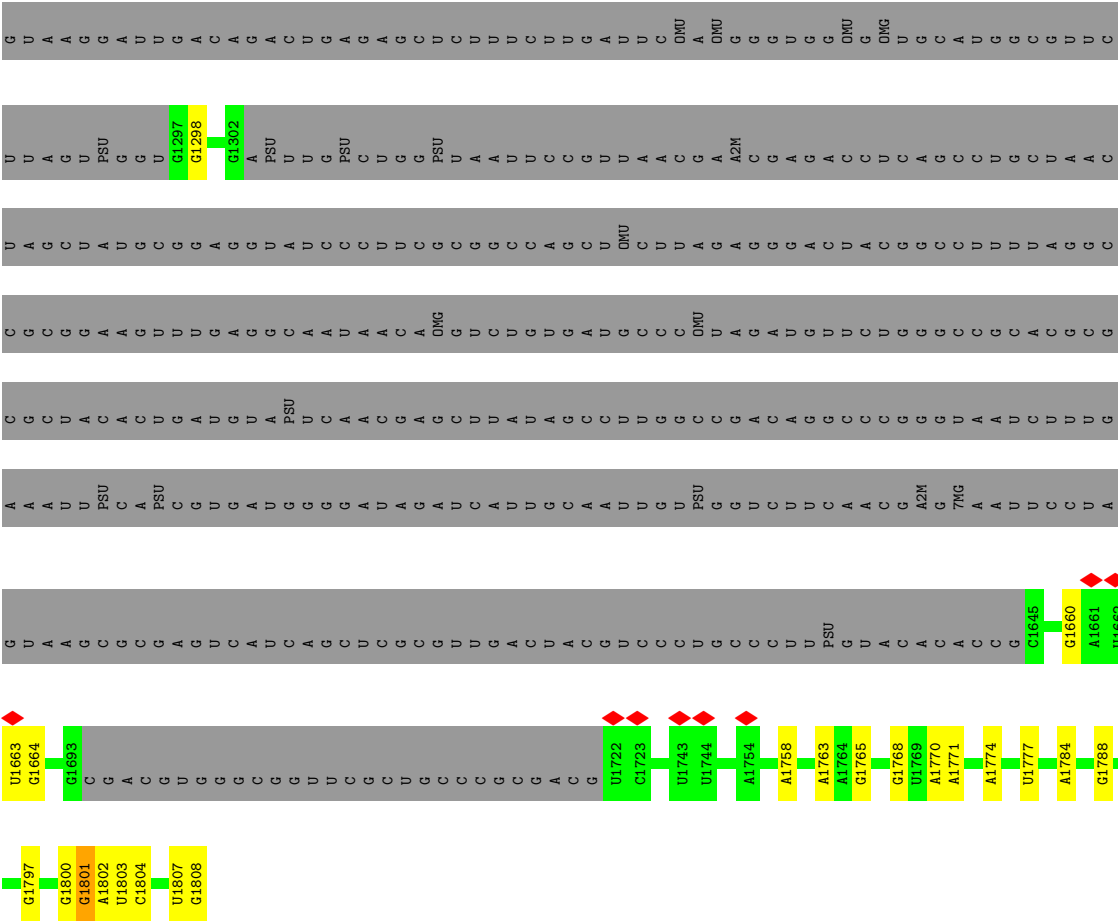
Mol	Chain	Residues	Atoms		AltConf
26	Q	12	Total 12	O 12	0
26	R	5	Total 5	O 5	0
26	S	5	Total 5	O 5	0
26	V	2	Total 2	O 2	0
26	W	2	Total 2	O 2	0
26	T	7	Total 7	O 7	0

3 Residue-property plots [i](#)

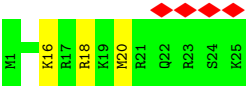
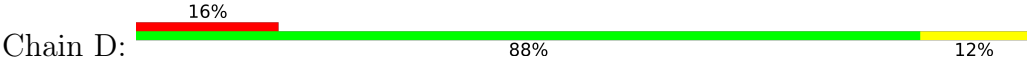
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 18S rRNA body

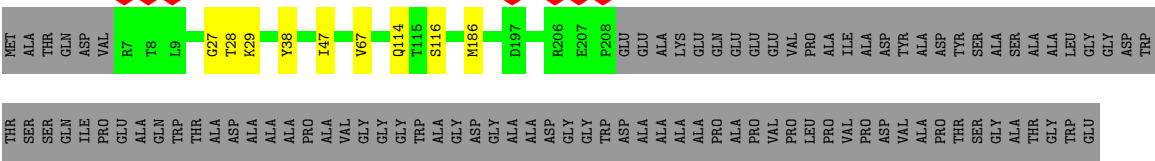




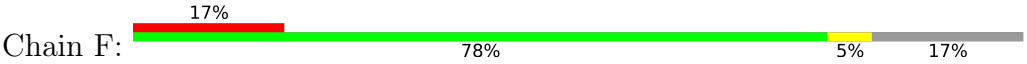
• Molecule 2: 60S ribosomal protein L41



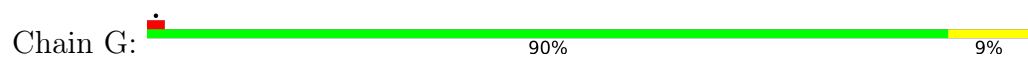
• Molecule 3: 40S ribosomal protein SA



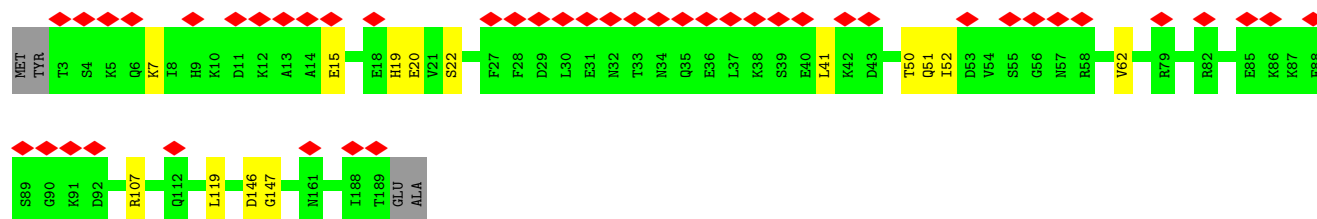
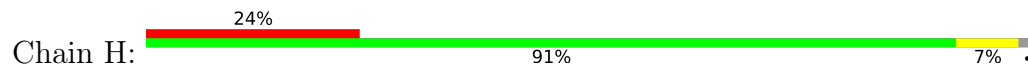
• Molecule 4: 40S ribosomal protein S3a



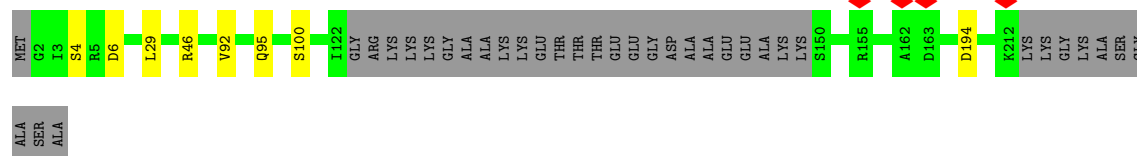
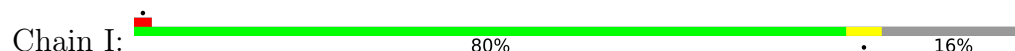
- Molecule 5: 40S body ribosomal protein eS4



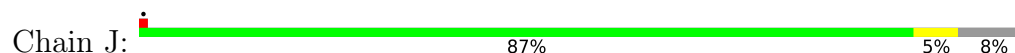
- Molecule 6: 40S ribosomal protein S7



- Molecule 7: 40S ribosomal protein S8

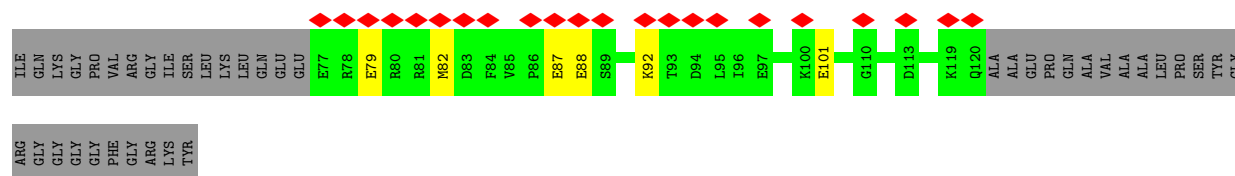


- Molecule 8: Ribosomal_S17_N domain-containing protein

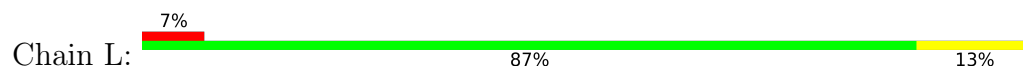


- Molecule 9: 40S ribosomal protein S17

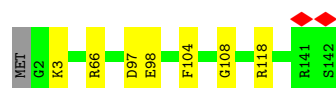




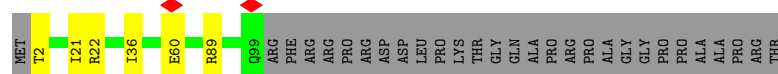
- Molecule 10: 40S ribosomal protein S21



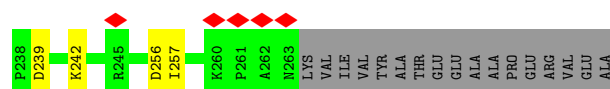
- Molecule 11: 40S body ribosomal protein uS12



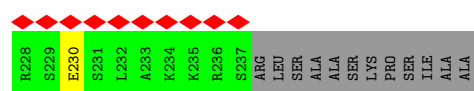
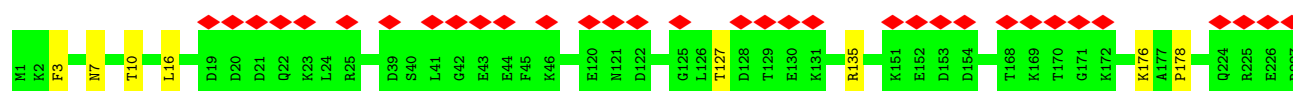
- Molecule 12: 40S ribosomal protein S26



- Molecule 13: S5 DRBM domain-containing protein

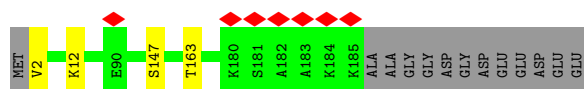


- Molecule 14: 40S ribosomal protein S6



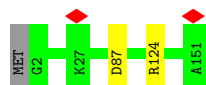
- Molecule 15: 40S body ribosomal protein uS4

Chain Q:  91% 7%




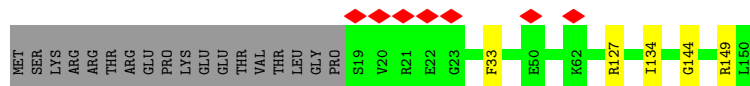
- Molecule 16: 30S ribosomal protein S15, chloroplastic

Chain R:  98%



- Molecule 17: Ribosomal protein S14

Chain S:  5% 85% 12%




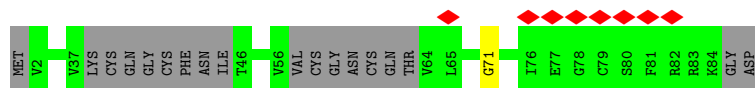
- Molecule 18: 40S ribosomal protein S24

Chain U:  7% 92% 5%



- Molecule 19: 40S ribosomal protein S27

Chain V:  9% 78% 21%



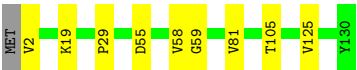
- Molecule 20: 40S ribosomal protein S30

Chain W:  5% 73% 5% 23%



- Molecule 21: 40S ribosomal protein S15a-1

Chain T:  92% 7%



● Molecule 22: Ribosomal protein L19



MET	VAL	ARG	SER	LEU	LEU	LYS	GLN	LYS	ARG	LEU	ALA	ALA	SER	VAL	LEU	LYS	CYS	GLY	ARG	GLY	LYS	VAL	TRP	LEU	ASP	PRO	ASN	GLY	ASN	GLY	ASN	GLY	ILE	SER	MET	ALA	ALA	ASN	SER	ARG	ARG	GLN	ASN	ILE	ARG	LYS	LYS	VAL	VAL	LYS	ASP	GLY	PHE	ILE	ILE	ARG	PRQ	THR	LYS	ILE	HIS	SER	ARG
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER	ARG	ALA	ARG	ARG	MET	LYS	GLU	ALA	LYS	ARG	LYS	GLY	ARG	HIS	GLY	TVR	GLY	LYS	ARG	GLU	ALA	ARG	PRO	THR	LYS	VAL	TRP	MET	ARG	ARG	LEU	ARG	VAL	LEU	ARG	LEU	LYS	TVR	ARG	GLU	SER	LYS	ILE	LYS	ASP	LYS	HIS	TYR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

HIS	ASP	MET	TYR	MET	LYS	VAL	LYS	GLY	ASN	VAL	PHE	LYS	ASN	LYS	VAL	LEU	MET	GLU	ASN	ILE	HIS	LYS	THR	LYS	ALA	E148	R151	E152	K153	D157	R162	R170	E171	R172	K173	F174	A175	R176	R177	K178	K179	ARG	LEU	ALA	GLN	GLY	PRO	PRO	GLY	GLY	GLU	LYS	PRO	VAL	GLN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

PRO	ALA	ALA	PRO	ALA	ALA	ALA	ALA	PRO	GLY	ALA	GLN	PRO	ALA	GLN	GLY	SER	LYS	LYS	SER	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	335806	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30.2	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.439	Depositor
Minimum map value	-0.205	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0316	Depositor
Map size (Å)	448.19998, 448.19998, 448.19998	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4AC, MG, 6MZ, OMC, UY1, A2M, OMG, K, MA6, PSU, IAS, ZN, OMU

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	0.30	0/25401	0.69	0/39567
2	D	0.25	0/239	0.69	0/302
3	E	0.24	0/1645	0.47	0/2228
4	F	0.24	0/1790	0.50	0/2402
5	G	0.25	0/2124	0.52	0/2849
6	H	0.24	0/1547	0.50	0/2081
7	I	0.25	0/1516	0.55	0/2026
8	J	0.27	0/1189	0.53	0/1591
9	K	0.23	0/348	0.47	0/466
10	L	0.25	0/649	0.47	0/871
11	M	0.25	0/1119	0.52	0/1487
12	N	0.25	0/810	0.56	0/1081
13	O	0.25	0/1743	0.48	0/2350
14	P	0.25	0/1930	0.54	0/2567
15	Q	0.24	0/1555	0.54	0/2078
16	R	0.24	0/1220	0.49	0/1639
17	S	0.24	0/1002	0.57	0/1339
18	U	0.25	0/1045	0.52	0/1385
19	V	0.24	0/549	0.48	0/737
20	W	0.24	0/387	0.57	0/508
21	T	0.26	0/1033	0.49	0/1388
22	X	0.23	0/276	0.57	0/358
All	All	0.28	0/49117	0.62	0/71300

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	23760	11982	11987	66	0
2	D	238	289	289	2	0
3	E	1609	1621	1620	6	0
4	F	1760	1810	1809	8	0
5	G	2084	2180	2185	16	0
6	H	1521	1582	1581	9	0
7	I	1493	1539	1537	6	0
8	J	1164	1217	1214	5	0
9	K	346	350	349	5	0
10	L	640	617	617	7	0
11	M	1100	1167	1165	4	0
12	N	797	831	830	7	0
13	O	1706	1809	1806	7	0
14	P	1906	2028	2028	7	0
15	Q	1529	1601	1600	4	0
16	R	1195	1285	1282	2	0
17	S	999	1032	1029	4	0
18	U	1030	1106	1105	2	0
19	V	540	558	555	1	0
20	W	383	411	409	3	0
21	T	1015	1047	1046	7	0
22	X	275	295	294	1	0
23	2	19	0	0	0	0
24	2	59	0	0	0	0
24	P	1	0	0	0	0
25	N	1	0	0	0	0
26	2	462	0	0	16	0
26	D	2	0	0	0	0
26	F	3	0	0	0	0
26	G	6	0	0	0	0
26	I	5	0	0	1	0
26	J	23	0	0	1	0
26	L	2	0	0	0	0
26	M	14	0	0	0	0
26	N	14	0	0	0	0
26	O	3	0	0	0	0
26	P	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	Q	12	0	0	0	0
26	R	5	0	0	0	0
26	S	5	0	0	0	0
26	T	7	0	0	0	0
26	V	2	0	0	1	0
26	W	2	0	0	2	0
All	All	47740	36357	36337	148	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.

All (148) 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)
1:2:945:G:OP2	26:2:2001:HOH:O	1.92	0.87
5:G:208:VAL:HG21	5:G:225:VAL:HG21	1.60	0.84
1:2:1060:C:HO2'	4:F:202:SER:HG	1.13	0.83
1:2:1037:C:HO2'	21:T:2:VAL:N	1.78	0.82
1:2:9:U:OP2	26:2:2002:HOH:O	2.00	0.80
13:O:237:THR:OG1	13:O:239:ASP:OD1	2.00	0.79
4:F:82:ARG:NH2	4:F:191:GLU:OE2	2.16	0.78
1:2:1298:G:N7	26:2:2011:HOH:O	2.17	0.77
11:M:108:GLY:O	11:M:118:ARG:NH1	2.23	0.72
1:2:792:U:OP1	5:G:106:LYS:NZ	2.20	0.71
6:H:20:GLU:OE1	6:H:20:GLU:N	2.24	0.71
8:J:129:CYS:O	26:J:201:HOH:O	2.07	0.71
4:F:72:ASP:OD1	17:S:127:ARG:NH1	2.24	0.70
1:2:610:G:OP1	26:2:2004:HOH:O	2.09	0.69
19:V:71:GLY:O	26:V:101:HOH:O	2.10	0.68
1:2:871:G:H1	1:2:963:U:H3	1.43	0.67
14:P:230:GLU:N	14:P:230:GLU:OE1	2.27	0.67
1:2:344:U:OP2	26:2:2006:HOH:O	2.13	0.66
1:2:820:G:N7	22:X:170:ARG:NH2	2.44	0.66
1:2:450:A:OP1	26:2:2005:HOH:O	2.12	0.66
18:U:99:ASP:OD1	18:U:100:THR:N	2.28	0.65
1:2:1801:G:OP2	26:2:2009:HOH:O	2.15	0.65
1:2:1793:U:OP1	17:S:149:ARG:NH1	2.30	0.65
5:G:212:ASP:OD1	5:G:213:SER:N	2.29	0.64
4:F:175:GLN:NE2	4:F:196:GLU:OE1	2.32	0.62
6:H:7:LYS:NZ	6:H:41:LEU:O	2.32	0.62
5:G:141:THR:OG1	5:G:143:ASP:OD1	2.06	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:211:G:O6	1:2:252:U:O2'	2.15	0.60
9:K:87:GLU:N	9:K:87:GLU:OE1	2.34	0.60
1:2:365:C:OP1	26:2:2010:HOH:O	2.16	0.60
21:T:29:PRO:HB2	21:T:58:VAL:HG11	1.84	0.59
9:K:79:GLU:N	9:K:79:GLU:OE1	2.36	0.58
1:2:1660:G:O6	26:2:2008:HOH:O	2.14	0.58
1:2:333:G:OP1	7:I:100:SER:OG	2.21	0.58
1:2:615:U:OP2	11:M:3:LYS:NZ	2.36	0.58
5:G:19:MET:SD	5:G:108:ARG:NE	2.77	0.57
1:2:807:G:O2'	6:H:107:ARG:NE	2.34	0.57
1:2:1298:G:O6	26:2:2007:HOH:O	2.14	0.57
26:2:2021:HOH:O	12:N:89:ARG:NH2	2.37	0.56
5:G:100:ARG:HB2	5:G:114:LEU:HD11	1.87	0.56
5:G:32:SER:OG	5:G:81:THR:OG1	2.21	0.55
20:W:10:ARG:NH2	26:W:101:HOH:O	2.39	0.55
1:2:370:A:OP1	1:2:762:PSU:O2'	2.18	0.55
1:2:265:A:OP1	7:I:46:ARG:NH1	2.41	0.54
1:2:506:G:H5'	20:W:45:VAL:HG11	1.89	0.54
6:H:15:GLU:OE1	6:H:15:GLU:N	2.41	0.54
10:L:22:ARG:NH2	21:T:19:LYS:O	2.41	0.54
10:L:1:MET:O	10:L:9:MET:N	2.39	0.53
13:O:256:ASP:OD1	13:O:257:ILE:HD12	2.08	0.53
1:2:465:G:OP1	15:Q:2:VAL:N	2.42	0.52
7:I:4:SER:OG	7:I:6:ASP:OD1	2.22	0.52
1:2:889:U:O2'	17:S:134:ILE:O	2.26	0.52
7:I:194:ASP:OD2	26:I:301:HOH:O	2.19	0.52
5:G:139:LEU:HD12	5:G:139:LEU:O	2.10	0.52
1:2:24:U:OP1	15:Q:12:LYS:NZ	2.31	0.51
1:2:542:G:OP2	1:2:542:G:N2	2.34	0.51
5:G:208:VAL:HG21	5:G:225:VAL:CG2	2.36	0.51
5:G:197:ASN:OD1	5:G:198:ARG:N	2.44	0.50
6:H:146:ASP:OD1	6:H:147:GLY:N	2.45	0.50
1:2:756:A:OP1	5:G:187:ARG:NH1	2.45	0.50
18:U:82:GLU:OE1	18:U:82:GLU:N	2.44	0.49
3:E:28:THR:HG22	3:E:29:LYS:N	2.28	0.49
1:2:452:C:OP2	5:G:49:ARG:NH1	2.36	0.48
2:D:16:LYS:O	2:D:20:MET:N	2.43	0.48
1:2:8:U:OP1	26:2:2002:HOH:O	2.20	0.48
3:E:67:VAL:HG11	3:E:186:MET:HB2	1.95	0.48
13:O:55:VAL:HG21	13:O:78:ILE:HG23	1.95	0.47
1:2:857:U:O4	1:2:858:A:N6	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:P:7:ASN:ND2	14:P:10:THR:OG1	2.48	0.47
3:E:38:TYR:OH	10:L:65:ASP:OD2	2.26	0.47
13:O:64:GLU:N	13:O:64:GLU:OE1	2.48	0.47
10:L:16:LYS:NZ	13:O:242:LYS:O	2.36	0.47
1:2:983:G:H4'	1:2:1784:A:H4'	1.96	0.46
8:J:113:SER:HG	8:J:115:CYS:HG	1.64	0.46
5:G:182:MET:HB2	5:G:228:LEU:HD11	1.97	0.46
11:M:97:ASP:OD1	11:M:98:GLU:N	2.48	0.46
5:G:139:LEU:HD12	5:G:139:LEU:C	2.36	0.46
6:H:52:ILE:HD12	6:H:62:VAL:HG21	1.97	0.46
7:I:92:VAL:O	7:I:95:GLN:NE2	2.49	0.46
1:2:254:A:N3	26:2:2032:HOH:O	2.35	0.46
7:I:29:LEU:C	7:I:29:LEU:HD12	2.36	0.46
6:H:19:HIS:O	6:H:22:SER:OG	2.24	0.46
21:T:105:THR:O	21:T:105:THR:HG23	2.16	0.45
14:P:3:PHE:N	14:P:16:LEU:O	2.50	0.45
1:2:185:G:N2	1:2:196:G:O6	2.50	0.45
3:E:114:GLN:NE2	3:E:116:SER:OG	2.49	0.45
14:P:127:THR:HG22	14:P:127:THR:O	2.17	0.45
21:T:55:ASP:OD1	21:T:59:GLY:N	2.46	0.44
1:2:970:A:OP2	16:R:124:ARG:NH2	2.41	0.44
1:2:1025:C:O2'	1:2:1128:A:N1	2.45	0.44
12:N:60:GLU:OE1	12:N:60:GLU:N	2.42	0.44
10:L:38:HIS:CE1	10:L:50:THR:HG23	2.52	0.44
1:2:67:G:O2'	1:2:69:A:OP1	2.23	0.43
10:L:30:ALA:O	10:L:59:ARG:NH1	2.49	0.43
15:Q:163:THR:HG22	15:Q:163:THR:O	2.19	0.43
1:2:581:OMU:O2	26:2:2012:HOH:O	2.20	0.43
1:2:105:A:O2'	26:2:2003:HOH:O	2.07	0.43
1:2:933:A:H2'	4:F:114:VAL:HG11	2.01	0.43
1:2:992:U:H2'	1:2:993:C:O4'	2.19	0.43
13:O:256:ASP:OD1	13:O:256:ASP:N	2.51	0.43
21:T:58:VAL:HG12	21:T:58:VAL:O	2.18	0.43
8:J:113:SER:OG	8:J:115:CYS:SG	2.75	0.43
1:2:15:U:H2'	1:2:16:G:O4'	2.19	0.42
3:E:28:THR:HG22	3:E:29:LYS:H	1.84	0.42
4:F:104:ASP:OD1	4:F:105:PHE:N	2.51	0.42
1:2:69:A:N7	14:P:176:LYS:NZ	2.66	0.42
12:N:21:ILE:HD12	12:N:21:ILE:C	2.39	0.42
20:W:43:ARG:NH1	26:W:102:HOH:O	2.51	0.42
1:2:385:C:O2'	1:2:759:A:N1	2.45	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:807:G:OP2	1:2:807:G:N2	2.45	0.42
16:R:87:ASP:N	16:R:87:ASP:OD1	2.51	0.42
1:2:572:C:H41	11:M:66:ARG:NH2	2.16	0.42
10:L:40:ASP:OD1	10:L:42:SER:N	2.51	0.42
1:2:1030:A:OP1	1:2:1797:G:O2'	2.28	0.42
1:2:1091:A:O3'	12:N:89:ARG:NH2	2.53	0.42
12:N:36:ILE:HD12	12:N:36:ILE:N	2.35	0.42
4:F:70:LEU:HD22	4:F:82:ARG:HD2	2.01	0.42
8:J:48:GLU:OE1	8:J:48:GLU:N	2.46	0.42
1:2:394:G:N3	1:2:394:G:H5''	2.35	0.42
1:2:1007:U:H3'	1:2:1008:A:H5''	2.02	0.42
1:2:1145:A:OP1	12:N:2:THR:N	2.53	0.42
1:2:164:C:O2	14:P:135:ARG:NH1	2.51	0.41
1:2:516:U:H2'	1:2:517:G:C8	2.55	0.41
6:H:50:THR:HG22	6:H:51:GLN:N	2.36	0.41
1:2:79:A:O2'	14:P:178:PRO:O	2.30	0.41
1:2:1128:A:OP1	2:D:18:ARG:NH1	2.51	0.41
1:2:96:G:HO2'	1:2:464:A:HO2'	1.52	0.41
1:2:642:U:OP1	6:H:119:LEU:N	2.47	0.41
9:K:82:MET:SD	9:K:82:MET:N	2.93	0.41
13:O:188:GLY:N	13:O:206:ASP:OD1	2.42	0.41
1:2:520:U:H2'	1:2:521:A:O4'	2.19	0.41
5:G:21:ASP:OD1	5:G:21:ASP:N	2.49	0.41
1:2:17:C:H2'	1:2:18:C:C6	2.56	0.41
1:2:871:G:OP2	26:2:2016:HOH:O	2.22	0.41
8:J:36:PHE:CE2	8:J:50:THR:HG23	2.56	0.41
1:2:616:G:H4'	1:2:617:C:OP1	2.20	0.41
1:2:1110:G:O2'	1:2:1111:G:H5'	2.21	0.41
3:E:27:GLY:O	3:E:47:ILE:HG23	2.21	0.41
9:K:101:GLU:OE1	9:K:101:GLU:N	2.49	0.41
1:2:463:G:O2'	1:2:464:A:OP1	2.34	0.40
9:K:88:GLU:OE2	9:K:92:LYS:NZ	2.36	0.40
21:T:81:VAL:HG21	21:T:125:VAL:CG2	2.50	0.40
1:2:478:A:OP1	15:Q:147:SER:OG	2.20	0.40
12:N:22:ARG:NH2	17:S:144:GLY:O	2.55	0.40
1:2:17:C:O2'	1:2:1140:A:N1	2.44	0.40
5:G:176:ASP:OD1	5:G:177:VAL:N	2.52	0.40
1:2:67:G:H2'	1:2:69:A:O5'	2.22	0.40
4:F:54:THR:O	4:F:54:THR:HG22	2.21	0.40

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	D	23/25 (92%)	23 (100%)	0	0	100	100
3	E	200/296 (68%)	199 (100%)	1 (0%)	0	100	100
4	F	213/260 (82%)	212 (100%)	1 (0%)	0	100	100
5	G	259/264 (98%)	258 (100%)	1 (0%)	0	100	100
6	H	185/191 (97%)	182 (98%)	3 (2%)	0	100	100
7	I	180/220 (82%)	179 (99%)	1 (1%)	0	100	100
8	J	145/159 (91%)	144 (99%)	1 (1%)	0	100	100
9	K	42/144 (29%)	39 (93%)	3 (7%)	0	100	100
10	L	80/82 (98%)	80 (100%)	0	0	100	100
11	M	139/142 (98%)	138 (99%)	1 (1%)	0	100	100
12	N	96/127 (76%)	95 (99%)	1 (1%)	0	100	100
13	O	218/280 (78%)	218 (100%)	0	0	100	100
14	P	235/249 (94%)	231 (98%)	4 (2%)	0	100	100
15	Q	182/197 (92%)	182 (100%)	0	0	100	100
16	R	148/151 (98%)	147 (99%)	1 (1%)	0	100	100
17	S	128/150 (85%)	127 (99%)	1 (1%)	0	100	100
18	U	124/133 (93%)	121 (98%)	3 (2%)	0	100	100
19	V	62/86 (72%)	61 (98%)	1 (2%)	0	100	100
20	W	44/62 (71%)	43 (98%)	1 (2%)	0	100	100
21	T	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
22	X	30/213 (14%)	30 (100%)	0	0	100	100
All	All	2860/3561 (80%)	2834 (99%)	26 (1%)	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	
2	D	24/24 (100%)	24 (100%)	0	100	100
3	E	170/229 (74%)	170 (100%)	0	100	100
4	F	196/229 (86%)	195 (100%)	1 (0%)	86	94
5	G	226/228 (99%)	225 (100%)	1 (0%)	89	96
6	H	168/171 (98%)	168 (100%)	0	100	100
7	I	158/181 (87%)	158 (100%)	0	100	100
8	J	125/132 (95%)	123 (98%)	2 (2%)	58	79
9	K	40/123 (32%)	40 (100%)	0	100	100
10	L	68/68 (100%)	68 (100%)	0	100	100
11	M	113/114 (99%)	112 (99%)	1 (1%)	75	89
12	N	87/109 (80%)	87 (100%)	0	100	100
13	O	185/222 (83%)	183 (99%)	2 (1%)	70	86
14	P	206/214 (96%)	206 (100%)	0	100	100
15	Q	162/170 (95%)	162 (100%)	0	100	100
16	R	130/131 (99%)	130 (100%)	0	100	100
17	S	103/120 (86%)	102 (99%)	1 (1%)	73	87
18	U	109/114 (96%)	109 (100%)	0	100	100
19	V	63/78 (81%)	63 (100%)	0	100	100
20	W	39/49 (80%)	39 (100%)	0	100	100
21	T	108/109 (99%)	108 (100%)	0	100	100
22	X	27/179 (15%)	27 (100%)	0	100	100
All	All	2507/2994 (84%)	2499 (100%)	8 (0%)	90	96

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	F	47	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	G	130	GLN
8	J	68	ARG
8	J	139	ASN
11	M	104	PHE
13	O	57	ASP
13	O	221	PHE
17	S	33	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	E	114	GLN
11	M	60	GLN
14	P	7	ASN
15	Q	92	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1091/1807 (60%)	127 (11%)	0

All (127) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	8	U
1	2	25	C
1	2	26	A
1	2	34	G
1	2	42	G
1	2	45	U
1	2	47	A
1	2	59	G
1	2	68	A
1	2	105	A
1	2	112	U
1	2	115	A
1	2	128	G
1	2	139	U
1	2	151	A
1	2	158	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	164	C
1	2	252	U
1	2	253	C
1	2	260	A
1	2	263	C
1	2	275	C
1	2	279	C
1	2	303	A
1	2	318	C
1	2	320	A
1	2	324	U
1	2	341	G
1	2	342	C
1	2	365	C
1	2	384	U
1	2	394	G
1	2	404	A
1	2	405	A
1	2	406	C
1	2	408	G
1	2	420	A
1	2	421	A
1	2	427	G
1	2	428	C
1	2	430	G
1	2	438	G
1	2	443	U
1	2	448	C
1	2	449	A
1	2	452	C
1	2	472	A
1	2	481	A
1	2	507	U
1	2	509	A
1	2	510	U
1	2	513	G
1	2	518	A
1	2	522	C
1	2	537	A
1	2	545	U
1	2	552	G
1	2	574	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	581	OMU
1	2	582	A
1	2	585	U
1	2	586	C
1	2	597	A
1	2	609	A
1	2	614	OMU
1	2	622	A2M
1	2	623	A
1	2	625	A
1	2	626	A
1	2	627	G
1	2	641	U
1	2	642	U
1	2	757	A
1	2	758	G
1	2	759	A
1	2	770	C
1	2	782	C
1	2	785	C
1	2	786	G
1	2	789	C
1	2	790	U
1	2	793	A
1	2	816	A
1	2	817	U
1	2	818	A
1	2	823	U
1	2	859	A
1	2	862	A
1	2	865	A
1	2	866	A
1	2	879	G
1	2	901	A
1	2	936	A
1	2	938	U
1	2	963	U
1	2	969	A
1	2	973	A
1	2	974	A
1	2	1007	U
1	2	1008	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	1029	A
1	2	1031	C
1	2	1057	U
1	2	1059	G
1	2	1060	C
1	2	1061	U
1	2	1085	U
1	2	1092	U
1	2	1095	A
1	2	1100	U
1	2	1141	A
1	2	1663	U
1	2	1664	G
1	2	1763	A
1	2	1765	G
1	2	1768	G
1	2	1770	A
1	2	1774	A
1	2	1777	U
1	2	1788	G
1	2	1800	G
1	2	1801	G
1	2	1802	A
1	2	1803	U
1	2	1804	C
1	2	1807	U
1	2	1808	G

There are no RNA pucker outliers to report.

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

51 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	PSU	2	753	1	18,21,22	0.50	0	22,30,33	0.58	0
1	OMU	2	614	1,23	19,22,23	0.29	0	26,31,34	0.38	0
1	A2M	2	544	1	18,25,26	0.66	0	18,36,39	0.78	1 (5%)
1	A2M	2	622	1,24	18,25,26	0.66	0	18,36,39	0.77	1 (5%)
1	PSU	2	121	1	18,21,22	0.46	0	22,30,33	0.56	0
1	A2M	2	977	1	18,25,26	0.67	0	18,36,39	0.78	1 (5%)
1	PSU	2	1002	1	18,21,22	0.48	0	22,30,33	0.54	0
1	PSU	2	1106	1	18,21,22	0.48	0	22,30,33	0.55	0
1	PSU	2	950	1	18,21,22	0.50	0	22,30,33	0.56	0
1	UY1	2	603	1	19,22,23	0.46	0	22,31,34	0.59	0
1	PSU	2	1120	1	18,21,22	0.48	0	22,30,33	0.56	0
1	PSU	2	300	1	18,21,22	0.49	0	22,30,33	0.54	0
1	6MZ	2	1771	1,23,24	18,25,26	0.73	0	16,36,39	0.74	1 (6%)
1	OMU	2	581	1	19,22,23	0.24	0	26,31,34	0.44	0
1	A2M	2	440	1	18,25,26	0.67	0	18,36,39	0.71	1 (5%)
1	A2M	2	1758	1	18,25,26	0.68	0	18,36,39	0.89	1 (5%)
1	PSU	2	103	1	18,21,22	0.50	0	22,30,33	0.55	0
1	PSU	2	255	1,24	18,21,22	0.50	0	22,30,33	0.59	0
1	A2M	2	162	1	18,25,26	0.67	0	18,36,39	0.87	1 (5%)
1	PSU	2	362	1	18,21,22	0.50	0	22,30,33	0.56	0
1	OMU	2	123	1	19,22,23	0.31	0	26,31,34	0.45	0
1	MA6	2	1789	1	18,26,27	0.73	0	19,38,41	0.57	0
1	PSU	2	306	1	18,21,22	0.50	0	22,30,33	0.57	0
1	A2M	2	468	1	18,25,26	0.68	0	18,36,39	0.85	1 (5%)
1	PSU	2	451	1,23	18,21,22	0.54	0	22,30,33	0.54	0
1	OMC	2	473	1	19,22,23	0.30	0	26,31,34	0.52	0
1	PSU	2	383	1,24	18,21,22	0.48	0	22,30,33	0.56	0
1	PSU	2	949	1	18,21,22	0.52	0	22,30,33	0.53	0
1	PSU	2	1027	1	18,21,22	0.56	0	22,30,33	0.65	1 (4%)
1	OMG	2	246	1	18,26,27	0.94	1 (5%)	19,38,41	0.64	0
1	PSU	2	912	1	18,21,22	0.49	0	22,30,33	0.57	0
1	PSU	2	635	1	18,21,22	0.54	0	22,30,33	0.56	0
1	MA6	2	1790	1	18,26,27	0.75	0	19,38,41	0.58	0
1	OMC	2	38	1	19,22,23	0.30	0	26,31,34	0.50	0
1	PSU	2	809	1	18,21,22	0.51	0	22,30,33	0.56	0
1	PSU	2	208	1	18,21,22	0.47	0	22,30,33	0.57	0
1	A2M	2	28	1,24	18,25,26	0.67	0	18,36,39	0.79	1 (5%)
1	PSU	2	258	1	18,21,22	0.49	0	22,30,33	0.56	0
1	PSU	2	605	1	18,21,22	0.49	0	22,30,33	0.58	0
1	OMG	2	598	1	18,26,27	0.94	2 (11%)	19,38,41	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	2	111	1,23	18,21,22	0.47	0	22,30,33	0.56	0
1	OMU	2	1012	1	19,22,23	0.28	0	26,31,34	0.49	0
1	4AC	2	1781	1	21,24,25	0.30	0	29,34,37	0.29	0
17	IAS	S	137	17	6,7,8	1.08	0	6,8,10	1.10	0
1	OMC	2	418	1	19,22,23	0.28	0	26,31,34	0.45	0
1	PSU	2	762	1	18,21,22	0.45	0	22,30,33	0.55	0
1	OMC	2	1645	1	19,22,23	0.27	0	26,31,34	0.45	0
1	A2M	2	800	1	18,25,26	0.67	0	18,36,39	0.83	1 (5%)
1	OMC	2	140	1	19,22,23	0.29	0	26,31,34	0.46	0
1	OMG	2	392	1	18,26,27	0.94	3 (16%)	19,38,41	0.63	0
1	PSU	2	584	1	18,21,22	0.48	0	22,30,33	0.57	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	PSU	2	753	1	-	0/7/25/26	0/2/2/2
1	OMU	2	614	1,23	-	0/9/27/28	0/2/2/2
1	A2M	2	544	1	-	0/5/27/28	0/3/3/3
1	A2M	2	622	1,24	-	2/5/27/28	0/3/3/3
1	PSU	2	121	1	-	0/7/25/26	0/2/2/2
1	A2M	2	977	1	-	0/5/27/28	0/3/3/3
1	PSU	2	1002	1	-	0/7/25/26	0/2/2/2
1	PSU	2	1106	1	-	0/7/25/26	0/2/2/2
1	PSU	2	950	1	-	0/7/25/26	0/2/2/2
1	UY1	2	603	1	-	0/9/27/28	0/2/2/2
1	PSU	2	1120	1	-	0/7/25/26	0/2/2/2
1	PSU	2	300	1	-	0/7/25/26	0/2/2/2
1	6MZ	2	1771	1,23,24	-	0/5/27/28	0/3/3/3
1	OMU	2	581	1	-	1/9/27/28	0/2/2/2
1	A2M	2	440	1	-	0/5/27/28	0/3/3/3
1	A2M	2	1758	1	-	0/5/27/28	0/3/3/3
1	PSU	2	103	1	-	0/7/25/26	0/2/2/2
1	PSU	2	255	1,24	-	0/7/25/26	0/2/2/2
1	A2M	2	162	1	-	0/5/27/28	0/3/3/3
1	PSU	2	362	1	-	0/7/25/26	0/2/2/2
1	OMU	2	123	1	-	0/9/27/28	0/2/2/2
1	MA6	2	1789	1	-	0/7/29/30	0/3/3/3
1	PSU	2	306	1	-	0/7/25/26	0/2/2/2
1	A2M	2	468	1	-	1/5/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	2	451	1,23	-	0/7/25/26	0/2/2/2
1	OMC	2	473	1	-	0/9/27/28	0/2/2/2
1	PSU	2	383	1,24	-	0/7/25/26	0/2/2/2
1	PSU	2	949	1	-	0/7/25/26	0/2/2/2
1	PSU	2	1027	1	-	0/7/25/26	0/2/2/2
1	OMG	2	246	1	-	0/5/27/28	0/3/3/3
1	PSU	2	912	1	-	0/7/25/26	0/2/2/2
1	PSU	2	635	1	-	0/7/25/26	0/2/2/2
1	MA6	2	1790	1	-	2/7/29/30	0/3/3/3
1	OMC	2	38	1	-	0/9/27/28	0/2/2/2
1	PSU	2	809	1	-	0/7/25/26	0/2/2/2
1	PSU	2	208	1	-	0/7/25/26	0/2/2/2
1	A2M	2	28	1,24	-	0/5/27/28	0/3/3/3
1	PSU	2	258	1	-	0/7/25/26	0/2/2/2
1	PSU	2	605	1	-	0/7/25/26	0/2/2/2
1	OMG	2	598	1	-	1/5/27/28	0/3/3/3
1	PSU	2	111	1,23	-	0/7/25/26	0/2/2/2
1	OMU	2	1012	1	-	0/9/27/28	0/2/2/2
1	4AC	2	1781	1	-	2/11/29/30	0/2/2/2
17	IAS	S	137	17	-	1/7/7/8	-
1	OMC	2	418	1	-	0/9/27/28	0/2/2/2
1	PSU	2	762	1	-	0/7/25/26	0/2/2/2
1	OMC	2	1645	1	-	0/9/27/28	0/2/2/2
1	A2M	2	800	1	-	0/5/27/28	0/3/3/3
1	OMC	2	140	1	-	0/9/27/28	0/2/2/2
1	OMG	2	392	1	-	0/5/27/28	0/3/3/3
1	PSU	2	584	1	-	3/7/25/26	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	246	OMG	C5-C6	-2.35	1.42	1.47
1	2	598	OMG	C5-C6	-2.27	1.42	1.47
1	2	392	OMG	C5-C6	-2.21	1.42	1.47
1	2	598	OMG	C8-N7	-2.05	1.31	1.35
1	2	392	OMG	C8-N7	-2.01	1.31	1.35
1	2	392	OMG	C5-C4	-2.00	1.38	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	800	A2M	C5-C6-N6	2.38	123.97	120.35
1	2	544	A2M	C5-C6-N6	2.36	123.94	120.35
1	2	622	A2M	C5-C6-N6	2.35	123.92	120.35
1	2	440	A2M	C5-C6-N6	2.33	123.89	120.35
1	2	1758	A2M	C5-C6-N6	2.31	123.86	120.35
1	2	28	A2M	C5-C6-N6	2.30	123.85	120.35
1	2	162	A2M	C5-C6-N6	2.29	123.84	120.35
1	2	468	A2M	C5-C6-N6	2.27	123.81	120.35
1	2	1771	6MZ	C2-N1-C6	2.22	118.50	116.59
1	2	977	A2M	C5-C6-N6	2.16	123.64	120.35
1	2	1027	PSU	O4'-C1'-C2'	2.10	108.10	105.14

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	581	OMU	O4'-C4'-C5'-O5'
1	2	584	PSU	C2'-C1'-C5-C4
1	2	622	A2M	O4'-C4'-C5'-O5'
1	2	622	A2M	C3'-C4'-C5'-O5'
1	2	1790	MA6	C5-C6-N6-C9
1	2	468	A2M	O4'-C4'-C5'-O5'
1	2	598	OMG	C4'-C5'-O5'-P
1	2	1790	MA6	C4'-C5'-O5'-P
17	S	137	IAS	CA-CB-CG-OD1
1	2	584	PSU	O4'-C1'-C5-C4
1	2	584	PSU	O4'-C1'-C5-C6
1	2	1781	4AC	N3-C4-N4-C7
1	2	1781	4AC	C5-C4-N4-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	581	OMU	1	0
1	2	762	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 80 ligands modelled in this entry, 80 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

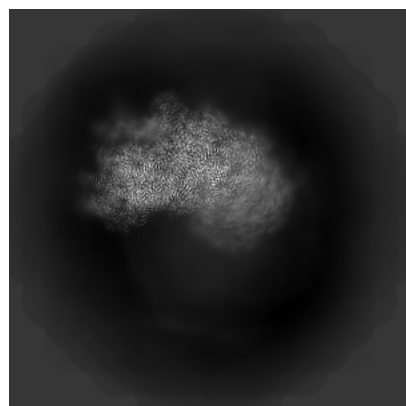
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14002. These allow visual inspection of the internal detail of the map and identification of artifacts.

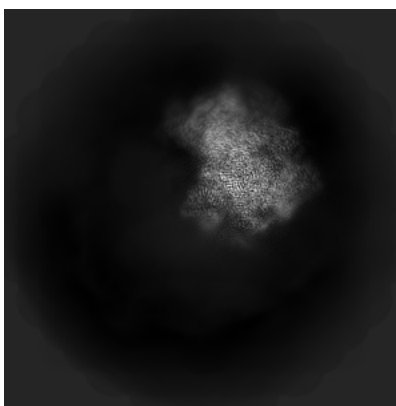
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

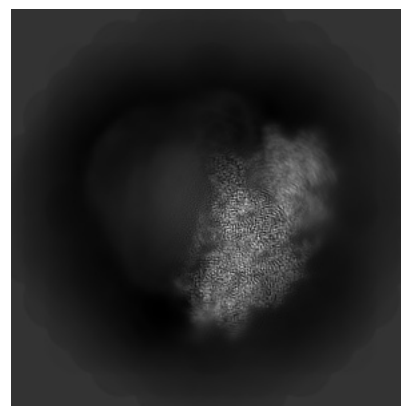
6.1.1 Primary map



X

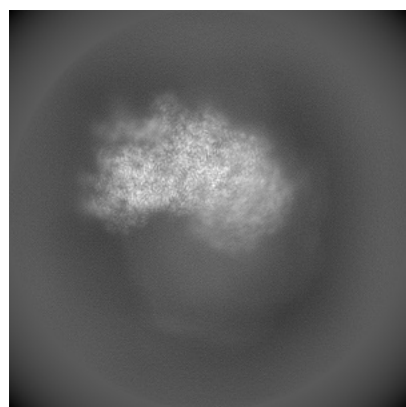


Y

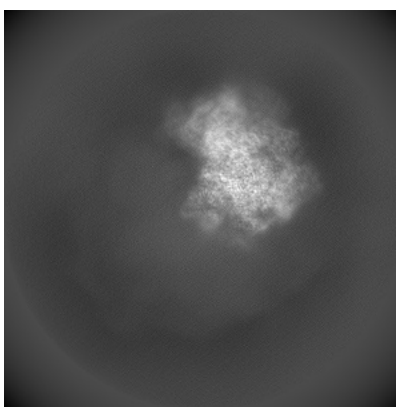


Z

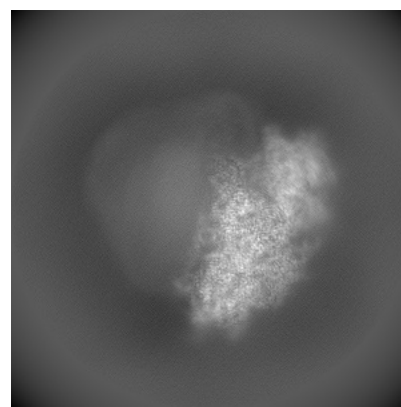
6.1.2 Raw map



X



Y



Z

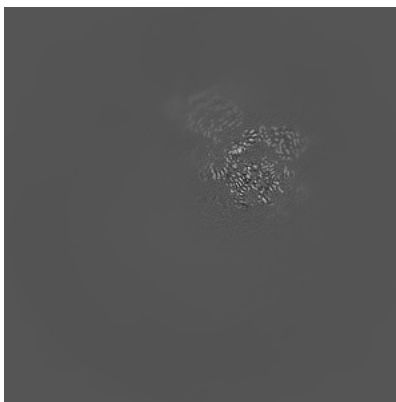
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

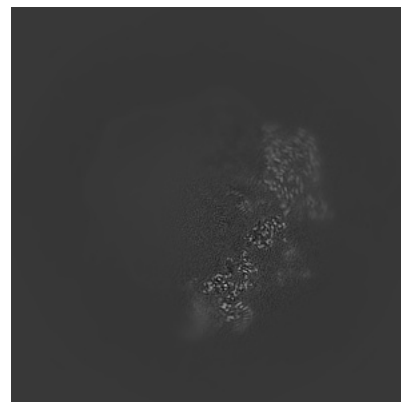
6.2.1 Primary map



X Index: 270

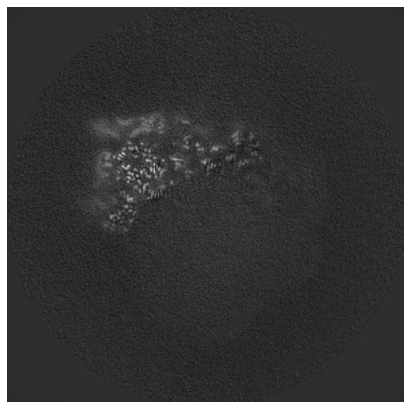


Y Index: 270

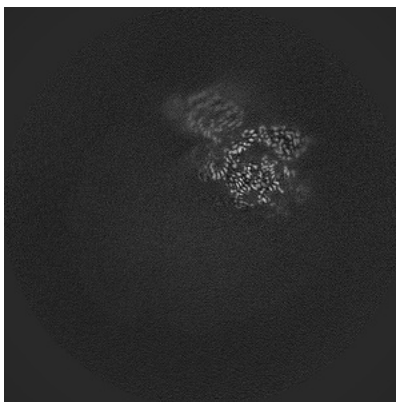


Z Index: 270

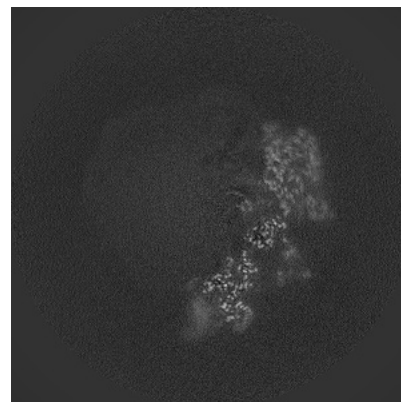
6.2.2 Raw map



X Index: 270



Y Index: 270

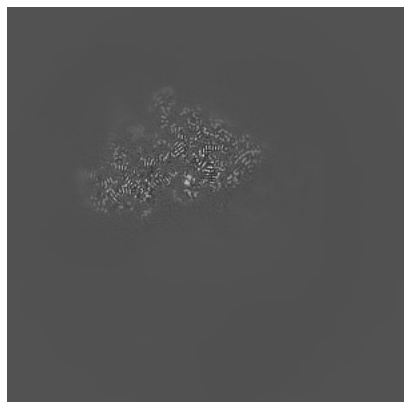


Z Index: 270

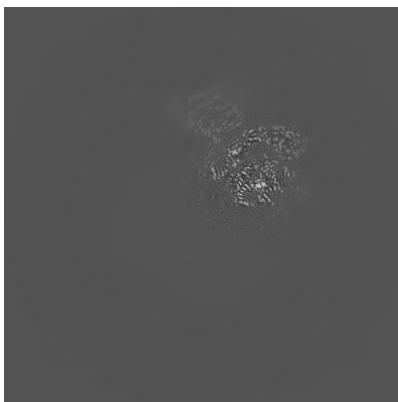
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

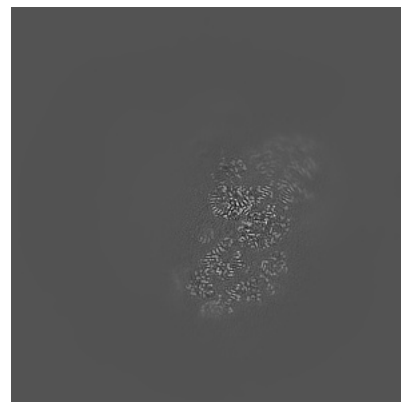
6.3.1 Primary map



X Index: 301

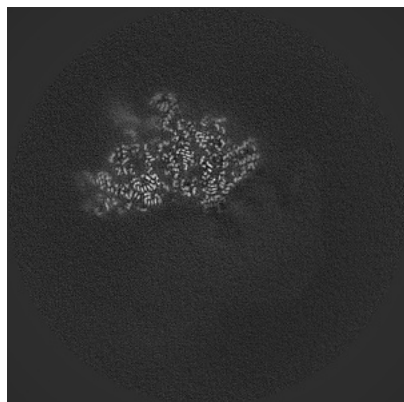


Y Index: 269

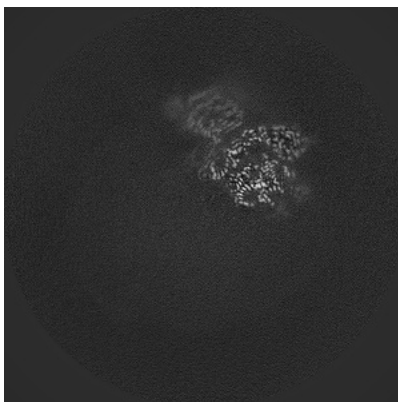


Z Index: 325

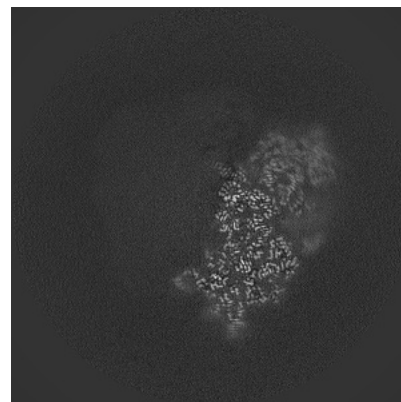
6.3.2 Raw map



X Index: 311



Y Index: 269

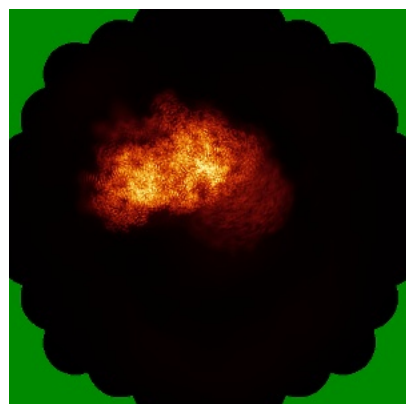


Z Index: 310

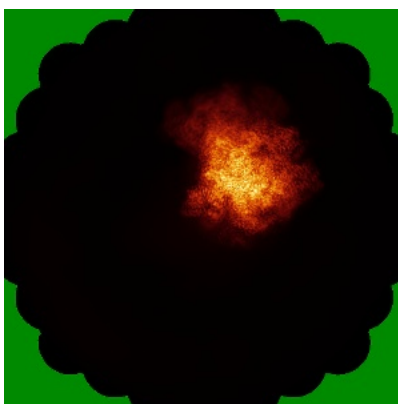
The images above show the largest variance slices of the map in three orthogonal directions.

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

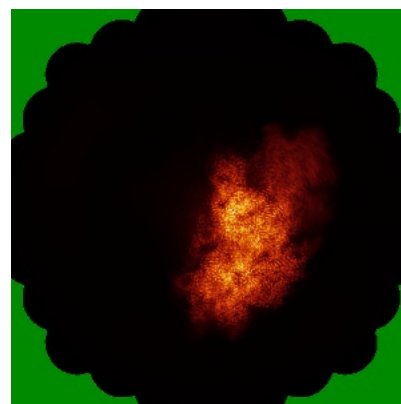
6.4.1 Primary map



X

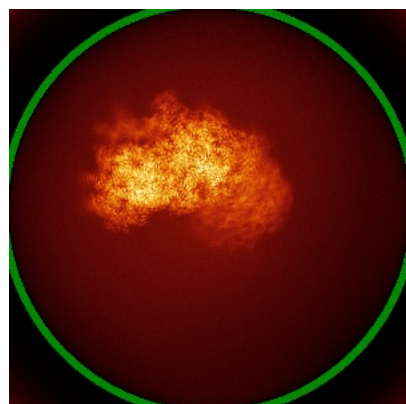


Y

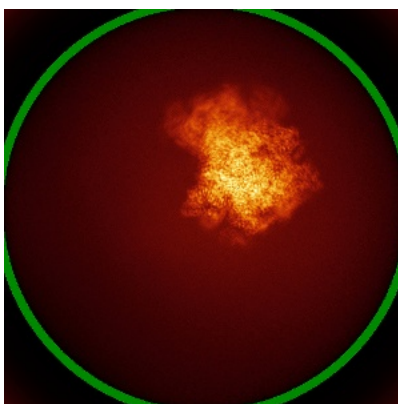


Z

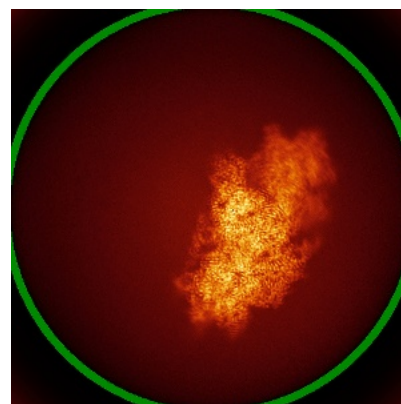
6.4.2 Raw map



X



Y

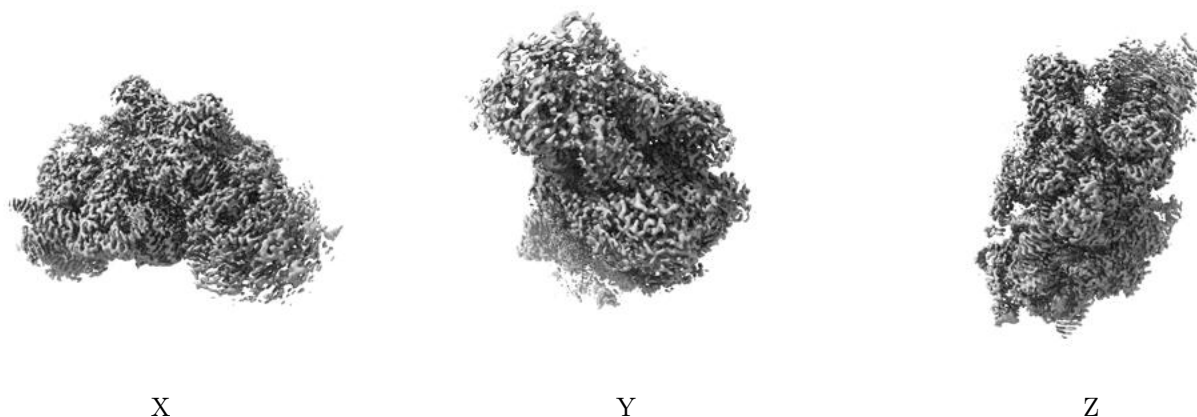


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0316. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

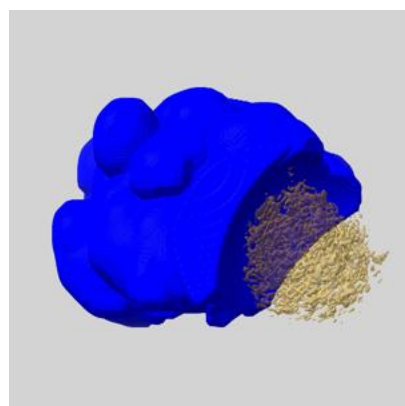
6.6 Mask visualisation [i](#)

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

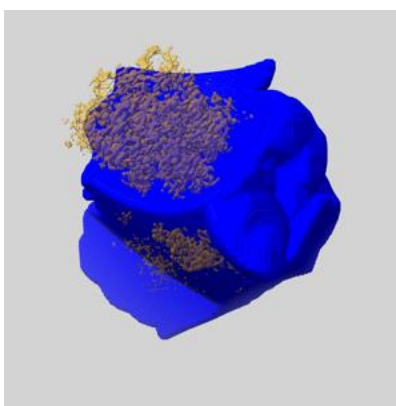
A mask typically either:

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

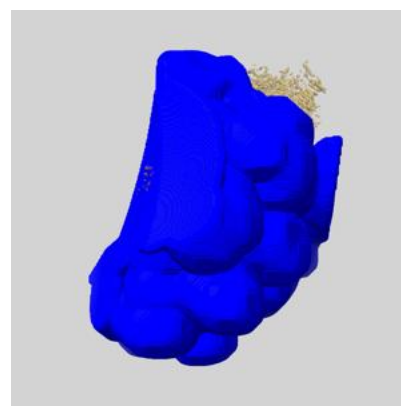
6.6.1 emd_14002_msk_1.map [i](#)



X



Y

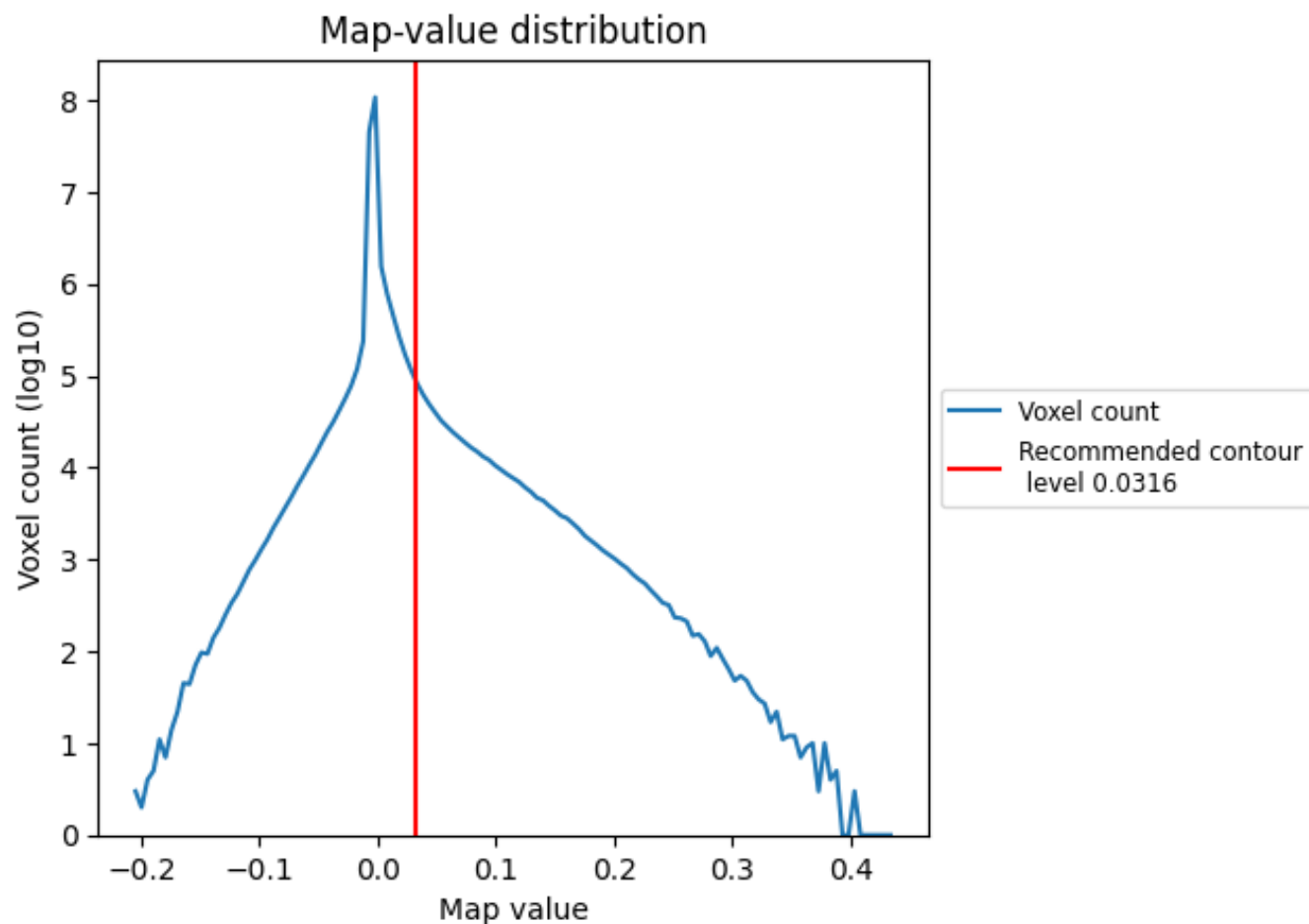


Z

7 Map analysis [i](#)

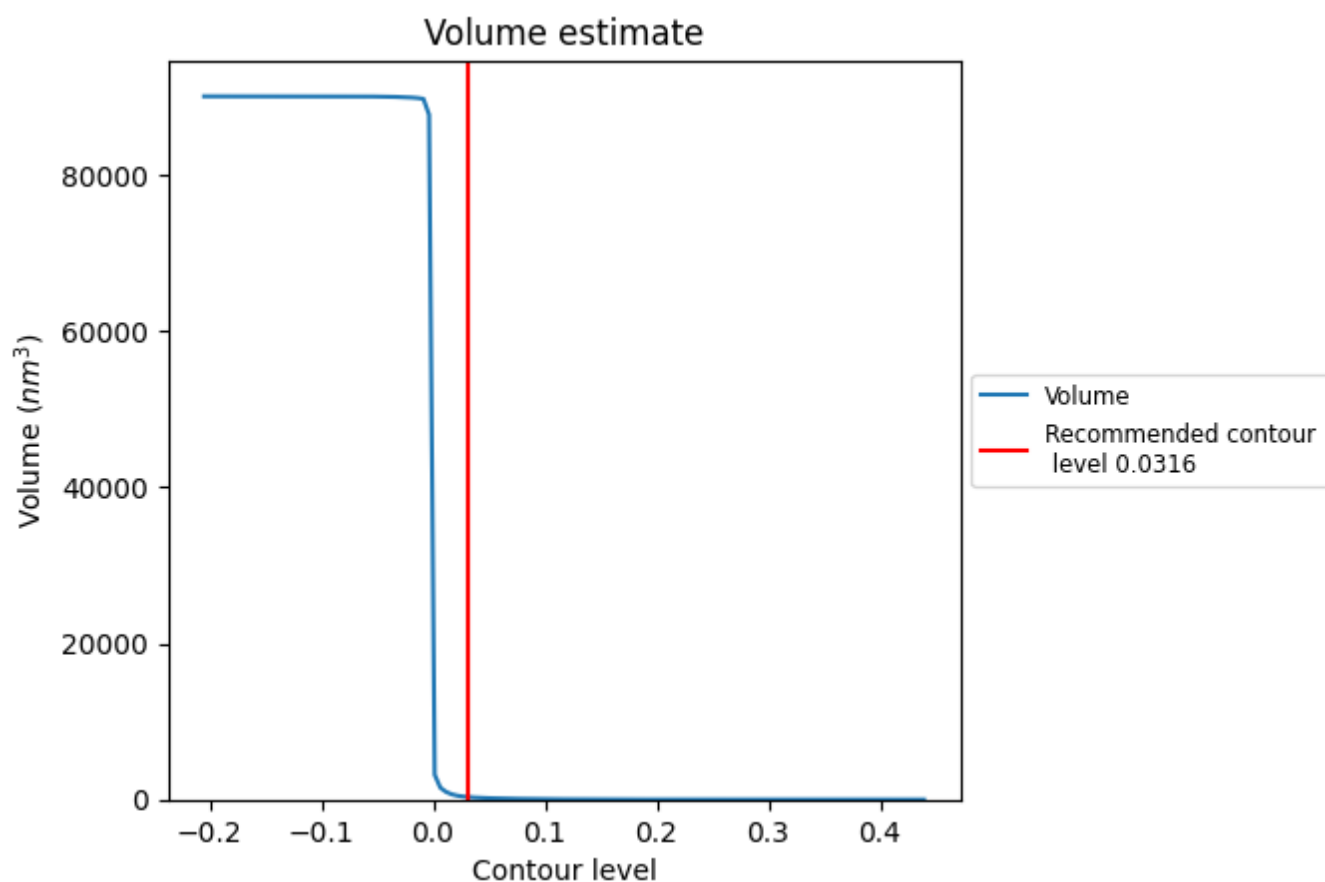
This section contains the results of statistical analysis of the map.

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.

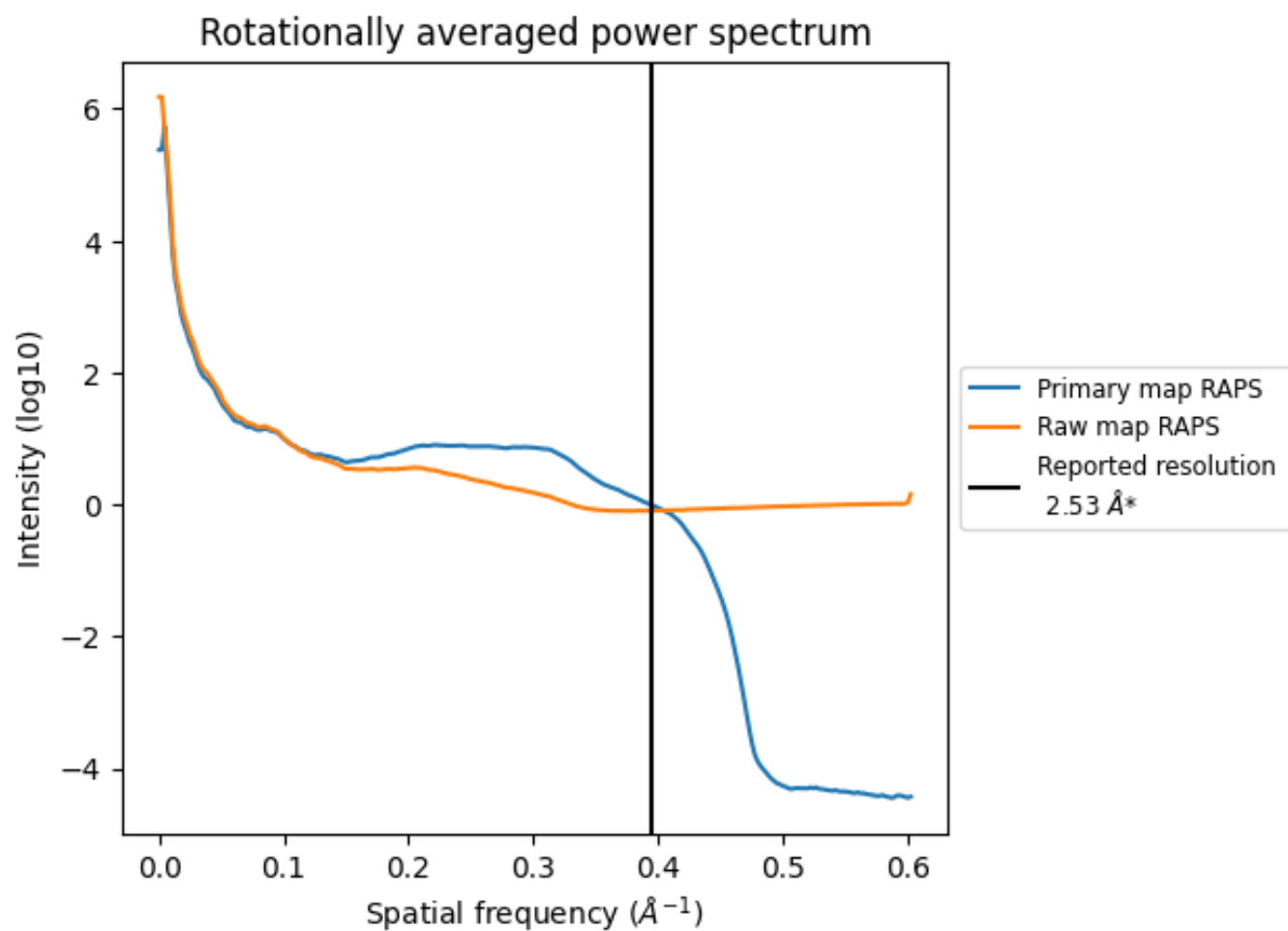
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 315 nm³; this corresponds to an approximate mass of 284 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 ⓘ

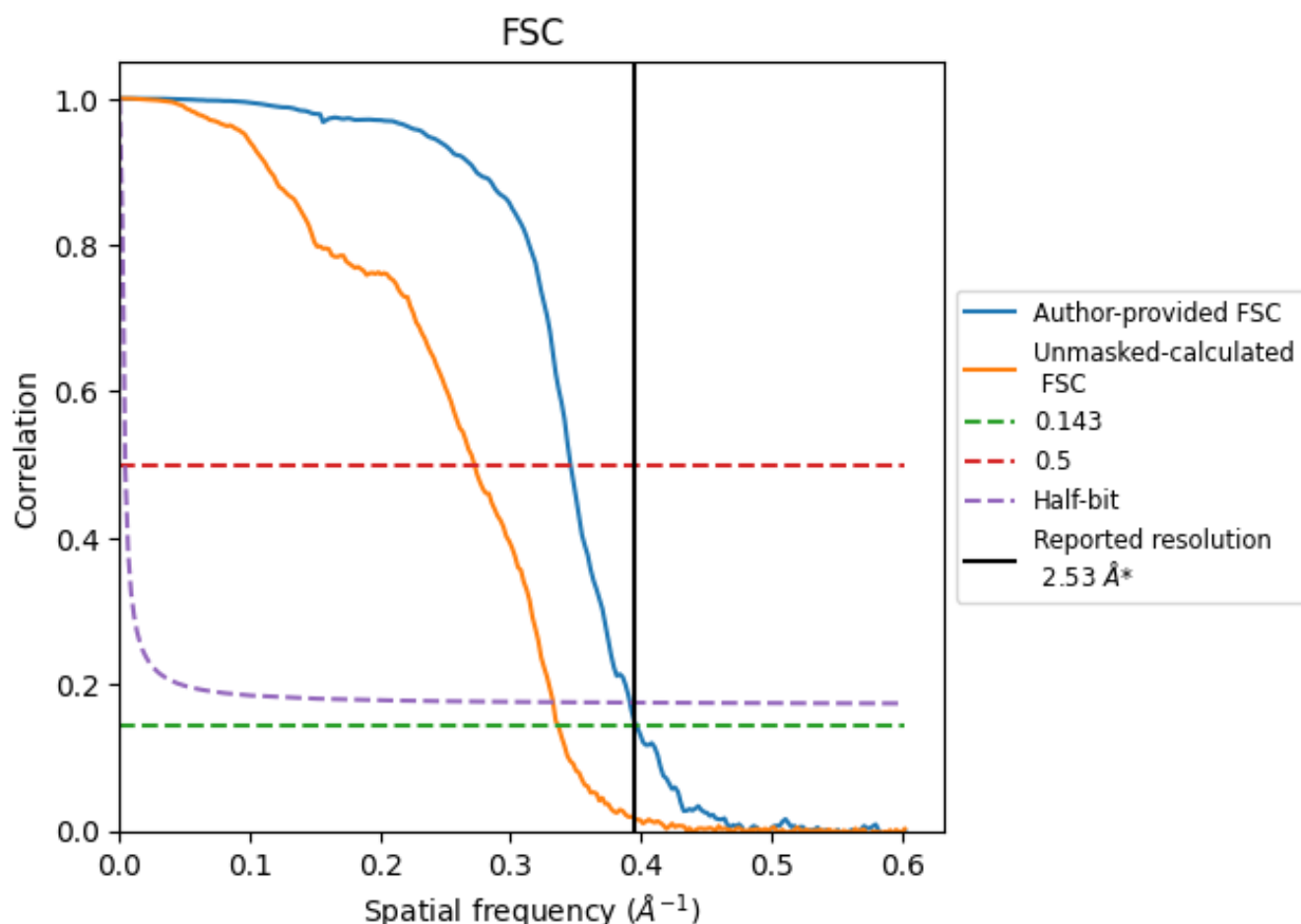


*Reported resolution corresponds to spatial frequency of 0.395 Å⁻¹

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 0.395 Å⁻¹

8.2 Resolution estimates [i](#)

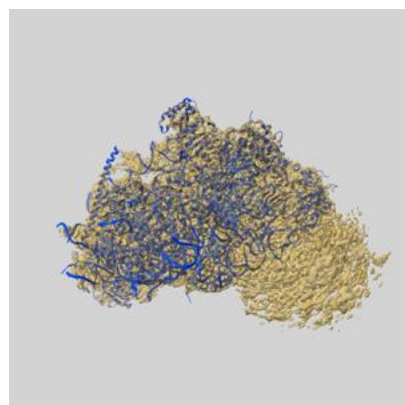
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.53	-	-
Author-provided FSC curve	2.52	2.89	2.55
Unmasked-calculated*	2.97	3.67	3.01

*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 2.97 differs from the reported value 2.53 by more than 10 %

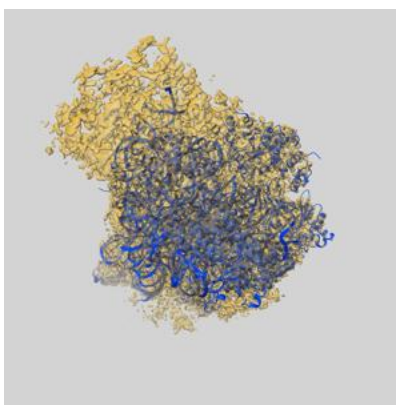
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14002 and PDB model 7QIX. Per-residue inclusion information can be found in section [3](#) on page [11](#).

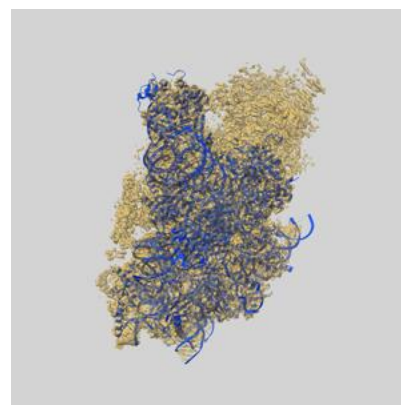
9.1 Map-model overlay [i](#)



X



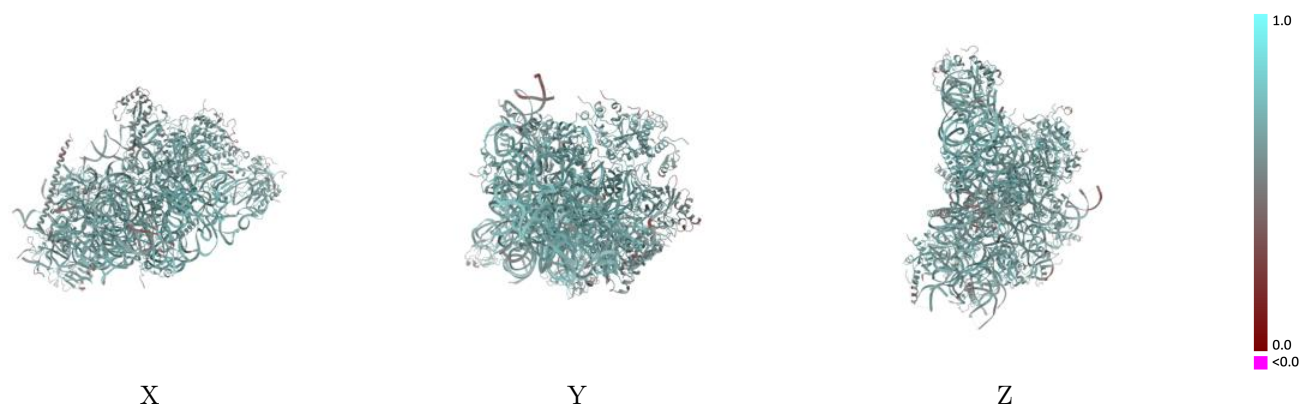
Y



Z

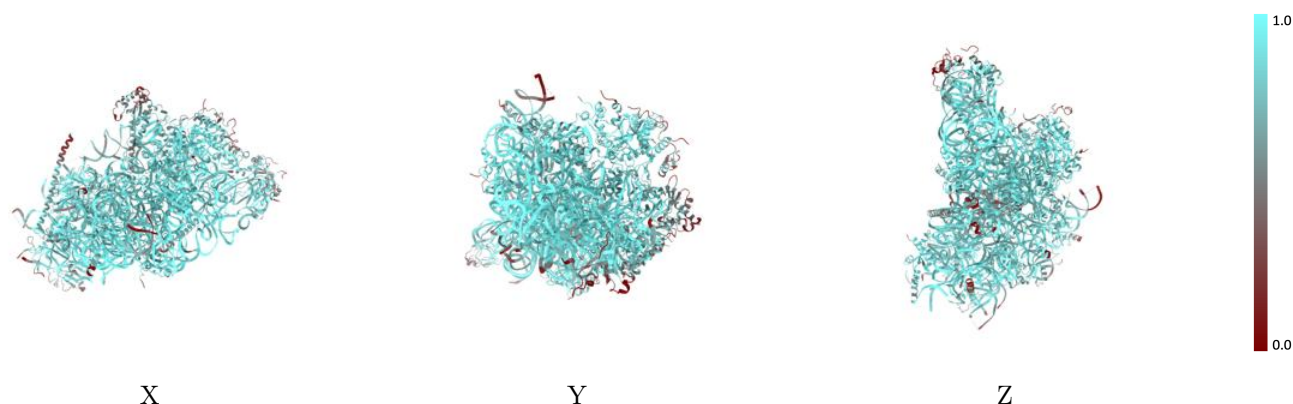
The images above show the 3D surface view of the map at the recommended contour level 0.0316 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



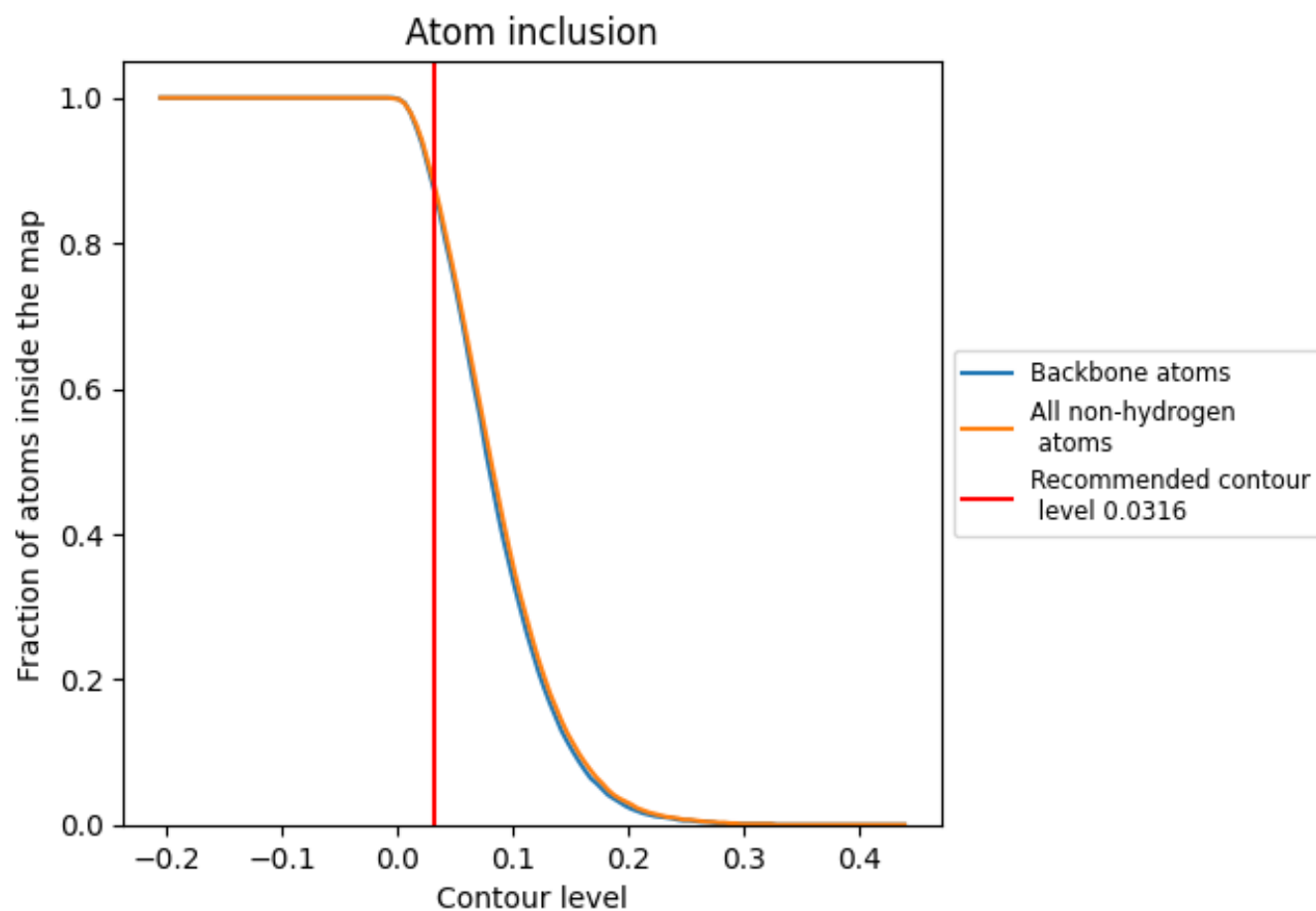
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0316).















































9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 88% 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 (0.0316) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8830	 0.6480
2	 0.9320	 0.6620
D	 0.7940	 0.6440
E	 0.8650	 0.6300
F	 0.7080	 0.6130
G	 0.9080	 0.6550
H	 0.6270	 0.5540
I	 0.9080	 0.6580
J	 0.9500	 0.6890
K	 0.4030	 0.4800
L	 0.8250	 0.6220
M	 0.9260	 0.6770
N	 0.9060	 0.6730
O	 0.9070	 0.6520
P	 0.7400	 0.5870
Q	 0.8820	 0.6400
R	 0.9050	 0.6630
S	 0.8430	 0.6470
T	 0.9650	 0.6880
U	 0.8240	 0.6210
V	 0.7790	 0.6370
W	 0.8140	 0.6130
X	 0.5170	 0.5050

