



Full wwPDB EM Validation Report ⓘ

Mar 13, 2025 – 03:51 pm GMT

PDB ID : 9G06
EMDB ID : EMD-50912
Title : Structure of 30S-IF1-IF3-mRNA-fMet-tRNA-GE81112A complex
Authors : Safdari, H.A.; Morici, M.; Wilson, D.N.
Deposited on : 2024-07-07
Resolution : 2.85 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:

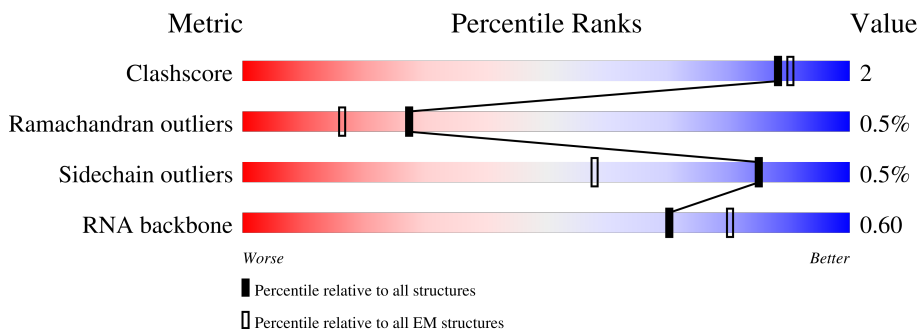
EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41

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 2.85 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	C	233	
2	D	206	
3	E	167	
4	F	135	
5	H	130	
6	I	72	
7	J	180	

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Mol	Chain	Length	Quality of chain
8	K	159	
9	L	124	
10	M	118	
11	N	101	
12	O	89	
13	P	82	
14	Q	84	
15	R	75	
16	S	92	
17	T	87	
18	U	71	
19	Y	40	
20	b	130	
21	B	1545	
22	a	73	
23	G	179	
24	c	103	

2 Entry composition i

There are 28 unique types of molecules in this entry. The entry contains 53636 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 Small ribosomal subunit protein uS3.

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

- Molecule 2 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 3 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	155	1143	712	216	209	6	0	0

- Molecule 4 is a protein called Small ribosomal subunit protein bS6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	F	100	816	515	148	148	5	0	0

- Molecule 5 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 6 is a protein called Translation initiation factor IF-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	I	70	557	350	99	105	3	0	0

- Molecule 7 is a protein called Translation initiation factor IF-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	J	102	832	524	152	152	4	0	0

- Molecule 8 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	K	117	876	540	173	160	3	0	0

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	conflict	UNP P0A7R9
K	130	GLY	-	expression tag	UNP P0A7R9
K	131	CYS	-	expression tag	UNP P0A7R9
K	132	ARG	-	expression tag	UNP P0A7R9
K	133	PRO	-	expression tag	UNP P0A7R9
K	134	PRO	-	expression tag	UNP P0A7R9
K	135	LYS	-	expression tag	UNP P0A7R9
K	136	LYS	-	expression tag	UNP P0A7R9
K	137	ARG	-	expression tag	UNP P0A7R9
K	138	ARG	-	expression tag	UNP P0A7R9
K	139	VAL	-	expression tag	UNP P0A7R9
K	140	GLY	-	expression tag	UNP P0A7R9
K	141	CYS	-	expression tag	UNP P0A7R9
K	142	ARG	-	expression tag	UNP P0A7R9
K	143	PRO	-	expression tag	UNP P0A7R9
K	144	PRO	-	expression tag	UNP P0A7R9
K	145	LYS	-	expression tag	UNP P0A7R9
K	146	LYS	-	expression tag	UNP P0A7R9
K	147	ARG	-	expression tag	UNP P0A7R9
K	148	ARG	-	expression tag	UNP P0A7R9
K	149	VAL	-	expression tag	UNP P0A7R9
K	150	GLY	-	expression tag	UNP P0A7R9
K	151	CYS	-	expression tag	UNP P0A7R9
K	152	ARG	-	expression tag	UNP P0A7R9
K	153	PRO	-	expression tag	UNP P0A7R9
K	154	PRO	-	expression tag	UNP P0A7R9
K	155	LYS	-	expression tag	UNP P0A7R9
K	156	LYS	-	expression tag	UNP P0A7R9
K	157	ARG	-	expression tag	UNP P0A7R9

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Chain	Residue	Modelled	Actual	Comment	Reference
K	158	ARG	-	expression tag	UNP P0A7R9
K	159	VAL	-	expression tag	UNP P0A7R9

- Molecule 9 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	L	121	942	582	193	162	5	0	0

- Molecule 10 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	M	113	876	541	177	155	3	0	0

- Molecule 11 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 12 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 13 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	P	79	629	394	124	110	1	0	0

- Molecule 14 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	Q	78	632	400	118	111	3	0	0

- Molecule 15 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	R	52	Total	C	N	O	0	0
			425	271	78	76		

- Molecule 16 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 17 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	84	Total	C	N	O	S	0	0
			656	405	136	112	3		

- Molecule 18 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	U	64	Total	C	N	O	S	0	0
			529	329	110	89	1		

- Molecule 19 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Y	6	Total	C	N	O	P	0	0
			131	58	24	43	6		

- Molecule 20 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	b	127	Total	C	N	O	S	0	0
			1021	634	206	178	3		

- Molecule 21 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	B	1504	Total	C	N	O	P	0	0
			32296	14411	5936	10445	1504		

- Molecule 22 is a RNA chain called fMet-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
22	a	68	1457	648	265	476	68	0	0

- Molecule 23 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	G	101	793	497	147	146	3	0	0

- Molecule 24 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
24	c	83	667	419	131	117	0	0

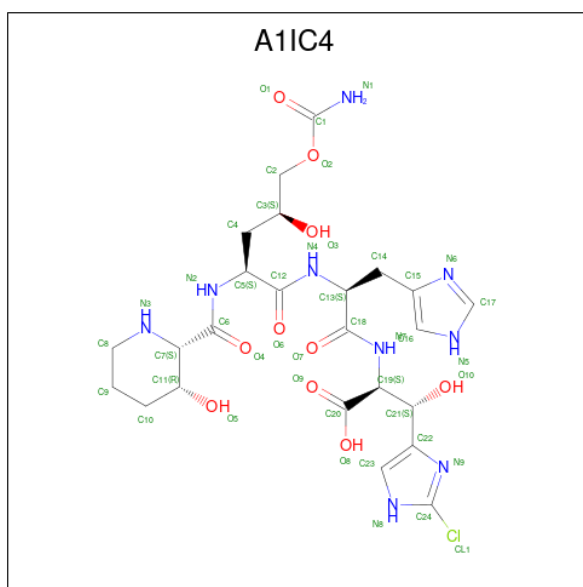
- Molecule 25 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
25	D	1	Total	K	0
			1	1	
25	F	1	Total	K	0
			1	1	
25	B	23	Total	K	0
			23	23	

- Molecule 26 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
26	B	49	Total	Mg	0
			49	49	

- Molecule 27 is (2S,3S)-2-[[[(2S)-2-[[[(2S,4S)-5-aminocarbonyloxy-4-oxidanyl-2-[[[(2S,3R)-3-oxidanylpiperidin-2-yl]carbonylamino]pentanoyl]amino]-3-(1H-imidazol-4-yl)propanoyl]amino]-3-(2-chloranyl-1H-imidazol-4-yl)-3-oxidanyl-propanoic acid (three-letter code: A1IC4) (formula: C₂₄H₃₄ClN₉O₁₀) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Cl	N	O	
27	B	1	44	24	1	9	10	0

- Molecule 28 is water.

Mol	Chain	Residues	Atoms		AltConf
28	D	40	Total	O	0
			40	40	
28	E	17	Total	O	0
			17	17	
28	F	1	Total	O	0
			1	1	
28	H	34	Total	O	0
			34	34	
28	I	3	Total	O	0
			3	3	
28	K	11	Total	O	0
			11	11	
28	L	42	Total	O	0
			42	42	
28	O	13	Total	O	0
			13	13	
28	P	33	Total	O	0
			33	33	
28	Q	13	Total	O	0
			13	13	
28	R	7	Total	O	0
			7	7	

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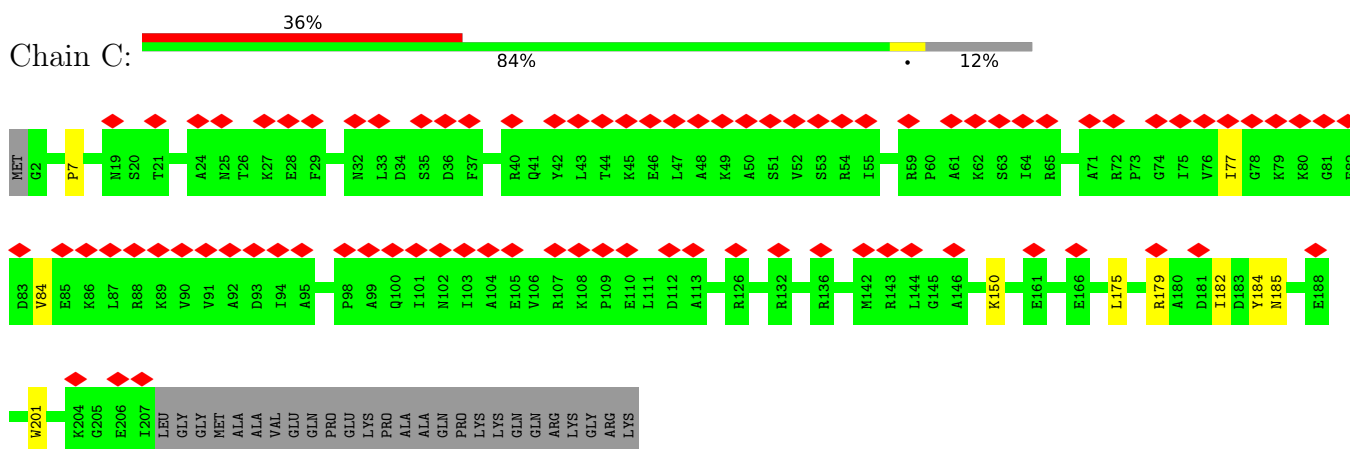
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Mol	Chain	Residues	Atoms		AltConf
28	T	26	Total 26	O 26	0
28	U	3	Total 3	O 3	0
28	Y	2	Total 2	O 2	0
28	B	1562	Total 1562	O 1562	0

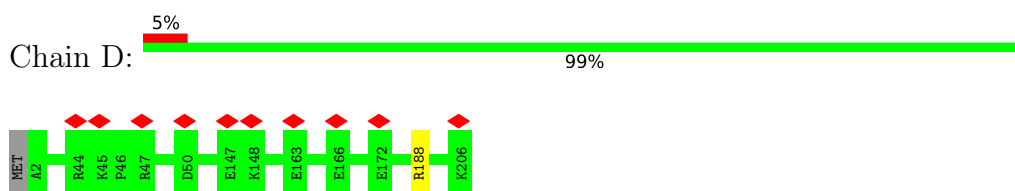
3 Residue-property plots

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

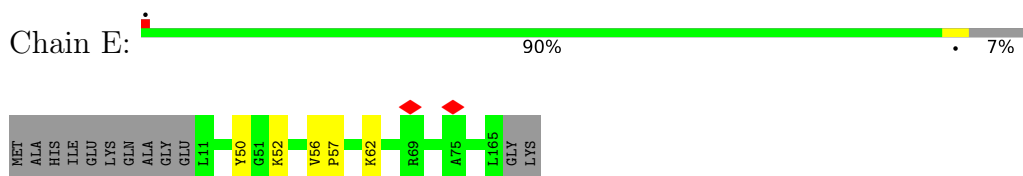
- Molecule 1: Small ribosomal subunit protein uS3



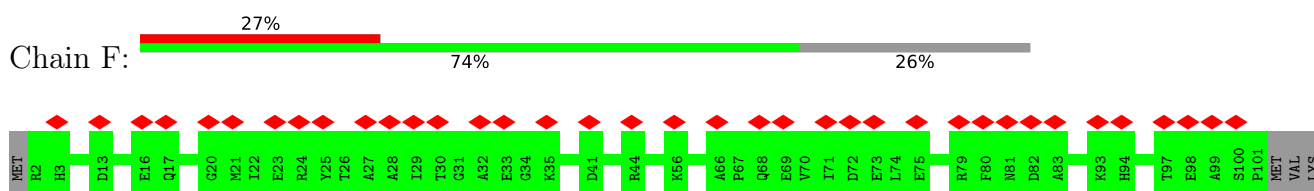
- Molecule 2: Small ribosomal subunit protein uS4

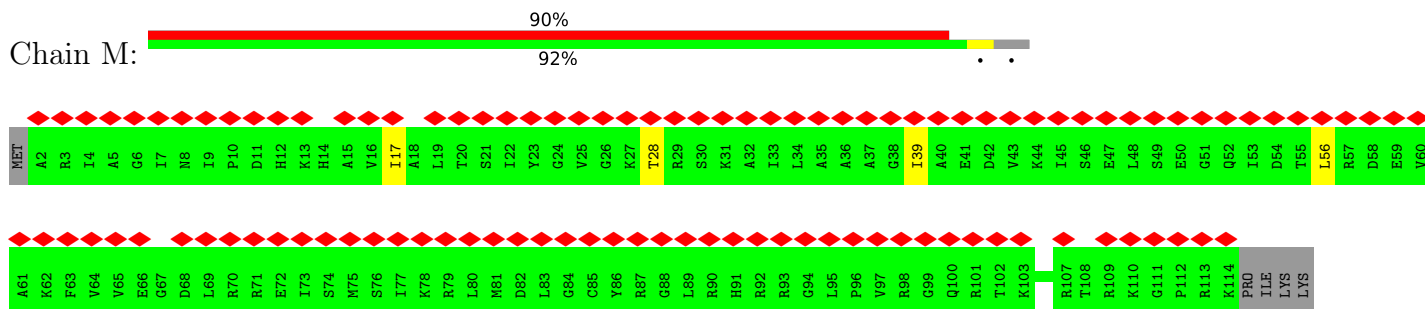


- Molecule 3: Small ribosomal subunit protein uS5

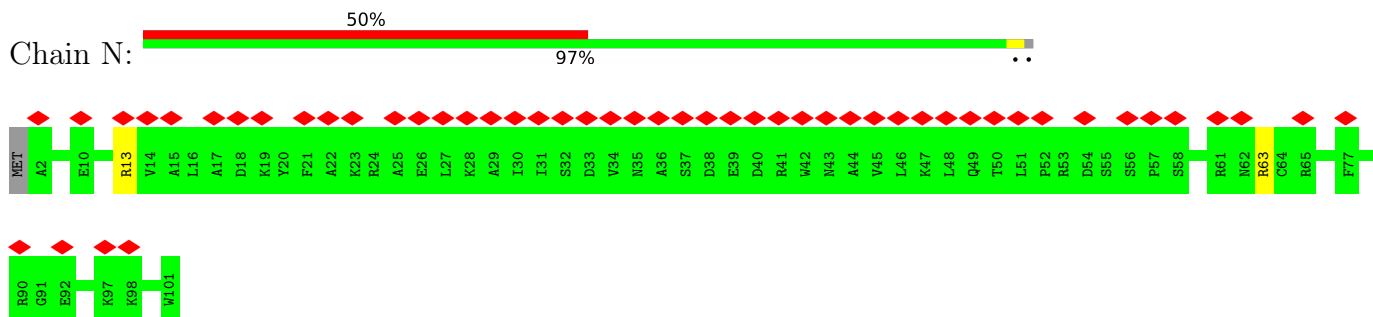


- Molecule 4: Small ribosomal subunit protein bS6, fully modified isoform

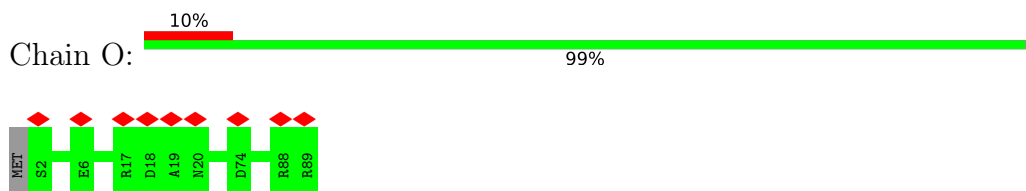




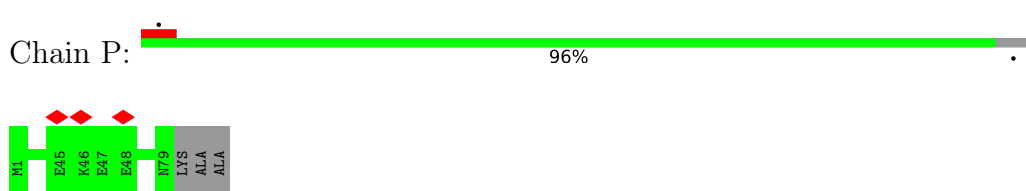
• Molecule 11: Small ribosomal subunit protein uS14



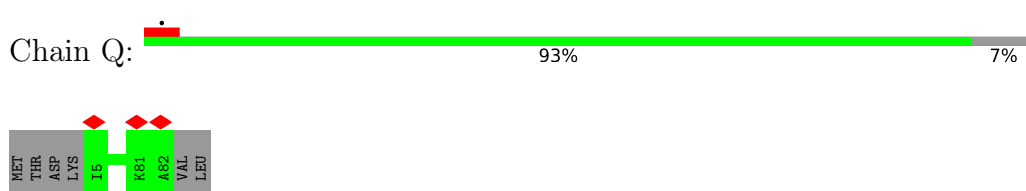
• Molecule 12: Small ribosomal subunit protein uS15



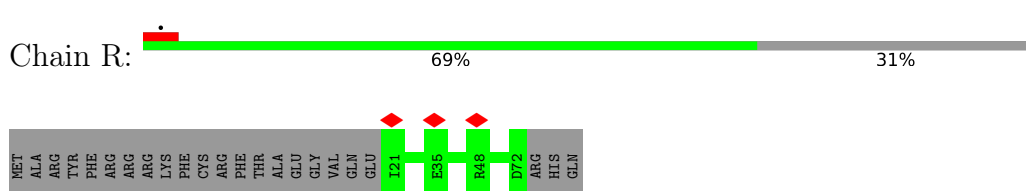
• Molecule 13: Small ribosomal subunit protein bS16



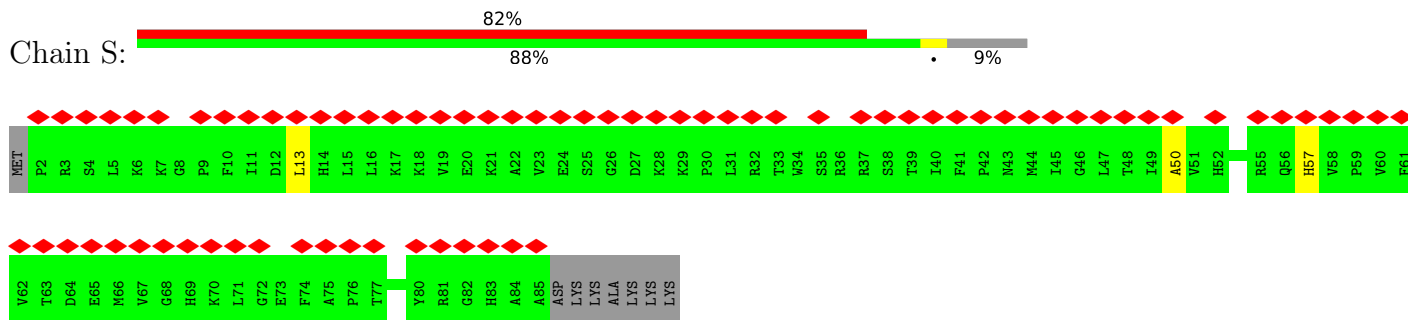
• Molecule 14: Small ribosomal subunit protein uS17



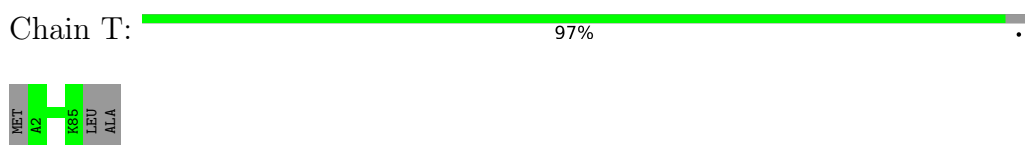
• Molecule 15: Small ribosomal subunit protein bS18



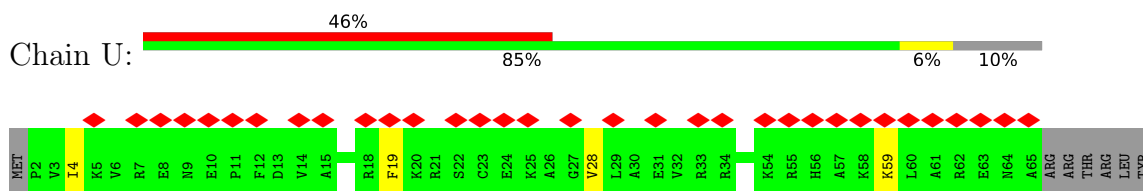
• Molecule 16: Small ribosomal subunit protein uS19



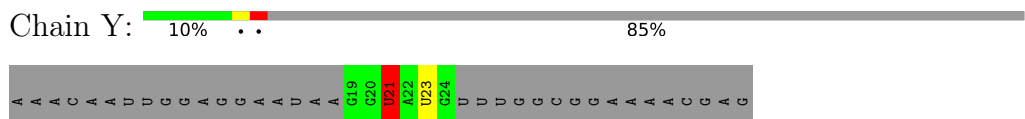
• Molecule 17: Small ribosomal subunit protein bS20



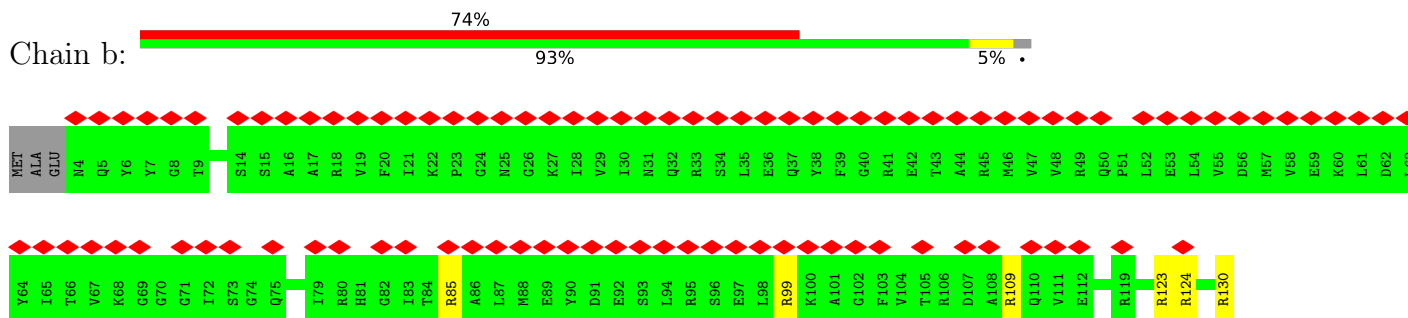
• Molecule 18: Small ribosomal subunit protein bS21



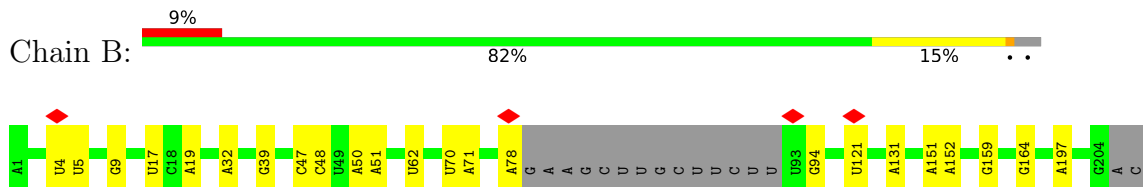
• Molecule 19: mRNA

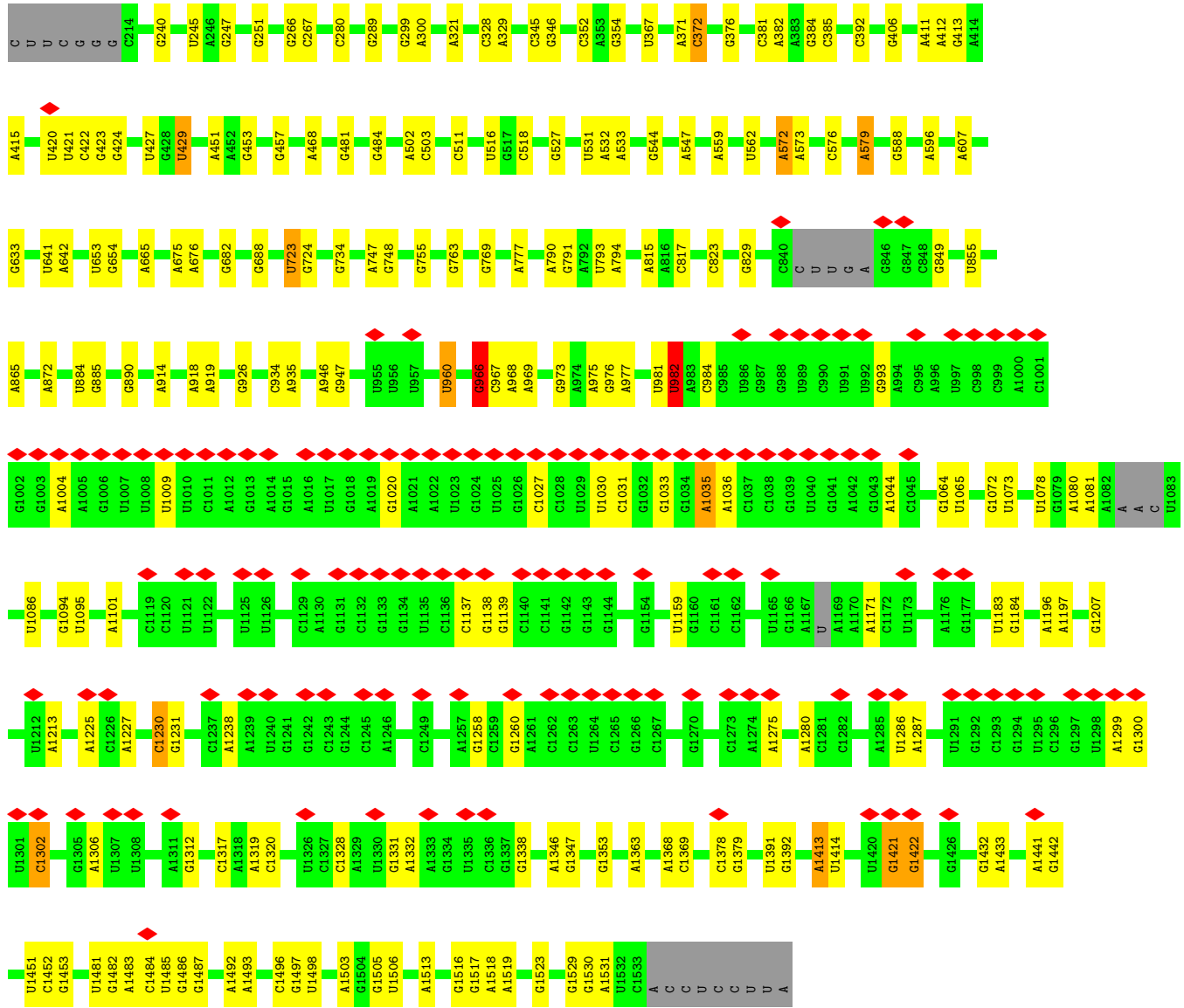


• Molecule 20: Small ribosomal subunit protein uS9

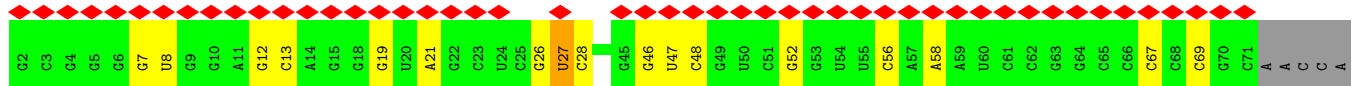


• Molecule 21: 16S ribosomal RNA

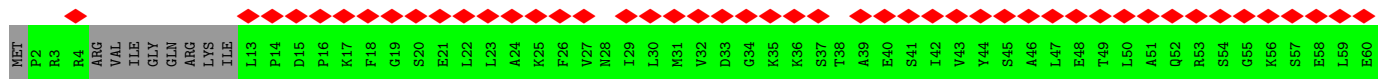


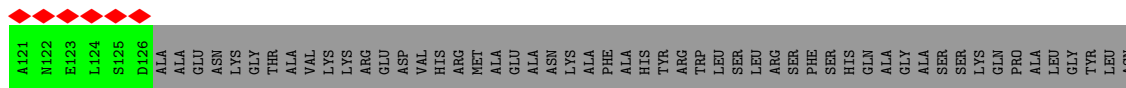


• Molecule 22: fMet-tRNA

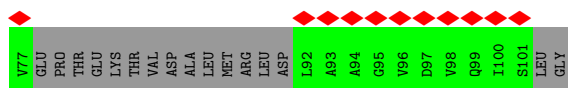
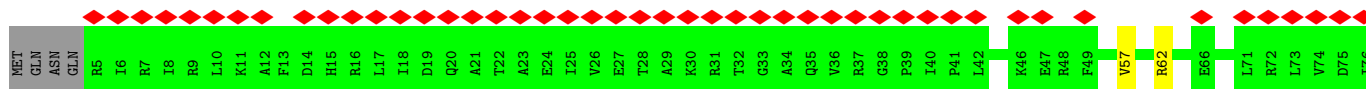
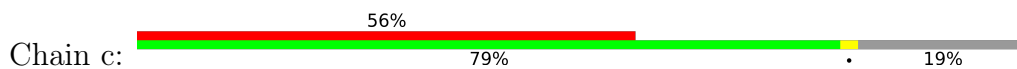


• Molecule 23: Small ribosomal subunit protein uS7





• Molecule 24: Small ribosomal subunit protein uS10



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	33966	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 ($e^-/\text{\AA}^2$)	1.14	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1100	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.093	Depositor
Minimum map value	-0.046	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0115	Depositor
Map size (Å)	359.424, 359.424, 359.424	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	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: MG, G7M, K, 5MC, IAS, 2MG, 4OC, D2T, PSU, UR3, MA6, A1IC4

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	C	0.29	0/1651	0.62	0/2225
2	D	0.36	0/1665	0.59	0/2227
3	E	0.34	0/1156	0.57	0/1556
4	F	0.35	0/835	0.58	0/1130
5	H	0.35	0/989	0.59	0/1326
6	I	0.33	0/564	0.57	0/759
7	J	0.62	0/840	0.70	0/1114
8	K	0.41	0/883	0.62	0/1191
9	L	0.42	1/945 (0.1%)	0.66	0/1268
10	M	0.30	0/884	0.64	0/1181
11	N	0.31	0/817	0.62	0/1088
12	O	0.35	0/722	0.54	0/964
13	P	0.33	0/639	0.62	0/859
14	Q	0.34	0/641	0.60	0/860
15	R	0.37	0/431	0.59	0/580
16	S	0.32	0/685	0.63	0/922
17	T	0.33	0/662	0.51	0/877
18	U	0.37	0/536	0.60	0/711
19	Y	0.67	0/146	1.19	1/226 (0.4%)
20	b	0.35	0/1033	0.78	0/1375
21	B	0.53	0/35882	1.02	15/55964 (0.0%)
22	a	0.73	0/1627	1.18	2/2534 (0.1%)
23	G	0.33	0/801	0.66	0/1073
24	c	0.32	0/675	0.68	0/911
All	All	0.49	1/55709 (0.0%)	0.93	18/82921 (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
1	C	0	1
7	J	0	2
11	N	0	1
20	b	0	6
24	c	0	1
All	All	0	11

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	L	45	PRO	N-CD	-7.10	1.38	1.47

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	981	U	OP1-P-O3'	11.24	129.92	105.20
21	B	982	U	O5'-P-OP2	-10.63	96.13	105.70
21	B	981	U	OP2-P-O3'	-10.61	81.87	105.20
21	B	973	G	O5'-P-OP2	-6.56	99.80	105.70
21	B	1331	G	O4'-C1'-N9	6.26	113.21	108.20
21	B	1369	C	O3'-P-O5'	-6.24	92.14	104.00
21	B	1035	A	P-O3'-C3'	6.09	127.01	119.70
21	B	1347	G	O3'-P-O5'	-6.01	92.57	104.00
21	B	982	U	OP1-P-OP2	-5.94	110.68	119.60
21	B	429	U	C3'-C2'-C1'	-5.67	96.97	101.50
21	B	960	U	C3'-C2'-C1'	-5.48	97.12	101.50
21	B	872	A	C1'-O4'-C4'	-5.29	105.66	109.90
21	B	1347	G	C3'-C2'-C1'	-5.15	97.38	101.50
22	a	56	C	OP1-P-O3'	5.13	116.50	105.20
21	B	872	A	O4'-C1'-N9	5.07	112.25	108.20
22	a	27	U	OP2-P-O3'	5.05	116.32	105.20
19	Y	21	U	OP1-P-OP2	-5.04	112.03	119.60
21	B	1230	C	OP1-P-OP2	-5.02	112.08	119.60

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	179	ARG	Sidechain
7	J	147	ARG	Sidechain
7	J	99	ARG	Sidechain
11	N	13	ARG	Sidechain

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Mol	Chain	Res	Type	Group
20	b	109	ARG	Sidechain
20	b	123	ARG	Sidechain
20	b	124	ARG	Sidechain
20	b	130	ARG	Sidechain
20	b	85	ARG	Sidechain
20	b	99	ARG	Sidechain
24	c	62	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1624	0	1696	11	0
2	D	1643	0	1706	0	0
3	E	1143	0	1190	7	0
4	F	816	0	803	0	0
5	H	979	0	1031	1	0
6	I	557	0	573	2	0
7	J	832	0	884	26	0
8	K	876	0	884	8	0
9	L	942	0	999	2	0
10	M	876	0	934	3	0
11	N	805	0	844	1	0
12	O	714	0	734	0	0
13	P	629	0	643	0	0
14	Q	632	0	669	0	0
15	R	425	0	452	0	0
16	S	668	0	693	1	0
17	T	656	0	703	0	0
18	U	529	0	563	5	0
19	Y	131	0	65	2	0
20	b	1021	0	1070	0	0
21	B	32296	0	16270	44	0
22	a	1457	0	739	0	0
23	G	793	0	827	0	0
24	c	667	0	704	0	0
25	B	23	0	0	0	0
25	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	F	1	0	0	0	0
26	B	49	0	0	0	0
27	B	44	0	0	0	0
28	B	1562	0	0	0	0
28	D	40	0	0	0	0
28	E	17	0	0	0	0
28	F	1	0	0	0	0
28	H	34	0	0	0	0
28	I	3	0	0	0	0
28	K	11	0	0	0	0
28	L	42	0	0	0	0
28	O	13	0	0	0	0
28	P	33	0	0	0	0
28	Q	13	0	0	0	0
28	R	7	0	0	0	0
28	T	26	0	0	0	0
28	U	3	0	0	0	0
28	Y	2	0	0	0	0
All	All	53636	0	35676	95	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 (95) 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:C:7:PRO:HG2	1:C:201:TRP:HE1	1.41	0.83
21:B:415:A:H61	21:B:427:U:H3	1.27	0.82
21:B:17:U:H4'	21:B:1080:A:O4'	1.80	0.82
3:E:62:LYS:NZ	21:B:1072:G:OP1	2.18	0.75
1:C:150:LYS:HD2	1:C:201:TRP:CE3	2.23	0.73
1:C:7:PRO:HG2	1:C:201:TRP:NE1	2.05	0.71
5:H:2:SER:N	21:B:823:C:HO2'	1.89	0.70
3:E:52:LYS:HE2	21:B:1081:A:C8	2.30	0.66
7:J:82:LYS:HA	7:J:85:LYS:HD2	1.78	0.66
3:E:52:LYS:HE2	21:B:1081:A:N7	2.12	0.65
21:B:1391:U:H2'	21:B:1392:G:C8	2.32	0.64
1:C:7:PRO:CG	1:C:201:TRP:HE1	2.11	0.63
1:C:150:LYS:HD2	1:C:201:TRP:CZ3	2.34	0.62
7:J:161:PHE:CD1	7:J:162:PRO:HD2	2.35	0.61
3:E:50:TYR:OH	21:B:1080:A:OP1	2.12	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:138:GLN:CD	7:J:165:ILE:HG13	2.23	0.59
9:L:44:LYS:HB3	9:L:45:PRO:HD3	1.86	0.58
21:B:17:U:H1'	21:B:1080:A:N3	2.19	0.57
7:J:158:VAL:HA	7:J:174:LEU:HD23	1.87	0.56
7:J:158:VAL:O	7:J:159:GLU:C	2.46	0.54
21:B:966:2MG:HM23	21:B:967:5MC:H1'	1.90	0.54
7:J:91:ILE:HG23	7:J:122:ASP:HA	1.90	0.53
8:K:110:ILE:HG23	18:U:4:ILE:HB	1.90	0.52
10:M:17:ILE:HG13	21:B:1302:C:C5	2.44	0.52
18:U:4:ILE:HG13	18:U:19:PHE:HA	1.92	0.52
7:J:116:ARG:O	7:J:117:PHE:C	2.47	0.52
7:J:76:GLU:C	7:J:78:SER:N	2.62	0.52
3:E:52:LYS:NZ	21:B:1081:A:OP2	2.25	0.51
1:C:175:LEU:HD23	1:C:182:ILE:HD13	1.91	0.51
21:B:769:G:H4'	21:B:1513:A:H4'	1.93	0.51
7:J:77:LYS:O	7:J:80:SER:N	2.43	0.50
16:S:50:ALA:HB1	16:S:57:HIS:HB3	1.93	0.50
21:B:17:U:C1'	21:B:1080:A:H1'	2.41	0.50
7:J:126:ILE:HD13	7:J:148:VAL:HG11	1.93	0.50
7:J:114:LEU:O	7:J:115:ILE:C	2.50	0.49
7:J:79:LYS:O	7:J:82:LYS:N	2.45	0.49
7:J:164:LYS:HE3	7:J:166:GLU:HB2	1.95	0.49
21:B:17:U:H1'	21:B:1080:A:H1'	1.94	0.49
21:B:1391:U:H2'	21:B:1392:G:H8	1.77	0.49
21:B:1421:G:H3'	21:B:1422:G:H5''	1.95	0.49
7:J:78:SER:O	7:J:81:SER:N	2.45	0.49
7:J:84:GLN:HA	7:J:87:LYS:HE2	1.95	0.48
7:J:89:LYS:HD3	7:J:90:VAL:H	1.78	0.48
21:B:1496:C:H2'	21:B:1497:G:O4'	2.12	0.48
19:Y:21:U:OP1	19:Y:21:U:H2'	2.13	0.48
1:C:184:TYR:HD1	1:C:201:TRP:CD1	2.31	0.48
21:B:1413:A:H2'	21:B:1414:U:O4'	2.14	0.48
3:E:62:LYS:HE2	21:B:1073:U:OP2	2.13	0.48
21:B:865:A:H5'	21:B:1078:U:C5	2.49	0.47
21:B:1230:C:H2'	21:B:1231:G:H8	1.79	0.47
21:B:790:A:H2'	21:B:791:G:C8	2.49	0.47
8:K:110:ILE:HG12	18:U:19:PHE:CG	2.50	0.46
7:J:80:SER:O	7:J:81:SER:C	2.54	0.46
7:J:130:PHE:CE1	7:J:138:GLN:HA	2.51	0.46
8:K:112:ASP:OD1	18:U:28:VAL:HG21	2.16	0.46
21:B:62:U:OP1	21:B:385:C:O2'	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:946:A:H2'	21:B:947:G:C8	2.52	0.45
1:C:184:TYR:CD1	1:C:201:TRP:CD1	3.04	0.45
19:Y:23:U:H5''	21:B:1498:UR3:C4	2.48	0.44
1:C:184:TYR:CD1	1:C:201:TRP:NE1	2.86	0.44
21:B:299:G:H2'	21:B:300:A:C8	2.53	0.44
21:B:918:A:H2'	21:B:919:A:O4'	2.17	0.44
21:B:17:U:O4'	21:B:1080:A:H1'	2.17	0.44
21:B:381:C:H2'	21:B:382:A:O4'	2.17	0.44
1:C:77:ILE:HA	1:C:84:VAL:HG22	2.00	0.44
21:B:19:A:O2'	21:B:572:A:N1	2.41	0.43
3:E:56:VAL:N	3:E:57:PRO:HD2	2.33	0.43
11:N:63:ARG:NH2	21:B:982:U:OP2	2.48	0.43
21:B:502:A:H2'	21:B:503:C:O4'	2.19	0.43
6:I:20:THR:OG1	6:I:41:ARG:NH2	2.51	0.43
7:J:78:SER:OG	7:J:79:LYS:N	2.52	0.43
8:K:110:ILE:HG12	18:U:19:PHE:CD1	2.53	0.43
7:J:79:LYS:O	7:J:80:SER:C	2.58	0.43
9:L:44:LYS:HB3	9:L:45:PRO:CD	2.48	0.43
7:J:78:SER:O	7:J:79:LYS:C	2.57	0.42
7:J:157:VAL:HG13	7:J:177:LYS:HG3	2.01	0.42
8:K:116:ILE:O	21:B:675:A:O2'	2.36	0.42
7:J:81:SER:HB2	7:J:85:LYS:HE3	2.01	0.42
8:K:97:ILE:HD13	8:K:110:ILE:HD12	2.01	0.42
8:K:128:ARG:NH2	21:B:1523:G:OP1	2.52	0.42
10:M:28:THR:HG21	21:B:1328:C:OP1	2.20	0.42
6:I:17:LEU:HB2	6:I:21:MET:HB2	2.01	0.42
21:B:723:U:H2'	21:B:855:U:H4'	2.02	0.42
21:B:151:A:H2'	21:B:152:A:O4'	2.20	0.41
21:B:1306:A:H1'	21:B:1332:A:C2	2.55	0.41
1:C:150:LYS:HZ2	1:C:201:TRP:HZ3	1.67	0.41
21:B:1485:U:H2'	21:B:1486:G:C8	2.56	0.41
7:J:92:GLN:HE21	7:J:94:LYS:HD3	1.86	0.41
7:J:77:LYS:HE3	7:J:77:LYS:HB3	1.80	0.41
7:J:82:LYS:O	7:J:86:LYS:N	2.36	0.41
21:B:579:A:C2	21:B:763:G:C2	3.08	0.41
10:M:39:ILE:HD12	10:M:56:LEU:HD21	2.02	0.40
8:K:115:PRO:HB3	21:B:676:A:H5''	2.02	0.40
21:B:371:A:H2'	21:B:372:C:O4'	2.21	0.40
21:B:502:A:C2	21:B:544:G:C2	3.09	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	
1	C	204/233 (88%)	197 (97%)	7 (3%)	0	100	100
2	D	203/206 (98%)	200 (98%)	3 (2%)	0	100	100
3	E	153/167 (92%)	143 (94%)	10 (6%)	0	100	100
4	F	98/135 (73%)	93 (95%)	5 (5%)	0	100	100
5	H	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
6	I	68/72 (94%)	68 (100%)	0	0	100	100
7	J	100/180 (56%)	73 (73%)	20 (20%)	7 (7%)	1	1
8	K	113/159 (71%)	106 (94%)	4 (4%)	3 (3%)	4	10
9	L	118/124 (95%)	114 (97%)	3 (2%)	1 (1%)	16	32
10	M	111/118 (94%)	108 (97%)	3 (3%)	0	100	100
11	N	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
12	O	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
13	P	77/82 (94%)	73 (95%)	4 (5%)	0	100	100
14	Q	76/84 (90%)	75 (99%)	1 (1%)	0	100	100
15	R	50/75 (67%)	49 (98%)	1 (2%)	0	100	100
16	S	82/92 (89%)	81 (99%)	1 (1%)	0	100	100
17	T	82/87 (94%)	82 (100%)	0	0	100	100
18	U	62/71 (87%)	58 (94%)	4 (6%)	0	100	100
20	b	125/130 (96%)	115 (92%)	10 (8%)	0	100	100
23	G	95/179 (53%)	92 (97%)	3 (3%)	0	100	100
24	c	79/103 (77%)	76 (96%)	2 (2%)	1 (1%)	10	22
All	All	2207/2617 (84%)	2105 (95%)	90 (4%)	12 (0%)	27	43

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	J	79	LYS
7	J	168	ARG
7	J	77	LYS
8	K	113	VAL
24	c	57	VAL
7	J	78	SER
8	K	108	THR
7	J	89	LYS
7	J	115	ILE
9	L	44	LYS
7	J	90	VAL
8	K	114	THR

5.3.2 Protein sidechains [i](#)

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	C	170/190 (90%)	169 (99%)	1 (1%)	84	92
2	D	172/173 (99%)	171 (99%)	1 (1%)	84	92
3	E	118/126 (94%)	118 (100%)	0	100	100
4	F	87/116 (75%)	87 (100%)	0	100	100
5	H	104/105 (99%)	104 (100%)	0	100	100
6	I	63/65 (97%)	63 (100%)	0	100	100
7	J	92/156 (59%)	88 (96%)	4 (4%)	25	47
8	K	89/125 (71%)	88 (99%)	1 (1%)	70	85
9	L	101/103 (98%)	101 (100%)	0	100	100
10	M	91/96 (95%)	91 (100%)	0	100	100
11	N	83/84 (99%)	83 (100%)	0	100	100
12	O	76/77 (99%)	76 (100%)	0	100	100
13	P	64/65 (98%)	64 (100%)	0	100	100
14	Q	72/78 (92%)	72 (100%)	0	100	100
15	R	45/65 (69%)	45 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	S	72/79 (91%)	71 (99%)	1 (1%)	62	82
17	T	64/66 (97%)	64 (100%)	0	100	100
18	U	54/61 (88%)	53 (98%)	1 (2%)	52	74
20	b	105/107 (98%)	105 (100%)	0	100	100
23	G	85/147 (58%)	85 (100%)	0	100	100
24	c	72/90 (80%)	72 (100%)	0	100	100
All	All	1879/2174 (86%)	1870 (100%)	9 (0%)	85	94

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	185	ASN
2	D	188	ARG
7	J	88	GLN
7	J	89	LYS
7	J	135	MET
7	J	161	PHE
8	K	109	ASN
16	S	13	LEU
18	U	59	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
7	J	92	GLN
7	J	108	GLN
7	J	146	ASN
8	K	109	ASN
8	K	118	HIS
16	S	14	HIS
16	S	56	GLN
16	S	83	HIS
24	c	58	ASN
24	c	64	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
19	Y	5/40 (12%)	1 (20%)	0
21	B	1496/1545 (96%)	176 (11%)	19 (1%)
22	a	66/73 (90%)	16 (24%)	0
All	All	1567/1658 (94%)	193 (12%)	19 (1%)

All (193) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
19	Y	21	U
21	B	4	U
21	B	5	U
21	B	9	G
21	B	32	A
21	B	39	G
21	B	47	C
21	B	48	C
21	B	50	A
21	B	51	A
21	B	71	A
21	B	78	A
21	B	94	G
21	B	121	U
21	B	131	A
21	B	159	G
21	B	164	G
21	B	197	A
21	B	240	G
21	B	245	U
21	B	247	G
21	B	251	G
21	B	266	G
21	B	267	C
21	B	280	C
21	B	289	G
21	B	321	A
21	B	328	C
21	B	329	A
21	B	345	C
21	B	346	G
21	B	352	C
21	B	354	G
21	B	367	U
21	B	372	C

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Mol	Chain	Res	Type
21	B	376	G
21	B	384	G
21	B	392	C
21	B	406	G
21	B	411	A
21	B	412	A
21	B	413	G
21	B	420	U
21	B	421	U
21	B	422	C
21	B	423	G
21	B	424	G
21	B	429	U
21	B	451	A
21	B	453	G
21	B	457	G
21	B	468	A
21	B	481	G
21	B	484	G
21	B	511	C
21	B	518	C
21	B	531	U
21	B	532	A
21	B	533	A
21	B	547	A
21	B	559	A
21	B	562	U
21	B	572	A
21	B	573	A
21	B	576	C
21	B	579	A
21	B	588	G
21	B	596	A
21	B	607	A
21	B	633	G
21	B	642	A
21	B	653	U
21	B	654	G
21	B	665	A
21	B	682	G
21	B	688	G
21	B	723	U

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Mol	Chain	Res	Type
21	B	724	G
21	B	734	G
21	B	747	A
21	B	748	G
21	B	755	G
21	B	777	A
21	B	793	U
21	B	794	A
21	B	815	A
21	B	817	C
21	B	829	G
21	B	849	G
21	B	885	G
21	B	890	G
21	B	914	A
21	B	926	G
21	B	934	C
21	B	935	A
21	B	960	U
21	B	966	2MG
21	B	968	A
21	B	969	A
21	B	975	A
21	B	976	G
21	B	977	A
21	B	982	U
21	B	984	C
21	B	993	G
21	B	1004	A
21	B	1009	U
21	B	1020	G
21	B	1027	C
21	B	1030	U
21	B	1031	C
21	B	1033	G
21	B	1035	A
21	B	1036	A
21	B	1044	A
21	B	1064	G
21	B	1065	U
21	B	1086	U
21	B	1094	G

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Mol	Chain	Res	Type
21	B	1095	U
21	B	1101	A
21	B	1137	C
21	B	1138	G
21	B	1139	G
21	B	1159	U
21	B	1171	A
21	B	1183	U
21	B	1184	G
21	B	1196	A
21	B	1197	A
21	B	1213	A
21	B	1227	A
21	B	1238	A
21	B	1258	G
21	B	1260	G
21	B	1275	A
21	B	1280	A
21	B	1286	U
21	B	1287	A
21	B	1299	A
21	B	1300	G
21	B	1302	C
21	B	1312	G
21	B	1317	C
21	B	1319	A
21	B	1320	C
21	B	1338	G
21	B	1346	A
21	B	1353	G
21	B	1363	A
21	B	1368	A
21	B	1378	C
21	B	1379	G
21	B	1413	A
21	B	1421	G
21	B	1422	G
21	B	1432	G
21	B	1433	A
21	B	1441	A
21	B	1442	G
21	B	1451	U

Continued on next page...

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Mol	Chain	Res	Type
21	B	1452	C
21	B	1453	G
21	B	1481	U
21	B	1482	G
21	B	1483	A
21	B	1484	C
21	B	1487	G
21	B	1492	A
21	B	1493	A
21	B	1503	A
21	B	1505	G
21	B	1506	U
21	B	1517	G
21	B	1529	G
21	B	1530	G
21	B	1531	A
22	a	7	G
22	a	8	U
22	a	12	G
22	a	13	C
22	a	19	G
22	a	21	A
22	a	26	G
22	a	27	U
22	a	28	C
22	a	46	G
22	a	47	U
22	a	48	C
22	a	52	G
22	a	58	A
22	a	67	C
22	a	69	C

All (19) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	B	5	U
21	B	70	U
21	B	251	G
21	B	345	C
21	B	412	A
21	B	421	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	B	641	U
21	B	653	U
21	B	793	U
21	B	884	U
21	B	993	G
21	B	1035	A
21	B	1137	C
21	B	1225	A
21	B	1319	A
21	B	1432	G
21	B	1452	C
21	B	1487	G
21	B	1492	A

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

13 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
21	MA6	B	1519	21	18,26,27	0.77	1 (5%)	19,38,41	0.66	0
21	5MC	B	967	21	18,22,23	0.33	0	26,32,35	0.55	0
21	5MC	B	1407	21	18,22,23	0.37	0	26,32,35	0.63	0
21	2MG	B	966	21	18,26,27	1.02	2 (11%)	16,38,41	0.78	0
21	PSU	B	516	21,26	18,21,22	1.08	1 (5%)	22,30,33	0.58	0
21	G7M	B	527	21	20,26,27	1.10	2 (10%)	17,39,42	0.50	0
9	D2T	L	89	9	7,9,10	0.92	0	6,11,13	1.73	3 (50%)
21	UR3	B	1498	21	19,22,23	0.32	0	26,32,35	0.68	0
8	IAS	K	119	8	6,7,8	0.88	0	6,8,10	0.95	0
21	2MG	B	1516	21	18,26,27	1.06	2 (11%)	16,38,41	0.80	0
21	2MG	B	1207	21	18,26,27	1.00	1 (5%)	16,38,41	0.73	0
21	MA6	B	1518	21	18,26,27	0.83	2 (11%)	19,38,41	0.52	0
21	4OC	B	1402	21	20,23,24	0.43	0	26,32,35	0.64	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
21	MA6	B	1519	21	-	2/7/29/30	0/3/3/3
21	5MC	B	967	21	-	0/7/25/26	0/2/2/2
21	5MC	B	1407	21	-	0/7/25/26	0/2/2/2
21	2MG	B	966	21	-	2/5/27/28	0/3/3/3
21	PSU	B	516	21,26	-	0/7/25/26	0/2/2/2
21	G7M	B	527	21	-	0/3/25/26	0/3/3/3
9	D2T	L	89	9	-	1/7/12/14	-
21	UR3	B	1498	21	-	0/7/25/26	0/2/2/2
8	IAS	K	119	8	-	0/7/7/8	-
21	2MG	B	1516	21	-	0/5/27/28	0/3/3/3
21	2MG	B	1207	21	-	0/5/27/28	0/3/3/3
21	MA6	B	1518	21	-	0/7/29/30	0/3/3/3
21	4OC	B	1402	21	-	0/9/29/30	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	516	PSU	C6-C5	4.17	1.40	1.35
21	B	527	G7M	C8-N9	3.39	1.39	1.33
21	B	966	2MG	C5-C6	-2.58	1.42	1.47
21	B	1516	2MG	C5-C6	-2.56	1.42	1.47
21	B	527	G7M	C8-N7	2.49	1.37	1.33
21	B	1518	MA6	C6-N1	2.28	1.36	1.33
21	B	1207	2MG	C5-C6	-2.21	1.42	1.47
21	B	966	2MG	C8-N7	-2.10	1.31	1.35
21	B	1518	MA6	C8-N7	-2.08	1.31	1.34
21	B	1519	MA6	C6-N1	2.08	1.36	1.33
21	B	1516	2MG	C8-N7	-2.01	1.31	1.35

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	L	89	D2T	OD1-CG-CB	-2.50	117.20	122.44
9	L	89	D2T	O-C-CA	-2.17	119.10	124.78
9	L	89	D2T	OD2-CG-CB	2.16	117.82	113.15

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	B	966	2MG	C3'-C4'-C5'-O5'
21	B	966	2MG	O4'-C4'-C5'-O5'
21	B	1519	MA6	O4'-C4'-C5'-O5'
9	L	89	D2T	CG-CB-SB-CB1
21	B	1519	MA6	C3'-C4'-C5'-O5'

There are no ring outliers.

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	967	5MC	1	0
21	B	966	2MG	1	0
21	B	1498	UR3	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 75 ligands modelled in this entry, 74 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
27	A1IC4	B	1673	-	38,46,46	0.51	0	39,63,63	0.69	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
27	A1IC4	B	1673	-	-	4/45/60/60	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

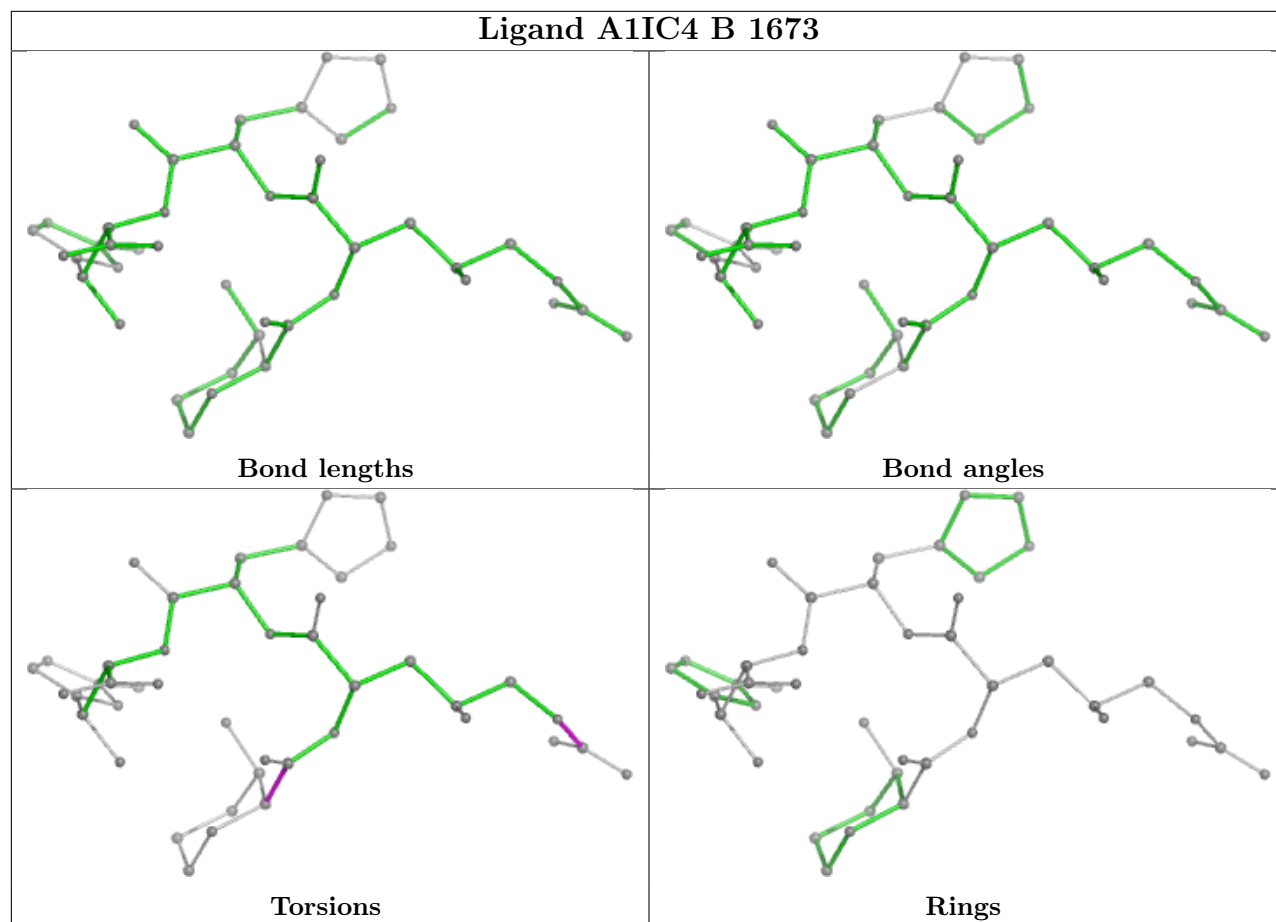
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	B	1673	A1IC4	N2-C6-C7-N3
27	B	1673	A1IC4	N1-C1-O2-C2
27	B	1673	A1IC4	O1-C1-O2-C2
27	B	1673	A1IC4	O4-C6-C7-C11

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	a	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	a	15:G	O3'	18:G	P	10.14

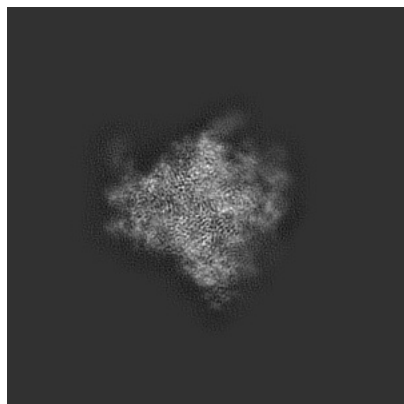
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50912. These allow visual inspection of the internal detail of the map and identification of artifacts.

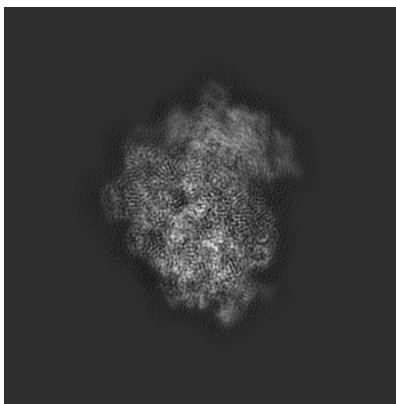
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

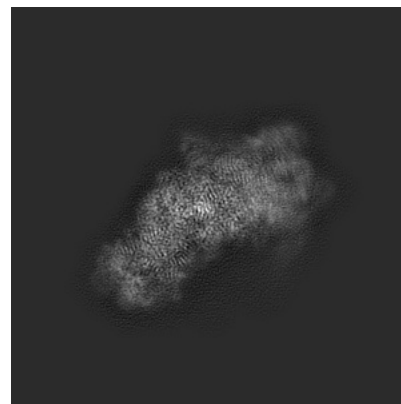
6.1.1 Primary map



X

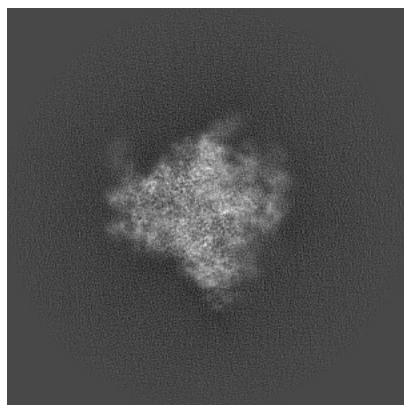


Y

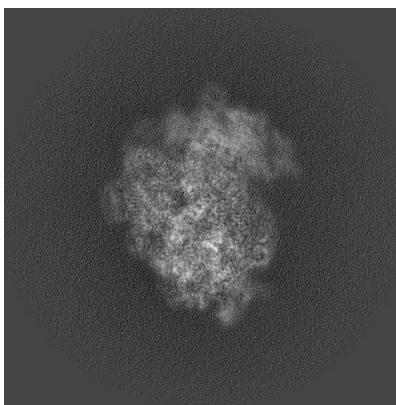


Z

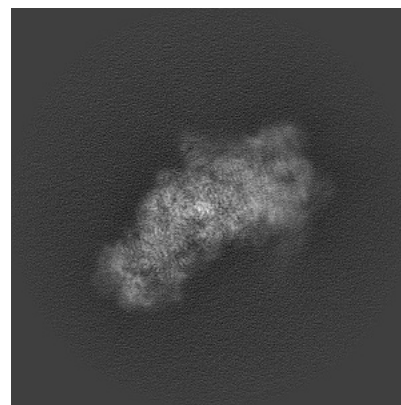
6.1.2 Raw map



X



Y

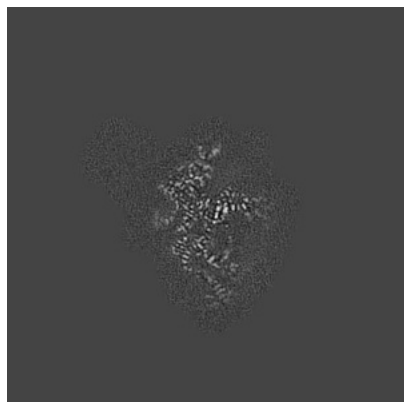


Z

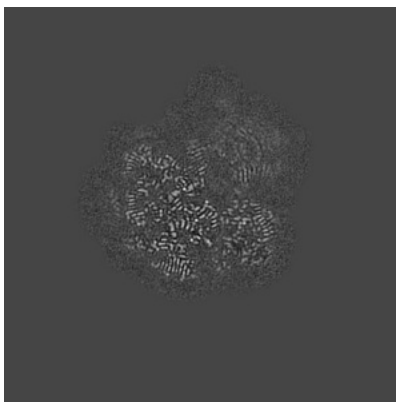
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

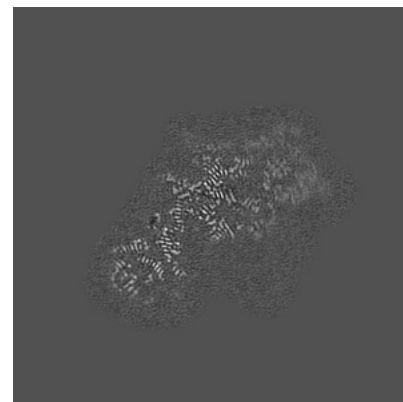
6.2.1 Primary map



X Index: 216

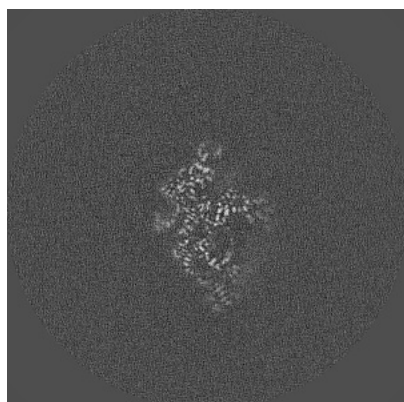


Y Index: 216

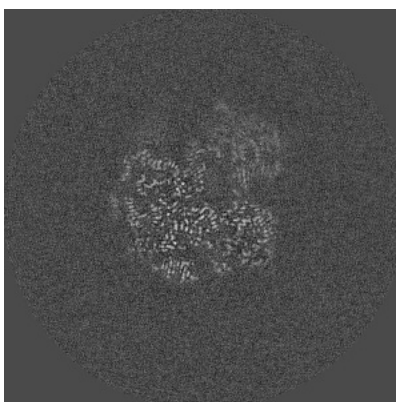


Z Index: 216

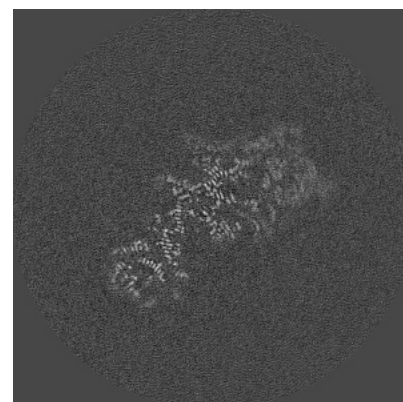
6.2.2 Raw map



X Index: 216



Y Index: 216

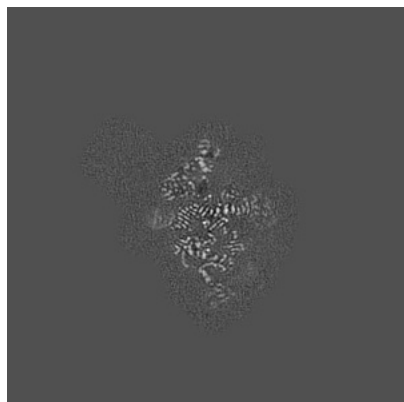


Z Index: 216

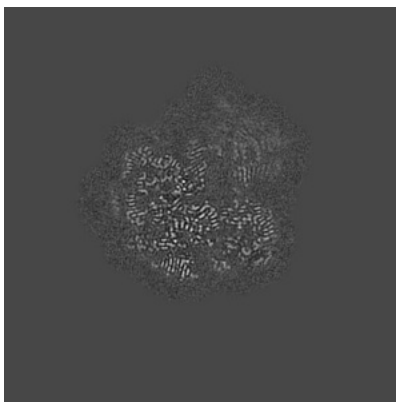
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

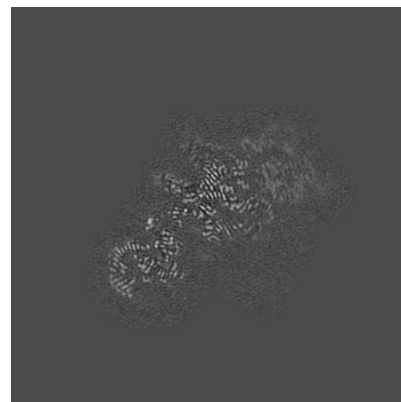
6.3.1 Primary map



X Index: 211

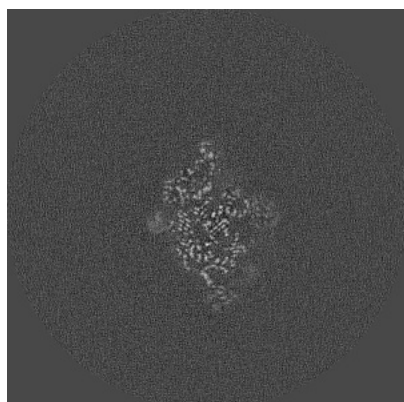


Y Index: 215

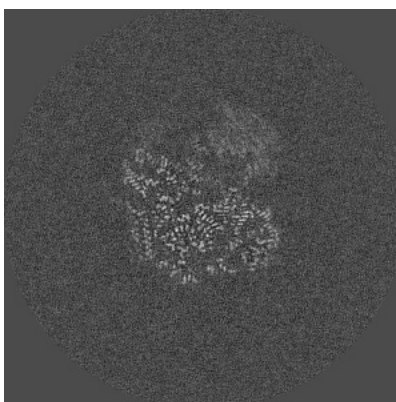


Z Index: 214

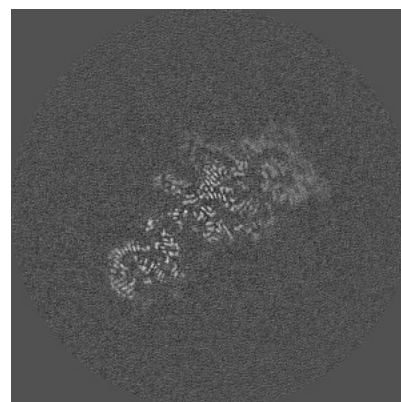
6.3.2 Raw map



X Index: 210



Y Index: 211

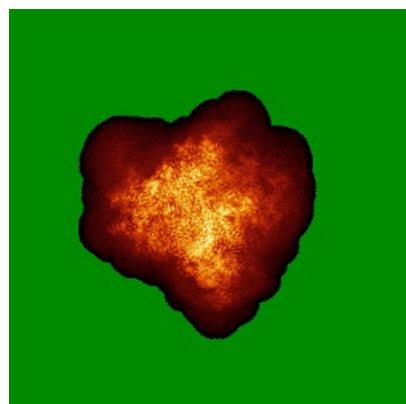


Z Index: 214

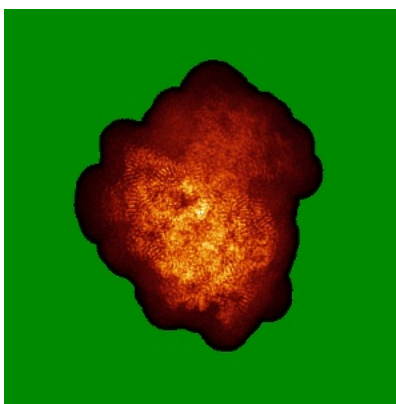
The images above show the largest variance slices of the map in three orthogonal directions.

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

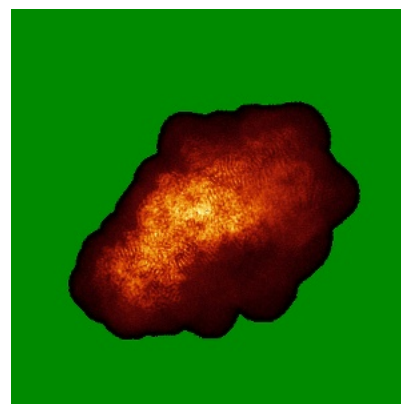
6.4.1 Primary map



X

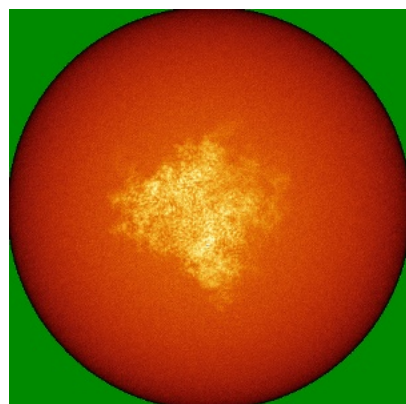


Y

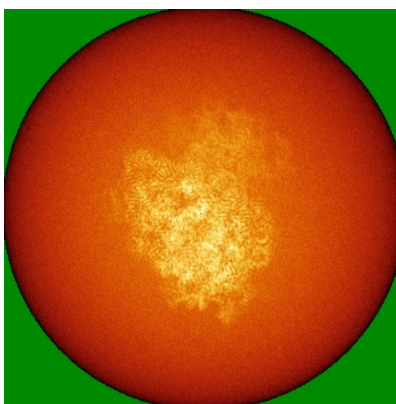


Z

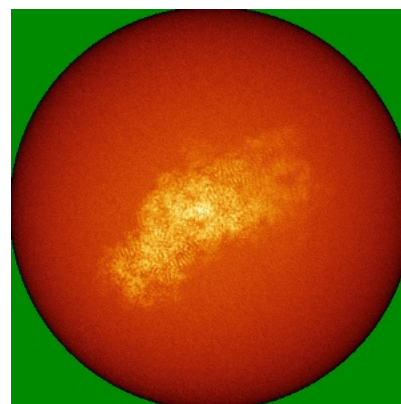
6.4.2 Raw map



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.

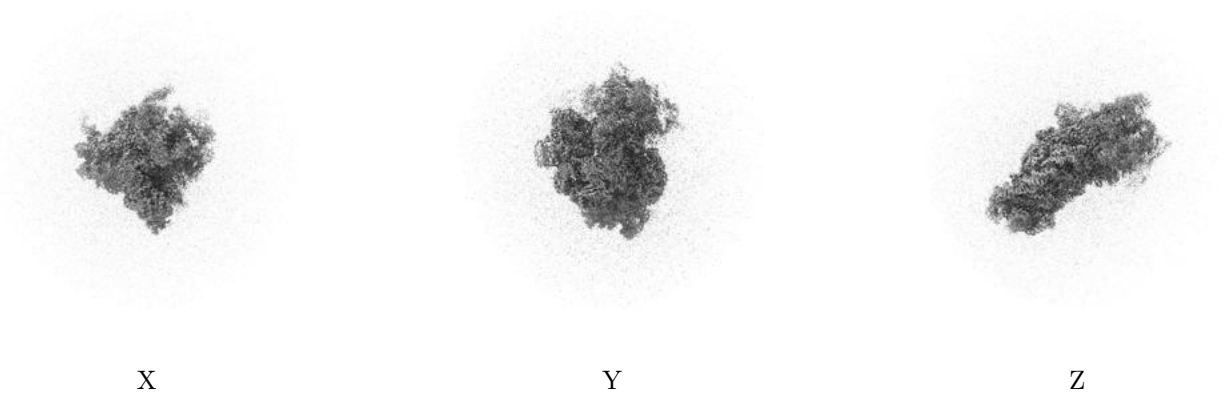
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0115. 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.

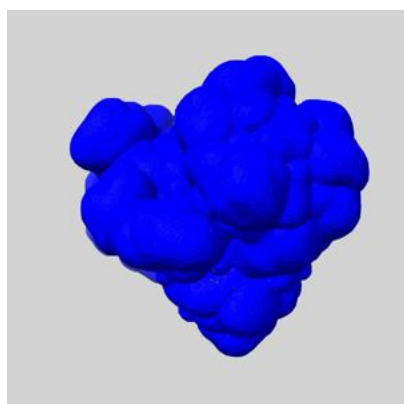
6.6 Mask visualisation [i](#)

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

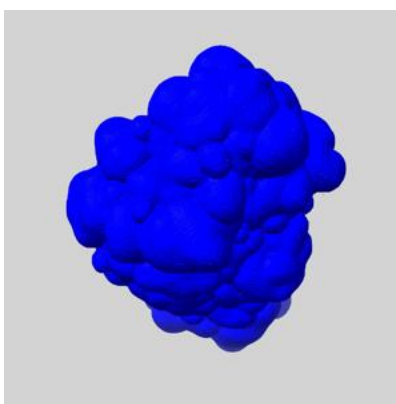
A mask typically either:

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

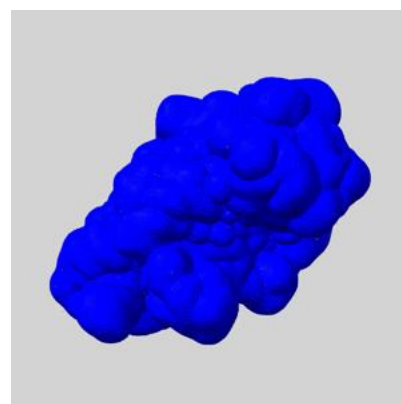
6.6.1 emd_50912_msk_1.map [i](#)



X



Y

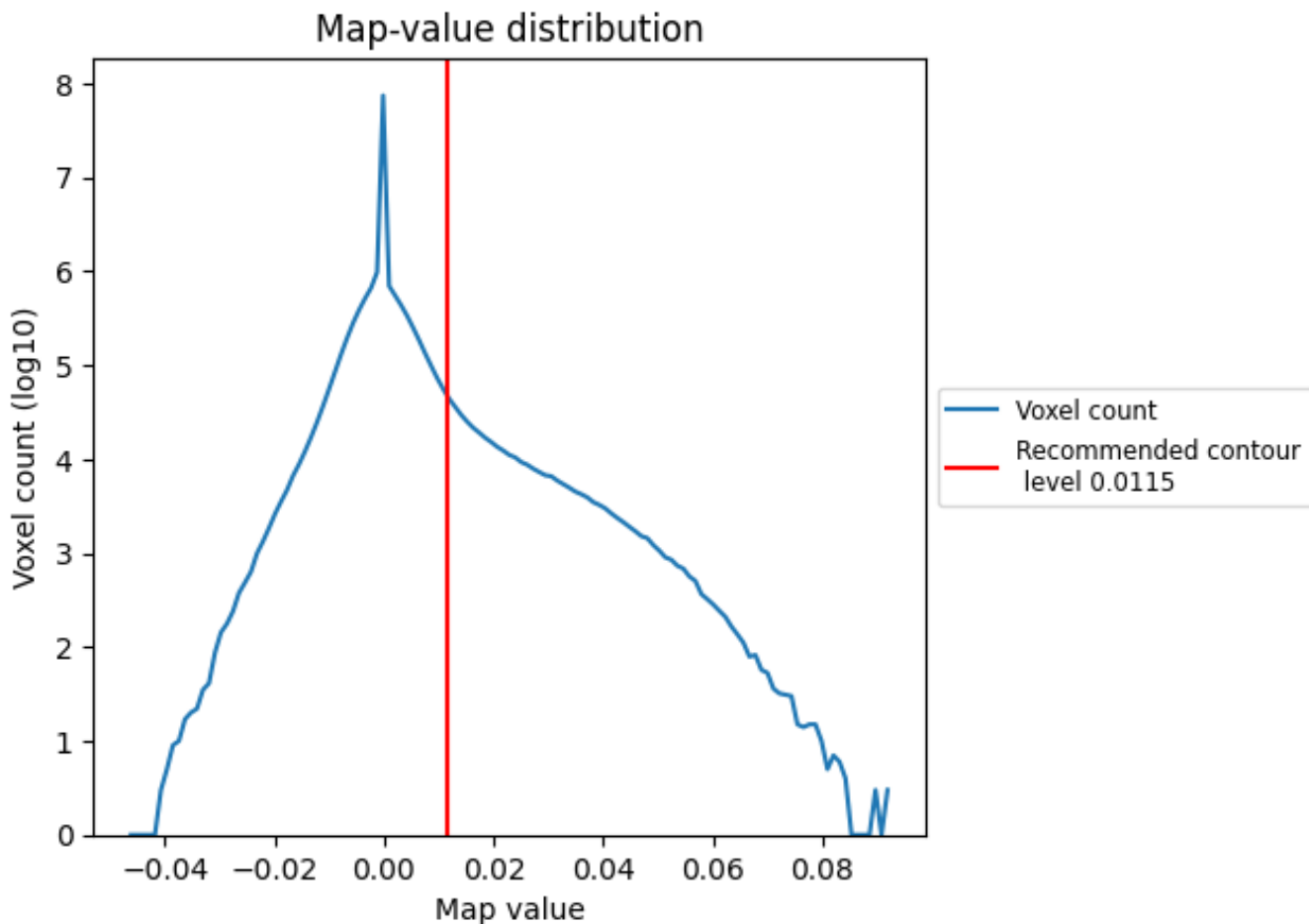


Z

7 Map analysis [i](#)

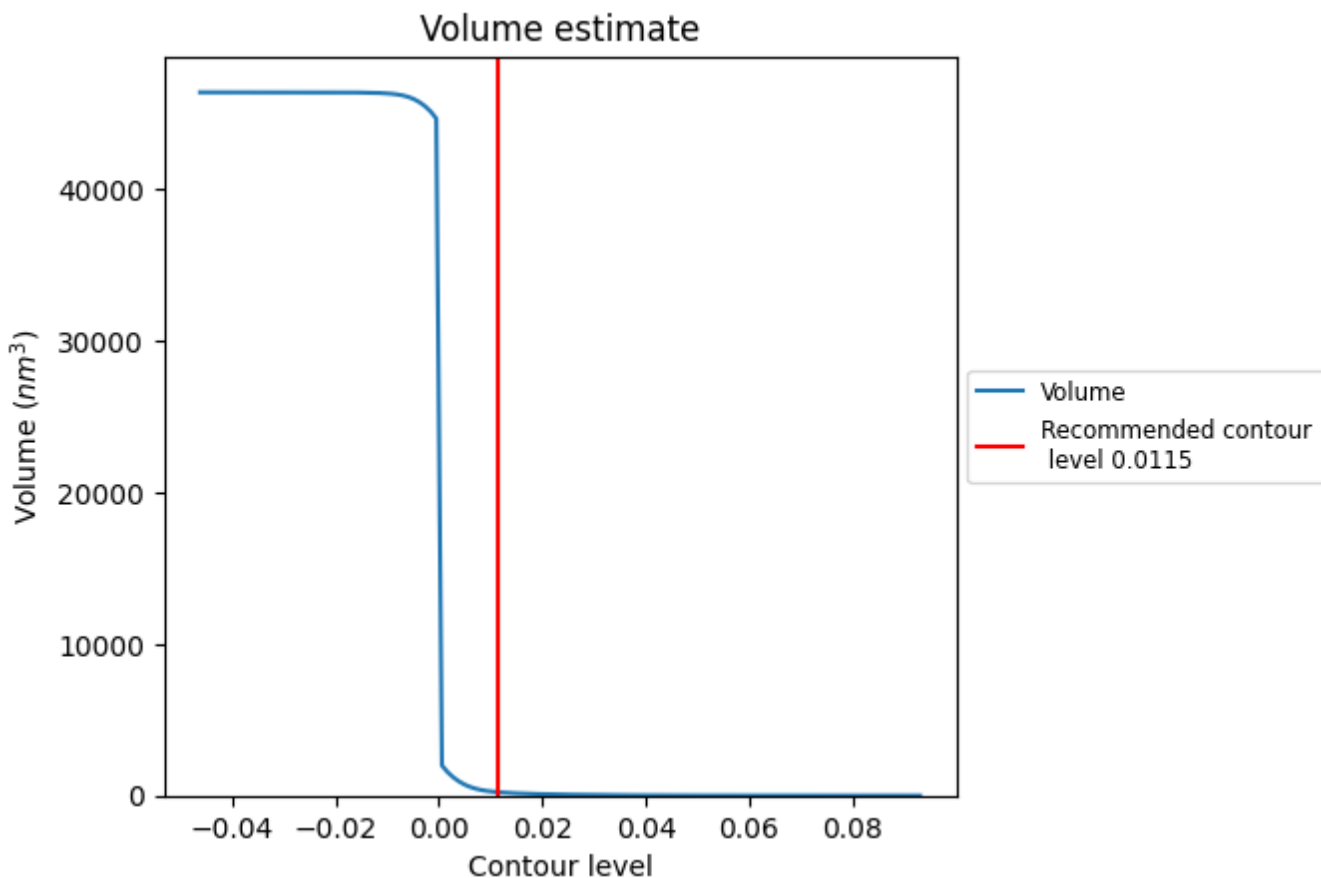
This section contains the results of statistical analysis of the map.

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.

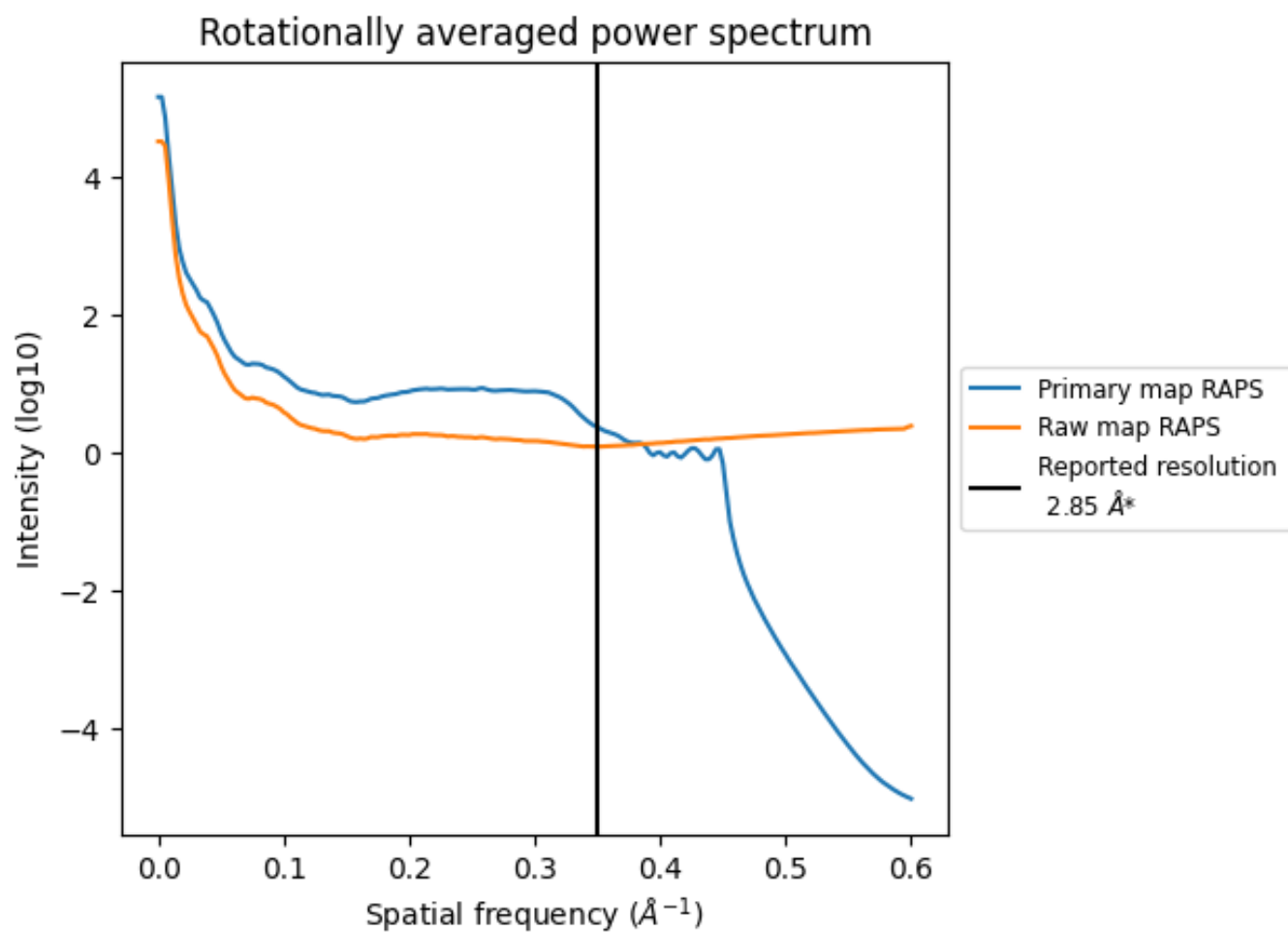
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 220 nm^3 ; this corresponds to an approximate mass of 199 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 i

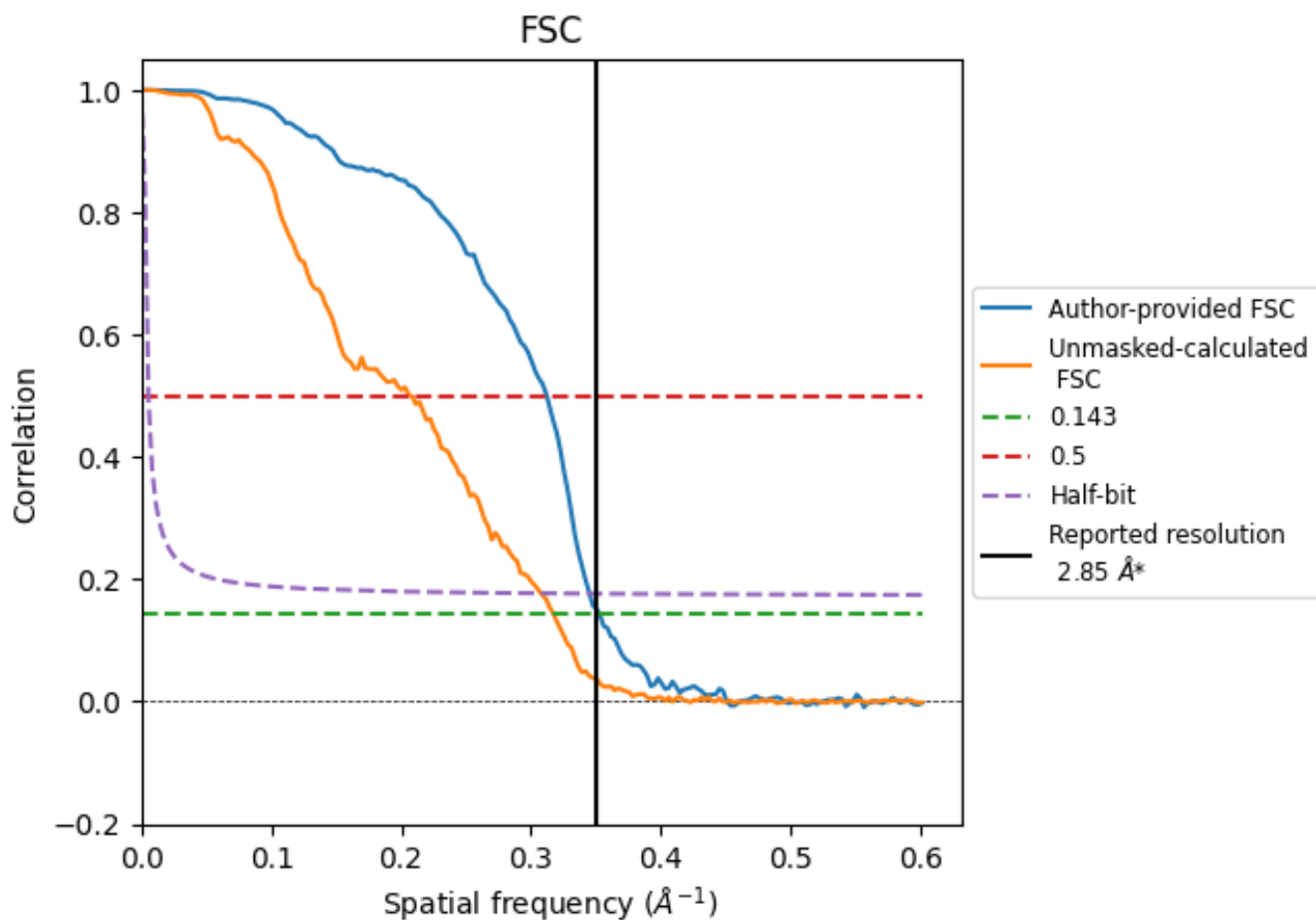


*Reported resolution corresponds to spatial frequency of 0.351 Å⁻¹

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 0.351 \AA^{-1}

8.2 Resolution estimates [i](#)

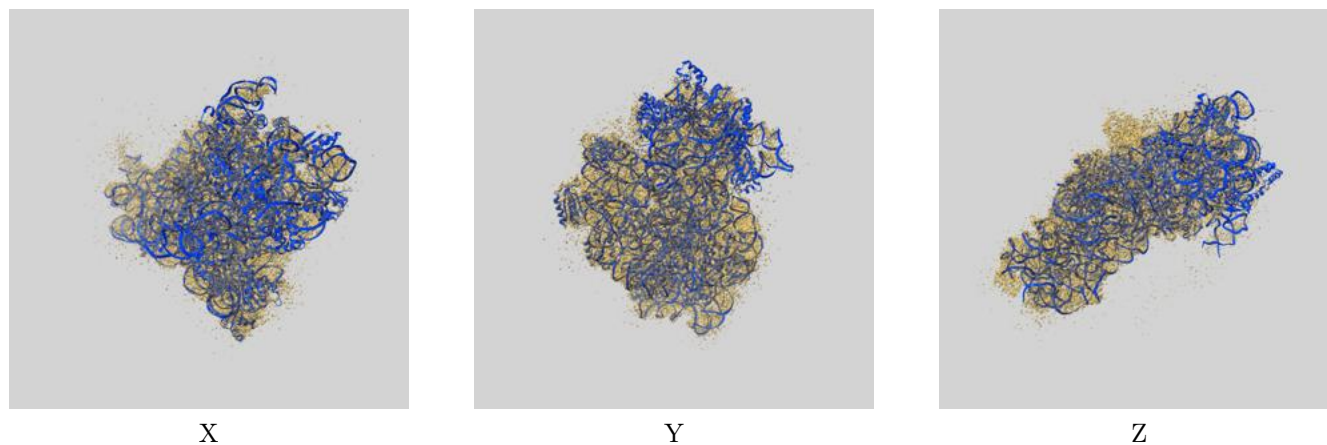
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.85	-	-
Author-provided FSC curve	2.84	3.20	2.90
Unmasked-calculated*	3.15	4.83	3.25

*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 3.15 differs from the reported value 2.85 by more than 10 %

9 Map-model fit [i](#)

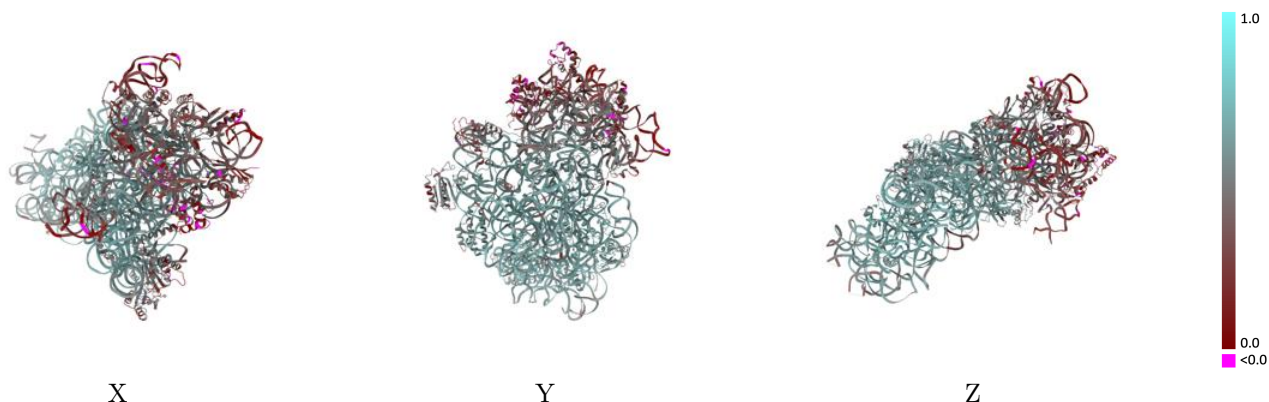
This section contains information regarding the fit between EMDB map EMD-50912 and PDB model 9G06. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



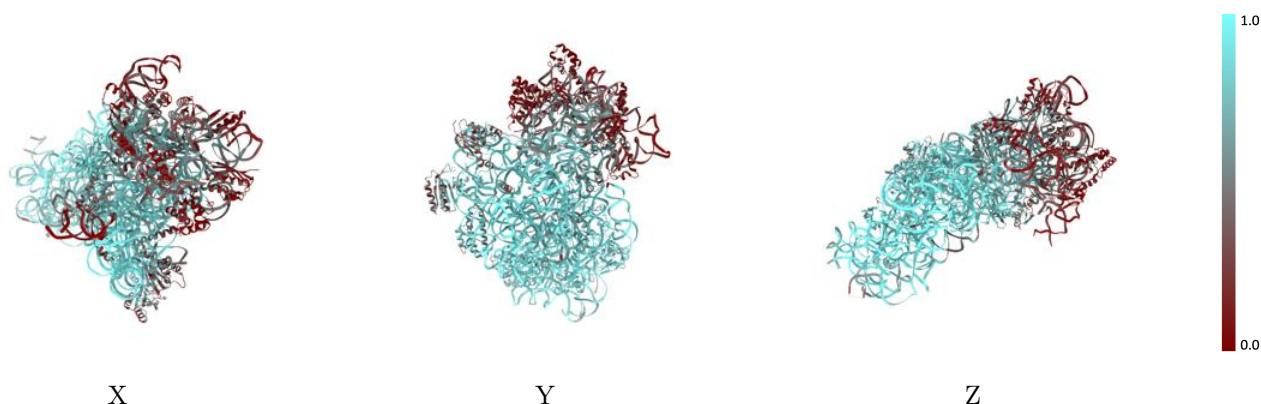
The images above show the 3D surface view of the map at the recommended contour level 0.0115 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



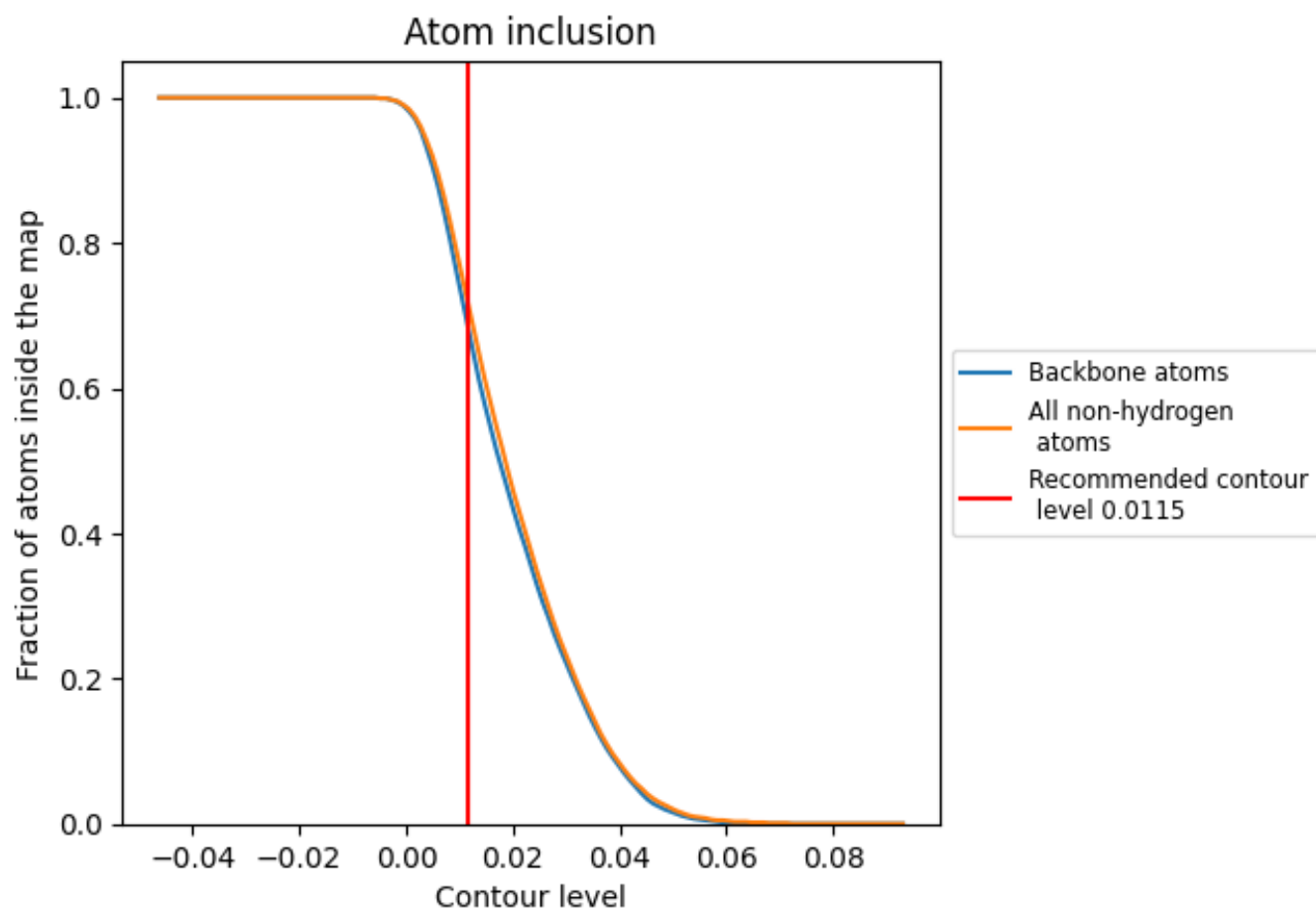
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0115).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 72% 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 (0.0115) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7210	 0.5320
B	 0.8210	 0.5670
C	 0.4720	 0.4760
D	 0.7820	 0.5840
E	 0.8640	 0.6250
F	 0.4800	 0.4230
G	 0.1080	 0.2030
H	 0.8700	 0.6270
I	 0.7410	 0.5760
J	 0.5290	 0.5180
K	 0.5810	 0.4180
L	 0.8910	 0.6420
M	 0.1410	 0.2290
N	 0.3860	 0.4090
O	 0.7230	 0.5660
P	 0.9040	 0.6480
Q	 0.8330	 0.6060
R	 0.6990	 0.5470
S	 0.1700	 0.3060
T	 0.8360	 0.6110
U	 0.4110	 0.3820
Y	 0.7710	 0.5580
a	 0.3070	 0.3420
b	 0.2710	 0.3210
c	 0.3010	 0.3600

