wwPDB EM Validation Summary Report

Feb 24, 2024 – 05:48 PM EST

PDB ID	:	7M4U
EMDB ID	:	EMD-23666
Title	:	A. baumannii Ribosome-Eravacycline complex: 30S
Authors	:	Morgan, C.E.; Yu, E.W.
Deposited on	:	2021-03-22
Resolution	:	2.71 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

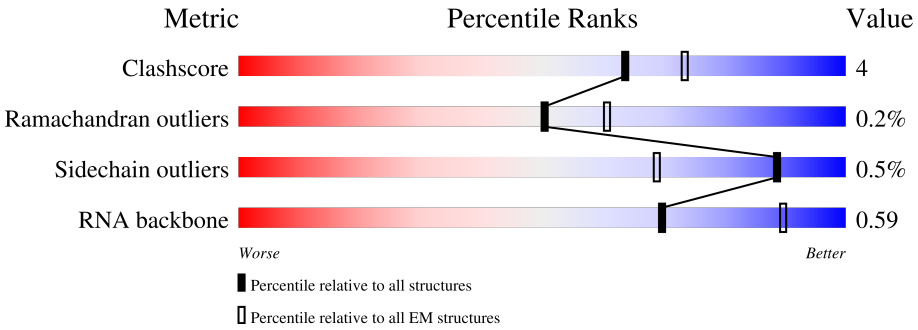
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.71 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	a	1544	5%, 83%, 16%
2	b	250	80%, 88%, 10%
3	c	250	86%, 14%
4	d	208	11%, 97%
5	e	165	94%, 6%
6	f	127	19%, 81%, 18%
7	g	156	19%, 90%, 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	h	131	99%
9	i	128	96%
10	j	103	97%
11	k	128	26% 91% 9%
12	l	124	97%
13	m	118	97%
14	n	101	99%
15	o	89	98%
16	p	101	82% 18%
17	q	85	92% 8%
18	r	75	69% 31%
19	s	91	90% 10%
20	t	88	98%
21	u	71	63% 89% 11%

2 Entry composition (i)

There are 24 unique types of molecules in this entry. The entry contains 51764 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16s Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	a	1528	32782	14631	5994	10630	1527	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	1007	U	C	conflict	GB 1211343212
a	1034	C	U	conflict	GB 1211343212

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	225	1769	1110	328	325	6	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	c	215	1690	1065	318	299	8	0	0

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	207	1631	1017	313	299	2	0	0

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	e	155	1129	700	217	207	5	0	0

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	104	Total	C	N	O	S	0	0
			867	546	158	159	4		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	141	Total	C	N	O	S	0	0
			1111	696	210	199	6		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	130	Total	C	N	O	S	0	0
			985	615	177	187	6		

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	124	Total	C	N	O	S	0	0
			970	606	191	172	1		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	100	Total	C	N	O	S	0	0
			801	500	150	148	3		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	117	Total	C	N	O	S	0	0
			862	535	167	159	1		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	122	Total	C	N	O	S	0	0
			945	580	193	167	5		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	115	Total	C	N	O	S	0	0
			903	558	184	158	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	100	Total	C	N	O	S	0	0
			792	493	158	137	4		

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	87	Total	C	N	O	S	0	0
			693	428	140	124	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	83	Total	C	N	O	S	0	0
			649	406	129	113	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	78	Total	C	N	O	S	0	0
			614	386	115	112	1		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	r	52	Total	C	N	O	0	0
			426	273	74	79		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	82	Total	C	N	O	S	0	0
			646	412	125	107	2		

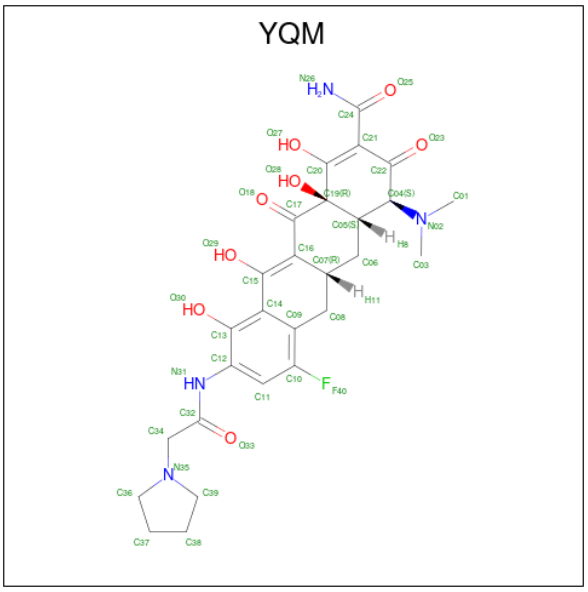
- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	86	Total	C	N	O	S	0	0
			663	409	139	113	2		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	u	63	Total	C	N	O	S	0	0
			522	327	105	89	1		

- Molecule 22 is Eravacycline (three-letter code: YQM) (formula: $C_{27}H_{31}FN_4O_8$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
22	a	1	Total	C	F	N	O	0
			40	27	1	4	8	

- Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
23	a	82	Total	Mg	0
			82	82	
23	e	1	Total	Mg	0
			1	1	

- Molecule 24 is water.

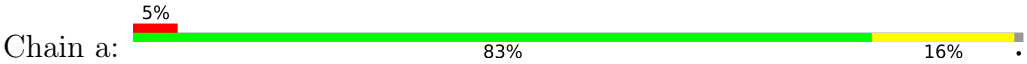
Mol	Chain	Residues	Atoms	AltConf
24	a	184	Total O 184 184	0
24	i	1	Total O 1 1	0
24	n	2	Total O 2 2	0
24	t	4	Total O 4 4	0

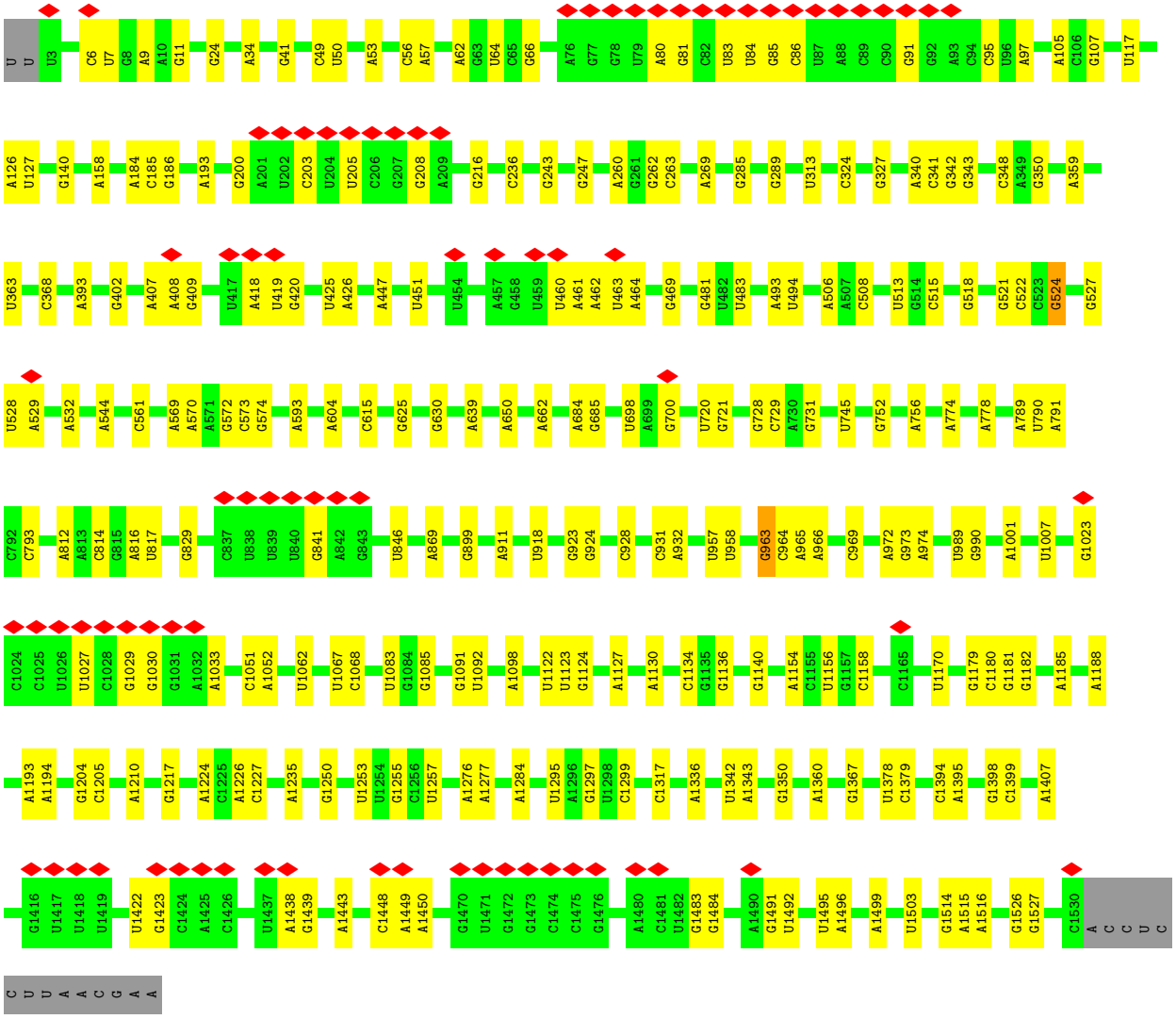
3 Residue-property plots (i)

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: 16s Ribosomal RNA

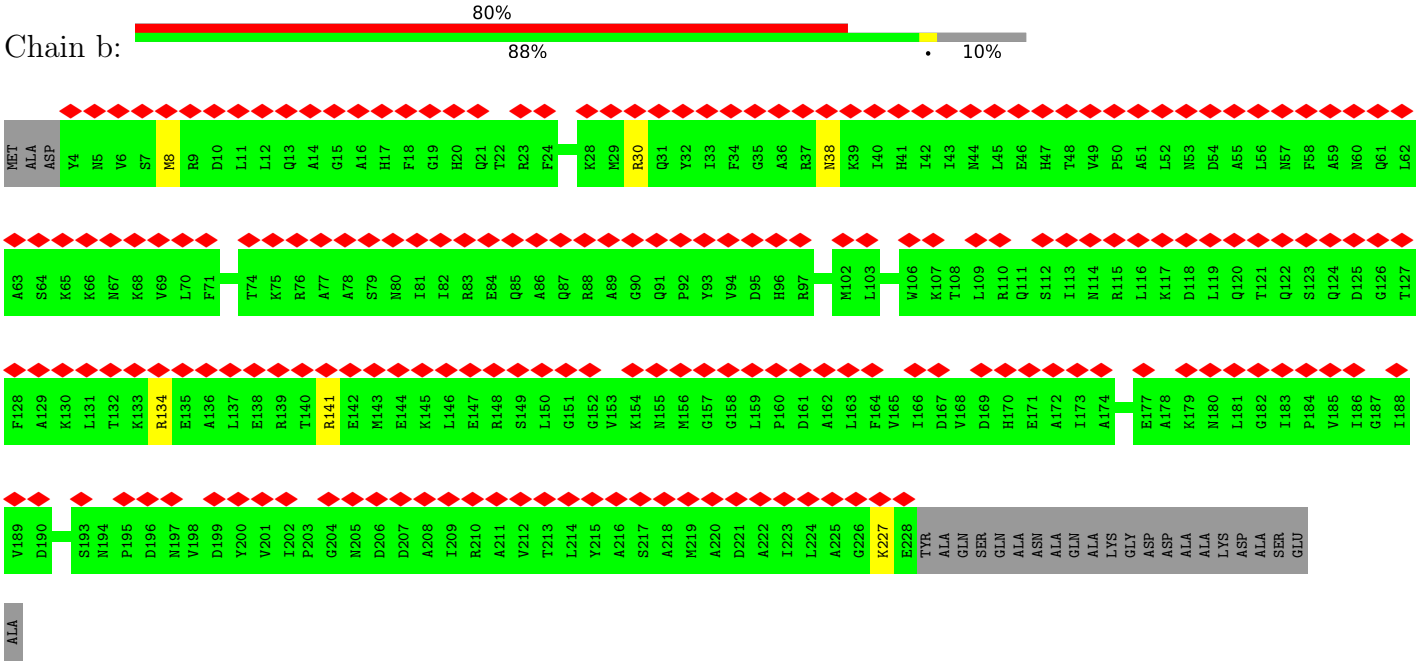
Chain a:





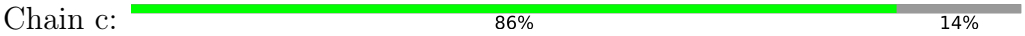
• Molecule 2: 30S ribosomal protein S2

Chain b:



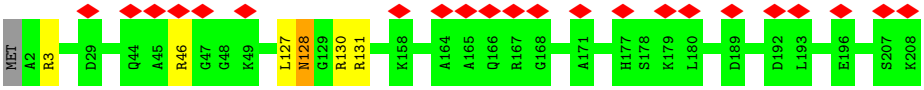
• Molecule 3: 30S ribosomal protein S3

Chain c:



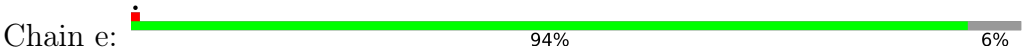
• Molecule 4: 30S ribosomal protein S4

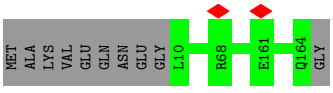
Chain d:



• Molecule 5: 30S ribosomal protein S5

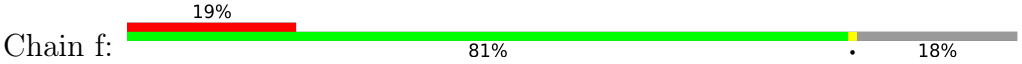
Chain e:

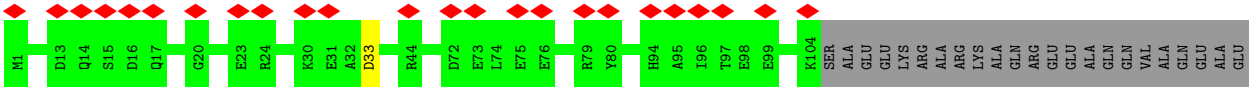




• Molecule 6: 30S ribosomal protein S6

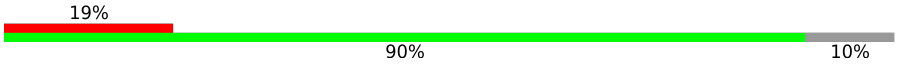
Chain f:

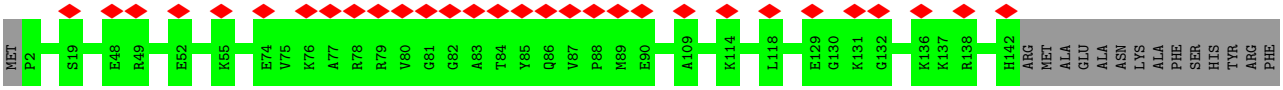




• Molecule 7: 30S ribosomal protein S7

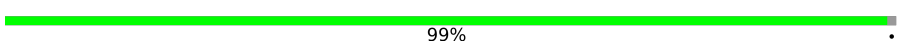
Chain g:





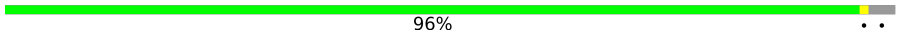
• Molecule 8: 30S ribosomal protein S8

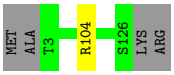
Chain h:



• Molecule 9: 30S ribosomal protein S9

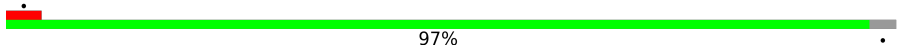
Chain i:

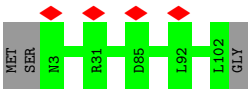




• Molecule 10: 30S ribosomal protein S10

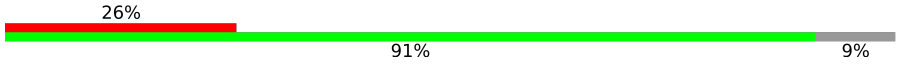
Chain j:

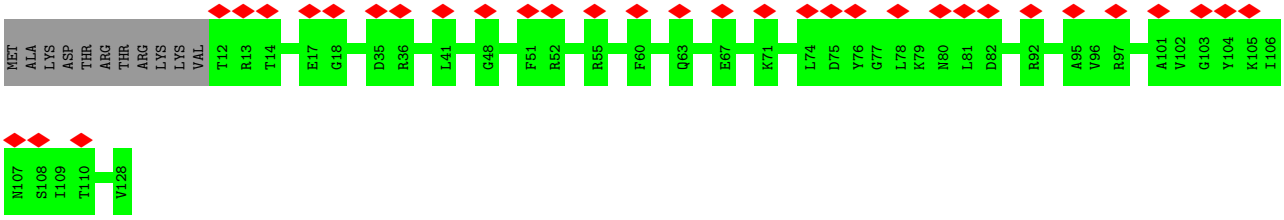




• Molecule 11: 30S ribosomal protein S11

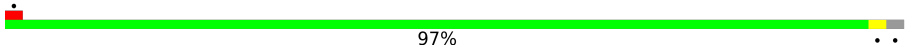
Chain k:

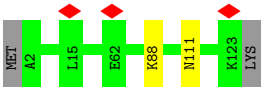




• Molecule 12: 30S ribosomal protein S12

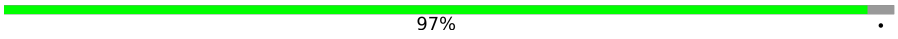
Chain l:

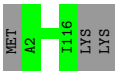




• Molecule 13: 30S ribosomal protein S13

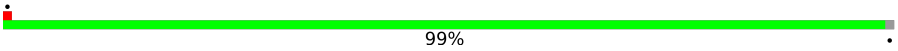
Chain m:

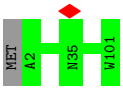




• Molecule 14: 30S ribosomal protein S14

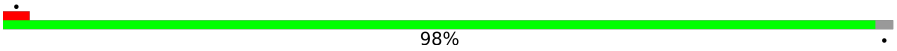
Chain n:

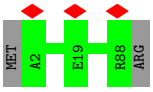




• Molecule 15: 30S ribosomal protein S15

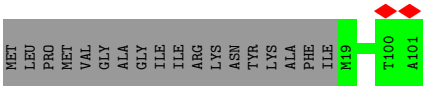
Chain o:





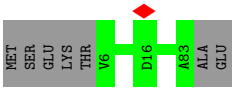
• Molecule 16: 30S ribosomal protein S16

Chain p:



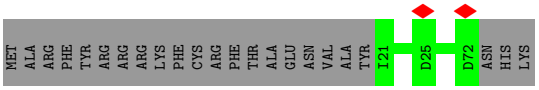
• Molecule 17: 30S ribosomal protein S17

Chain q:



• Molecule 18: 30S ribosomal protein S18

Chain r:

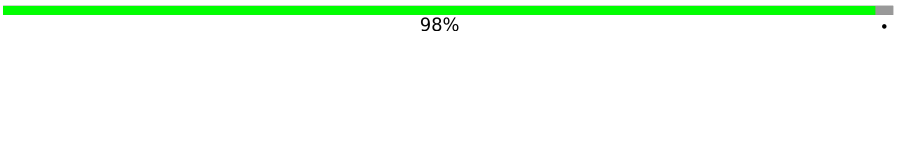


• Molecule 19: 30S ribosomal protein S19

Chain s:

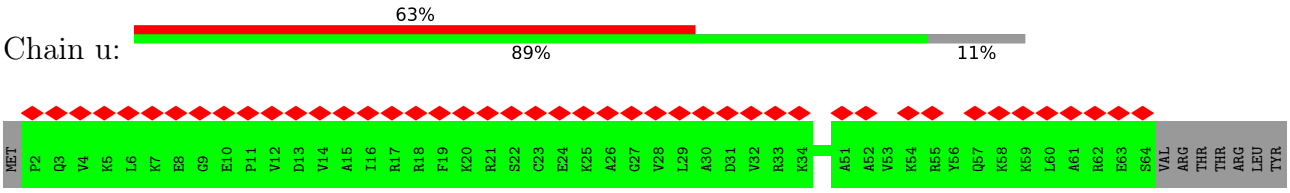
• Molecule 20: 30S ribosomal protein S20

Chain t:



• Molecule 21: 30S ribosomal protein S21

Chain u:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47367	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 ($e^-/Å^2$)	46	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.987	Depositor
Minimum map value	-1.036	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.053	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	434.176, 434.176, 434.176	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.848, 0.848, 0.848	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: 4OC, MA6, PSU, YQM, UR3, MG, 5MC, 7MG, 2MG

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	a	0.27	0/36476	0.75	1/56895 (0.0%)
2	b	0.26	0/1799	0.53	0/2429
3	c	0.25	0/1714	0.54	0/2304
4	d	0.27	0/1653	0.57	2/2213 (0.1%)
5	e	0.25	0/1141	0.55	0/1537
6	f	0.24	0/882	0.50	0/1189
7	g	0.25	0/1127	0.54	0/1511
8	h	0.24	0/993	0.52	0/1331
9	i	0.26	0/981	0.60	0/1314
10	j	0.25	0/811	0.55	0/1096
11	k	0.25	0/878	0.54	0/1189
12	l	0.25	0/958	0.60	0/1284
13	m	0.24	0/913	0.59	0/1226
14	n	0.27	0/803	0.58	0/1071
15	o	0.25	0/703	0.51	0/944
16	p	0.24	0/660	0.57	0/886
17	q	0.23	0/621	0.52	0/837
18	r	0.25	0/432	0.53	0/583
19	s	0.25	0/664	0.53	0/897
20	t	0.25	0/669	0.52	0/892
21	u	0.25	0/528	0.53	0/697
All	All	0.26	0/55406	0.70	3/82325 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	d	128	ASN	CB-CA-C	7.22	124.83	110.40
4	d	131	ARG	CB-CA-C	7.20	124.80	110.40
1	a	1123	U	P-O3'-C3'	5.10	125.83	119.70

There are no chirality outliers.

There are no planarity outliers.

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	a	32782	0	16508	0	0
2	b	1769	0	1787	0	0
3	c	1690	0	1774	0	0
4	d	1631	0	1691	0	0
5	e	1129	0	1174	0	0
6	f	867	0	868	0	0
7	g	1111	0	1163	0	0
8	h	985	0	1047	0	0
9	i	970	0	1022	0	0
10	j	801	0	832	0	0
11	k	862	0	877	0	0
12	l	945	0	998	0	0
13	m	903	0	962	0	0
14	n	792	0	833	0	0
15	o	693	0	699	0	0
16	p	649	0	660	0	0
17	q	614	0	658	0	0
18	r	426	0	447	0	0
19	s	646	0	663	0	0
20	t	663	0	715	0	0
21	u	522	0	565	0	0
22	a	40	0	0	0	0
23	a	82	0	0	0	0
23	e	1	0	0	0	0
24	a	184	0	0	0	0
24	i	1	0	0	0	0
24	n	2	0	0	0	0
24	t	4	0	0	0	0
All	All	51764	0	35943	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	b	223/250 (89%)	211 (95%)	9 (4%)	3 (1%)	12 28
3	c	213/250 (85%)	202 (95%)	11 (5%)	0	100 100
4	d	205/208 (99%)	201 (98%)	4 (2%)	0	100 100
5	e	153/165 (93%)	150 (98%)	3 (2%)	0	100 100
6	f	102/127 (80%)	96 (94%)	5 (5%)	1 (1%)	15 35
7	g	139/156 (89%)	134 (96%)	5 (4%)	0	100 100
8	h	128/131 (98%)	126 (98%)	2 (2%)	0	100 100
9	i	122/128 (95%)	119 (98%)	3 (2%)	0	100 100
10	j	98/103 (95%)	94 (96%)	4 (4%)	0	100 100
11	k	115/128 (90%)	109 (95%)	6 (5%)	0	100 100
12	l	120/124 (97%)	111 (92%)	8 (7%)	1 (1%)	19 41
13	m	113/118 (96%)	107 (95%)	6 (5%)	0	100 100
14	n	98/101 (97%)	94 (96%)	4 (4%)	0	100 100
15	o	85/89 (96%)	84 (99%)	1 (1%)	0	100 100
16	p	81/101 (80%)	81 (100%)	0	0	100 100
17	q	76/85 (89%)	76 (100%)	0	0	100 100
18	r	50/75 (67%)	50 (100%)	0	0	100 100
19	s	80/91 (88%)	78 (98%)	2 (2%)	0	100 100
20	t	84/88 (96%)	84 (100%)	0	0	100 100
21	u	61/71 (86%)	61 (100%)	0	0	100 100
All	All	2346/2589 (91%)	2268 (97%)	73 (3%)	5 (0%)	50 72

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	30	ARG
6	f	33	ASP
12	l	88	LYS
2	b	8	MET
2	b	38	ASN

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
2	b	185/200 (92%)	182 (98%)	3 (2%)	62 83
3	c	175/198 (88%)	175 (100%)	0	100 100
4	d	170/171 (99%)	165 (97%)	5 (3%)	42 70
5	e	113/120 (94%)	113 (100%)	0	100 100
6	f	94/111 (85%)	94 (100%)	0	100 100
7	g	116/128 (91%)	116 (100%)	0	100 100
8	h	108/109 (99%)	108 (100%)	0	100 100
9	i	97/100 (97%)	96 (99%)	1 (1%)	76 90
10	j	89/91 (98%)	89 (100%)	0	100 100
11	k	88/98 (90%)	88 (100%)	0	100 100
12	l	104/106 (98%)	103 (99%)	1 (1%)	76 90
13	m	95/98 (97%)	95 (100%)	0	100 100
14	n	81/82 (99%)	81 (100%)	0	100 100
15	o	70/72 (97%)	70 (100%)	0	100 100
16	p	63/77 (82%)	63 (100%)	0	100 100
17	q	70/76 (92%)	70 (100%)	0	100 100
18	r	46/66 (70%)	46 (100%)	0	100 100
19	s	70/78 (90%)	70 (100%)	0	100 100
20	t	65/67 (97%)	65 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
21	u	54/62 (87%)	54 (100%)	0	100 100
All	All	1953/2110 (93%)	1943 (100%)	10 (0%)	89 95

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	d	130	ARG
9	i	104	ARG
12	l	111	ASN
4	d	3	ARG
4	d	46	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
18	r	54	GLN
12	l	72	HIS
10	j	56	HIS
7	g	29	HIS
11	k	21	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1524/1544 (98%)	239 (15%)	0

5 of 239 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	6	C
1	a	7	U
1	a	9	A
1	a	11	G
1	a	24	G

There are no RNA pucker outliers to report.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	7MG	a	524	1	22,26,27	1.18	1 (4%)	29,39,42	0.80	2 (6%)
1	2MG	a	1204	1	18,26,27	1.17	2 (11%)	16,38,41	0.88	1 (6%)
1	MA6	a	1515	1	19,26,27	1.04	2 (10%)	18,38,41	3.47	2 (11%)
1	PSU	a	513	1	18,21,22	1.11	1 (5%)	22,30,33	1.80	5 (22%)
1	5MC	a	964	1	18,22,23	0.56	0	26,32,35	0.59	0
1	2MG	a	963	1	18,26,27	1.18	2 (11%)	16,38,41	0.89	1 (6%)
1	4OC	a	1399	1	20,23,24	3.16	8 (40%)	26,32,35	0.90	1 (3%)
1	MA6	a	1516	1	19,26,27	1.04	2 (10%)	18,38,41	3.45	2 (11%)
1	UR3	a	1495	1	19,22,23	2.89	7 (36%)	26,32,35	1.31	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	7MG	a	524	1	-	2/7/37/38	0/3/3/3
1	2MG	a	1204	1	-	0/5/27/28	0/3/3/3
1	MA6	a	1515	1	-	2/7/29/30	0/3/3/3
1	PSU	a	513	1	-	3/7/25/26	0/2/2/2
1	5MC	a	964	1	-	2/7/25/26	0/2/2/2
1	2MG	a	963	1	-	0/5/27/28	0/3/3/3
1	4OC	a	1399	1	-	1/9/29/30	0/2/2/2
1	MA6	a	1516	1	-	2/7/29/30	0/3/3/3
1	UR3	a	1495	1	-	0/7/25/26	0/2/2/2

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	1399	4OC	C4-N3	6.85	1.44	1.32
1	a	1495	UR3	C2-N1	6.85	1.48	1.38
1	a	1495	UR3	C6-C5	6.79	1.50	1.35
1	a	1399	4OC	C6-C5	6.29	1.49	1.35
1	a	1399	4OC	C2-N3	6.08	1.48	1.36

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	1515	MA6	N1-C6-N6	-13.45	102.90	117.06
1	a	1516	MA6	N1-C6-N6	-13.40	102.96	117.06
1	a	1515	MA6	N3-C2-N1	-5.62	119.89	128.68
1	a	1516	MA6	N3-C2-N1	-5.46	120.14	128.68
1	a	1495	UR3	C4-N3-C2	-4.94	119.91	124.56

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	513	PSU	C2'-C1'-C5-C4
1	a	524	7MG	C3'-C4'-C5'-O5'
1	a	964	5MC	O4'-C4'-C5'-O5'
1	a	964	5MC	C3'-C4'-C5'-O5'
1	a	524	7MG	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 84 ligands modelled in this entry, 83 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	$\#\|Z\| > 2$
22	YQM	a	1601	23	42,44,44	3.28	20 (47%)	47,69,69	2.71	20 (42%)

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
22	YQM	a	1601	23	-	2/16/81/81	0/5/5/5

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	1601	YQM	C19-C20	13.86	1.64	1.52
22	a	1601	YQM	C19-C17	6.75	1.64	1.55
22	a	1601	YQM	C21-C24	4.99	1.57	1.47
22	a	1601	YQM	C32-N31	3.90	1.44	1.35
22	a	1601	YQM	C09-C10	3.88	1.44	1.38

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	a	1601	YQM	C34-C32-N31	6.90	127.09	114.12
22	a	1601	YQM	C11-C12-C13	-5.66	114.87	120.49
22	a	1601	YQM	O18-C17-C19	-4.71	109.87	119.08
22	a	1601	YQM	C34-N35-C39	-4.54	107.22	113.25
22	a	1601	YQM	O33-C32-C34	-4.54	113.13	121.08

There are no chirality outliers.

All (2) torsion outliers are listed below:

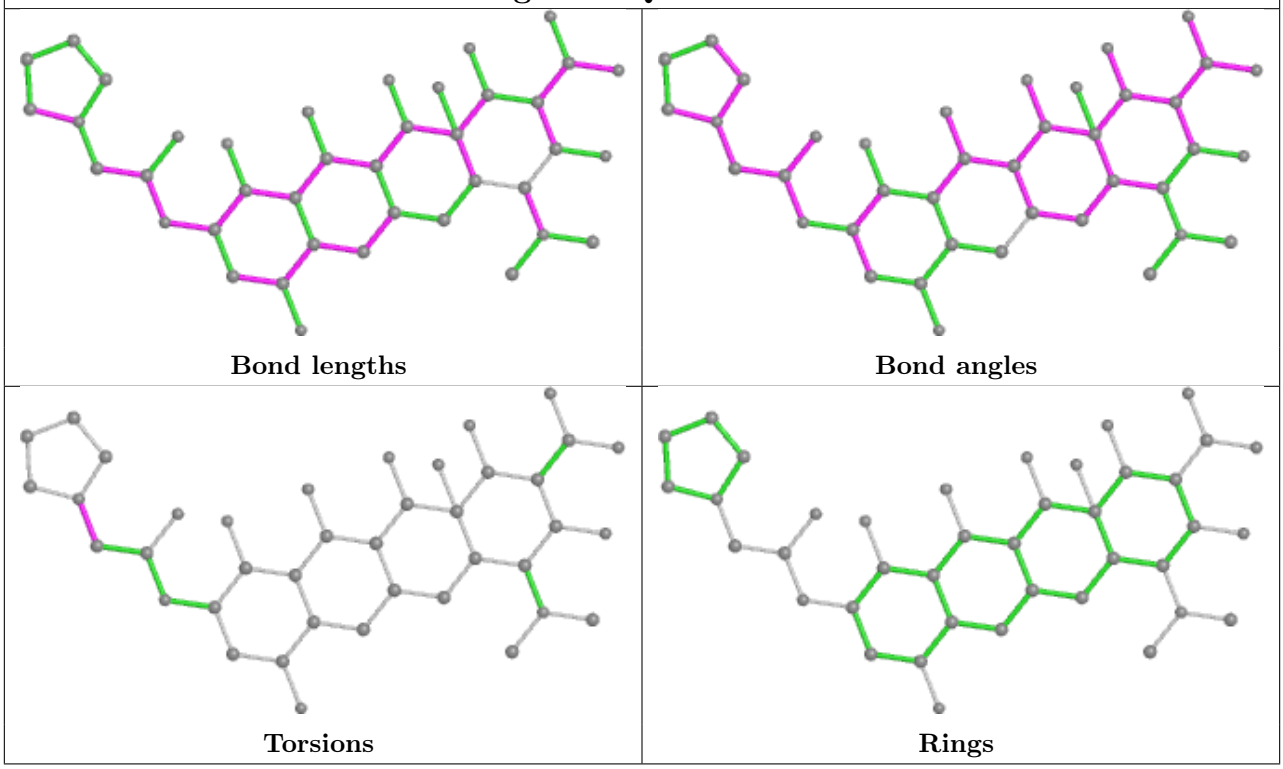
Mol	Chain	Res	Type	Atoms
22	a	1601	YQM	C32-C34-N35-C36
22	a	1601	YQM	C32-C34-N35-C39

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 then 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.

Ligand YQM a 1601



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

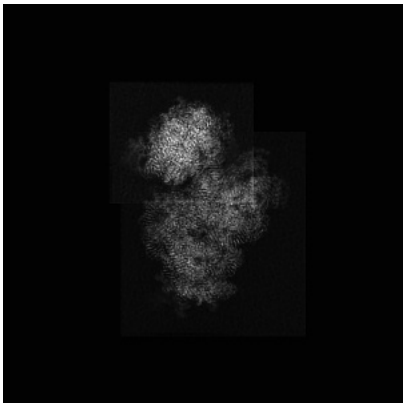
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23666. These allow visual inspection of the internal detail of the map and identification of artifacts.

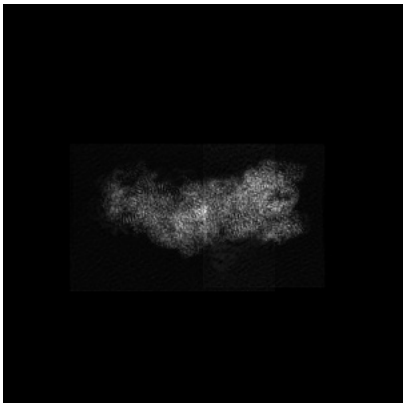
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

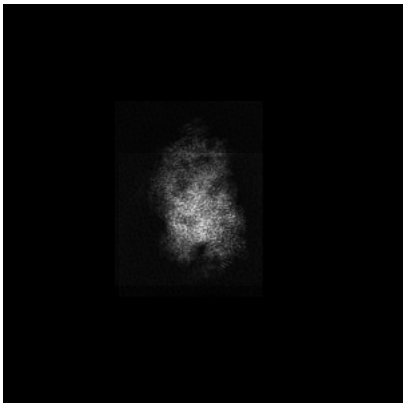
6.1.1 Primary map



X



Y



Z

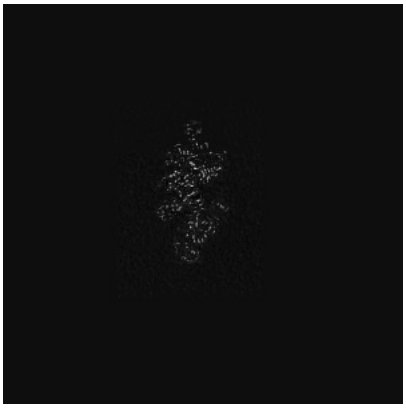
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map

X Index: 256

Y Index: 256



Z Index: 256

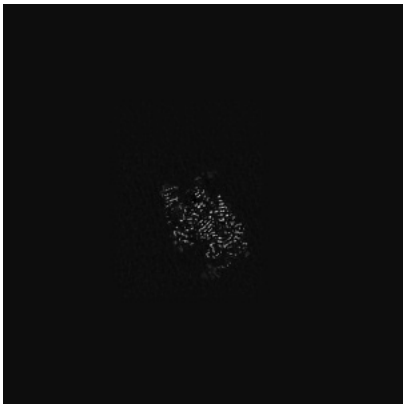
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 258

Y Index: 222

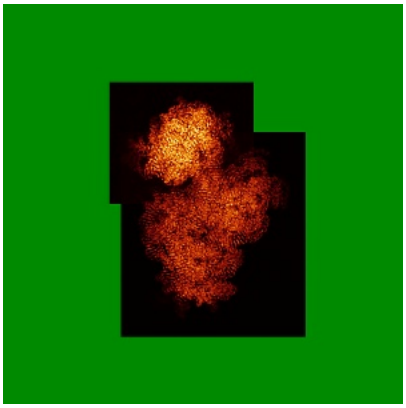


Z Index: 335

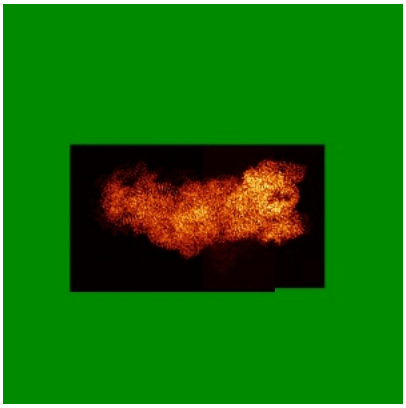
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

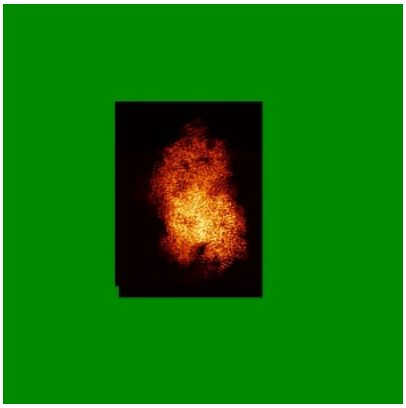
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

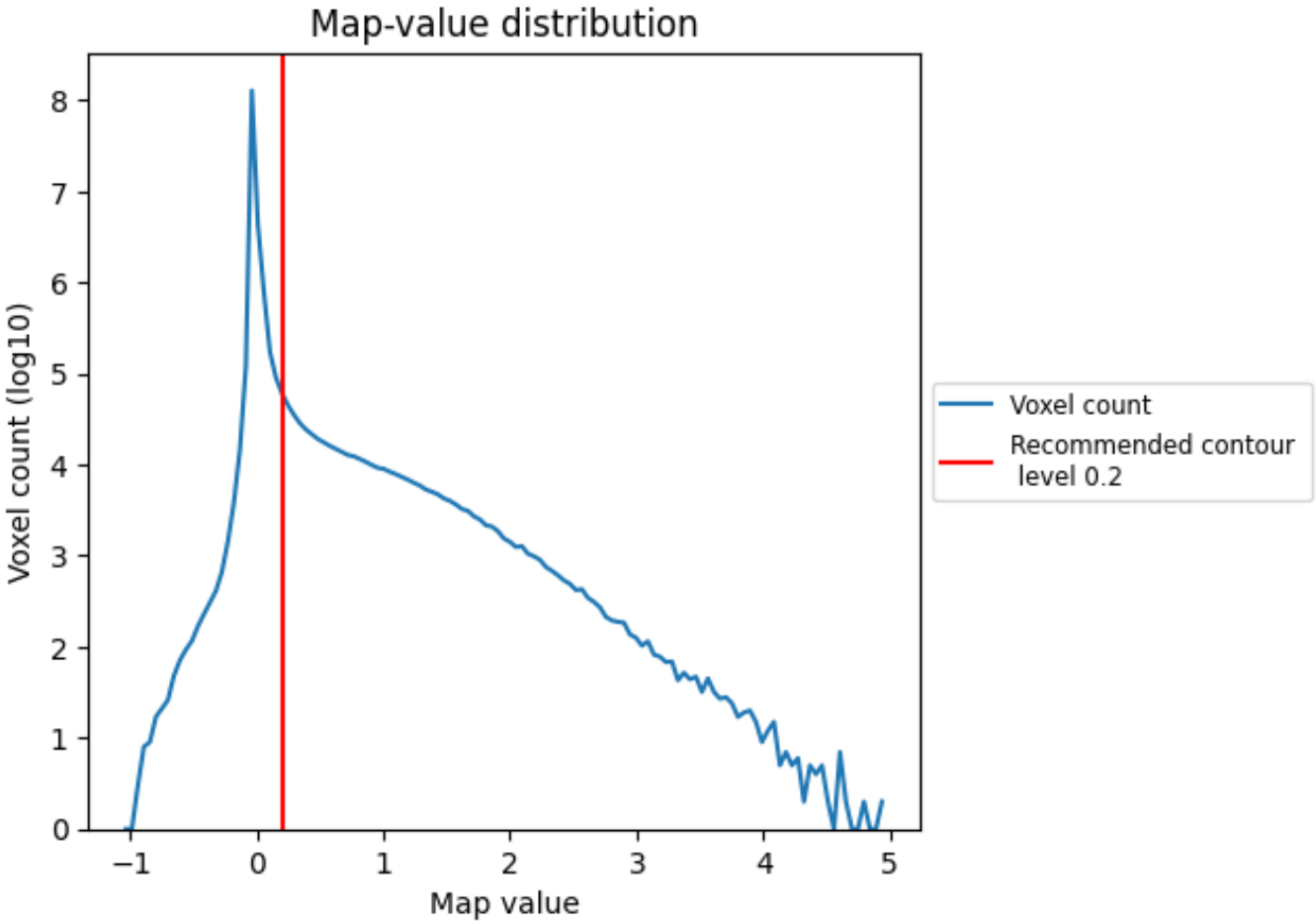
6.6 Mask visualisation (i)

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

7 Map analysis

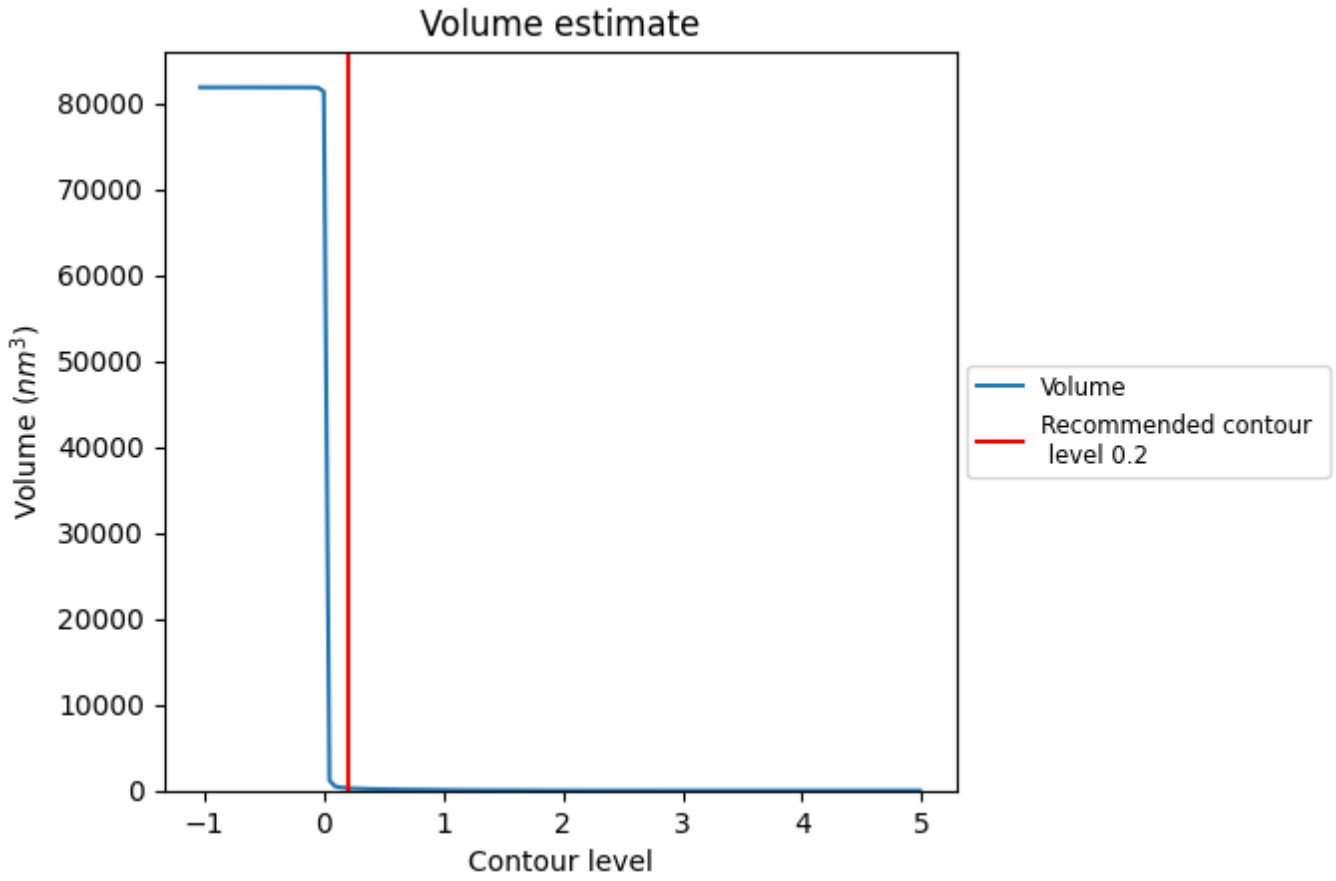
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

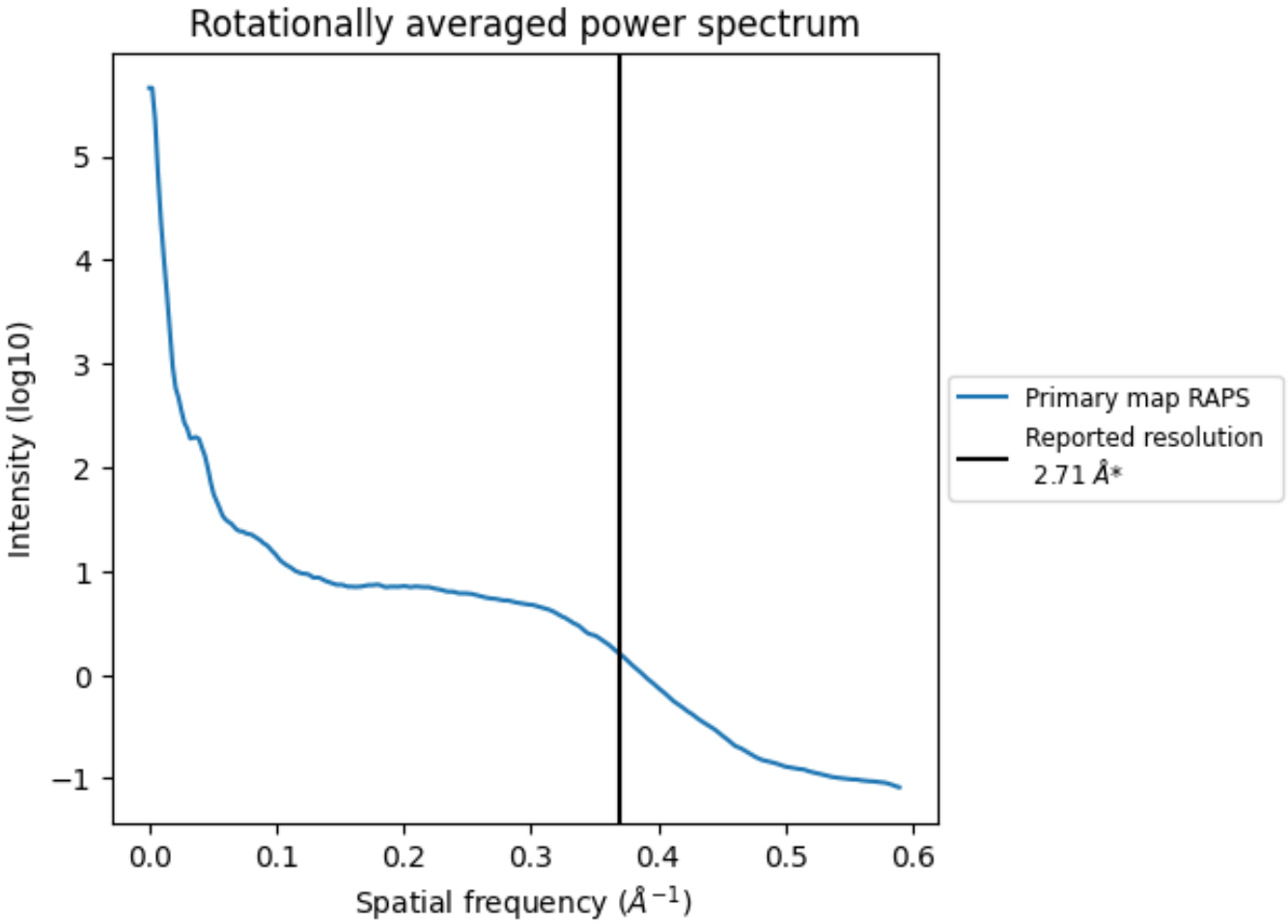
7.2 Volume estimate (i)



The volume at the recommended contour level is 288 nm^3; this corresponds to an approximate mass of 260 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 0.369 $Å^{-1}$

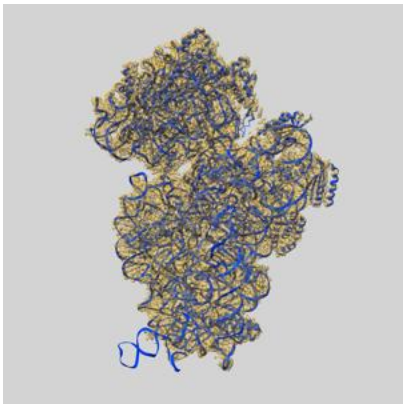
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

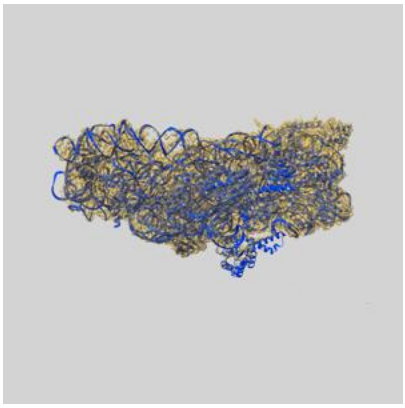
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23666 and PDB model 7M4U. Per-residue inclusion information can be found in section 3 on page 9.

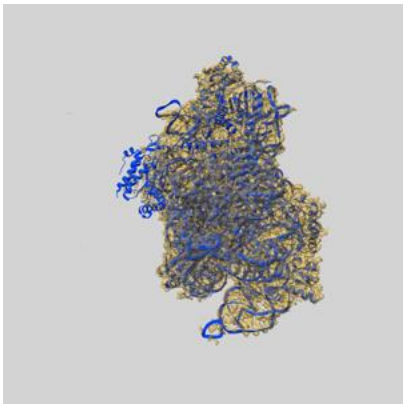
9.1 Map-model overlay



X



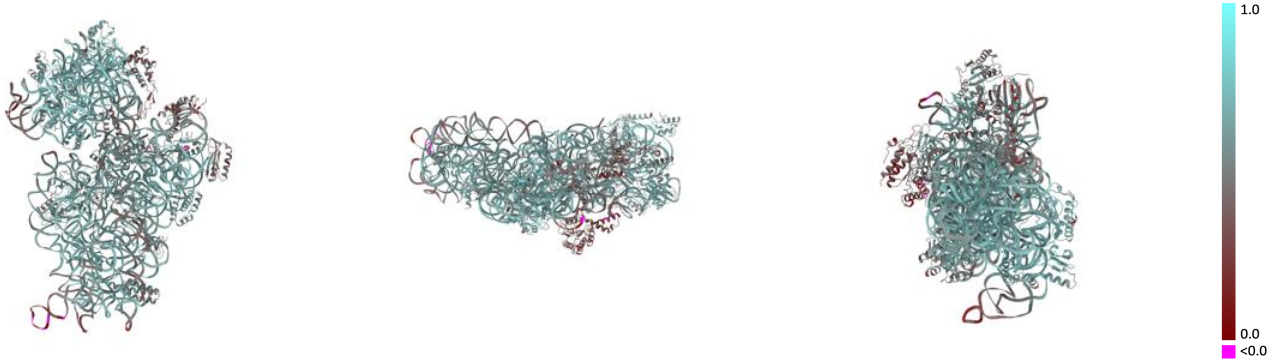
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 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.

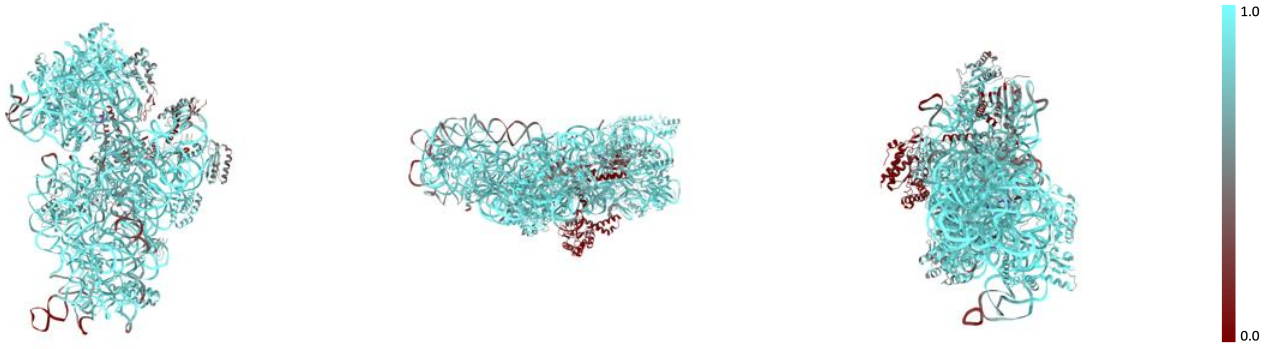
9.2 Q-score mapped to coordinate model



X Y Z

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.

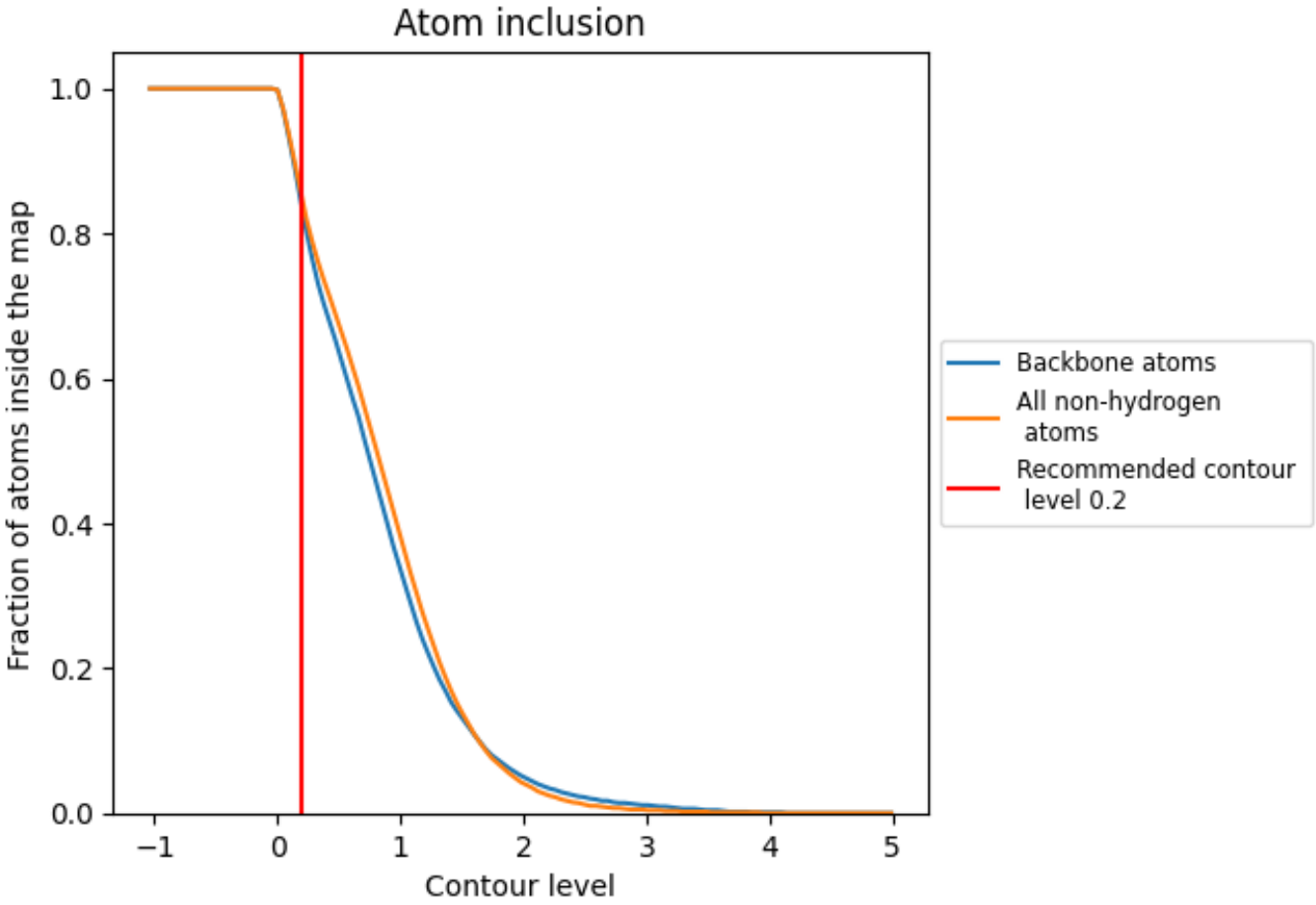
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 85% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8460	0.5870
a	0.9000	0.6050
b	0.1500	0.3220
c	0.9150	0.6300
d	0.7500	0.5420
e	0.8790	0.6010
f	0.6060	0.4630
g	0.6650	0.4570
h	0.9190	0.6490
i	0.9470	0.6670
j	0.8750	0.6130
k	0.5850	0.4410
l	0.8500	0.5960
m	0.9110	0.6110
n	0.9280	0.6640
o	0.8970	0.6120
p	0.9120	0.6730
q	0.8220	0.5630
r	0.8160	0.5640
s	0.9570	0.6720
t	0.9030	0.6210
u	0.2530	0.3760