wwPDB EM Validation Summary Report (i)

May 13, 2025 – 04:30 pm BST

PDB ID	:	9H90 / pdb_00009h90
EMDB ID	:	EMD-51946
Title	:	Cryo-EM structure of the Vibrio natrigens 30S ribosomal subunit in complex with spectinomycin.
Authors	:	Raulf, K.F.; Koller, T.O.; Beckert, B.; Morici, M.; Lepak, A.; Bange, G.; Wilson, D.N.
Deposited on	:	2024-10-29
Resolution	:	2.80 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 (i)) were used in the production of this report:

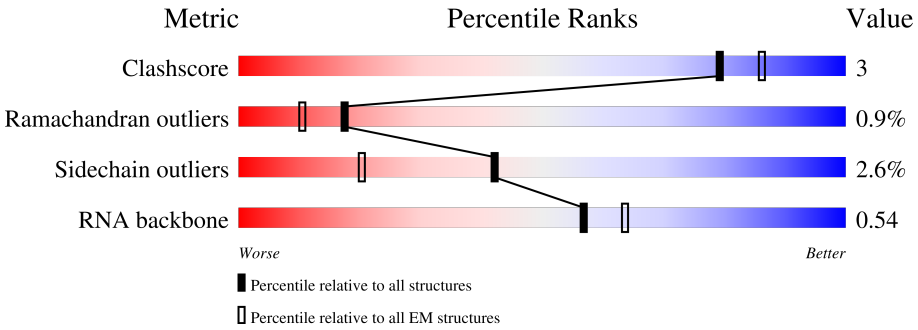
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 2.80 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 <=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	u	71	35% 77% 10% · 11%
2	C	232	9% 78% 9% 12%
3	G	156	10% 66% 10% · 23%
4	o	89	· 82% 16% ··
5	h	130	92% 8% ·
6	f	129	· 66% 15% · 19%
7	e	167	· 85% 9% 6%

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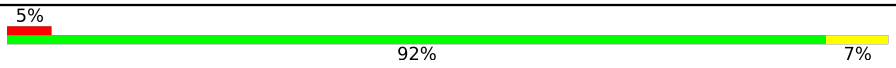
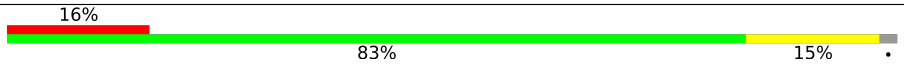
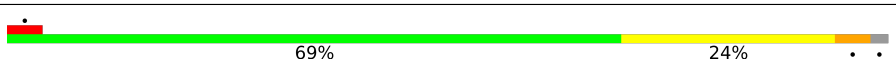
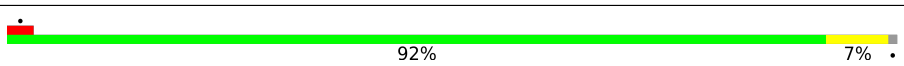
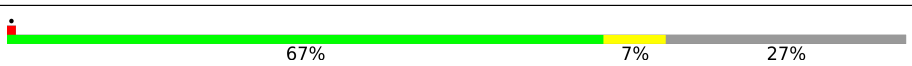
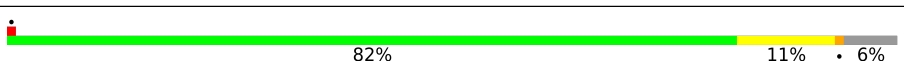
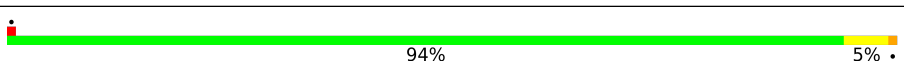
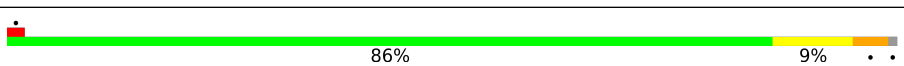
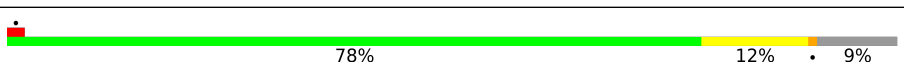
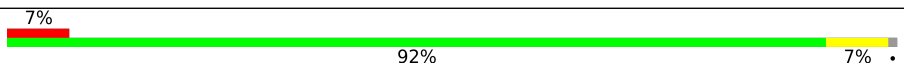
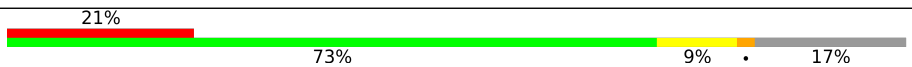
Mol	Chain	Length	Quality of chain
8	d	206	
9	I	130	
10	a	1544	
11	t	86	
12	r	75	
13	q	84	
14	p	82	
15	l	124	
16	k	129	
17	D	101	
18	J	103	

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 47463 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 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	u	63	Total	C	N	O	S	0	0
			526	328	114	83	1		

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	203	Total	C	N	O	S	0	0
			1580	1000	300	277	3		

- Molecule 3 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	120	Total	C	N	O	S	0	0
			944	592	175	172	5		

- Molecule 4 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	o	88	Total	C	N	O	S	0	0
			699	433	142	123	1		

- Molecule 5 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	h	129	Total	C	N	O	S	0	0
			970	617	171	176	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	105	Total	C	N	O	S	0	0
			854	537	155	155	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	e	157	Total	C	N	O	S	0	0
			1150	713	216	214	7		

- Molecule 8 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	d	205	Total	C	N	O	S	0	0
			1632	1020	311	296	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	127	Total	C	N	O	S	0	0
			998	620	197	178	3		

- Molecule 10 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	a	1509	Total	C	N	O	P	0	0
			32388	14445	5938	10496	1509		

- Molecule 11 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	t	85	Total	C	N	O	S	0	0
			660	406	136	114	4		

- Molecule 12 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	r	55	Total	C	N	O	0	0
			446	284	81	81		

- Molecule 13 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	q	79	Total	C	N	O	S	0	0
			632	396	117	116	3		

- Molecule 14 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	p	82	Total	C	N	O	S	0	0
			640	401	125	113	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	l	123	Total	C	N	O	S	0	0
			953	588	194	167	4		

- Molecule 16 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	k	117	Total	C	N	O	S	0	0
			876	540	174	158	4		

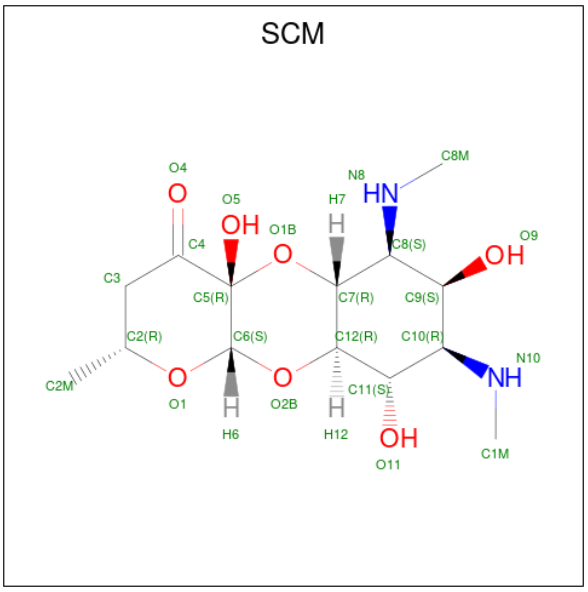
- Molecule 17 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	D	100	Total	C	N	O	S	0	0
			794	488	163	139	4		

- Molecule 18 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	86	Total	C	N	O	S	0	0
			694	436	134	123	1		

- Molecule 19 is SPECTINOMYCIN (CCD ID: SCM) (formula: $C_{14}H_{24}N_2O_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
19	a	1	Total	C	N	O	0
			23	14	2	7	

- Molecule 20 is water.

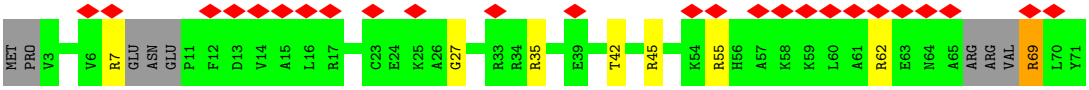
Mol	Chain	Residues	Atoms		AltConf
20	a	4	Total	O	0
			4	4	

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.

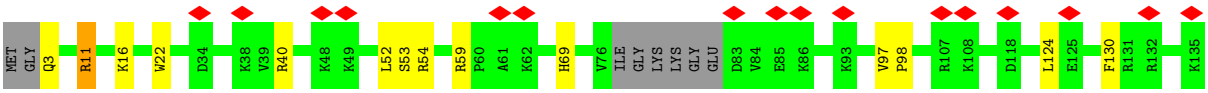
• Molecule 1: 30S ribosomal protein S21

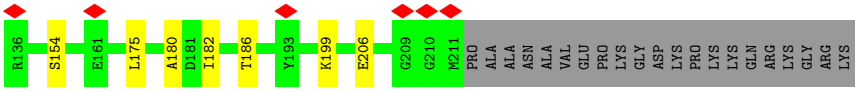
Chain u:



• Molecule 2: 30S ribosomal protein S3

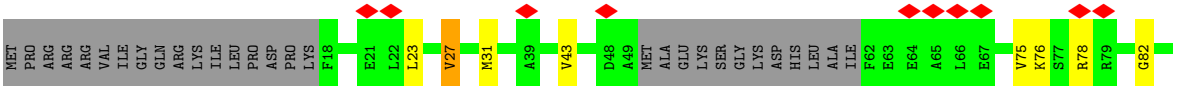
Chain C:

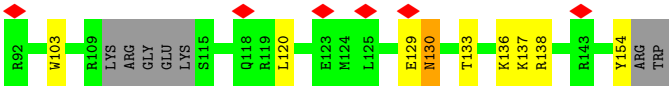




• Molecule 3: Small ribosomal subunit protein uS7

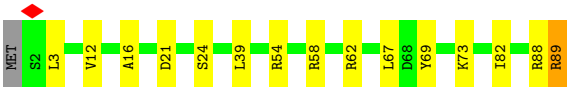
Chain G:





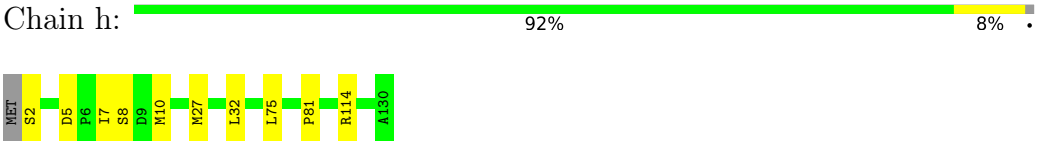
• Molecule 4: 30S ribosomal protein S15

Chain o:



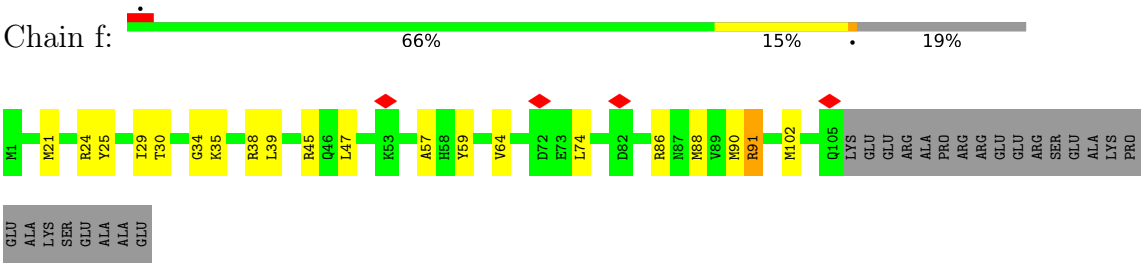
• Molecule 5: 30S ribosomal protein S8

Chain h:



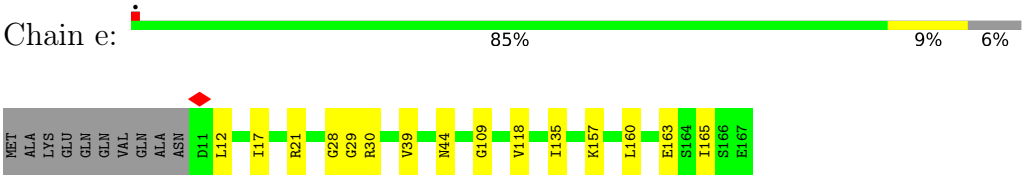
• Molecule 6: 30S ribosomal protein S6

Chain f:



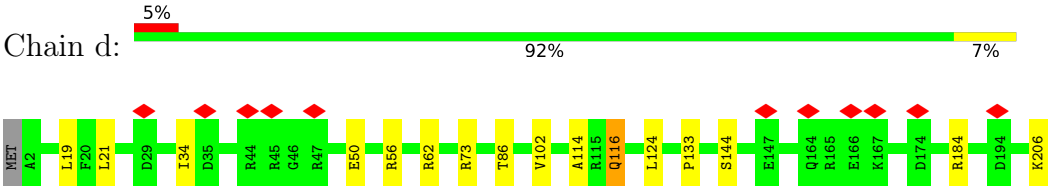
• Molecule 7: 30S ribosomal protein S5

Chain e:



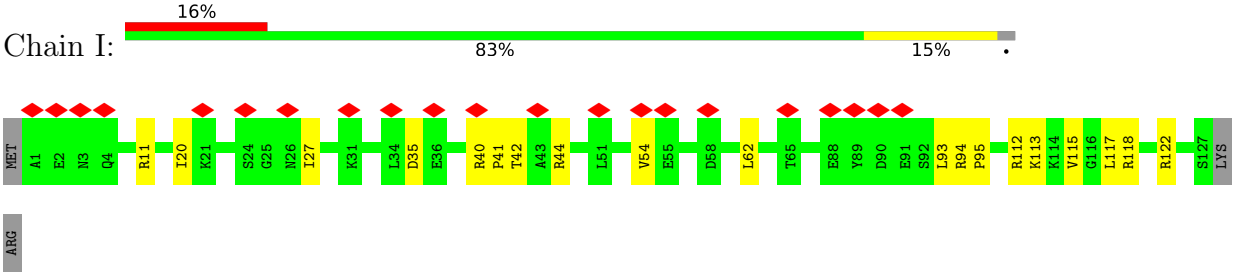
• Molecule 8: 30S ribosomal protein S4

Chain d:



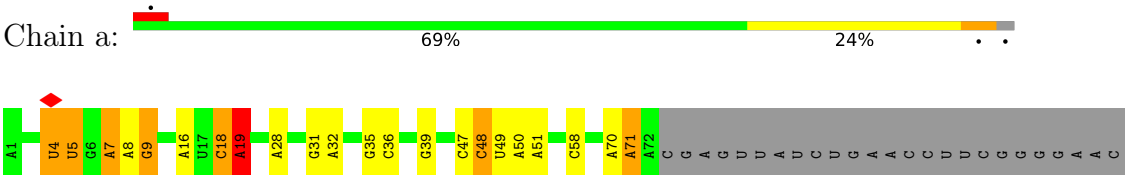
• Molecule 9: 30S ribosomal protein S9

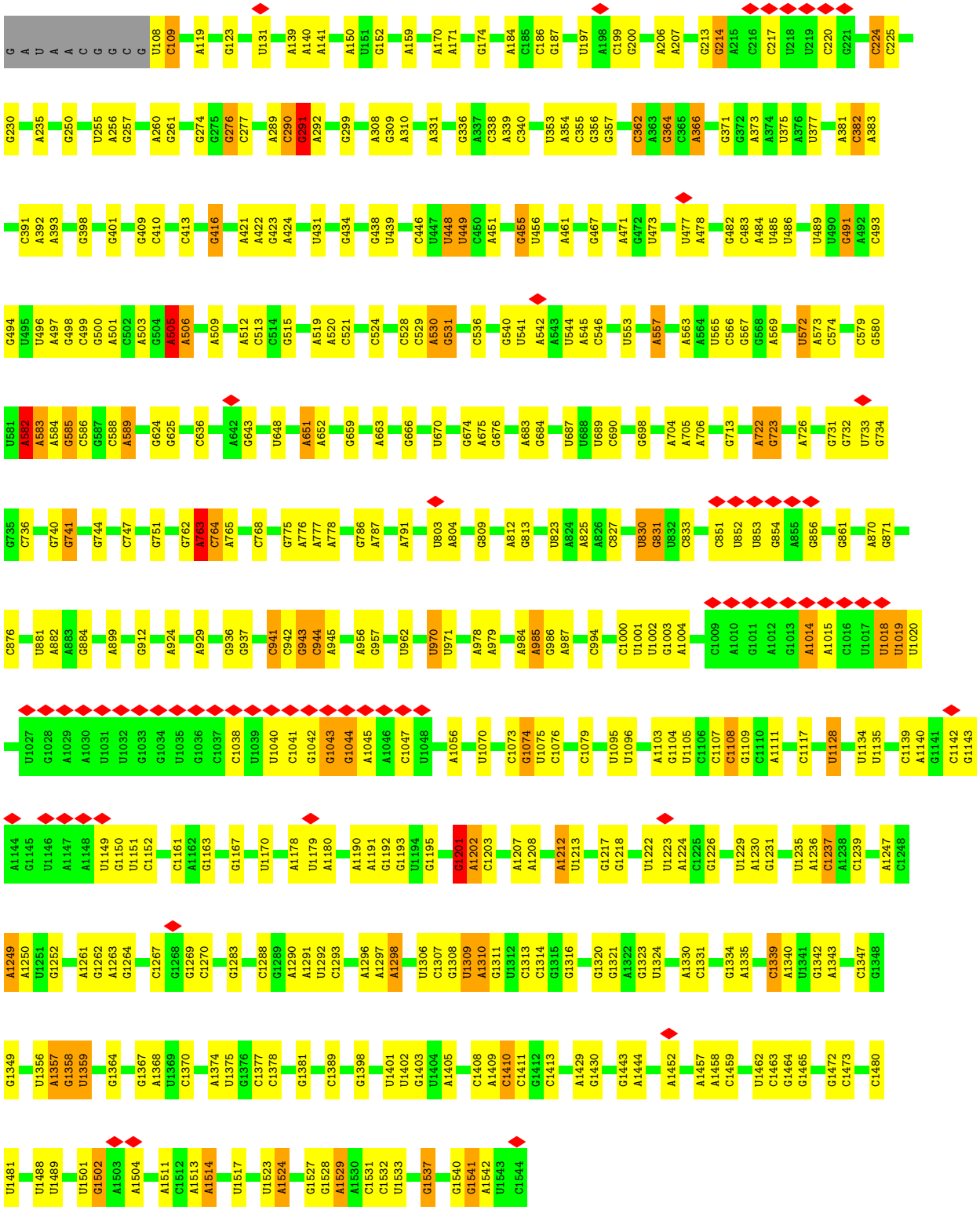
Chain I:



• Molecule 10: 16S ribosomal RNA

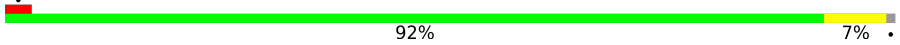
Chain a:

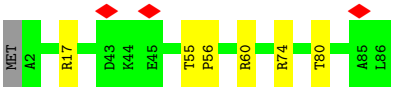




• Molecule 11: 30S ribosomal protein S20

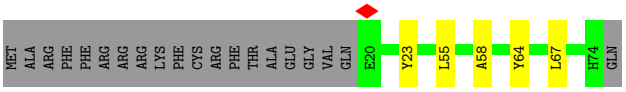
Chain t:





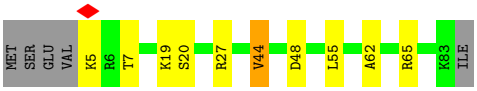
• Molecule 12: 30S ribosomal protein S18

Chain r:



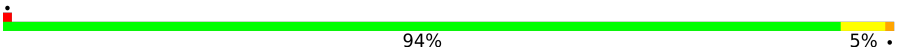
• Molecule 13: 30S ribosomal protein S17

Chain q:



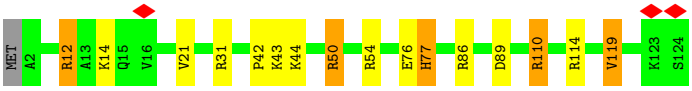
• Molecule 14: 30S ribosomal protein S16

Chain p:



• Molecule 15: 30S ribosomal protein S12

Chain l:

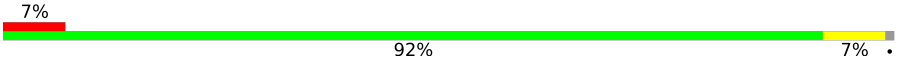


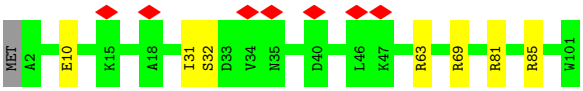
• Molecule 16: 30S ribosomal protein S11

Chain k:

• Molecule 17: 30S ribosomal protein S14

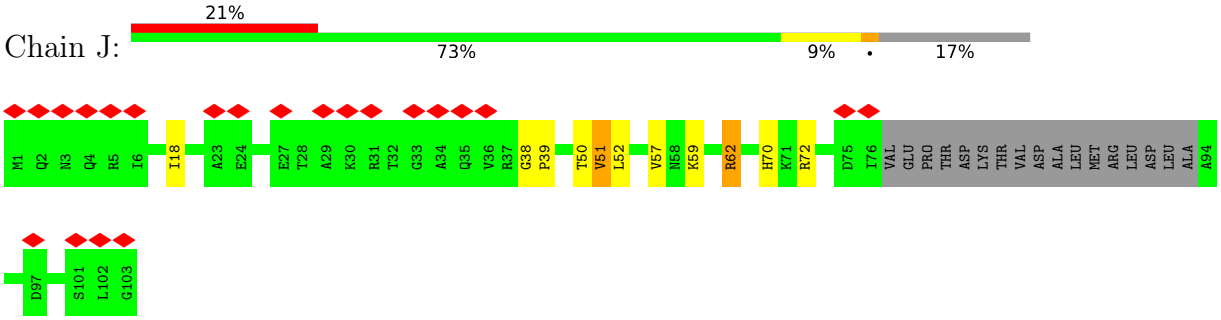
Chain D:





• Molecule 18: 30S ribosomal protein S10

Chain J:


21%
73%
9%
17%
M1 Q2 N3 Q4 R5 I6 I18 A23 E24 E27 T28 A29 K30 R31 T32 G33 A34 Q35 V36 R37 G38 P39 T50 V51 L52 V57 N58 K59 R62 H70 K71 R72 D75 I76 VAL GLU PRO THR ASP LYS THR VAL ASP ALA LEU MET ARG LEU ASP LEU ALA A94
D97 S101 L102 G103

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	294068	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 ($e^-/Å^2$)	1.0	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.454	Depositor
Minimum map value	-0.226	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	441.376, 441.376, 441.376	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.061, 1.061, 1.061	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: SCM

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	u	0.56	0/531	1.01	0/700
2	C	0.58	0/1606	0.90	0/2163
3	G	0.59	0/955	0.97	0/1280
4	o	0.69	0/708	0.97	0/946
5	h	0.69	0/981	0.95	0/1316
6	f	0.59	0/869	0.90	0/1169
7	e	0.67	0/1163	0.94	0/1564
8	d	0.55	0/1652	0.94	1/2209 (0.0%)
9	I	0.56	0/1012	0.96	0/1357
10	a	0.57	0/36268	0.95	77/56578 (0.1%)
11	t	0.64	0/666	1.01	0/883
12	r	0.67	0/453	0.95	0/610
13	q	0.56	0/641	0.90	0/859
14	p	0.68	0/650	0.92	1/871 (0.1%)
15	l	0.66	0/967	0.91	0/1299
16	k	0.63	0/892	0.91	0/1203
17	D	0.57	0/804	0.94	0/1068
18	J	0.57	0/702	0.90	0/941
All	All	0.58	0/51520	0.95	79/77016 (0.1%)

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	u	0	5
2	C	0	2
3	G	0	1
4	o	0	2
5	h	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	f	0	4
7	e	0	1
8	d	0	3
9	I	0	6
10	a	0	1
11	t	0	3
14	p	0	1
15	l	0	7
16	k	0	1
18	J	0	2
All	All	0	40

There are no bond length outliers.

The worst 5 of 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	a	584	A	O3'-P-O5'	-10.71	87.94	104.00
10	a	584	A	C4'-C3'-O3'	-8.93	99.60	113.00
10	a	18	C	O3'-P-O5'	-8.07	91.89	104.00
10	a	970	U	C4'-C3'-O3'	8.02	121.44	109.40
10	a	583	A	C4'-C3'-O3'	-7.98	101.03	113.00

There are no chirality outliers.

5 of 40 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	u	35	ARG	Sidechain
1	u	55	ARG	Sidechain
1	u	62	ARG	Sidechain
1	u	69	ARG	Sidechain
1	u	7	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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	u	526	0	569	2	0
2	C	1580	0	1641	7	0
3	G	944	0	967	6	0
4	o	699	0	726	7	0
5	h	970	0	1043	5	0
6	f	854	0	854	9	0
7	e	1150	0	1198	6	0
8	d	1632	0	1698	6	0
9	I	998	0	1034	6	0
10	a	32388	0	16284	137	0
11	t	660	0	709	2	0
12	r	446	0	468	4	0
13	q	632	0	661	3	0
14	p	640	0	658	3	0
15	l	953	0	1006	7	0
16	k	876	0	887	8	0
17	D	794	0	834	4	0
18	J	694	0	739	6	0
19	a	23	0	24	2	0
20	a	4	0	0	0	0
All	All	47463	0	32000	196	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 3.

The worst 5 of 196 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)
5:h:2:SER:N	10:a:833:C:HO2'	1.81	0.77
2:C:175:LEU:HD23	2:C:182:ILE:HD13	1.81	0.63
10:a:674:G:H22	10:a:751:G:H1	1.46	0.63
10:a:705:A:H2'	10:a:706:A:C8	2.35	0.61
10:a:1309:U:H5"	10:a:1310:A:H5'	1.82	0.60

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
1	u	57/71 (80%)	52 (91%)	4 (7%)	1 (2%)	7 24
2	C	199/232 (86%)	186 (94%)	11 (6%)	2 (1%)	13 39
3	G	114/156 (73%)	100 (88%)	12 (10%)	2 (2%)	7 24
4	o	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	11 34
5	h	127/130 (98%)	121 (95%)	6 (5%)	0	100 100
6	f	103/129 (80%)	96 (93%)	7 (7%)	0	100 100
7	e	155/167 (93%)	147 (95%)	5 (3%)	3 (2%)	6 23
8	d	203/206 (98%)	200 (98%)	3 (2%)	0	100 100
9	I	125/130 (96%)	111 (89%)	14 (11%)	0	100 100
11	t	83/86 (96%)	81 (98%)	2 (2%)	0	100 100
12	r	53/75 (71%)	50 (94%)	3 (6%)	0	100 100
13	q	77/84 (92%)	72 (94%)	4 (5%)	1 (1%)	10 32
14	p	80/82 (98%)	78 (98%)	2 (2%)	0	100 100
15	l	121/124 (98%)	114 (94%)	6 (5%)	1 (1%)	16 44
16	k	115/129 (89%)	104 (90%)	9 (8%)	2 (2%)	7 26
17	D	98/101 (97%)	90 (92%)	6 (6%)	2 (2%)	6 21
18	J	82/103 (80%)	70 (85%)	10 (12%)	2 (2%)	5 18
All	All	1878/2094 (90%)	1751 (93%)	110 (6%)	17 (1%)	17 42

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	k	119	ASN
18	J	57	VAL
17	D	32	SER
3	G	130	ASN
2	C	98	PRO

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	u	53/61 (87%)	52 (98%)	1 (2%)	52 82
2	C	161/183 (88%)	156 (97%)	5 (3%)	35 69
3	G	97/128 (76%)	92 (95%)	5 (5%)	19 50
4	o	72/73 (99%)	69 (96%)	3 (4%)	25 58
5	h	103/104 (99%)	102 (99%)	1 (1%)	73 91
6	f	90/109 (83%)	87 (97%)	3 (3%)	33 67
7	e	119/127 (94%)	116 (98%)	3 (2%)	42 75
8	d	171/172 (99%)	166 (97%)	5 (3%)	37 71
9	I	102/105 (97%)	100 (98%)	2 (2%)	50 81
11	t	65/66 (98%)	65 (100%)	0	100 100
12	r	47/64 (73%)	47 (100%)	0	100 100
13	q	71/76 (93%)	66 (93%)	5 (7%)	12 36
14	p	64/64 (100%)	64 (100%)	0	100 100
15	l	104/105 (99%)	100 (96%)	4 (4%)	28 62
16	k	88/98 (90%)	87 (99%)	1 (1%)	70 90
17	D	82/83 (99%)	82 (100%)	0	100 100
18	J	75/90 (83%)	73 (97%)	2 (3%)	40 74
All	All	1564/1708 (92%)	1524 (97%)	40 (3%)	42 75

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	q	5	LYS
15	l	86	ARG
13	q	20	SER
13	q	55	LEU
16	k	16	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11

such sidechains are listed below:

Mol	Chain	Res	Type
14	p	63	GLN
15	l	15	GLN
18	J	58	ASN
16	k	15	GLN
6	f	17	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	a	1507/1544 (97%)	255 (16%)	0

5 of 255 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	a	4	U
10	a	5	U
10	a	7	A
10	a	9	G
10	a	19	A

There are no RNA pucker outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand is 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	$\#\|Z\| > 2$
19	SCM	a	1601	-	23,25,25	0.48	0	26,39,39	0.53	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
19	SCM	a	1601	-	-	0/4/57/57	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

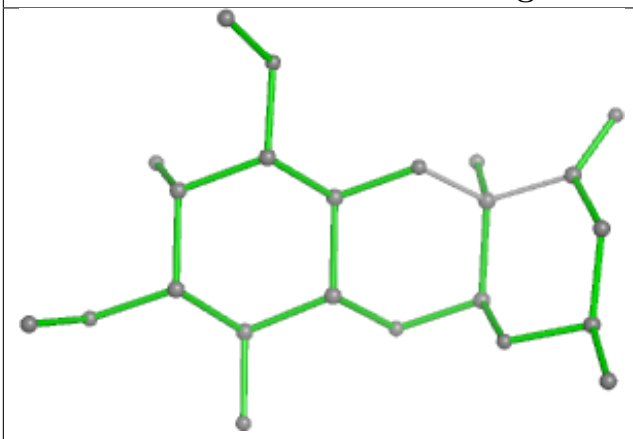
There are no ring outliers.

1 monomer is involved in 2 short contacts:

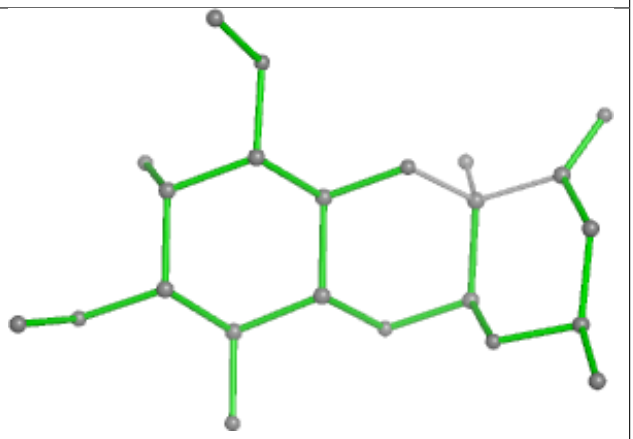
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	a	1601	SCM	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

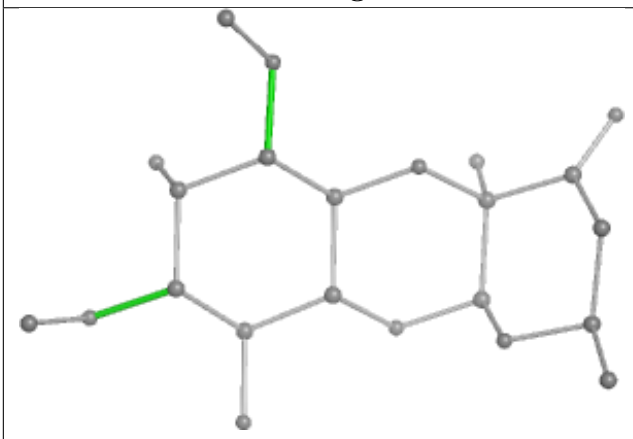
Ligand SCM a 1601



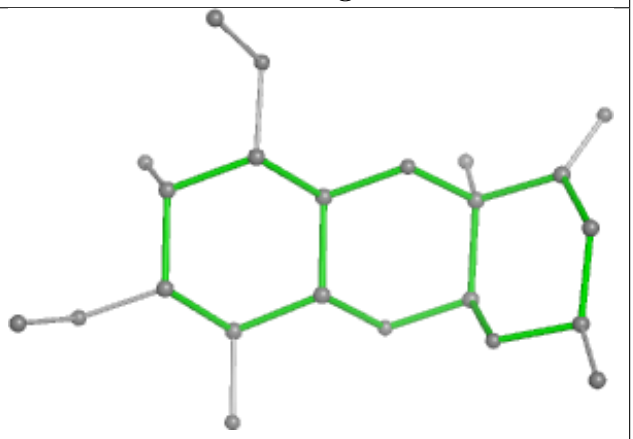
Bond lengths



Bond angles



Torsions



Rings

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.

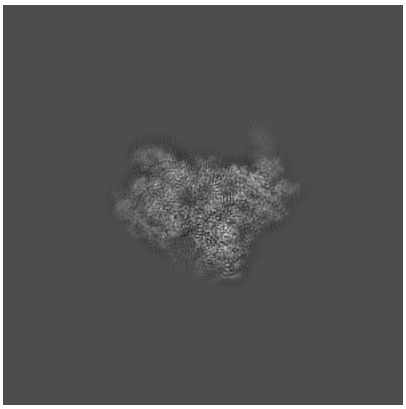
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-51946. These allow visual inspection of the internal detail of the map and identification of artifacts.

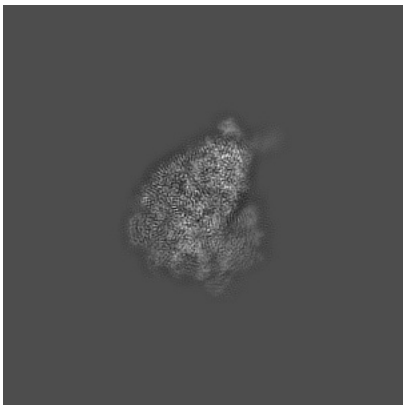
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

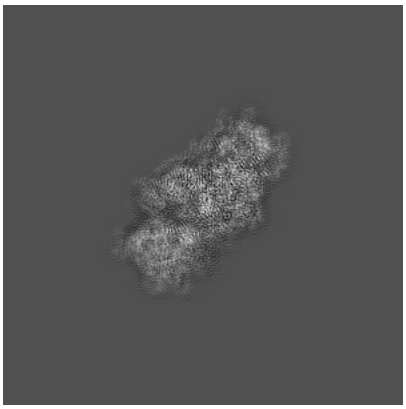
6.1.1 Primary map



X

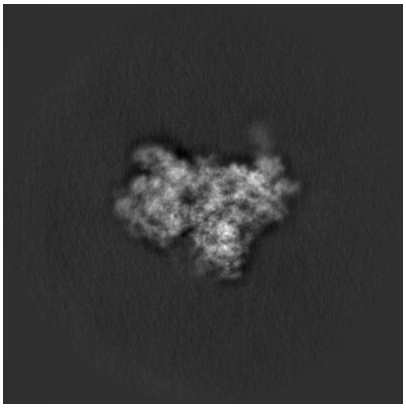


Y

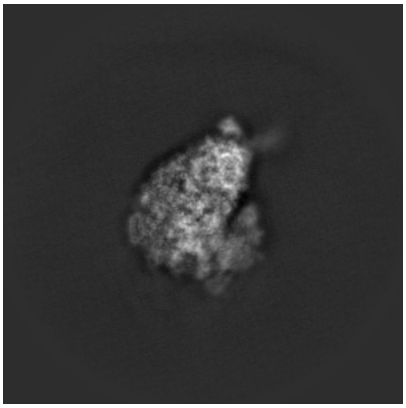


Z

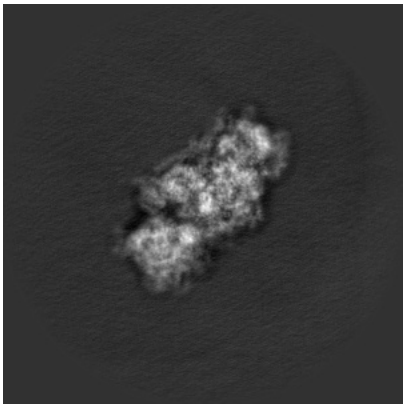
6.1.2 Raw map



X



Y

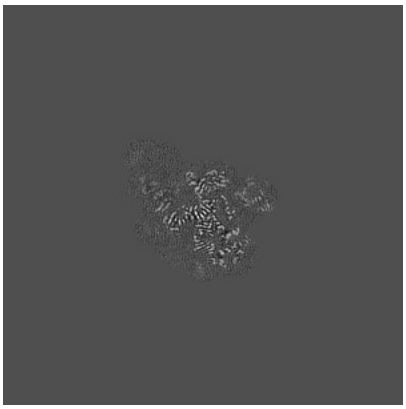


Z

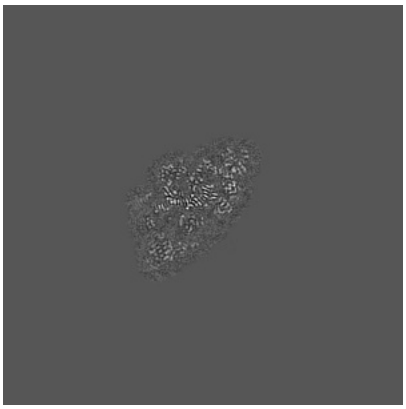
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

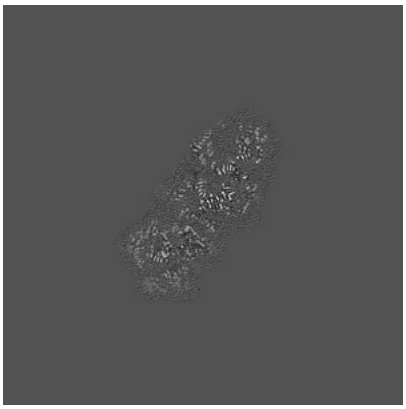
6.2.1 Primary map



X Index: 208

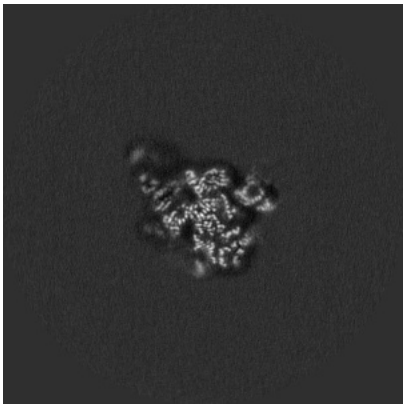


Y Index: 208

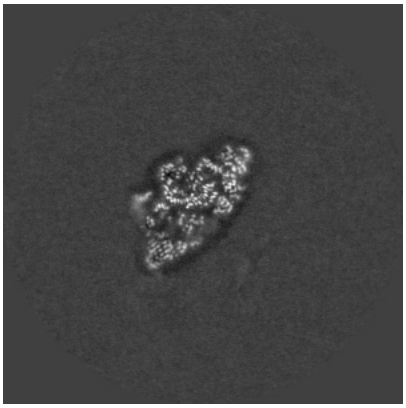


Z Index: 208

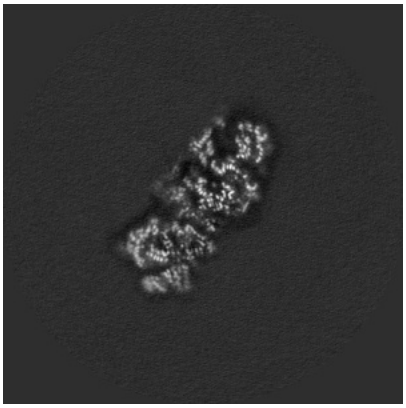
6.2.2 Raw map



X Index: 208



Y Index: 208

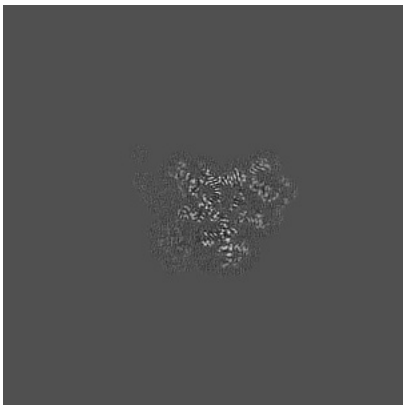


Z Index: 208

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

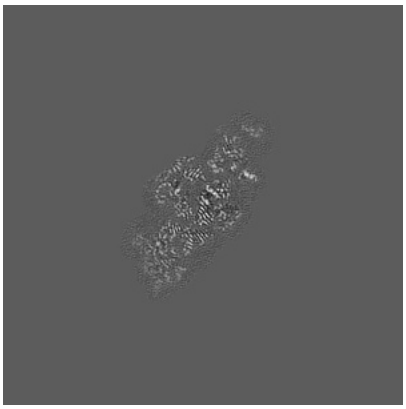
6.3 Largest variance slices (i)

6.3.1 Primary map



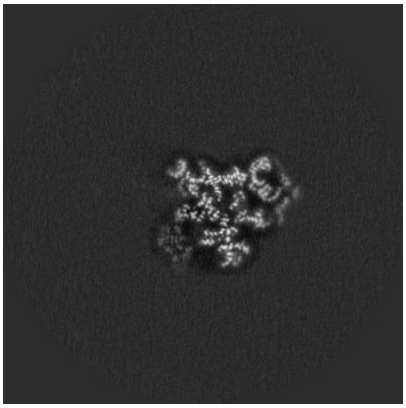
X Index: 226

Y Index: 231

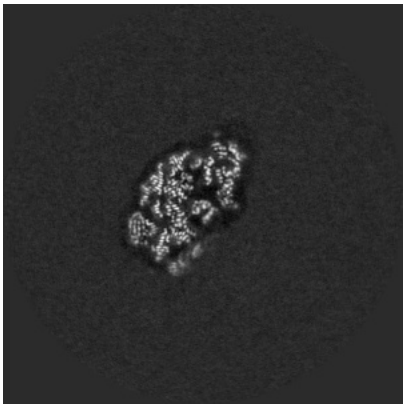


Z Index: 194

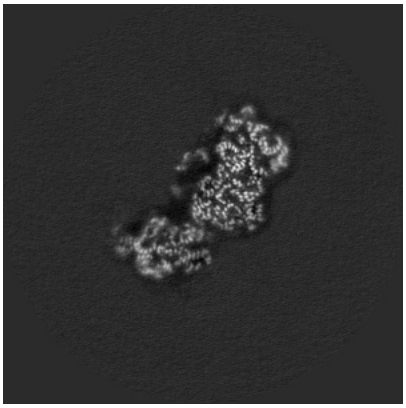
6.3.2 Raw map



X Index: 226



Y Index: 231

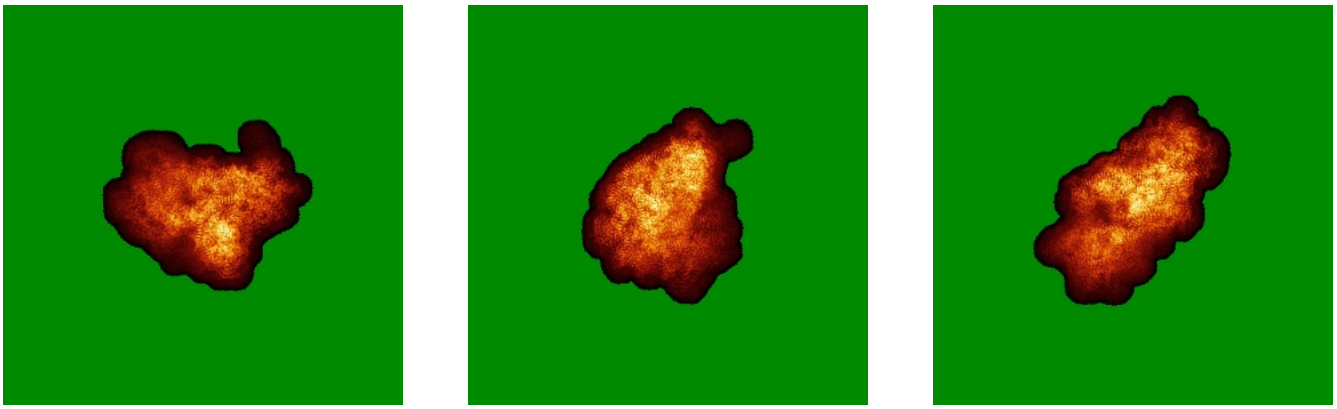


Z Index: 229

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

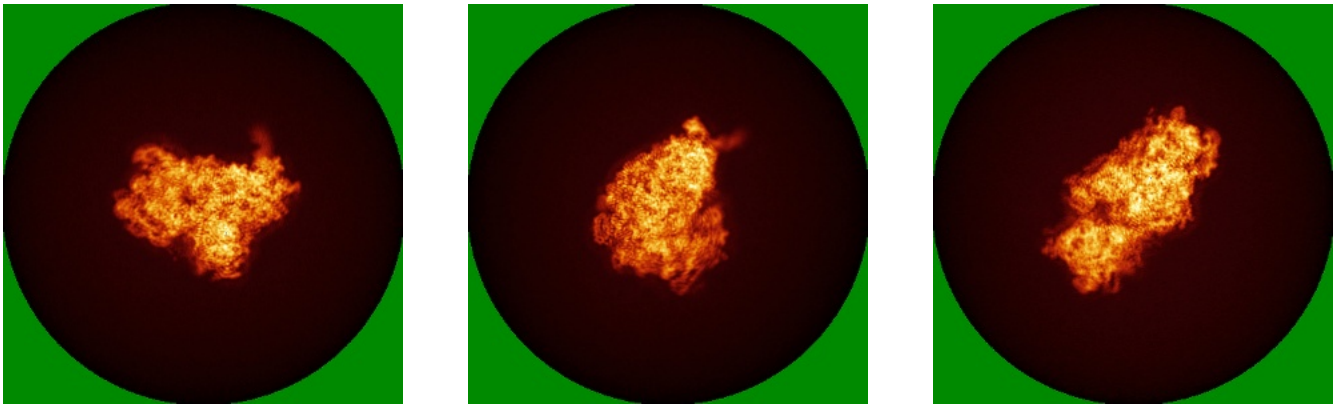
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map



X Y Z

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

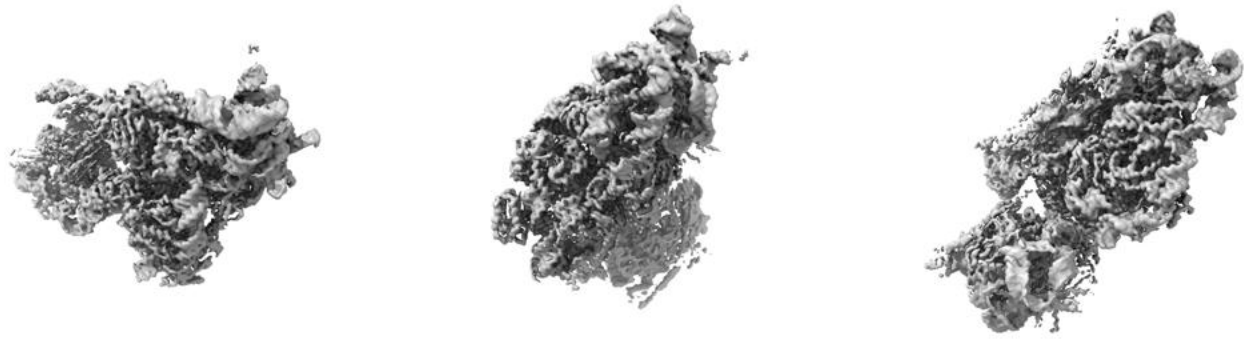
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

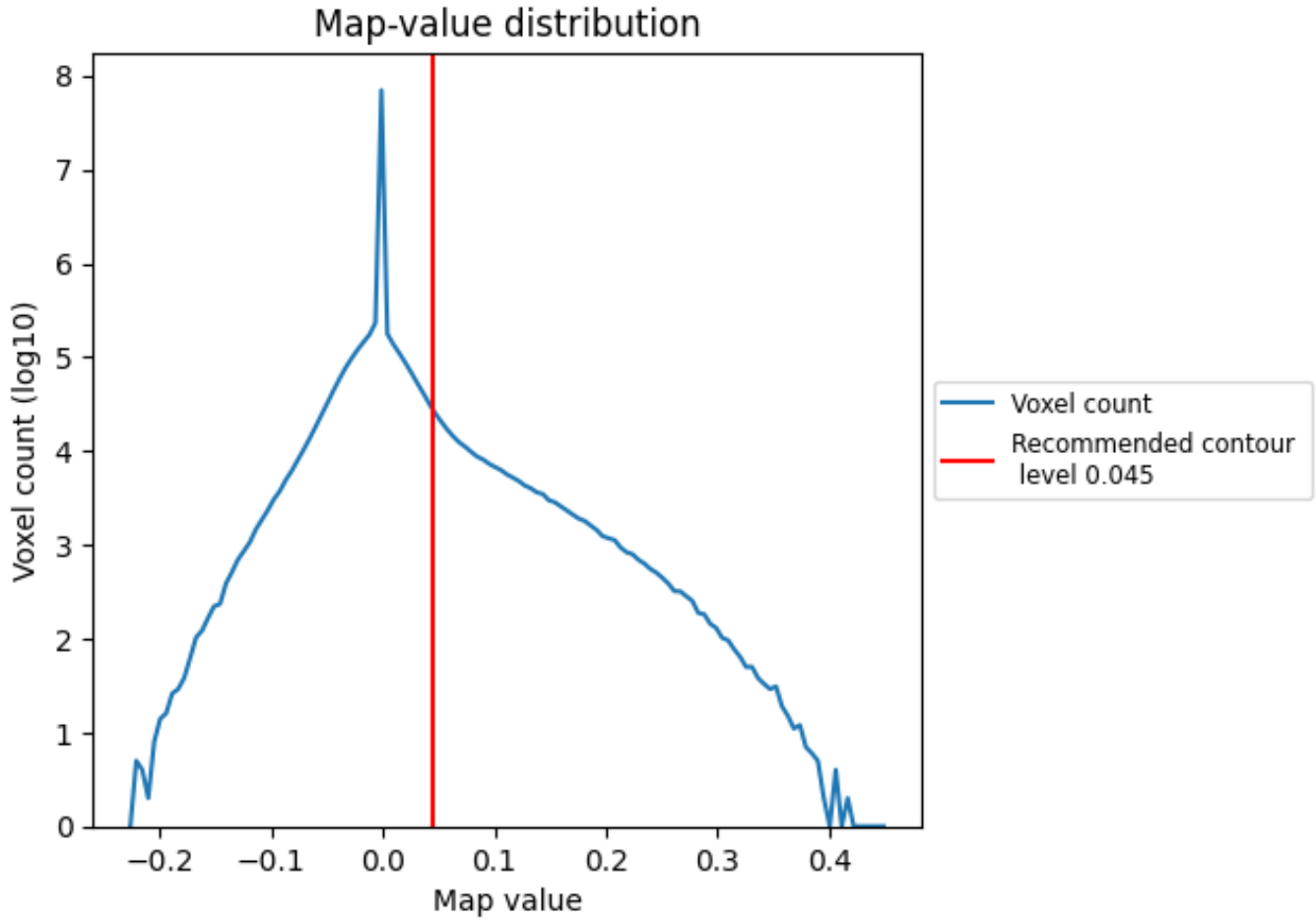
6.6 Mask visualisation (i)

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

7 Map analysis

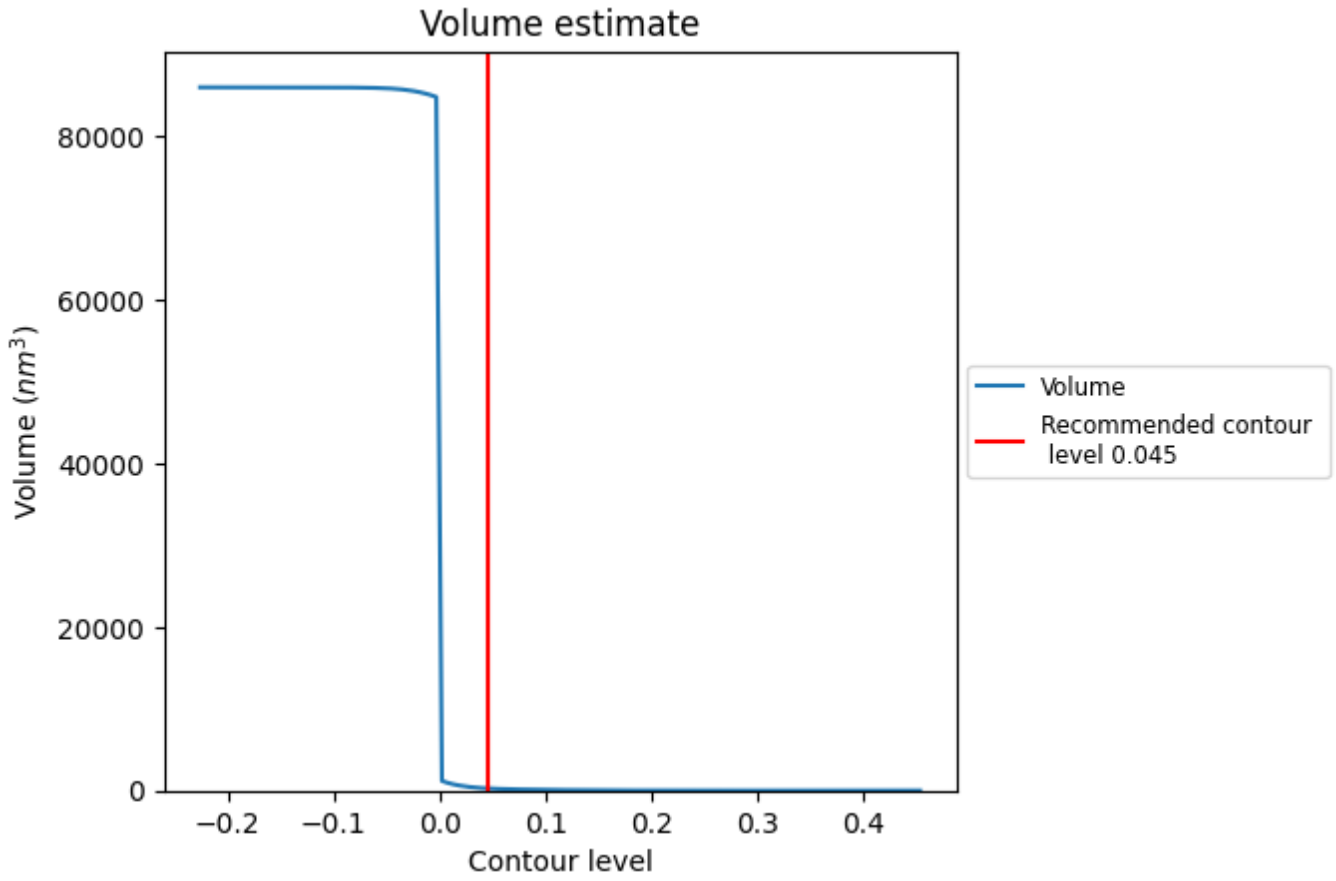
This section contains the results of statistical analysis of the map.

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.

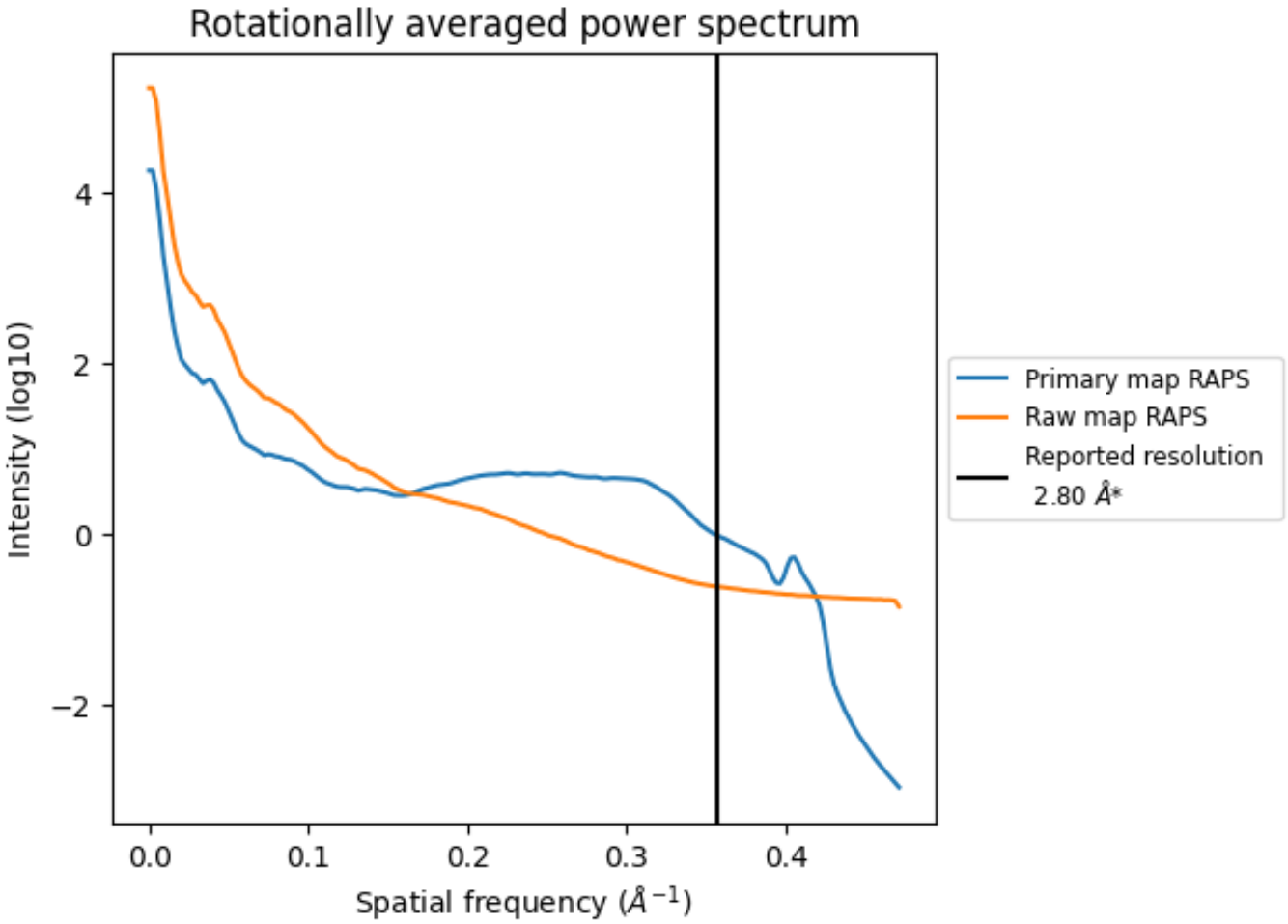
7.2 Volume estimate (i)



The volume at the recommended contour level is 264 nm^3; this corresponds to an approximate mass of 238 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)

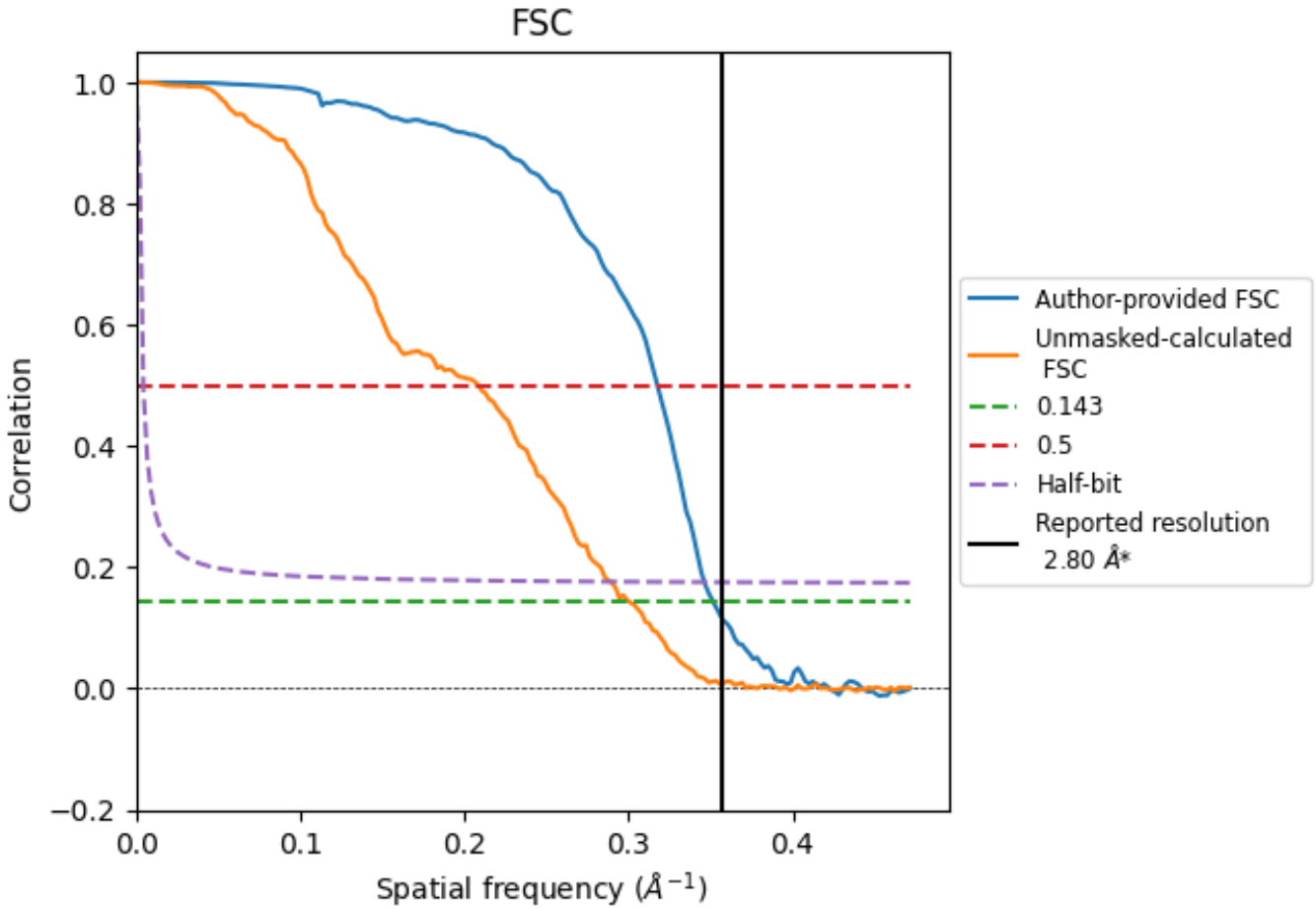


*Reported resolution corresponds to spatial frequency of 0.357 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8.2 Resolution estimates (i)

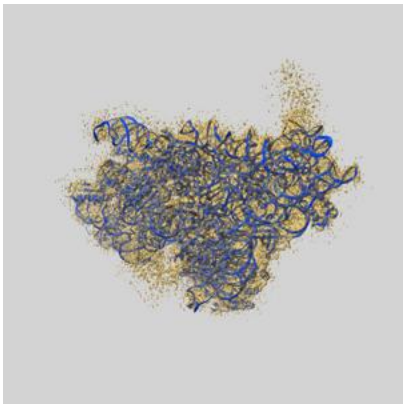
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.84	3.15	2.89
Unmasked-calculated*	3.33	4.79	3.46

*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 3.33 differs from the reported value 2.8 by more than 10 %

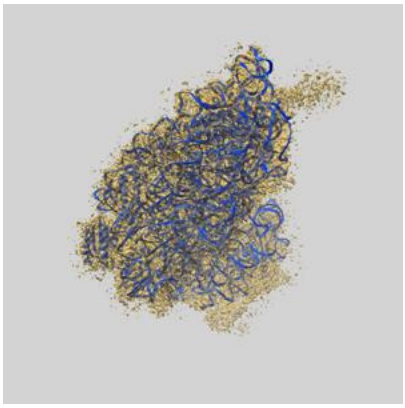
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-51946 and PDB model 9H90. Per-residue inclusion information can be found in section 3 on page 8.

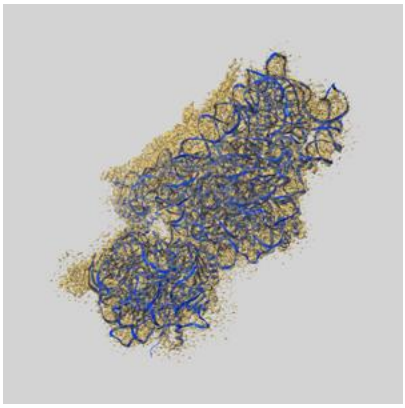
9.1 Map-model overlay



X



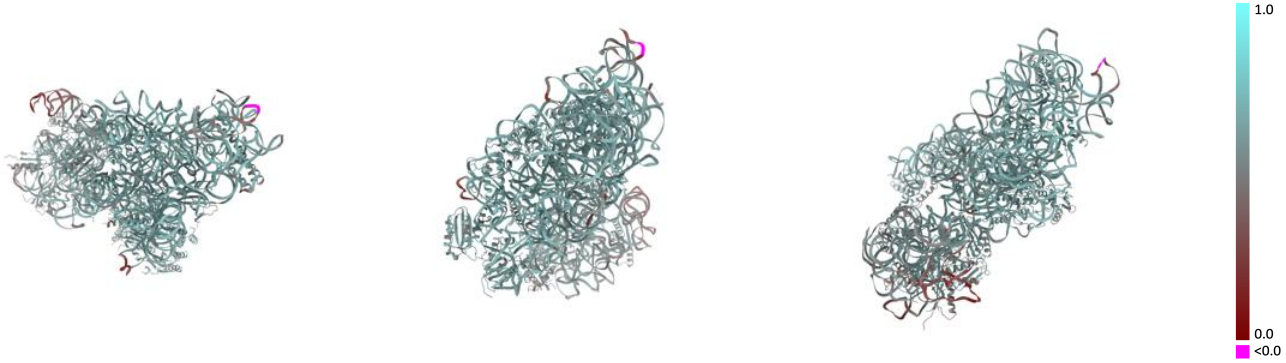
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.045 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.

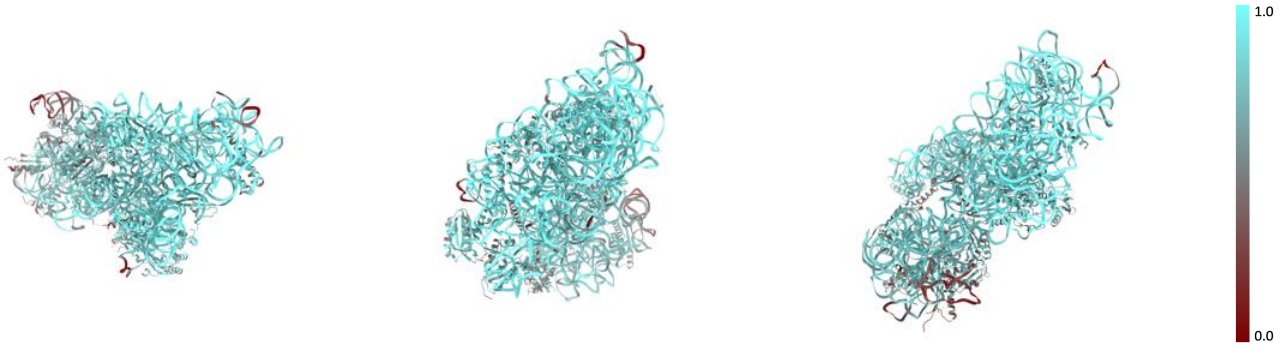
9.2 Q-score mapped to coordinate model (i)



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.

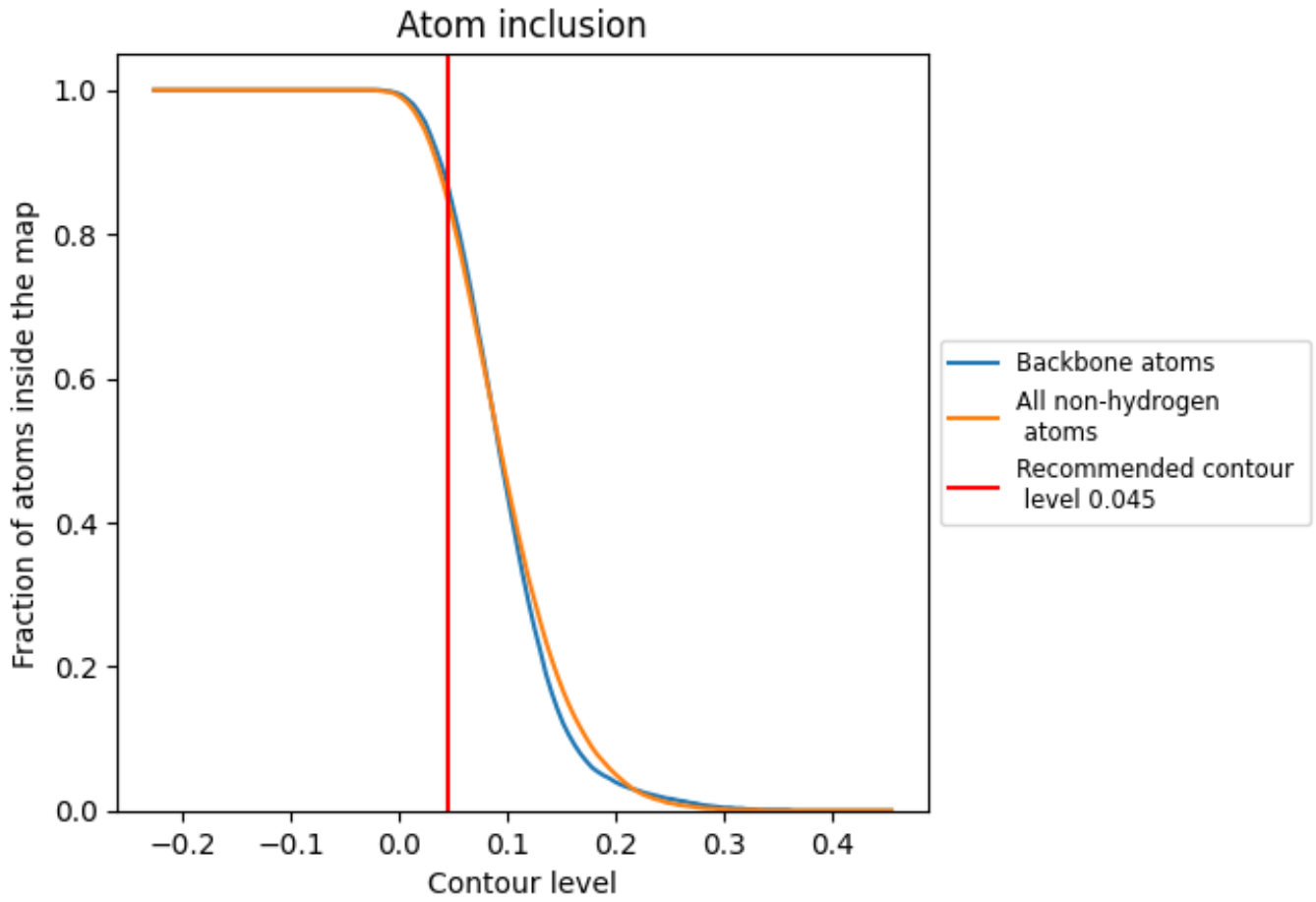
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.045).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 84% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8450	0.5940
C	0.6900	0.5710
D	0.7090	0.5670
G	0.6220	0.5180
I	0.6450	0.5320
J	0.6310	0.5440
a	0.8870	0.5980
d	0.7680	0.5970
e	0.8610	0.6210
f	0.7590	0.5750
h	0.8810	0.6360
k	0.7880	0.5910
l	0.8610	0.6230
o	0.8550	0.6140
p	0.8750	0.6330
q	0.8010	0.5970
r	0.8330	0.6150
t	0.7940	0.5980
u	0.4660	0.5180