wwPDB EM Validation Summary Report

Apr 17, 2024 – 01:38 pm BST

PDB ID	:	8CEP
EMDB ID	:	EMD-16612
Title	:	Kasugamycin bound to the 30S body
Authors	:	Paternoga, H.; Beckert, B.; Wilson, D.N.
Deposited on	:	2023-02-02
Resolution	:	2.04 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 ⓘ 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:

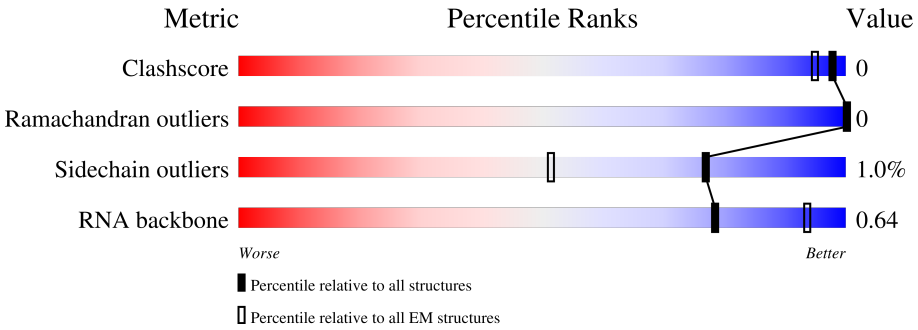
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.04 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	1540	58% 9% 32%
2	D	206	12% 92% 7%
3	E	167	5% 90% 7%
4	F	131	25% 76% 24%
5	H	130	98%
6	K	129	19% 88% 9%
7	L	124	6% 94% 5%

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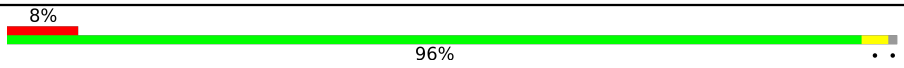
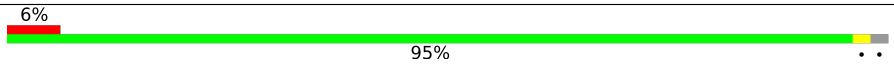
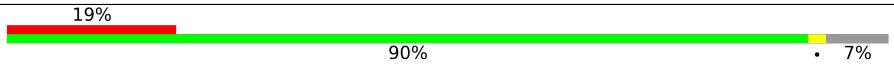
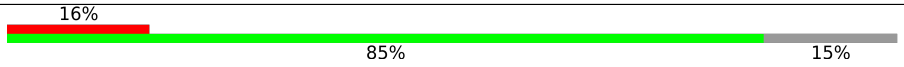
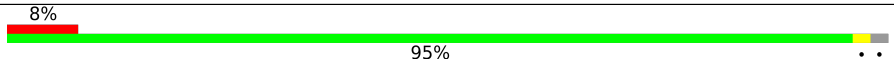
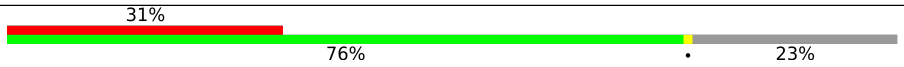
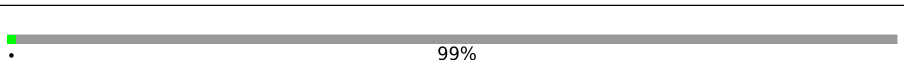
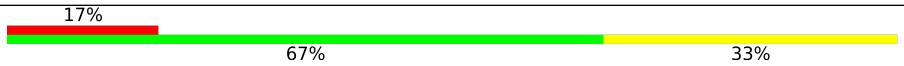
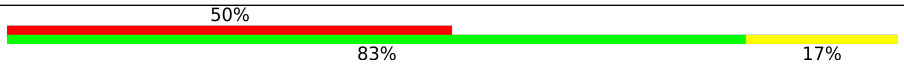
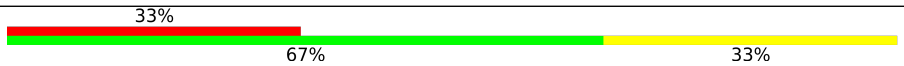
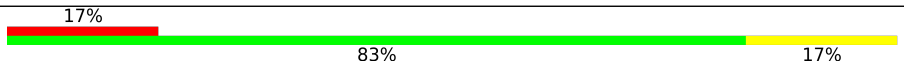
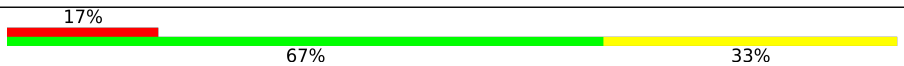
Mol	Chain	Length	Quality of chain
8	O	89	
9	P	82	
10	Q	84	
11	R	75	
12	T	87	
13	U	71	
14	a	2904	
15	B	6	
15	C	6	
15	G	6	
15	I	6	
15	V	6	

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 35490 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 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	1046	22497	10036	4157	7258	1046	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	156	1152	717	217	212	6	0	0

- Molecule 4 is a protein called Small ribosomal subunit protein bS6, non-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 Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	K	117	877	540	173	161	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	modified residue	UNP P0A7R9

- Molecule 7 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 8 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 9 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	P	80	Total	C	N	O	S	0	0
			638	400	126	111	1		

- Molecule 10 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 11 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	R	64	Total	C	N	O	S	0	0
			524	330	99	94	1		

- Molecule 12 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	85	Total	C	N	O	S	0	0
			664	411	137	113	3		

- Molecule 13 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	U	55	Total	C	N	O	S	0	0
			460	287	95	77	1		

- Molecule 14 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	a	31	Total	C	N	O	P	0	0
			664	297	121	215	31		

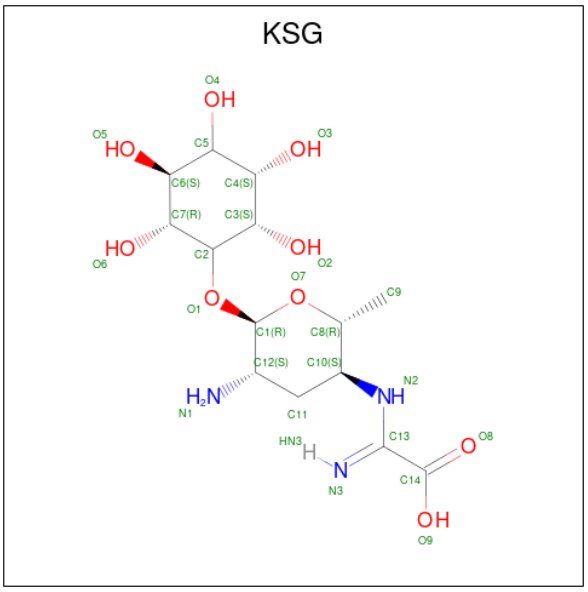
- Molecule 15 is a protein called Capreomycin IA.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	V	6	Total	C	N	O	0	0
			47	25	14	8		
15	B	6	Total	C	N	O	0	0
			47	25	14	8		
15	C	6	Total	C	N	O	0	0
			47	25	14	8		
15	G	6	Total	C	N	O	0	0
			47	25	14	8		
15	I	6	Total	C	N	O	0	0
			47	25	14	8		

- Molecule 16 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
16	A	23	Total	K	0
			23	23	
16	D	1	Total	K	0
			1	1	
16	F	1	Total	K	0
			1	1	

- Molecule 17 is (1S,2R,3S,4R,5S,6S)-2,3,4,5,6-PENTAHYDROXYCYCLOHEXYL 2-AMIN O-4-{[CARBOXY(IMINO)METHYL]AMINO}-2,3,4,6-TETRADEOXY-ALPHA-D-ARA BINO-HEXOPYRANOSIDE (three-letter code: KSG) (formula: $C_{14}H_{25}N_3O_9$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
17	A	1	Total	C	N	O	0
			26	14	3	9	

- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
18	A	54	Total	Mg	0
			54	54	

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		AltConf
19	A	1660	Total	O	0
			1660	1660	
19	D	40	Total	O	0
			40	40	
19	E	35	Total	O	0
			35	35	
19	F	2	Total	O	0
			2	2	
19	H	27	Total	O	0
			27	27	
19	K	17	Total	O	0
			17	17	
19	L	43	Total	O	0
			43	43	

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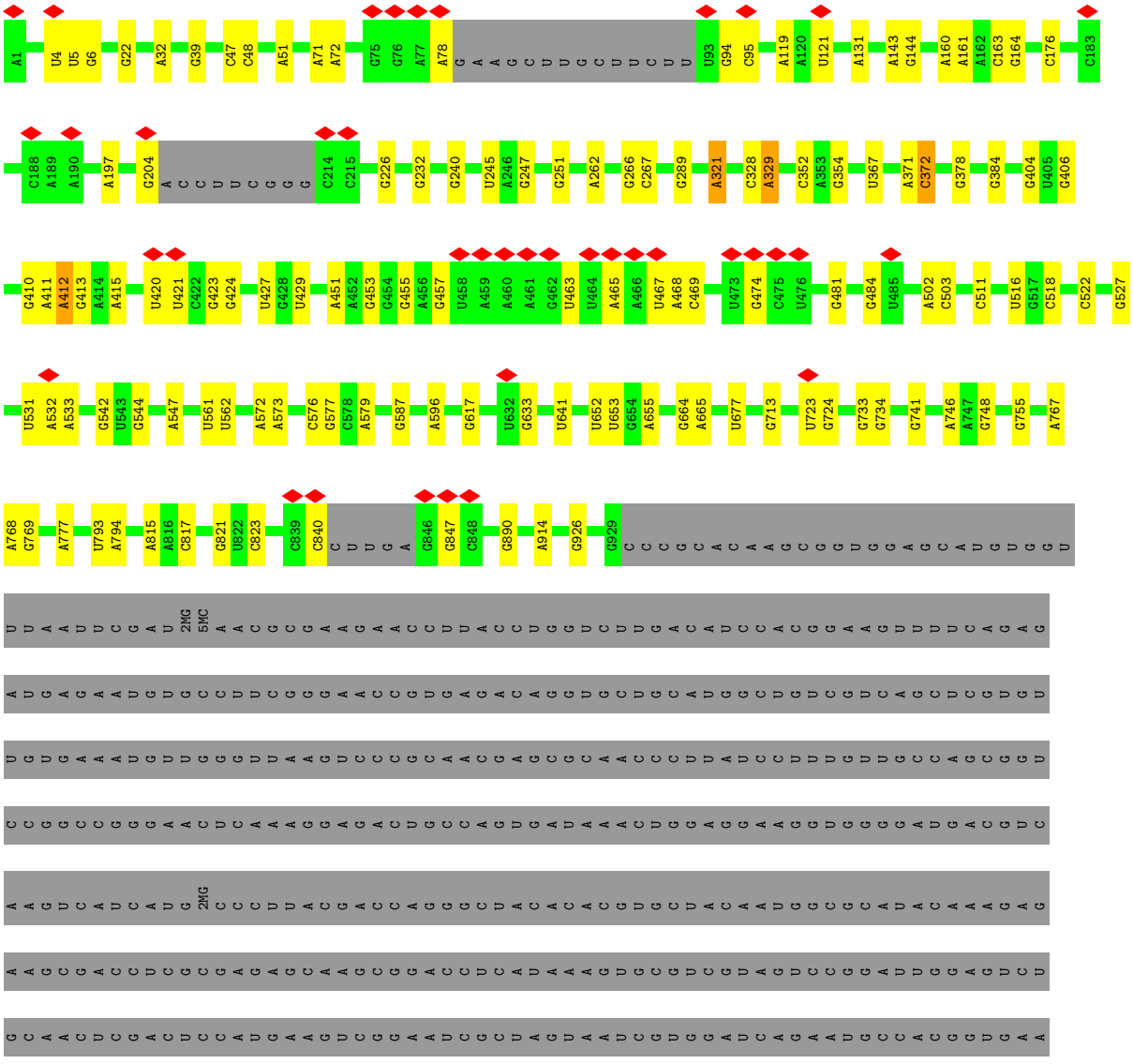
Mol	Chain	Residues	Atoms	AltConf
19	O	18	Total O 18 18	0
19	P	33	Total O 33 33	0
19	Q	15	Total O 15 15	0
19	R	6	Total O 6 6	0
19	T	25	Total O 25 25	0
19	U	4	Total O 4 4	0
19	a	1	Total O 1 1	0
19	V	2	Total O 2 2	0
19	B	1	Total O 1 1	0
19	C	1	Total O 1 1	0
19	I	3	Total O 3 3	0

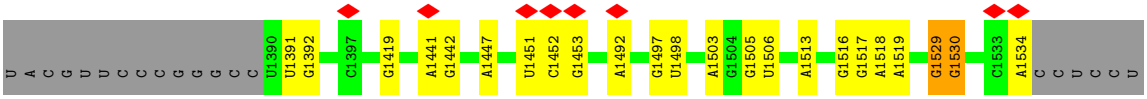
3 Residue-property plots (i)

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.

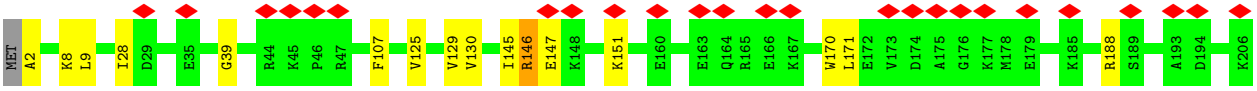
- Molecule 1: 16S rRNA

Chain A:

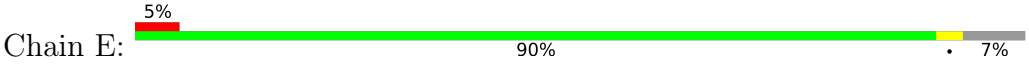


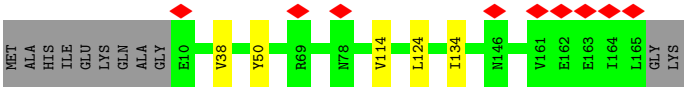


• Molecule 2: Small ribosomal subunit protein uS4

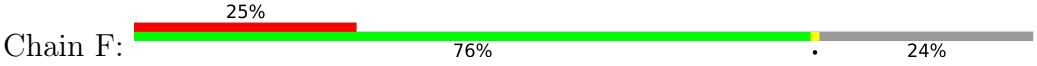


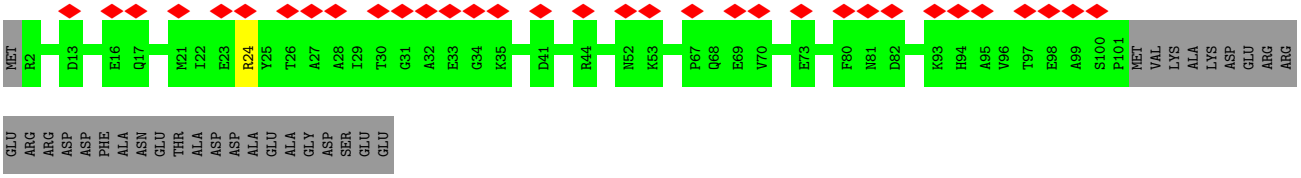
• Molecule 3: Small ribosomal subunit protein uS5



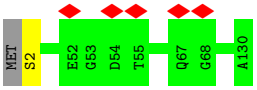


• Molecule 4: Small ribosomal subunit protein bS6, non-modified isoform

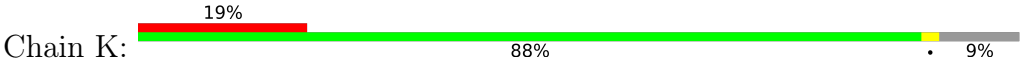


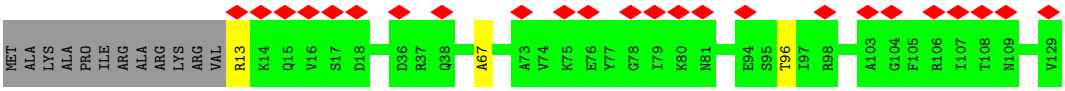


• Molecule 5: Small ribosomal subunit protein uS8

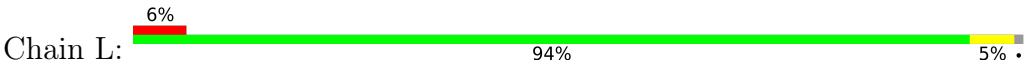


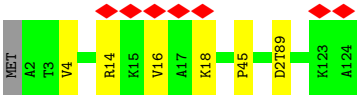
• Molecule 6: Small ribosomal subunit protein uS11





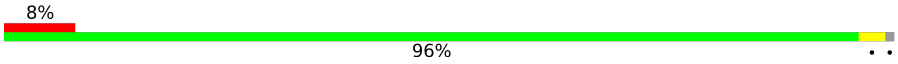
• Molecule 7: Small ribosomal subunit protein uS12

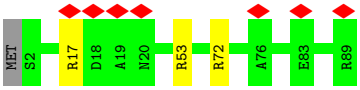




• Molecule 8: Small ribosomal subunit protein uS15

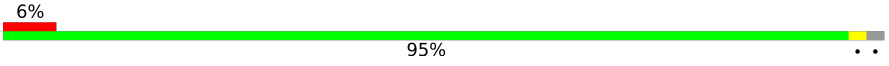
Chain O:

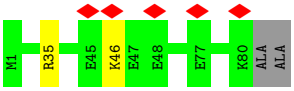




• Molecule 9: 30S ribosomal protein S16

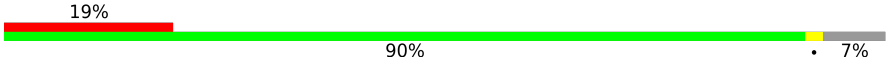
Chain P:

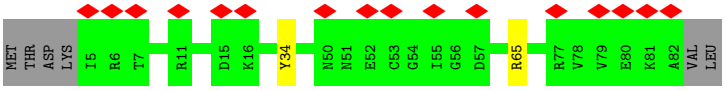




• Molecule 10: Small ribosomal subunit protein uS17

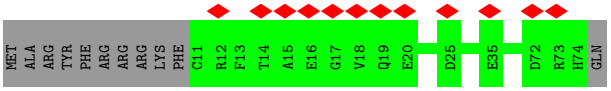
Chain Q:





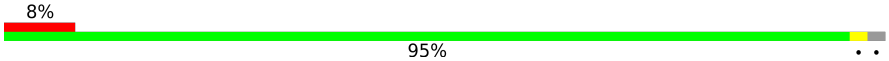
• Molecule 11: Small ribosomal subunit protein bS18

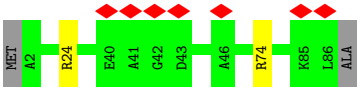
Chain R:



• Molecule 12: 30S ribosomal protein S20

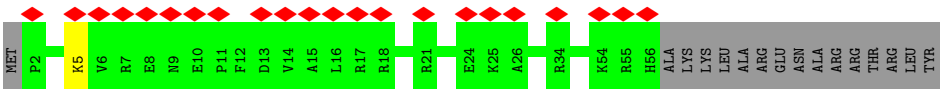
Chain T:





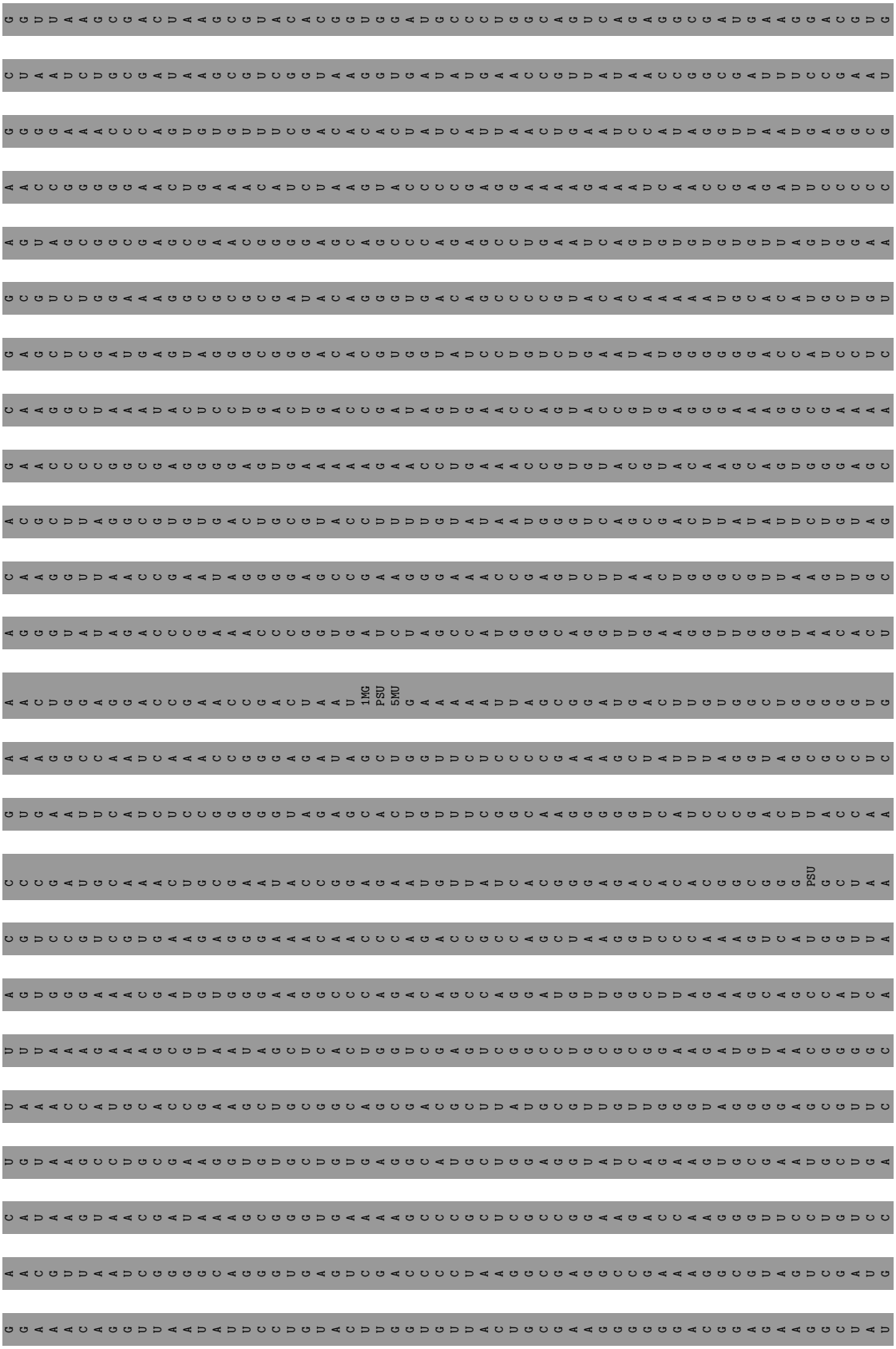
• Molecule 13: Small ribosomal subunit protein bS21

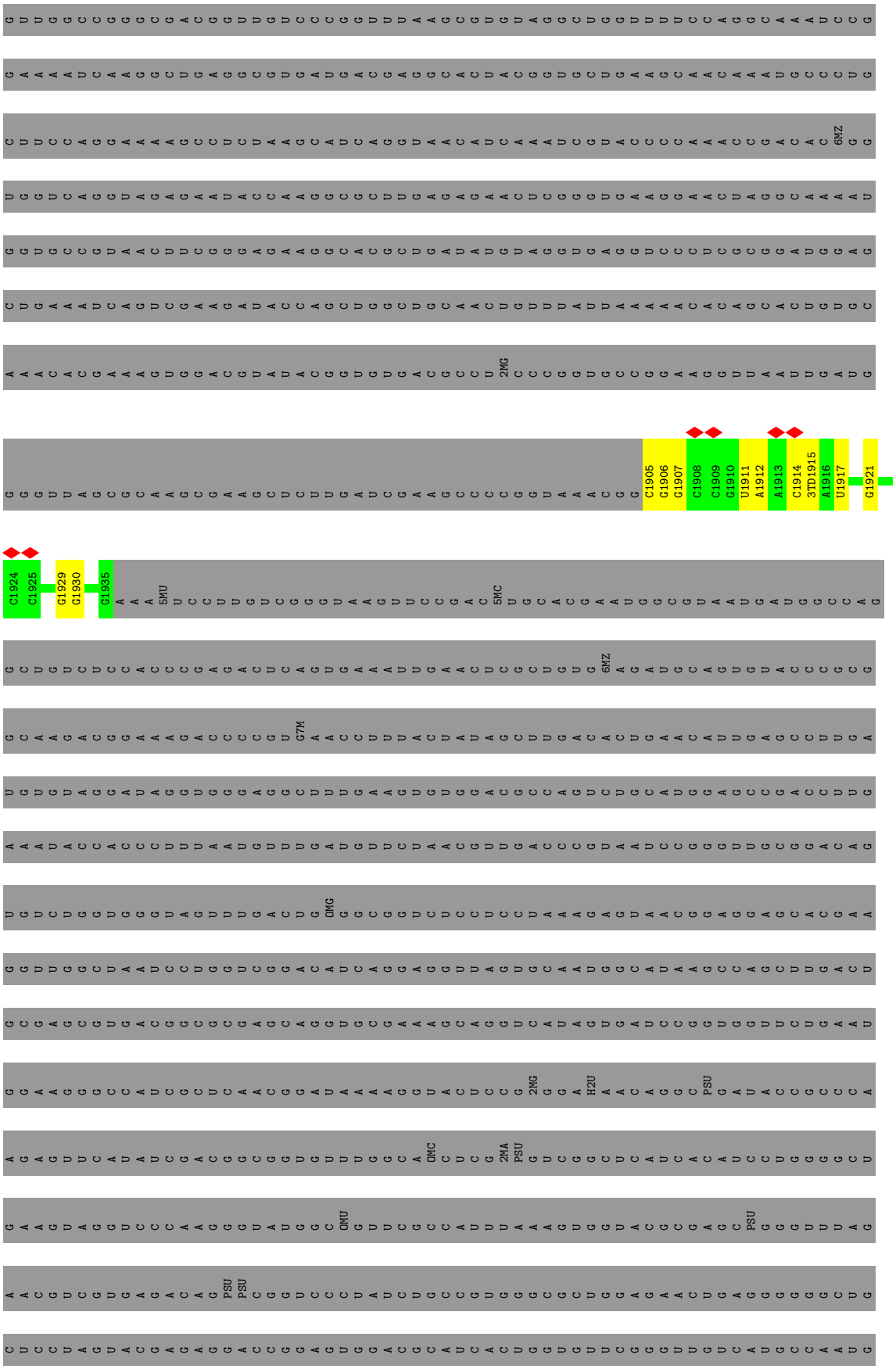
Chain U:

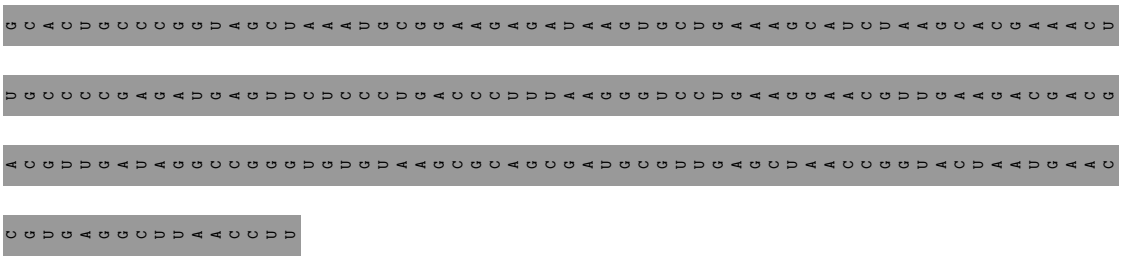


• Molecule 14: 23S rRNA

Chain a: 99%

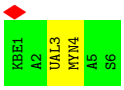



6MZ
2MG
C1905
G1906
G1907
C1908
C1909
G1910
U1911
A1912
A1913
C1914
3TD1915
A1916
U1917
G1921
C1924
C1925
G1929
G1930
G1935
5MU
5MC
6MZ
G7M
DMG
2MG
H2U
PSU
OMC
2MA
PSU
OMU
PSU
PSU



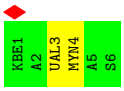
• Molecule 15: Capreomycin IA

Chain V:



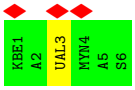
• Molecule 15: Capreomycin IA

Chain B:



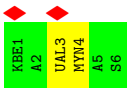
• Molecule 15: Capreomycin IA

Chain C:



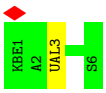
• Molecule 15: Capreomycin IA

Chain G:



• Molecule 15: Capreomycin IA

Chain I:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	179724	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.079	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0122	Depositor
Map size (Å)	518.4, 518.4, 518.4	wwPDB
Map dimensions	720, 720, 720	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.72, 0.72, 0.72	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: DPP, UR3, UAL, G7M, IAS, PSU, 3TD, K, D2T, MYN, 5MC, 2MG, KSG, KBE, MA6, 4OC, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.48	0/24994	1.14	20/38986 (0.1%)
2	D	0.29	0/1665	0.64	0/2227
3	E	0.30	0/1165	0.65	0/1568
4	F	0.29	0/835	0.66	0/1130
5	H	0.30	0/989	0.63	0/1326
6	K	0.32	0/884	0.66	0/1191
7	L	0.29	0/960	0.73	0/1286
8	O	0.29	0/722	0.58	0/964
9	P	0.29	0/648	0.69	0/870
10	Q	0.28	0/641	0.65	0/860
11	R	0.30	0/532	0.65	0/715
12	T	0.27	0/670	0.56	0/888
13	U	0.29	0/467	0.67	0/620
14	a	0.54	0/674	1.20	2/1047 (0.2%)
15	B	0.19	0/5	0.38	0/5
15	C	0.07	0/5	0.36	0/5
15	G	0.15	0/5	0.29	0/5
15	I	0.12	0/5	0.51	0/5
15	V	0.17	0/5	0.22	0/5
All	All	0.44	0/35871	1.04	22/53703 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1
4	F	0	1
7	L	0	1
8	O	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
9	P	0	1
10	Q	0	1
12	T	0	2
All	All	0	9

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	22	G	O5'-P-OP2	-7.44	99.00	105.70
1	A	321	A	O5'-P-OP2	-7.34	99.09	105.70
1	A	176	C	O3'-P-O5'	-7.34	90.06	104.00
1	A	329	A	O5'-P-OP2	-7.09	99.32	105.70
14	a	1905	C	O3'-P-O5'	-7.05	90.61	104.00

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	146	ARG	Sidechain
4	F	24	ARG	Sidechain
7	L	14	ARG	Sidechain
8	O	53	ARG	Sidechain
8	O	72	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	A	22497	0	11322	14	0
2	D	1643	0	1706	7	0
3	E	1152	0	1196	3	0
4	F	816	0	803	0	0
5	H	979	0	1031	1	0
6	K	877	0	884	1	0
7	L	957	0	1017	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	O	714	0	734	0	0
9	P	638	0	656	0	0
10	Q	632	0	669	1	0
11	R	524	0	543	0	0
12	T	664	0	714	0	0
13	U	460	0	486	0	0
14	a	664	0	338	0	0
15	B	47	0	39	0	0
15	C	47	0	39	0	0
15	G	47	0	39	0	0
15	I	47	0	39	0	0
15	V	47	0	39	0	0
16	A	23	0	0	0	0
16	D	1	0	0	0	0
16	F	1	0	0	0	0
17	A	26	0	23	0	0
18	A	54	0	0	0	0
19	A	1660	0	0	0	0
19	B	1	0	0	0	0
19	C	1	0	0	0	0
19	D	40	0	0	0	0
19	E	35	0	0	0	0
19	F	2	0	0	0	0
19	H	27	0	0	0	0
19	I	3	0	0	0	0
19	K	17	0	0	0	0
19	L	43	0	0	0	0
19	O	18	0	0	0	0
19	P	33	0	0	0	0
19	Q	15	0	0	0	0
19	R	6	0	0	0	0
19	T	25	0	0	0	0
19	U	4	0	0	0	0
19	V	2	0	0	0	0
19	a	1	0	0	0	0
All	All	35490	0	22317	23	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 0.

The worst 5 of 23 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:A:415:A:H61	1:A:427:U:H3	1.34	0.76
1:A:823:C:HO2'	5:H:2:SER:N	1.93	0.66
7:L:4:VAL:HG23	10:Q:34:TYR:HB3	1.88	0.54
1:A:664:G:H22	1:A:741:G:H1	1.55	0.54
1:A:769:G:H4'	1:A:1513:A:H4'	1.90	0.53

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	D	203/206 (98%)	199 (98%)	4 (2%)	0	100	100
3	E	154/167 (92%)	148 (96%)	6 (4%)	0	100	100
4	F	98/131 (75%)	95 (97%)	3 (3%)	0	100	100
5	H	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
6	K	113/129 (88%)	110 (97%)	3 (3%)	0	100	100
7	L	120/124 (97%)	119 (99%)	1 (1%)	0	100	100
8	O	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
9	P	78/82 (95%)	75 (96%)	3 (4%)	0	100	100
10	Q	76/84 (90%)	75 (99%)	1 (1%)	0	100	100
11	R	62/75 (83%)	60 (97%)	2 (3%)	0	100	100
12	T	83/87 (95%)	83 (100%)	0	0	100	100
13	U	53/71 (75%)	51 (96%)	2 (4%)	0	100	100
All	All	1253/1375 (91%)	1224 (98%)	29 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	D	172/173 (99%)	168 (98%)	4 (2%)	50 44
3	E	119/126 (94%)	119 (100%)	0	100 100
4	F	87/112 (78%)	87 (100%)	0	100 100
5	H	104/105 (99%)	104 (100%)	0	100 100
6	K	89/98 (91%)	88 (99%)	1 (1%)	73 73
7	L	102/103 (99%)	99 (97%)	3 (3%)	42 35
8	O	76/77 (99%)	75 (99%)	1 (1%)	69 67
9	P	65/65 (100%)	64 (98%)	1 (2%)	65 62
10	Q	72/78 (92%)	72 (100%)	0	100 100
11	R	55/65 (85%)	55 (100%)	0	100 100
12	T	65/66 (98%)	65 (100%)	0	100 100
13	U	48/61 (79%)	47 (98%)	1 (2%)	53 48
15	B	1/1 (100%)	1 (100%)	0	100 100
15	C	1/1 (100%)	1 (100%)	0	100 100
15	G	1/1 (100%)	1 (100%)	0	100 100
15	I	1/1 (100%)	1 (100%)	0	100 100
15	V	1/1 (100%)	1 (100%)	0	100 100
All	All	1059/1134 (93%)	1048 (99%)	11 (1%)	77 75

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	L	45	PRO
8	O	17	ARG
13	U	5	LYS
9	P	46	LYS
6	K	13	ARG

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

sidechains are listed below:

Mol	Chain	Res	Type
2	D	136	GLN
6	K	81	ASN
9	P	9	HIS
11	R	19	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1038/1540 (67%)	102 (9%)	11 (1%)
14	a	29/2904 (0%)	6 (20%)	0
All	All	1067/4444 (24%)	108 (10%)	11 (1%)

5 of 108 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	5	U
1	A	32	A
1	A	39	G
1	A	47	C

5 of 11 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	653	U
1	A	733	G
1	A	1452	C
1	A	1447	A
1	A	468	A

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

38 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	$\#\|Z\|>2$
15	MYN	G	4	15	7,11,12	0.47	0	6,14,16	1.34	1 (16%)
1	2MG	A	1516	1	18,26,27	1.02	2 (11%)	16,38,41	0.79	0
15	DPP	B	2	15	3,5,6	0.71	0	1,5,7	0.08	0
15	DPP	G	5	15	3,5,6	0.64	0	1,5,7	0.19	0
1	UR3	A	1498	1	19,22,23	0.26	0	26,32,35	0.75	1 (3%)
15	KBE	G	1	15	8,8,9	0.59	0	7,8,10	0.62	0
1	PSU	A	516	1,18	18,21,22	0.95	1 (5%)	22,30,33	0.63	0
1	MA6	A	1518	1	18,26,27	0.78	2 (11%)	19,38,41	0.62	0
15	DPP	B	5	15	3,5,6	0.64	0	1,5,7	0.24	0
14	PSU	a	1911	14	18,21,22	0.94	1 (5%)	22,30,33	0.70	0
15	UAL	B	3	15	7,8,9	1.40	1 (14%)	5,9,11	2.04	1 (20%)
1	G7M	A	527	1	20,26,27	1.09	2 (10%)	17,39,42	0.69	0
7	D2T	L	89	7	7,9,10	1.01	0	6,11,13	1.79	3 (50%)
15	UAL	I	3	15	7,8,9	1.38	1 (14%)	5,9,11	2.32	1 (20%)
15	KBE	C	1	15	8,8,9	0.63	0	7,8,10	0.76	0
1	4OC	A	1402	1	20,23,24	0.42	0	26,32,35	0.75	0
15	DPP	V	2	15	3,5,6	0.71	0	1,5,7	0.47	0
15	KBE	B	1	15	8,8,9	0.57	0	7,8,10	0.71	0
15	MYN	B	4	15	7,11,12	0.56	0	6,14,16	1.29	1 (16%)
15	KBE	V	1	15	8,8,9	0.57	0	7,8,10	0.56	0
15	DPP	V	5	15	3,5,6	0.65	0	1,5,7	0.20	0
15	UAL	V	3	15	7,8,9	1.38	1 (14%)	5,9,11	2.07	1 (20%)
14	3TD	a	1915	14	18,22,23	1.00	1 (5%)	22,32,35	0.74	0
15	DPP	C	2	15	3,5,6	0.73	0	1,5,7	0.17	0
15	DPP	C	5	15	3,5,6	0.66	0	1,5,7	0.31	0
15	DPP	G	2	15	3,5,6	0.73	0	1,5,7	0.06	0
15	MYN	I	4	15	7,11,12	0.48	0	6,14,16	0.98	0
1	MA6	A	1519	1	18,26,27	0.79	1 (5%)	19,38,41	0.77	0
14	PSU	a	1917	14	18,21,22	0.98	1 (5%)	22,30,33	0.64	0
15	DPP	I	2	15	3,5,6	0.74	0	1,5,7	0.09	0
15	UAL	G	3	15	7,8,9	1.40	1 (14%)	5,9,11	2.13	1 (20%)
15	DPP	I	5	15	3,5,6	0.65	0	1,5,7	0.27	0
6	IAS	K	119	6	6,7,8	0.89	0	6,8,10	0.93	0
15	UAL	C	3	15	7,8,9	1.45	1 (14%)	5,9,11	2.17	1 (20%)
1	5MC	A	1407	1	18,22,23	0.34	0	26,32,35	0.80	0
15	KBE	I	1	15	8,8,9	0.57	0	7,8,10	0.66	0
15	MYN	V	4	15	7,11,12	0.55	0	6,14,16	1.35	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	MYN	C	4	15	7,11,12	0.50	0	6,14,16	1.14	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
15	MYN	G	4	15	-	1/1/16/18	0/1/1/1
1	2MG	A	1516	1	-	0/5/27/28	0/3/3/3
15	DPP	B	2	15	-	0/2/4/6	-
15	DPP	G	5	15	-	0/2/4/6	-
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
15	KBE	G	1	15	-	4/7/7/8	-
1	PSU	A	516	1,18	-	0/7/25/26	0/2/2/2
1	MA6	A	1518	1	-	0/7/29/30	0/3/3/3
15	DPP	B	5	15	-	0/2/4/6	-
14	PSU	a	1911	14	-	2/7/25/26	0/2/2/2
15	UAL	B	3	15	-	0/3/7/9	-
1	G7M	A	527	1	-	0/3/25/26	0/3/3/3
7	D2T	L	89	7	-	4/7/12/14	-
15	UAL	I	3	15	-	2/3/7/9	-
15	KBE	C	1	15	-	2/7/7/8	-
1	4OC	A	1402	1	-	0/9/29/30	0/2/2/2
15	DPP	V	2	15	-	2/2/4/6	-
15	KBE	B	1	15	-	2/7/7/8	-
15	MYN	B	4	15	-	0/1/16/18	0/1/1/1
15	KBE	V	1	15	-	1/7/7/8	-
15	DPP	V	5	15	-	0/2/4/6	-
15	UAL	V	3	15	-	0/3/7/9	-
14	3TD	a	1915	14	-	0/7/25/26	0/2/2/2
15	DPP	C	2	15	-	0/2/4/6	-
15	DPP	C	5	15	-	0/2/4/6	-
15	DPP	G	2	15	-	2/2/4/6	-
15	MYN	I	4	15	-	0/1/16/18	0/1/1/1
1	MA6	A	1519	1	-	2/7/29/30	0/3/3/3
14	PSU	a	1917	14	-	0/7/25/26	0/2/2/2
15	DPP	I	2	15	-	0/2/4/6	-
15	UAL	G	3	15	-	0/3/7/9	-
15	DPP	I	5	15	-	0/2/4/6	-
6	IAS	K	119	6	-	1/7/7/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	UAL	C	3	15	-	2/3/7/9	-
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
15	KBE	I	1	15	-	1/7/7/8	-
15	MYN	V	4	15	-	0/1/16/18	0/1/1/1
15	MYN	C	4	15	-	0/1/16/18	0/1/1/1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1917	PSU	C6-C5	3.91	1.39	1.35
14	a	1915	3TD	C6-C5	3.88	1.39	1.35
1	A	516	PSU	C6-C5	3.82	1.39	1.35
14	a	1911	PSU	C6-C5	3.71	1.39	1.35
1	A	527	G7M	C8-N9	3.52	1.39	1.33

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	I	3	UAL	O-C-CA	-4.90	119.15	125.39
15	G	3	UAL	O-C-CA	-4.73	119.38	125.39
15	C	3	UAL	O-C-CA	-4.62	119.52	125.39
15	V	3	UAL	O-C-CA	-4.56	119.59	125.39
15	B	3	UAL	O-C-CA	-4.51	119.65	125.39

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	L	89	D2T	CG-CB-SB-CB1
7	L	89	D2T	CA-CB-CG-OD1
7	L	89	D2T	CA-CB-CG-OD2
14	a	1911	PSU	O4'-C1'-C5-C4
14	a	1911	PSU	O4'-C1'-C5-C6

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 80 ligands modelled in this entry, 79 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	$\#\|Z\| > 2$
17	KSG	A	1603	-	25,27,27	0.54	1 (4%)	30,40,40	0.59	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
17	KSG	A	1603	-	-	1/10/52/52	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	1603	KSG	O9-C14	-2.18	1.24	1.30

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	A	1603	KSG	O7-C1-O1-C2

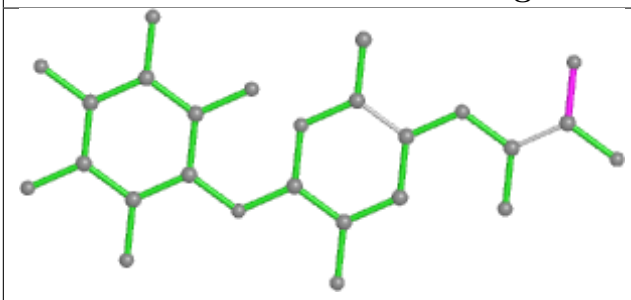
There are no ring outliers.

No monomer is involved in short contacts.

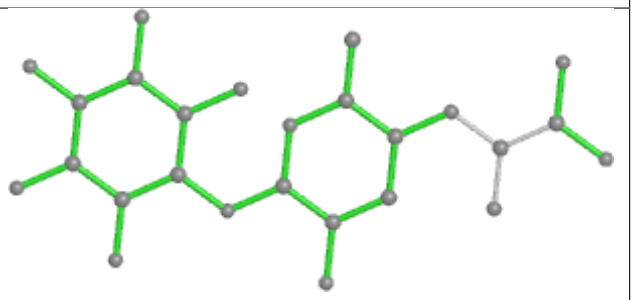
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

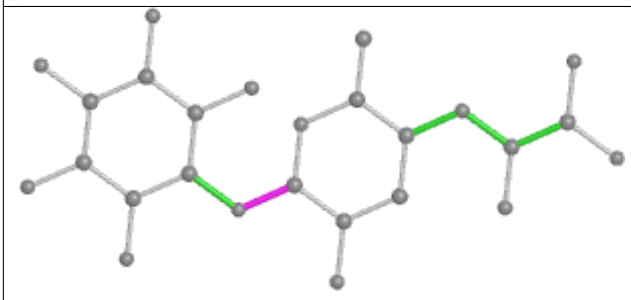
Ligand KSG A 1603



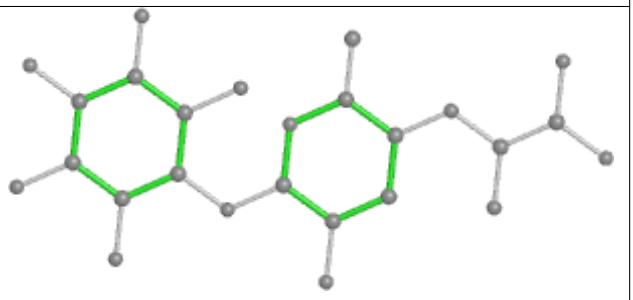
Bond lengths



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.

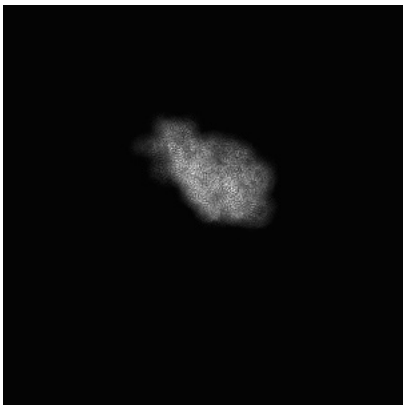
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16612. These allow visual inspection of the internal detail of the map and identification of artifacts.

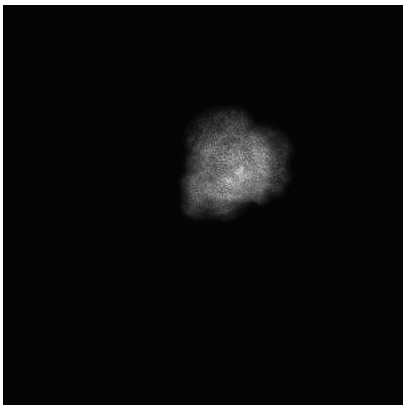
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

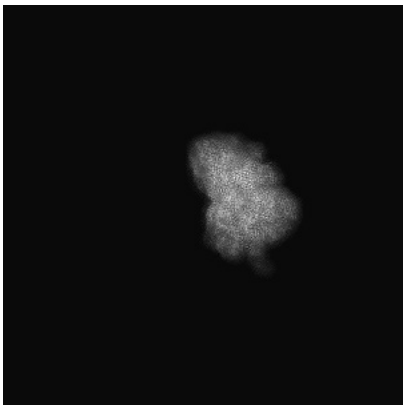
6.1.1 Primary map



X

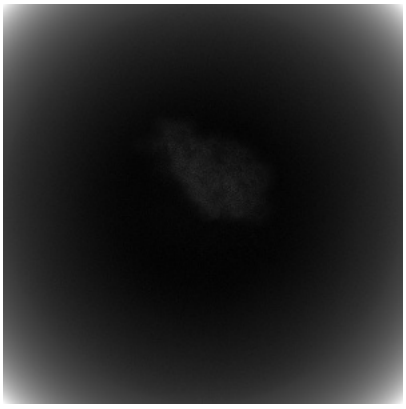


Y

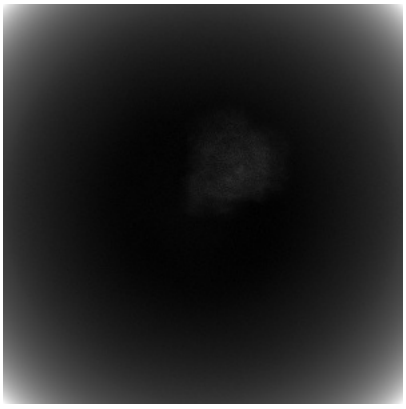


Z

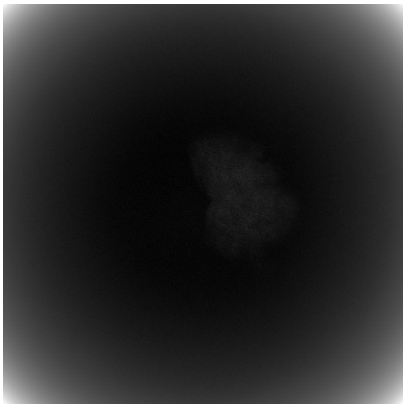
6.1.2 Raw map



X



Y

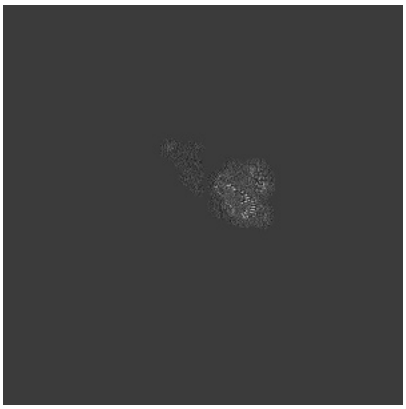


Z

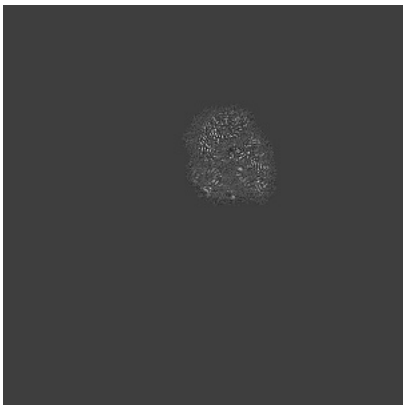
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

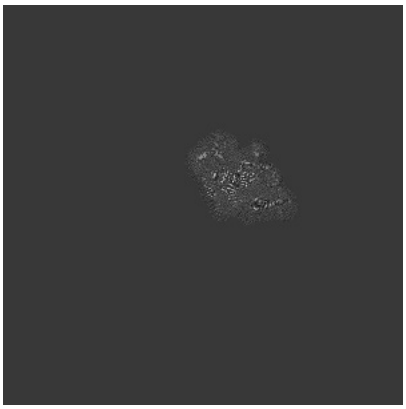
6.2.1 Primary map



X Index: 360

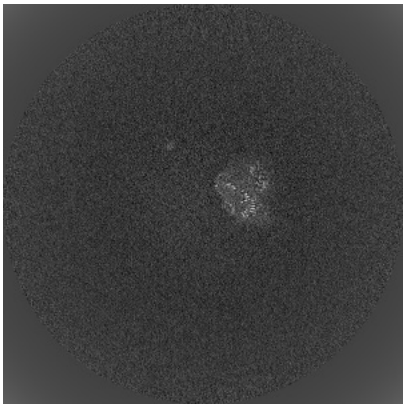


Y Index: 360

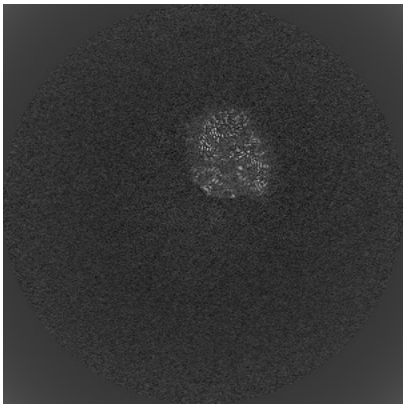


Z Index: 360

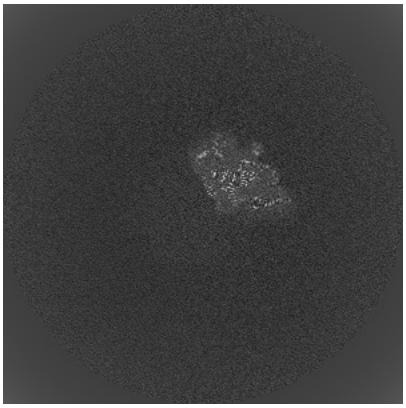
6.2.2 Raw map



X Index: 360



Y Index: 360

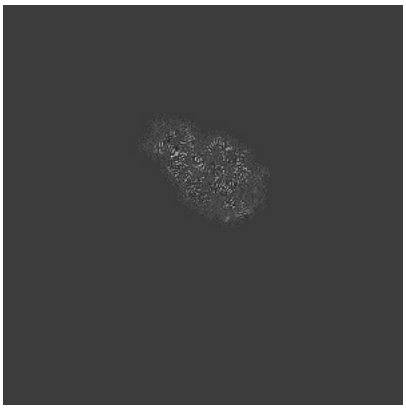


Z Index: 360

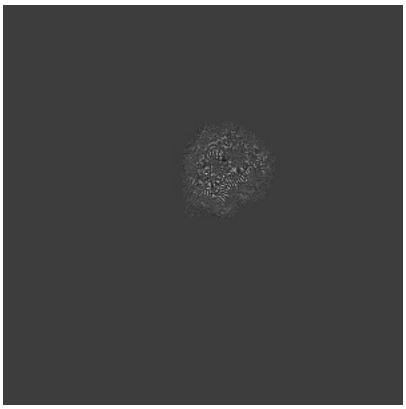
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

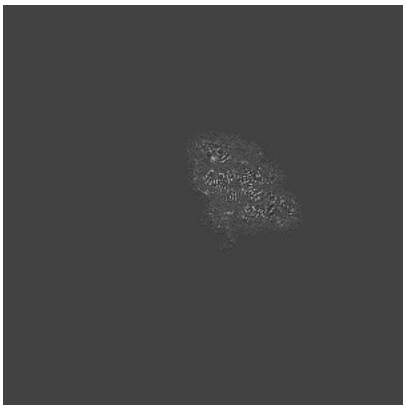
6.3.1 Primary map



X Index: 444



Y Index: 405

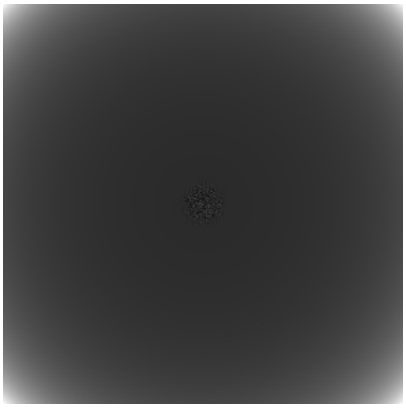


Z Index: 396

6.3.2 Raw map

X Index: 0

Y Index: 0

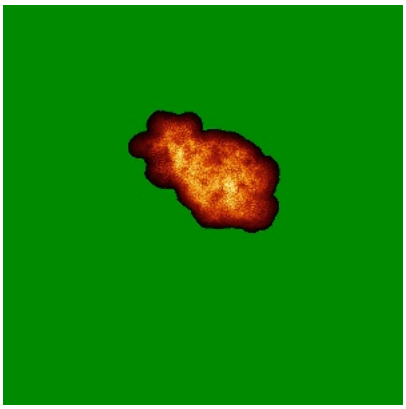


Z Index: 0

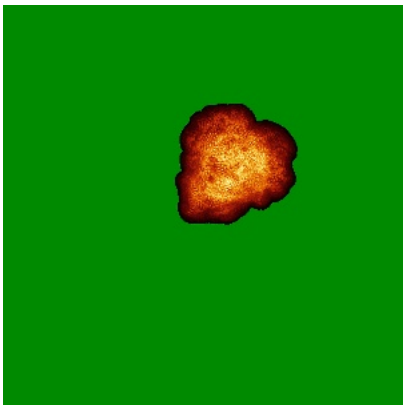
The images above show the largest variance slices of the map in three orthogonal directions.

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

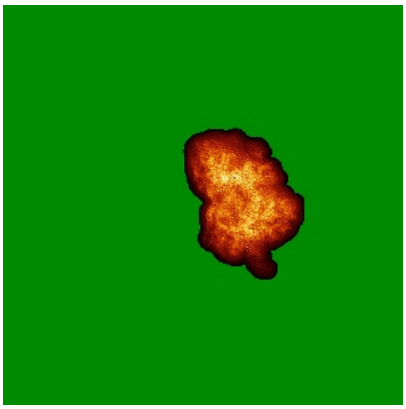
6.4.1 Primary map



X

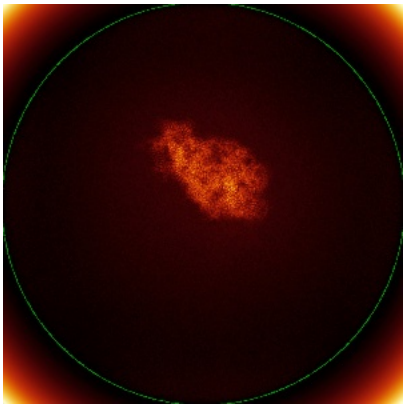


Y

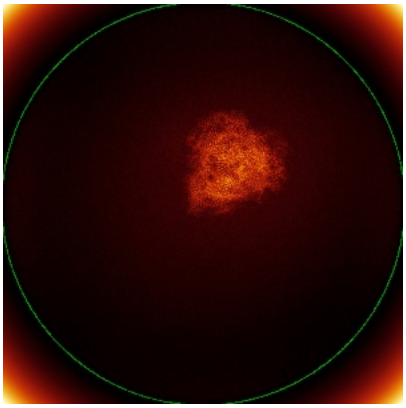


Z

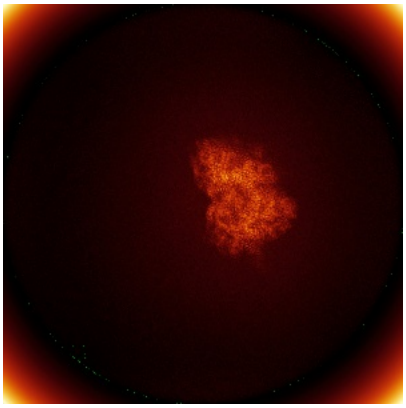
6.4.2 Raw map



X



Y

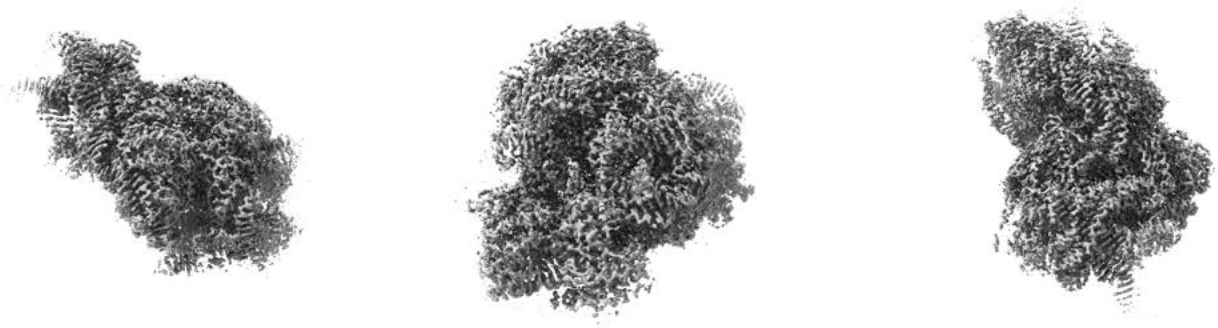


Z

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

6.5 Orthogonal surface views (i)

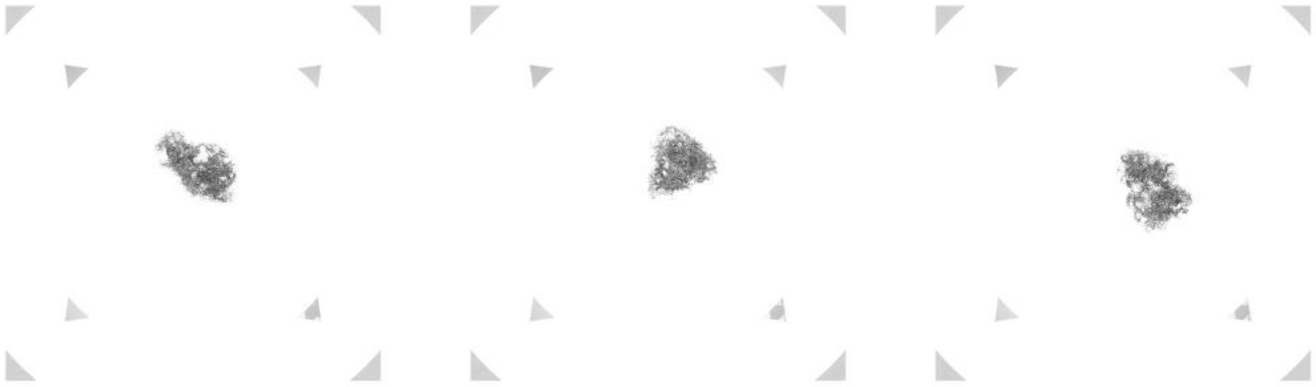
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0122. 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.

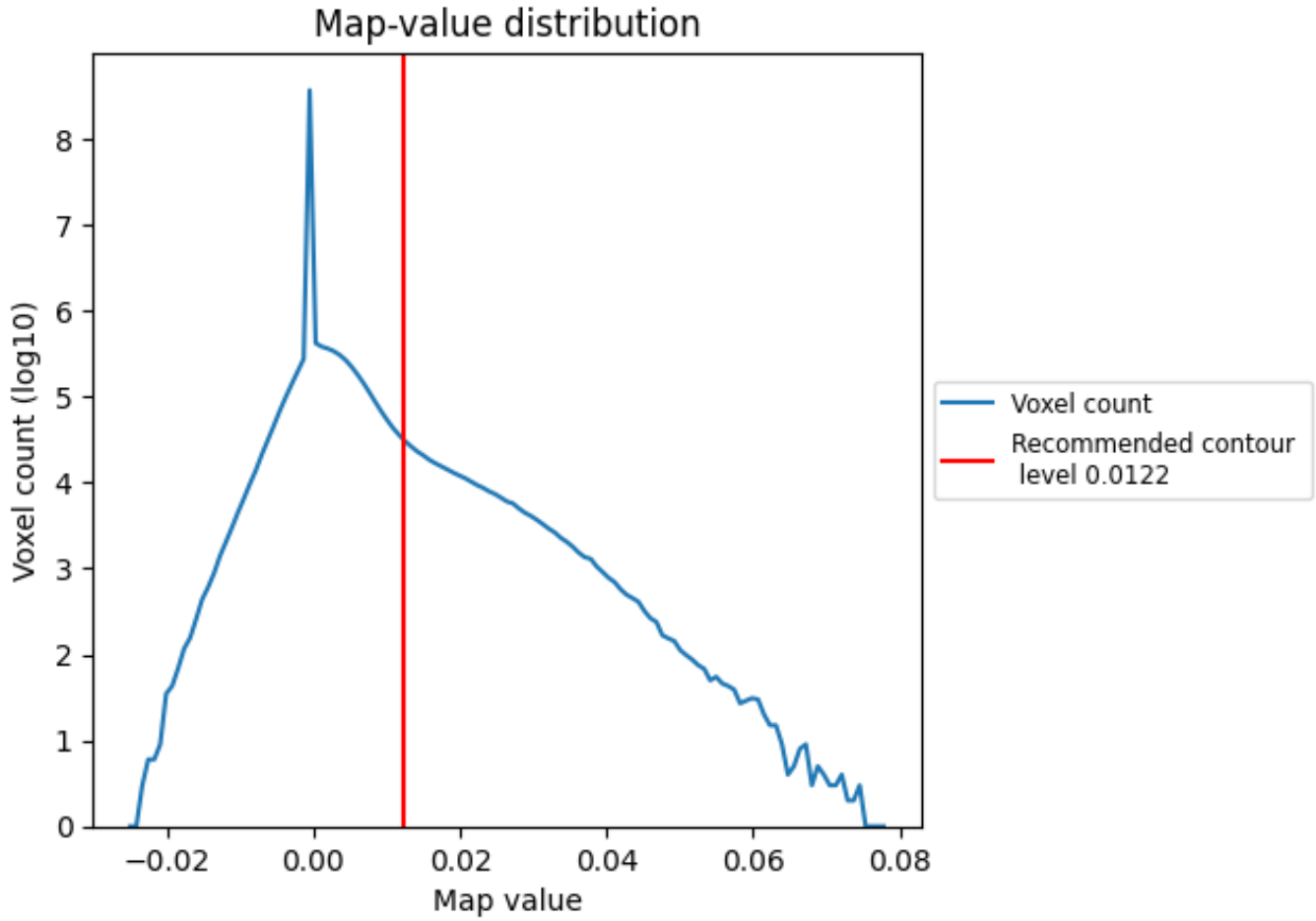
6.6 Mask visualisation (i)

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

7 Map analysis

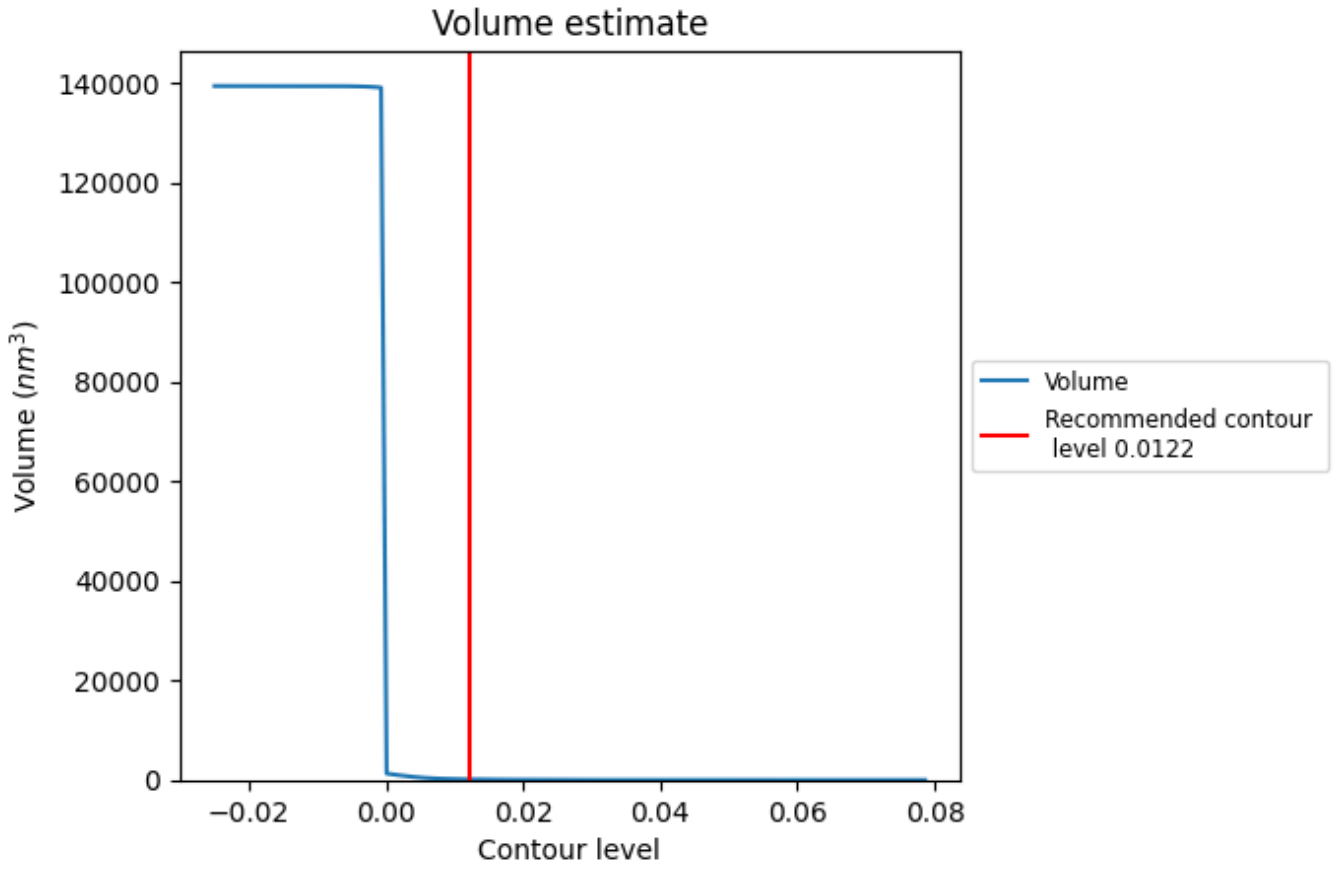
This section contains the results of statistical analysis of the map.

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.

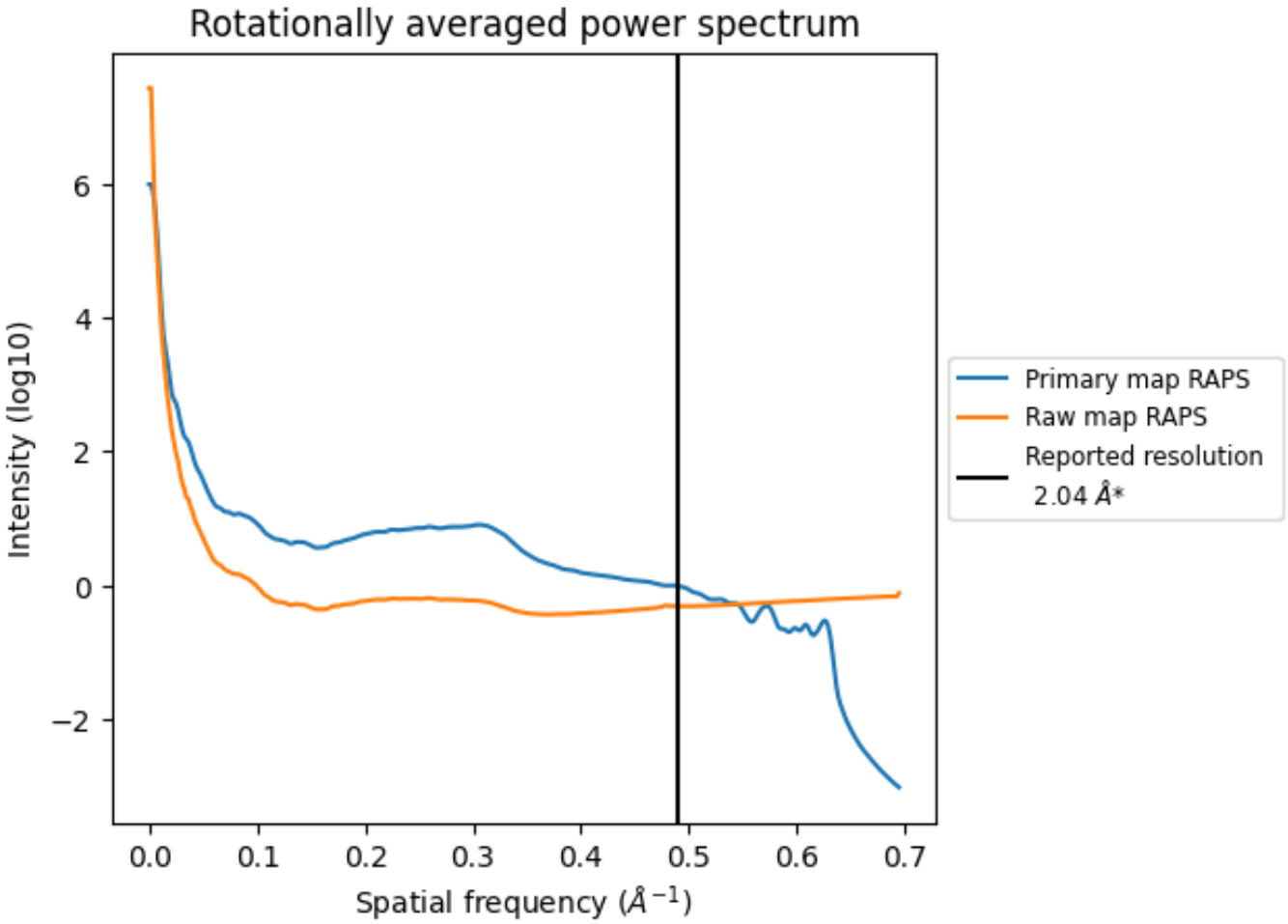
7.2 Volume estimate (i)



The volume at the recommended contour level is 120 nm^3; this corresponds to an approximate mass of 109 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)

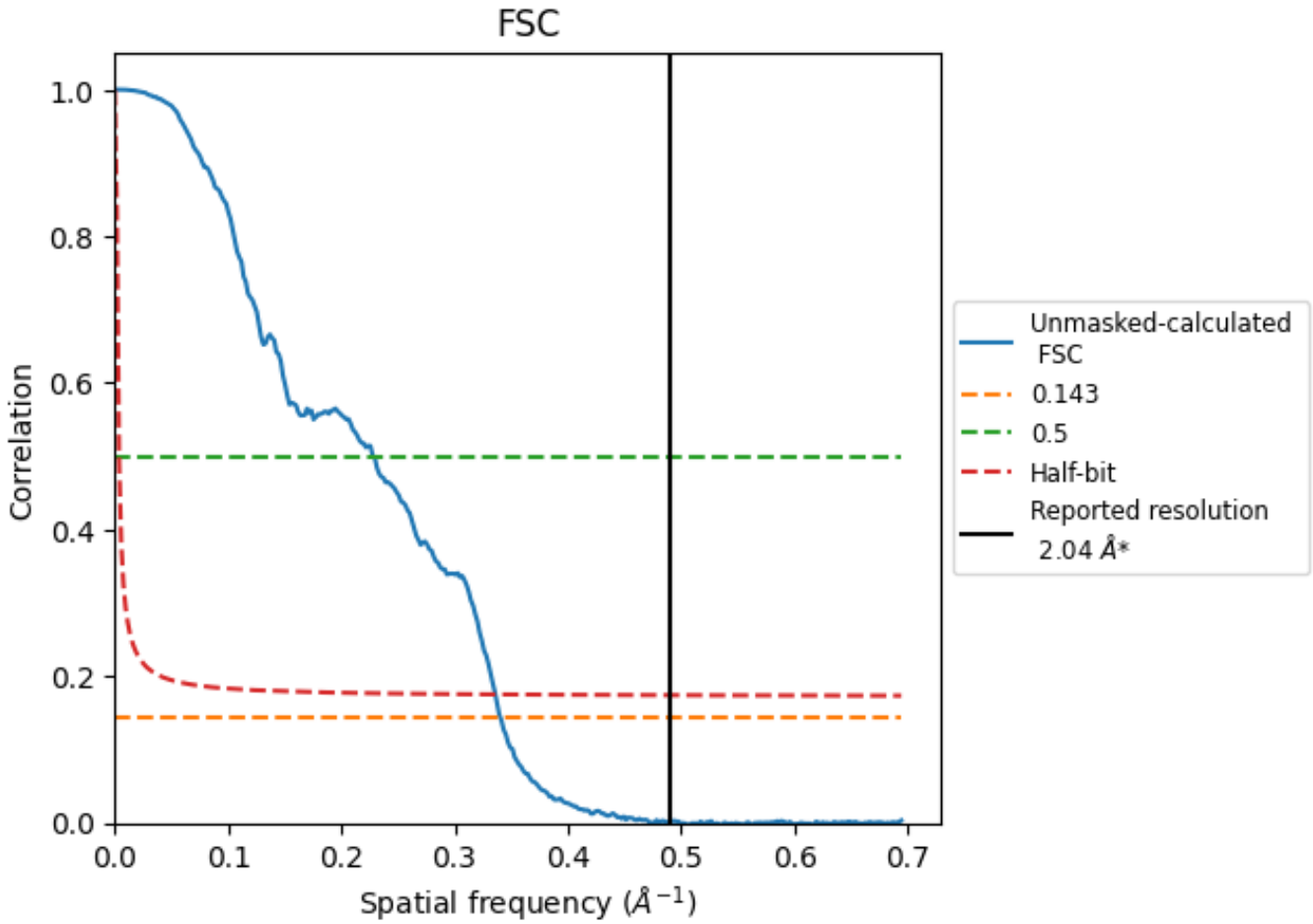


*Reported resolution corresponds to spatial frequency of 0.490 Å^{-1}

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 0.490 Å^{-1}

8.2 Resolution estimates (i)

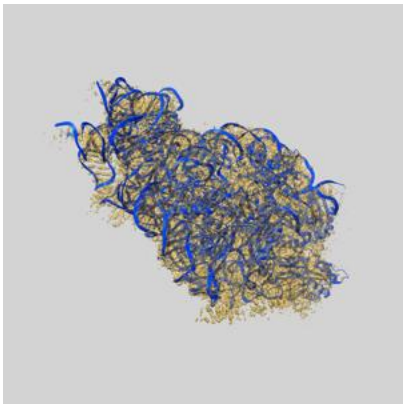
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.04	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.94	4.38	2.98

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.94 differs from the reported value 2.04 by more than 10 %

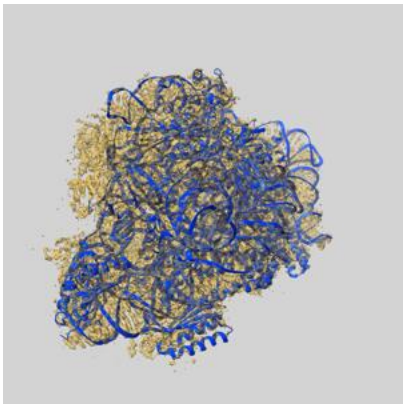
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16612 and PDB model 8CEP. Per-residue inclusion information can be found in section 3 on page 9.

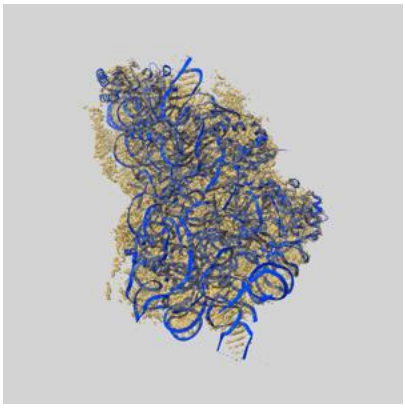
9.1 Map-model overlay



X



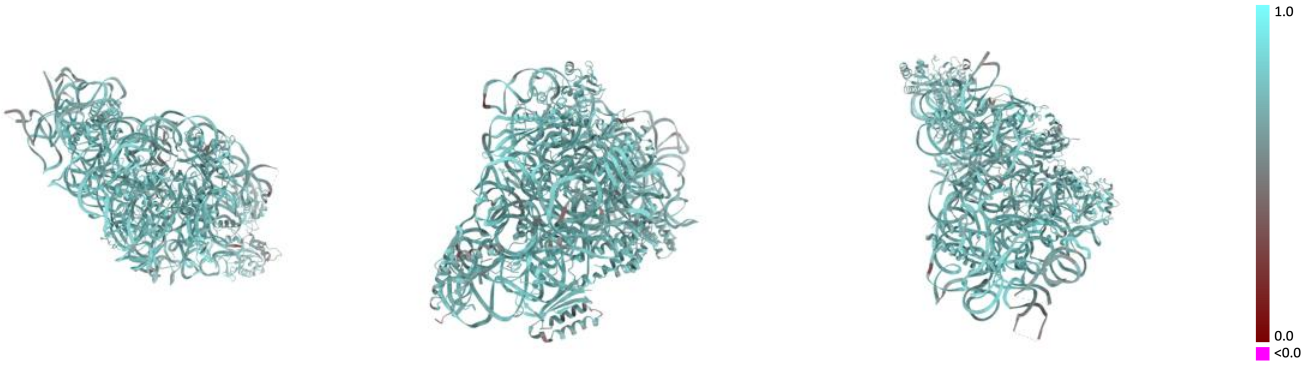
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0122 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.

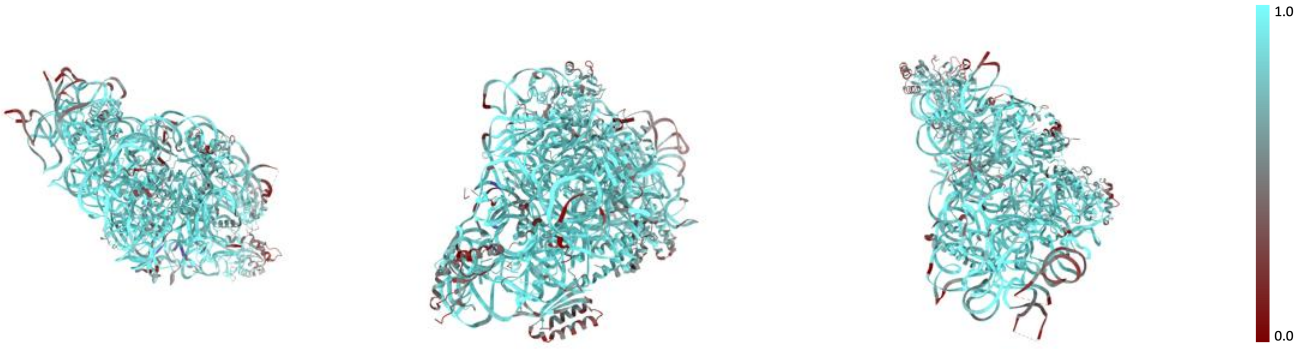
9.2 Q-score mapped to coordinate model (i)



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.

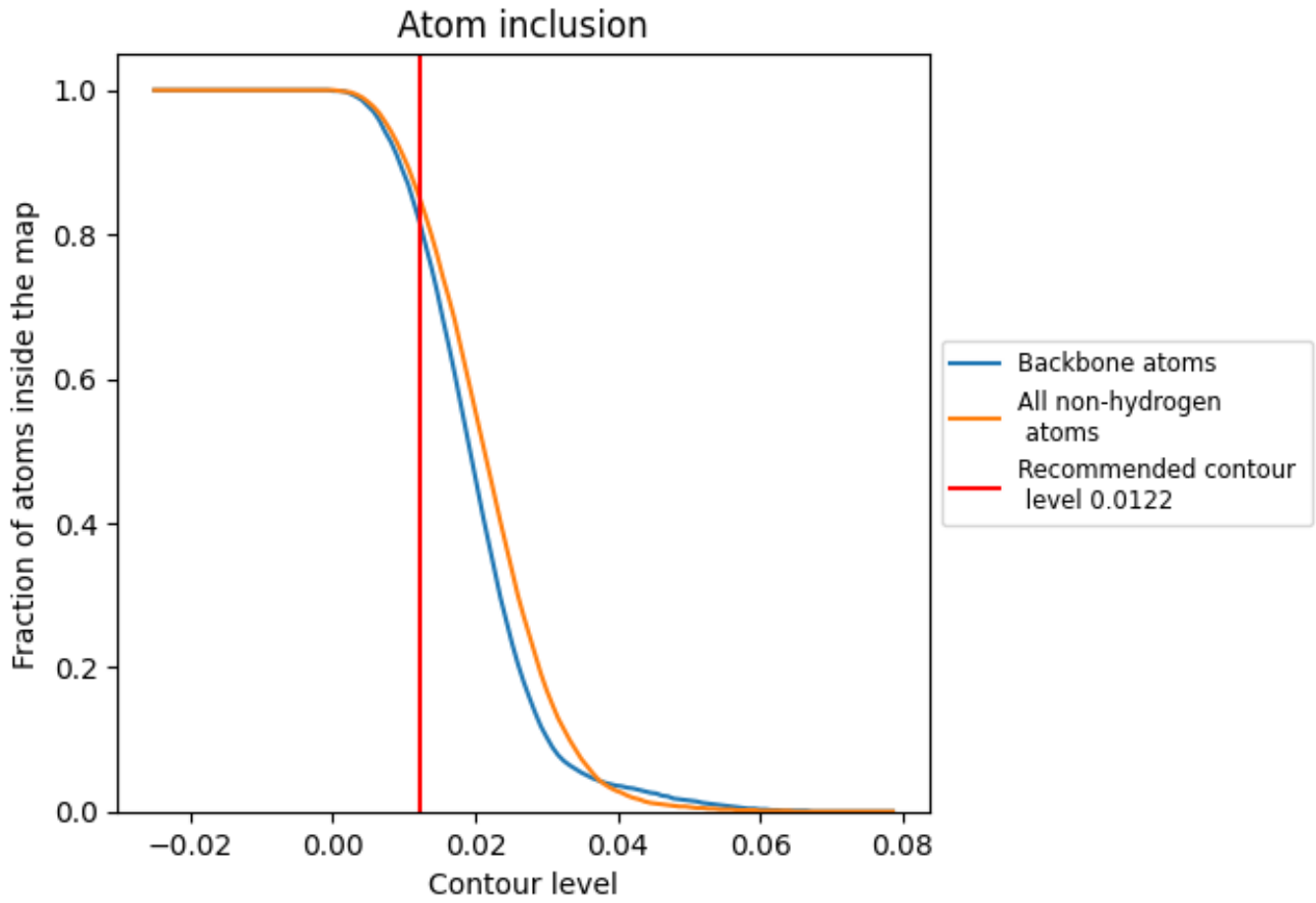
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0122).

9.4 Atom inclusion (i)



At the recommended contour level, 82% 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 (0.0122) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8520	0.7340
A	0.9050	0.7440
B	0.5110	0.6040
C	0.4250	0.6340
D	0.7870	0.7300
E	0.8230	0.7330
F	0.5590	0.6530
G	0.4250	0.6440
H	0.8390	0.7480
I	0.5750	0.6660
K	0.7000	0.6920
L	0.8450	0.7460
O	0.7780	0.7330
P	0.8650	0.7670
Q	0.7010	0.6960
R	0.7320	0.6970
T	0.8430	0.7520
U	0.4810	0.6110
V	0.5750	0.6560
a	0.6580	0.6500