wwPDB EM Validation Summary Report

Nov 6, 2023 – 12:36 am GMT

PDB ID	:	8CGD
EMDB ID	:	EMD-16641
Title	:	Clindamycin bound to the 50S subunit
Authors	:	Paternoga, H.; Koller, T.O.; Beckert, B.; Wilson, D.N.
Deposited on	:	2023-02-03
Resolution	:	1.98 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:

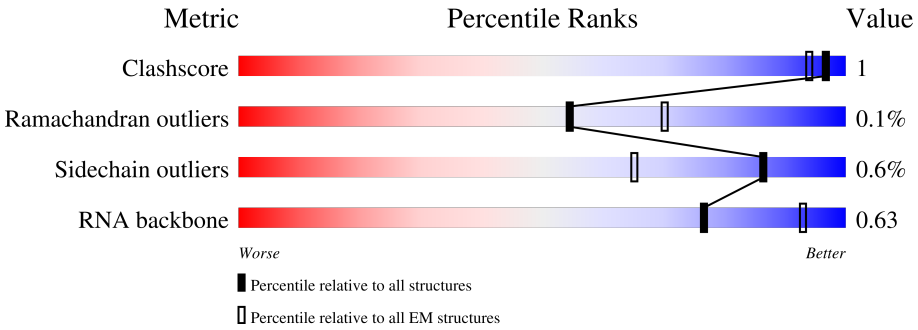
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.98 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	0	55	91% 9%
2	1	46	96%
3	2	65	95%
4	3	38	95% 5%
5	a	2904	82% 12% 5%
6	b	120	5% 88% 10%
7	c	273	99%

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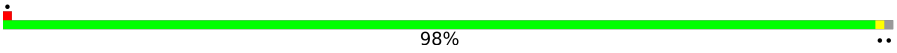
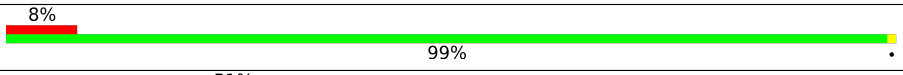
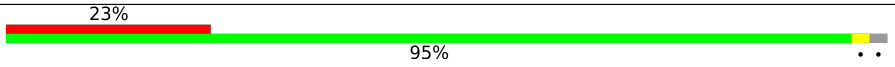
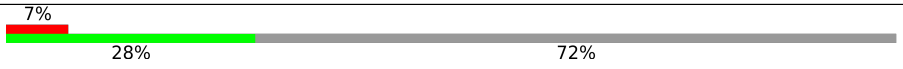
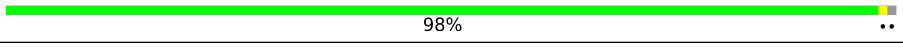
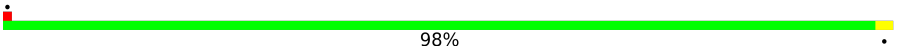
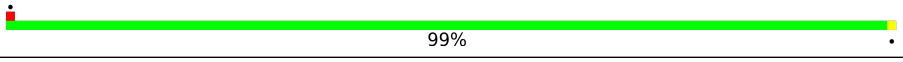
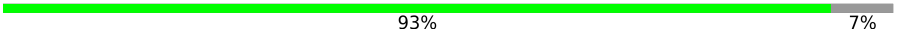
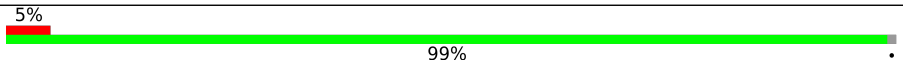
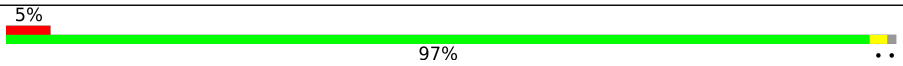
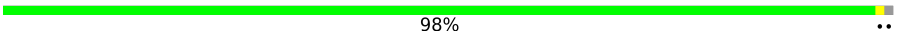
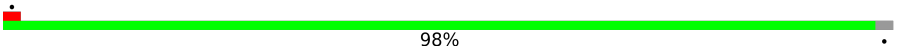
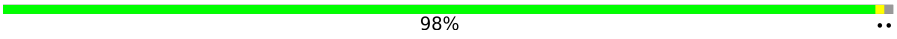
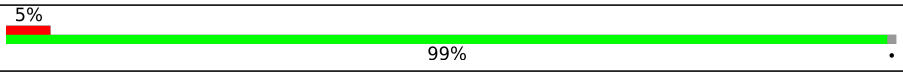
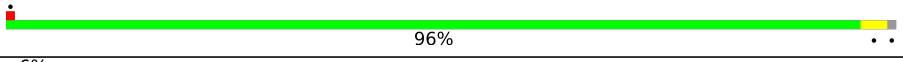
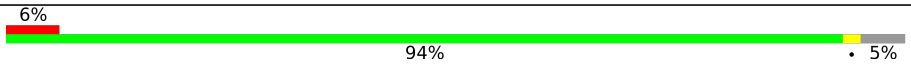
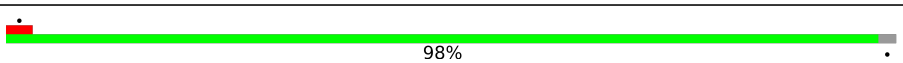
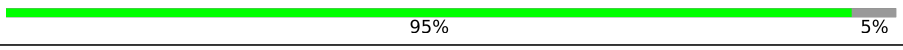
Mol	Chain	Length	Quality of chain
8	d	209	
9	e	201	
10	f	179	
11	g	177	
12	h	149	
13	i	142	
14	j	123	
15	k	144	
16	l	136	
17	m	127	
18	n	117	
19	o	115	
20	p	118	
21	q	103	
22	r	110	
23	s	100	
24	t	104	
25	u	94	
26	v	85	
27	w	78	
28	x	63	
29	y	59	
30	z	57	

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 94181 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 Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	50	Total	C	N	O	0	0
			413	267	75	71		

- Molecule 2 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	45	Total	C	N	O	S	0	0
			367	222	88	55	2		

- Molecule 3 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 4 is a protein called Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 5 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	a	2748	Total	C	N	O	P	0	0
			59025	26337	10880	19060	2748		

- Molecule 6 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	b	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 7 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	c	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 8 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	d	207	Total	C	N	O	S	0	0
			1552	972	286	291	3		

- Molecule 9 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	e	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 10 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	f	154	Total	C	N	O	S	0	0
			1211	773	210	222	6		

- Molecule 11 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	g	173	Total	C	N	O	S	0	0
			1295	814	237	242	2		

- Molecule 12 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	h	41	Total	C	N	O	S	0	0
			303	194	54	54	1		

- Molecule 13 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	i	141	Total	C	N	O	S	0	0
			1121	709	211	198	3		

- Molecule 14 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	j	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 15 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	k	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 16 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	l	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	82	MS6	MET	modified residue	UNP P0ADY7

- Molecule 17 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 18 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	n	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 19 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	o	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 20 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	p	117	Total 947	C 604	N 192	O 151	0	0

- Molecule 21 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	q	101	Total 803	C 509	N 151	O 141	S 2	0	0

- Molecule 22 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	r	109	Total 845	C 526	N 162	O 154	S 3	0	0

- Molecule 23 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	s	88	Total 700	C 444	N 132	O 122	S 2	0	0

- Molecule 24 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	t	92	Total 708	C 446	N 133	O 129	0	0

- Molecule 25 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	u	93	Total 745	C 474	N 136	O 133	S 2	0	0

- Molecule 26 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	v	75	Total 569	C 353	N 113	O 102	S 1	0	0

- Molecule 27 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	w	77	Total 625	C 388	N 129	O 106	S 2	0	0

- Molecule 28 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	x	60	Total 491	C 303	N 96	O 91	S 1	0	0

- Molecule 29 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	y	58	Total 449	C 281	N 87	O 79	S 2	0	0

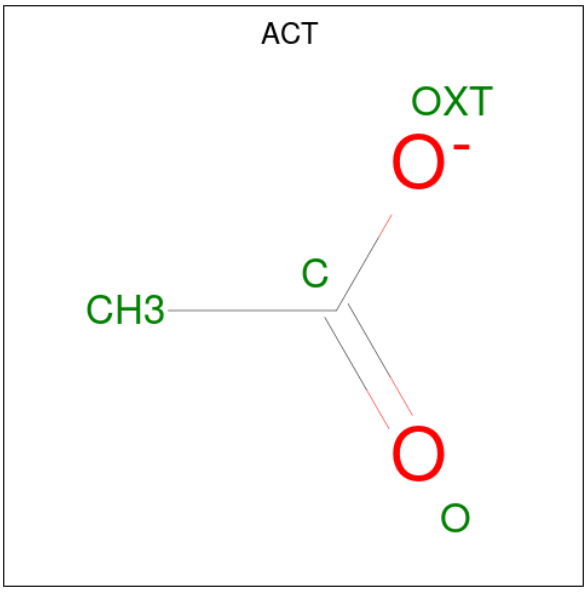
- Molecule 30 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	z	54	Total 429	C 260	N 91	O 77	S 1	0	0

- Molecule 31 is ZINC ION (three-letter code: ZN) (formula: Zn).

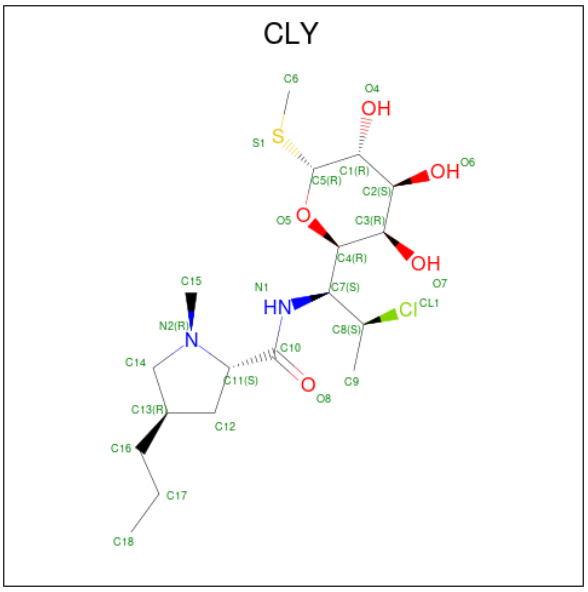
Mol	Chain	Residues	Atoms		AltConf
31	3	1	Total 1	Zn 1	0
31	f	1	Total 1	Zn 1	0

- Molecule 32 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



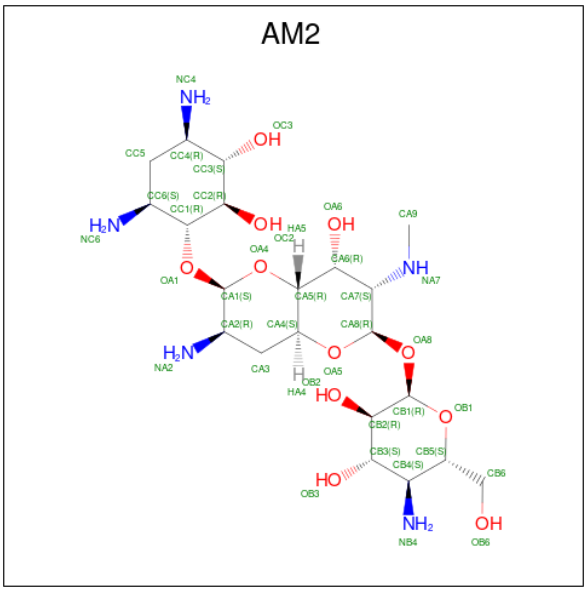
Mol	Chain	Residues	Atoms			AltConf
32	a	1	Total	C	O	0
			4	2	2	

- Molecule 33 is CLINDAMYCIN (three-letter code: CLY) (formula: $C_{18}H_{33}ClN_2O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
33	a	1	Total	C	Cl	N	O	S	0
			27	18	1	2	5	1	

- Molecule 34 is APRAMYCIN (three-letter code: AM2) (formula: $C_{21}H_{41}N_5O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
34	a	1	Total C N O 37 21 5 11	0

- Molecule 35 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
35	a	246	Total Mg 246 246	0
35	b	4	Total Mg 4 4	0
35	c	1	Total Mg 1 1	0
35	d	1	Total Mg 1 1	0
35	p	1	Total Mg 1 1	0
35	z	1	Total Mg 1 1	0

- Molecule 36 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
36	a	79	Total K 79 79	0
36	c	4	Total K 4 4	0

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Mol	Chain	Residues	Atoms	AltConf
36	e	1	Total K 1 1	0
36	t	1	Total K 1 1	0

- Molecule 37 is water.

Mol	Chain	Residues	Atoms	AltConf
37	0	6	Total O 6 6	0
37	1	44	Total O 44 44	0
37	2	40	Total O 40 40	0
37	3	16	Total O 16 16	0
37	a	7060	Total O 7060 7060	0
37	b	111	Total O 111 111	0
37	c	155	Total O 155 155	0
37	d	115	Total O 115 115	0
37	e	72	Total O 72 72	0
37	g	3	Total O 3 3	0
37	h	1	Total O 1 1	0
37	i	53	Total O 53 53	0
37	j	38	Total O 38 38	0
37	k	69	Total O 69 69	0
37	l	70	Total O 70 70	0
37	m	59	Total O 59 59	0
37	n	8	Total O 8 8	0

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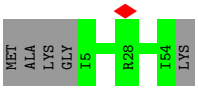
Mol	Chain	Residues	Atoms	AltConf
37	o	50	Total O 50 50	0
37	p	68	Total O 68 68	0
37	q	39	Total O 39 39	0
37	r	59	Total O 59 59	0
37	s	31	Total O 31 31	0
37	t	24	Total O 24 24	0
37	u	23	Total O 23 23	0
37	v	37	Total O 37 37	0
37	w	30	Total O 30 30	0
37	x	11	Total O 11 11	0
37	y	21	Total O 21 21	0
37	z	44	Total O 44 44	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.

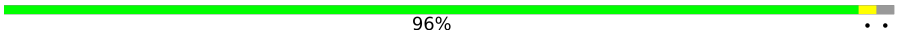
• Molecule 1: Large ribosomal subunit protein bL33

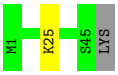
Chain 0:



• Molecule 2: Large ribosomal subunit protein bL34

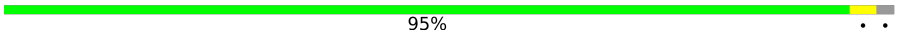
Chain 1:

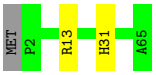




• Molecule 3: Large ribosomal subunit protein bL35

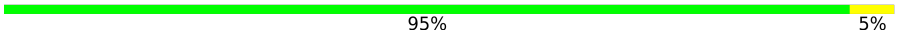
Chain 2:

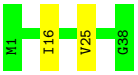




• Molecule 4: Large ribosomal subunit protein bL36A

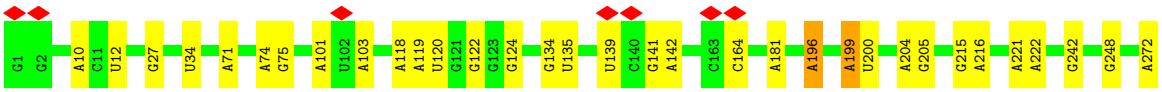
Chain 3:

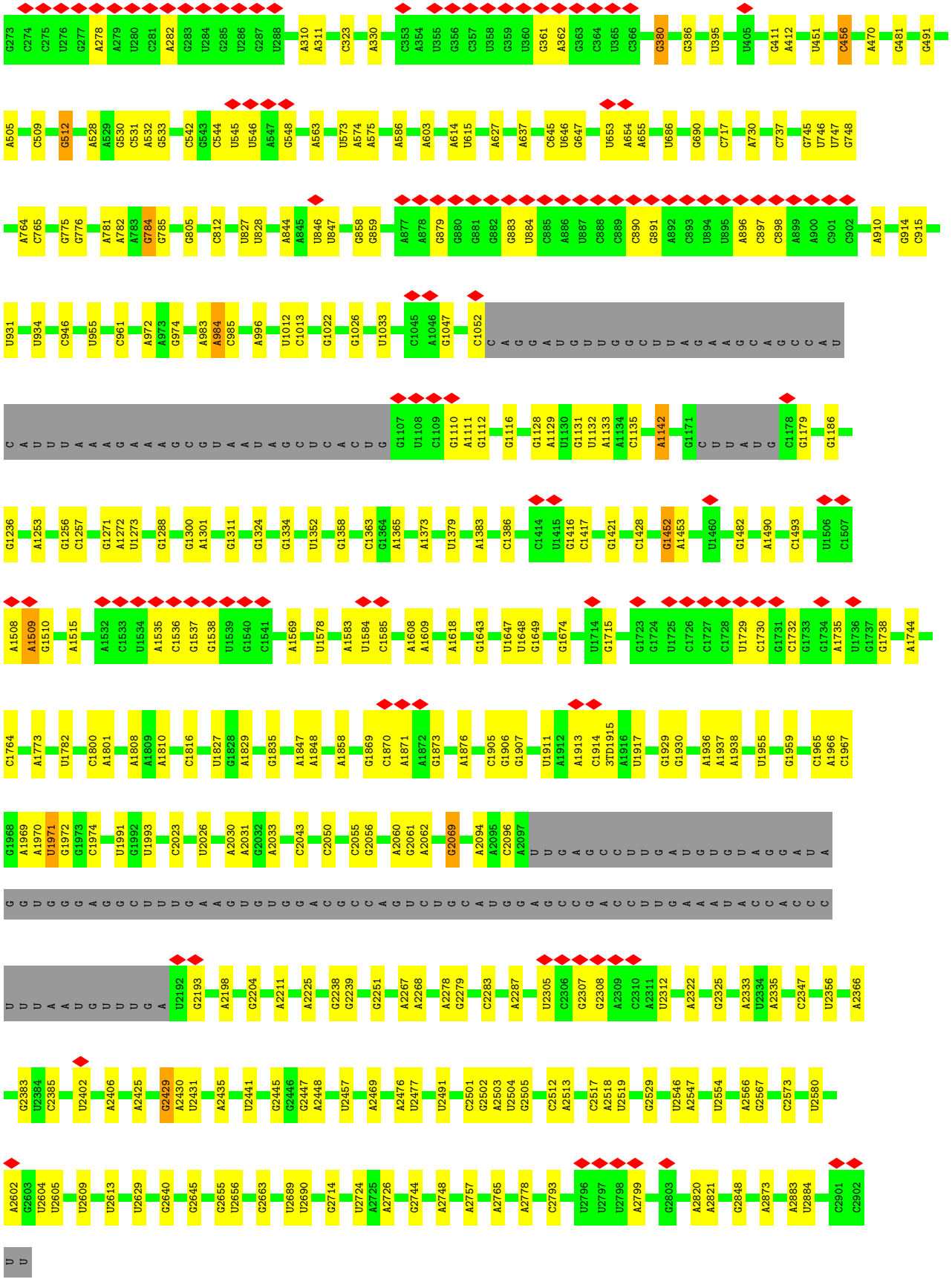




• Molecule 5: 23S rRNA

Chain a:



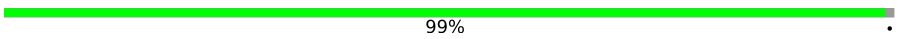


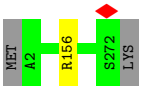
• Molecule 6: 5S rRNA

Chain b:

• Molecule 7: Large ribosomal subunit protein uL2

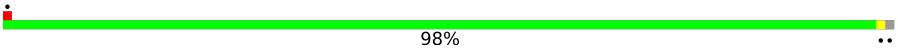
Chain c:

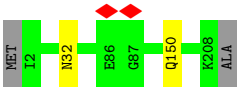




• Molecule 8: Large ribosomal subunit protein uL3

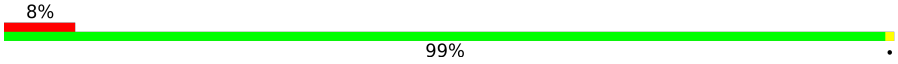
Chain d:

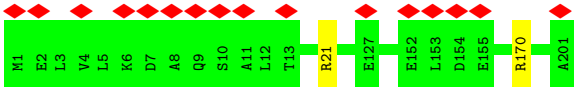




• Molecule 9: Large ribosomal subunit protein uL4

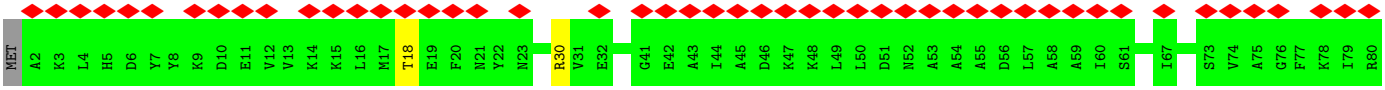
Chain e:

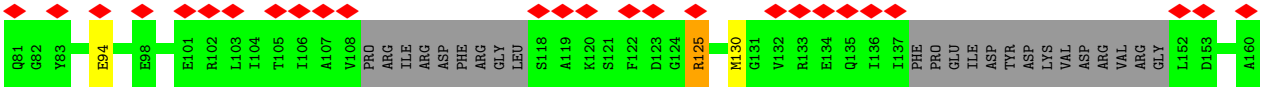


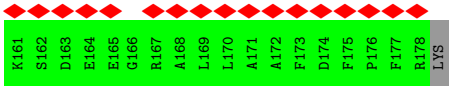


• Molecule 10: Large ribosomal subunit protein uL5

Chain f:

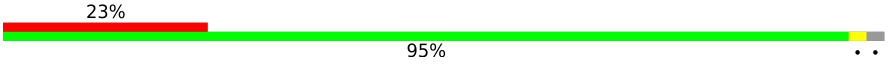


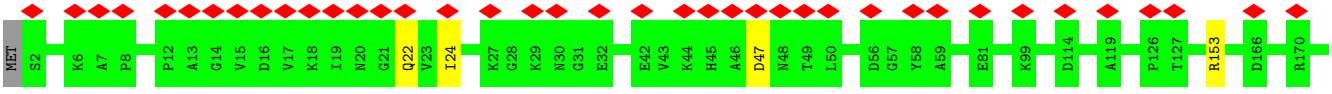


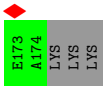


• Molecule 11: Large ribosomal subunit protein uL6

Chain g:

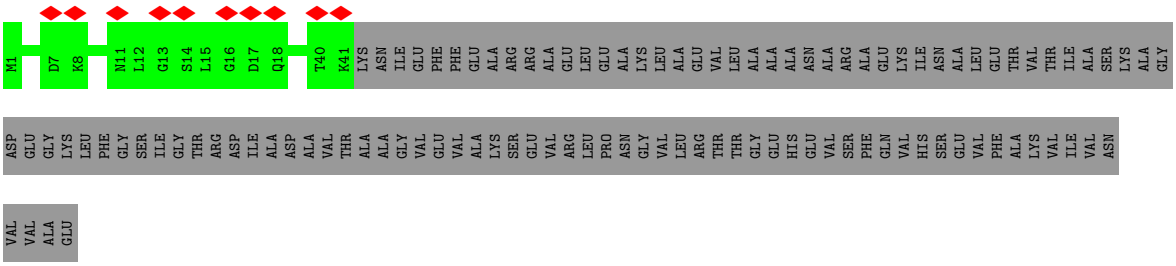






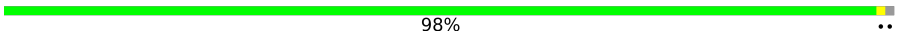
• Molecule 12: Large ribosomal subunit protein bL9

Chain h:



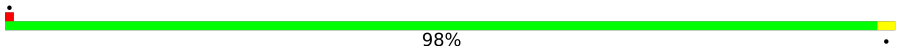
• Molecule 13: Large ribosomal subunit protein uL13

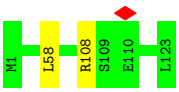
Chain i:



• Molecule 14: Large ribosomal subunit protein uL14

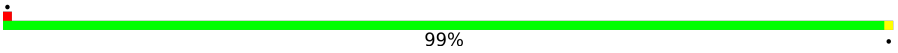
Chain j:

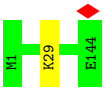




• Molecule 15: 50S ribosomal protein L15

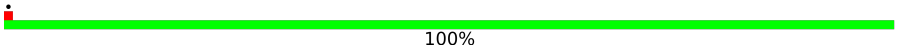
Chain k:

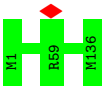




• Molecule 16: Large ribosomal subunit protein uL16

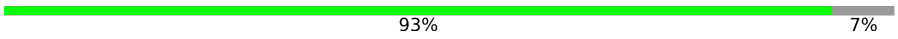
Chain l:

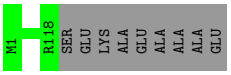




• Molecule 17: Large ribosomal subunit protein bL17

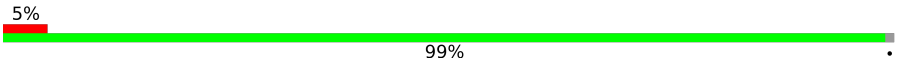
Chain m:

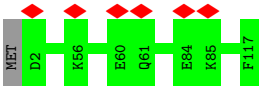




• Molecule 18: Large ribosomal subunit protein uL18

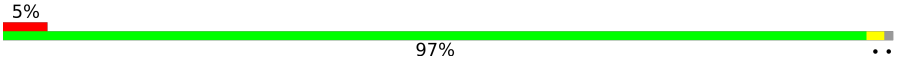
Chain n:

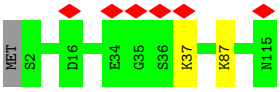




• Molecule 19: Large ribosomal subunit protein bL19

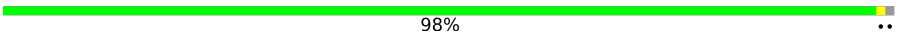
Chain o:





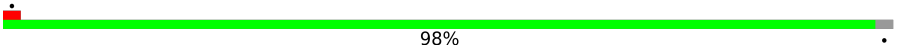
• Molecule 20: Large ribosomal subunit protein bL20

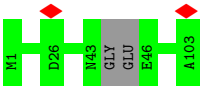
Chain p:



• Molecule 21: Large ribosomal subunit protein bL21

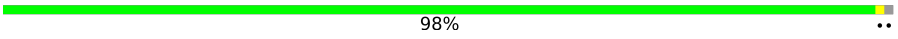
Chain q:

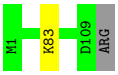




• Molecule 22: Large ribosomal subunit protein uL22

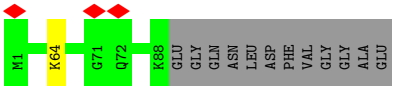
Chain r:





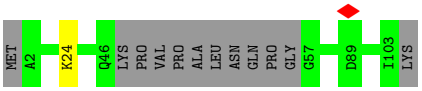
• Molecule 23: Large ribosomal subunit protein uL23

Chain s:



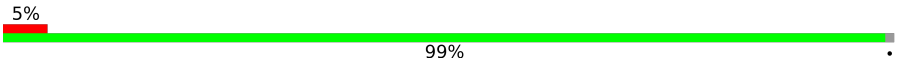
• Molecule 24: Large ribosomal subunit protein uL24

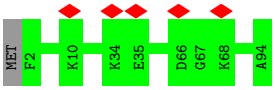
Chain t:



• Molecule 25: 50S ribosomal protein L25

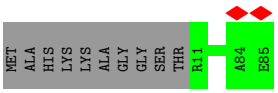
Chain u:





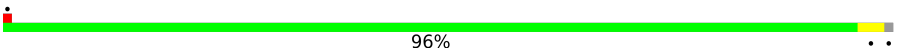
• Molecule 26: Large ribosomal subunit protein bL27

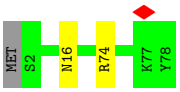
Chain v:



• Molecule 27: Large ribosomal subunit protein bL28

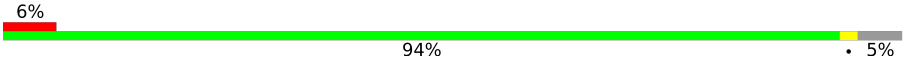
Chain w:

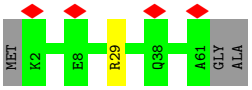




• Molecule 28: Large ribosomal subunit protein uL29

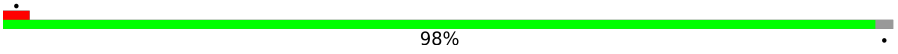
Chain x:





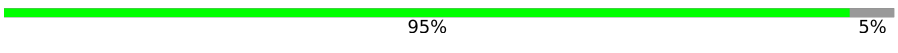
• Molecule 29: Large ribosomal subunit protein uL30

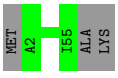
Chain y:



• Molecule 30: Large ribosomal subunit protein bL32

Chain z:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	275137	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	0.178	Depositor
Minimum map value	-0.073	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0147	Depositor
Map size (Å)	460.80002, 460.80002, 460.80002	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.768, 0.768, 0.768	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: 2MA, 1MG, PSU, 5MC, H2U, K, 6MZ, OMG, ZN, MG, 2MG, 3TD, MS6, ACT, MEQ, 4D4, 5MU, OMU, AM2, G7M, OMC, CLY

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	0	0.32	0/420	0.64	0/560
2	1	0.30	0/370	0.78	0/487
3	2	0.31	0/513	0.69	0/676
4	3	0.30	0/303	0.75	0/397
5	a	0.48	0/65534	1.14	80/102231 (0.1%)
6	b	0.51	0/2850	1.14	2/4444 (0.0%)
7	c	0.31	0/2121	0.70	0/2852
8	d	0.30	0/1562	0.66	0/2102
9	e	0.29	0/1571	0.61	0/2113
10	f	0.31	0/1228	0.66	0/1646
11	g	0.30	0/1315	0.63	0/1783
12	h	0.31	0/306	0.69	0/413
13	i	0.29	0/1144	0.64	0/1541
14	j	0.30	0/955	0.70	0/1279
15	k	0.33	0/1062	0.65	0/1413
16	l	0.29	0/1073	0.67	0/1433
17	m	0.30	0/958	0.67	0/1281
18	n	0.29	0/902	0.63	0/1209
19	o	0.32	0/929	0.68	0/1242
20	p	0.30	0/960	0.67	0/1278
21	q	0.32	0/815	0.68	0/1087
22	r	0.29	0/852	0.65	0/1142
23	s	0.26	0/706	0.62	0/943
24	t	0.28	0/712	0.66	0/945
25	u	0.29	0/758	0.65	0/1015
26	v	0.34	0/576	0.69	0/762
27	w	0.32	0/635	0.72	0/848
28	x	0.26	0/492	0.58	0/655
29	y	0.28	0/453	0.62	0/605
30	z	0.32	0/435	0.67	0/581
All	All	0.44	0/92510	1.05	82/138963 (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
3	2	0	1
5	a	0	1
7	c	0	1
9	e	0	2
10	f	0	1
11	g	0	1
13	i	0	2
14	j	0	1
20	p	0	1
27	w	0	2
28	x	0	1
All	All	0	14

There are no bond length outliers.

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	a	512	G	O4'-C1'-N9	11.80	117.64	108.20
5	a	1905	C	O3'-P-O5'	-7.99	88.83	104.00
5	a	2848	G	O4'-C1'-N9	7.68	114.34	108.20
5	a	196	A	O5'-P-OP1	-7.53	98.93	105.70
5	a	395	U	O4'-C1'-N1	7.49	114.19	108.20

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	2	13	ARG	Sidechain
5	a	512	G	Sidechain
7	c	156	ARG	Sidechain
9	e	170	ARG	Sidechain
9	e	21	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	0	413	0	448	0	0
2	1	367	0	405	0	0
3	2	504	0	572	0	0
4	3	302	0	340	1	0
5	a	59025	0	29689	0	0
6	b	2549	0	1291	0	0
7	c	2082	0	2153	0	0
8	d	1552	0	1601	0	0
9	e	1552	0	1619	0	0
10	f	1211	0	1244	0	0
11	g	1295	0	1332	0	0
12	h	303	0	327	0	0
13	i	1121	0	1150	0	0
14	j	946	0	1023	0	0
15	k	1053	0	1129	0	0
16	l	1075	0	1145	0	0
17	m	945	0	989	0	0
18	n	892	0	923	0	0
19	o	917	0	962	0	0
20	p	947	0	1019	0	0
21	q	803	0	829	0	0
22	r	845	0	909	0	0
23	s	700	0	773	0	0
24	t	708	0	753	0	0
25	u	745	0	768	0	0
26	v	569	0	581	0	0
27	w	625	0	652	0	0
28	x	491	0	523	0	0
29	y	449	0	488	0	0
30	z	429	0	440	0	0
31	3	1	0	0	0	0
31	f	1	0	0	0	0
32	a	4	0	3	0	0
33	a	27	0	32	0	0
34	a	37	0	41	0	0
35	a	246	0	0	0	0
35	b	4	0	0	0	0
35	c	1	0	0	0	0
35	d	1	0	0	0	0
35	p	1	0	0	0	0
35	z	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	a	79	0	0	0	0
36	c	4	0	0	0	0
36	e	1	0	0	0	0
36	t	1	0	0	0	0
37	0	6	0	0	0	0
37	1	44	0	0	0	0
37	2	40	0	0	0	0
37	3	16	0	0	0	0
37	a	7060	0	0	0	0
37	b	111	0	0	0	0
37	c	155	0	0	0	0
37	d	115	0	0	0	0
37	e	72	0	0	0	0
37	g	3	0	0	0	0
37	h	1	0	0	0	0
37	i	53	0	0	0	0
37	j	38	0	0	0	0
37	k	69	0	0	0	0
37	l	70	0	0	0	0
37	m	59	0	0	0	0
37	n	8	0	0	0	0
37	o	50	0	0	0	0
37	p	68	0	0	0	0
37	q	39	0	0	0	0
37	r	59	0	0	0	0
37	s	31	0	0	0	0
37	t	24	0	0	0	0
37	u	23	0	0	0	0
37	v	37	0	0	0	0
37	w	30	0	0	0	0
37	x	11	0	0	0	0
37	y	21	0	0	0	0
37	z	44	0	0	0	0
All	All	94181	0	56153	1	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 1.

All (1) 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)
4:3:16:ILE:HD13	4:3:25:VAL:HG22	1.93	0.49

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	0	48/55 (87%)	46 (96%)	2 (4%)	0	100	100
2	1	43/46 (94%)	43 (100%)	0	0	100	100
3	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
7	c	269/273 (98%)	261 (97%)	8 (3%)	0	100	100
8	d	204/209 (98%)	198 (97%)	6 (3%)	0	100	100
9	e	199/201 (99%)	193 (97%)	6 (3%)	0	100	100
10	f	148/179 (83%)	138 (93%)	10 (7%)	0	100	100
11	g	171/177 (97%)	164 (96%)	6 (4%)	1 (1%)	25	14
12	h	39/149 (26%)	36 (92%)	3 (8%)	0	100	100
13	i	139/142 (98%)	139 (100%)	0	0	100	100
14	j	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
15	k	142/144 (99%)	136 (96%)	5 (4%)	1 (1%)	22	11
16	l	132/136 (97%)	128 (97%)	4 (3%)	0	100	100
17	m	116/127 (91%)	111 (96%)	5 (4%)	0	100	100
18	n	114/117 (97%)	109 (96%)	5 (4%)	0	100	100
19	o	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
20	p	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
21	q	97/103 (94%)	96 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	r	107/110 (97%)	106 (99%)	1 (1%)	0	100	100
23	s	86/100 (86%)	84 (98%)	2 (2%)	0	100	100
24	t	88/104 (85%)	87 (99%)	1 (1%)	0	100	100
25	u	91/94 (97%)	90 (99%)	1 (1%)	0	100	100
26	v	73/85 (86%)	72 (99%)	1 (1%)	0	100	100
27	w	75/78 (96%)	75 (100%)	0	0	100	100
28	x	58/63 (92%)	58 (100%)	0	0	100	100
29	y	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
30	z	52/57 (91%)	51 (98%)	1 (2%)	0	100	100
All	All	2993/3267 (92%)	2913 (97%)	78 (3%)	2 (0%)	54	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	g	47	ASP
15	k	29	LYS

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	0	46/49 (94%)	46 (100%)	0	100	100
2	1	37/38 (97%)	36 (97%)	1 (3%)	44	35
3	2	51/52 (98%)	50 (98%)	1 (2%)	55	48
4	3	34/34 (100%)	34 (100%)	0	100	100
7	c	216/218 (99%)	216 (100%)	0	100	100
8	d	162/163 (99%)	161 (99%)	1 (1%)	86	85
9	e	165/165 (100%)	165 (100%)	0	100	100
10	f	127/150 (85%)	122 (96%)	5 (4%)	32	19
11	g	134/138 (97%)	132 (98%)	2 (2%)	65	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
12	h	32/114 (28%)	32 (100%)	0	100 100
13	i	115/116 (99%)	115 (100%)	0	100 100
14	j	104/104 (100%)	103 (99%)	1 (1%)	76 73
15	k	103/103 (100%)	103 (100%)	0	100 100
16	l	107/107 (100%)	107 (100%)	0	100 100
17	m	98/103 (95%)	98 (100%)	0	100 100
18	n	86/87 (99%)	86 (100%)	0	100 100
19	o	99/100 (99%)	97 (98%)	2 (2%)	55 48
20	p	89/90 (99%)	89 (100%)	0	100 100
21	q	83/84 (99%)	83 (100%)	0	100 100
22	r	92/93 (99%)	91 (99%)	1 (1%)	73 70
23	s	76/84 (90%)	75 (99%)	1 (1%)	69 64
24	t	75/85 (88%)	74 (99%)	1 (1%)	69 64
25	u	77/78 (99%)	77 (100%)	0	100 100
26	v	56/63 (89%)	56 (100%)	0	100 100
27	w	67/68 (98%)	67 (100%)	0	100 100
28	x	54/55 (98%)	54 (100%)	0	100 100
29	y	48/49 (98%)	48 (100%)	0	100 100
30	z	46/48 (96%)	46 (100%)	0	100 100
All	All	2479/2638 (94%)	2463 (99%)	16 (1%)	86 85

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	s	64	LYS
22	r	83	LYS
11	g	22	GLN
19	o	87	LYS
10	f	130	MET

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

Mol	Chain	Res	Type
7	c	90	ASN

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Mol	Chain	Res	Type
17	m	73	ASN
19	o	115	ASN
28	x	45	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	a	2740/2904 (94%)	276 (10%)	0
6	b	118/120 (98%)	13 (11%)	0
All	All	2858/3024 (94%)	289 (10%)	0

5 of 289 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	a	10	A
5	a	12	U
5	a	34	U
5	a	71	A
5	a	74	A

There are no RNA pucker outliers to report.

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

26 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	$\#\|Z\| > 2$
5	PSU	a	2605	5	18,21,22	0.98	1 (5%)	22,30,33	0.85	0
5	H2U	a	2449	5	18,21,22	0.61	0	21,30,33	0.71	0
5	OMU	a	2552	5	19,22,23	0.23	0	26,31,34	0.45	0
5	PSU	a	1911	5	18,21,22	0.97	1 (5%)	22,30,33	0.64	0
5	2MG	a	2445	5	18,26,27	1.03	2 (11%)	16,38,41	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	2MG	a	1835	5	18,26,27	1.05	2 (11%)	16,38,41	0.67	0
5	PSU	a	1917	5	18,21,22	0.97	1 (5%)	22,30,33	0.61	0
5	PSU	a	746	35,5	18,21,22	0.98	1 (5%)	22,30,33	0.67	0
5	3TD	a	1915	5	19,22,23	0.96	1 (5%)	21,32,35	0.72	0
5	PSU	a	2604	5	18,21,22	0.94	1 (5%)	22,30,33	0.78	1 (4%)
5	5MU	a	747	5	19,22,23	0.34	0	28,32,35	0.46	0
5	OMC	a	2498	35,5	19,22,23	0.26	0	26,31,34	0.60	0
5	5MU	a	1939	36,5	19,22,23	0.34	0	28,32,35	0.58	0
16	4D4	l	81	16	9,11,12	0.46	0	8,13,15	0.79	0
5	PSU	a	2457	5	18,21,22	1.01	1 (5%)	22,30,33	0.74	0
5	PSU	a	955	5	18,21,22	0.93	1 (5%)	22,30,33	0.72	0
5	PSU	a	2504	36,5	18,21,22	0.91	1 (5%)	22,30,33	0.76	0
5	6MZ	a	2030	5	18,25,26	0.75	0	16,36,39	1.15	1 (6%)
5	5MC	a	1962	5	18,22,23	0.37	0	26,32,35	0.74	0
5	G7M	a	2069	5	20,26,27	1.10	2 (10%)	17,39,42	0.70	0
5	OMG	a	2251	36,5	18,26,27	1.01	2 (11%)	19,38,41	0.77	0
5	PSU	a	2580	36,5	18,21,22	1.00	1 (5%)	22,30,33	0.62	0
8	MEQ	d	150	8	8,9,10	0.52	0	5,10,12	1.36	1 (20%)
5	2MA	a	2503	35,5,36	17,25,26	0.97	2 (11%)	17,37,40	1.08	1 (5%)
5	6MZ	a	1618	5	18,25,26	0.69	0	16,36,39	0.86	1 (6%)
5	1MG	a	745	5	18,26,27	1.04	3 (16%)	19,39,42	0.57	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PSU	a	2605	5	-	0/7/25/26	0/2/2/2
5	H2U	a	2449	5	-	0/7/38/39	0/2/2/2
5	OMU	a	2552	5	-	0/9/27/28	0/2/2/2
5	PSU	a	1911	5	-	0/7/25/26	0/2/2/2
5	2MG	a	2445	5	-	0/5/27/28	0/3/3/3
5	2MG	a	1835	5	-	0/5/27/28	0/3/3/3
5	PSU	a	1917	5	-	0/7/25/26	0/2/2/2
5	PSU	a	746	35,5	-	1/7/25/26	0/2/2/2
5	3TD	a	1915	5	-	0/7/25/26	0/2/2/2
5	PSU	a	2604	5	-	0/7/25/26	0/2/2/2
5	5MU	a	747	5	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	OMC	a	2498	35,5	-	0/9/27/28	0/2/2/2
5	5MU	a	1939	36,5	-	0/7/25/26	0/2/2/2
16	4D4	l	81	16	-	1/11/12/14	-
5	PSU	a	2457	5	-	0/7/25/26	0/2/2/2
5	PSU	a	955	5	-	0/7/25/26	0/2/2/2
5	PSU	a	2504	36,5	-	0/7/25/26	0/2/2/2
5	6MZ	a	2030	5	-	2/5/27/28	0/3/3/3
5	5MC	a	1962	5	-	1/7/25/26	0/2/2/2
5	G7M	a	2069	5	-	2/3/25/26	0/3/3/3
5	OMG	a	2251	36,5	-	0/5/27/28	0/3/3/3
5	PSU	a	2580	36,5	-	0/7/25/26	0/2/2/2
8	MEQ	d	150	8	-	2/8/9/11	-
5	2MA	a	2503	35,5,36	-	2/3/25/26	0/3/3/3
5	6MZ	a	1618	5	-	0/5/27/28	0/3/3/3
5	1MG	a	745	5	-	0/3/25/26	0/3/3/3

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	a	2457	PSU	C6-C5	4.01	1.40	1.35
5	a	746	PSU	C6-C5	3.92	1.39	1.35
5	a	2580	PSU	C6-C5	3.90	1.39	1.35
5	a	1917	PSU	C6-C5	3.88	1.39	1.35
5	a	1911	PSU	C6-C5	3.87	1.39	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	a	2503	2MA	CM2-C2-N1	3.35	123.68	116.23
5	a	2030	6MZ	C2-N1-C6	2.94	119.11	116.59
5	a	1618	6MZ	C2-N1-C6	2.57	118.80	116.59
5	a	2604	PSU	C2'-C3'-C4'	-2.36	98.06	102.64
8	d	150	MEQ	OE1-CD-CG	-2.15	118.09	122.02

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	d	150	MEQ	NE2-CD-CG-CB
8	d	150	MEQ	OE1-CD-CG-CB
5	a	2030	6MZ	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
5	a	2069	G7M	C4'-C5'-O5'-P
5	a	2030	6MZ	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 344 ligands modelled in this entry, 341 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
32	ACT	a	3001	-	3,3,3	0.97	0	3,3,3	0.79	0
33	CLY	a	3002	-	25,28,28	0.34	0	29,40,40	0.95	3 (10%)
34	AM2	a	3003	-	40,40,40	0.45	0	53,60,60	0.72	1 (1%)

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
33	CLY	a	3002	-	-	0/21/53/53	0/2/2/2
34	AM2	a	3003	-	-	2/12/84/84	0/4/4/4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	a	3002	CLY	C15-N2-C14	2.46	115.78	112.45
33	a	3002	CLY	C12-C13-C16	-2.26	111.86	114.60
33	a	3002	CLY	C14-N2-C11	2.16	108.12	104.84
34	a	3003	AM2	CB3-CB4-CB5	2.09	115.02	110.67

There are no chirality outliers.

All (2) torsion outliers are listed below:

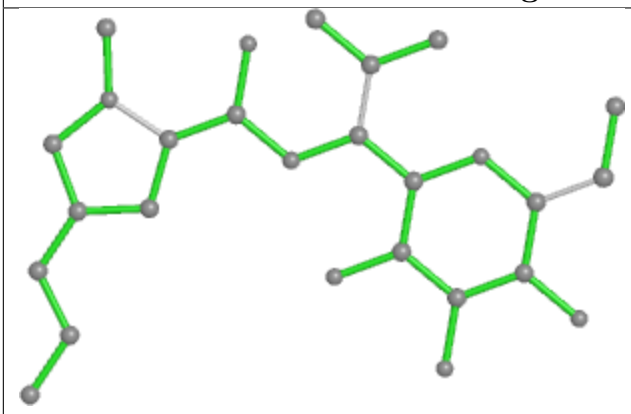
Mol	Chain	Res	Type	Atoms
34	a	3003	AM2	OA5-CA8-OA8-CB1
34	a	3003	AM2	OB1-CB5-CB6-OB6

There are no ring outliers.

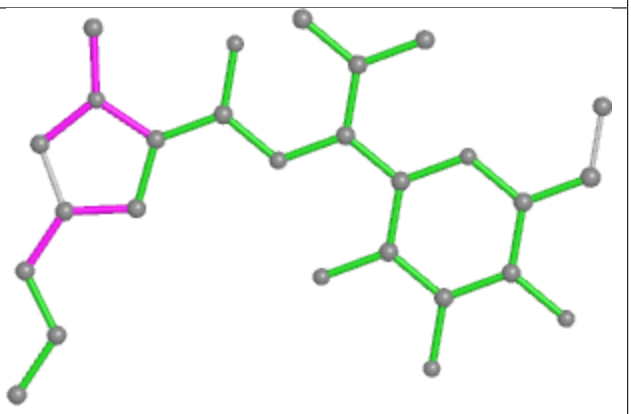
No monomer is involved in short contacts.

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.

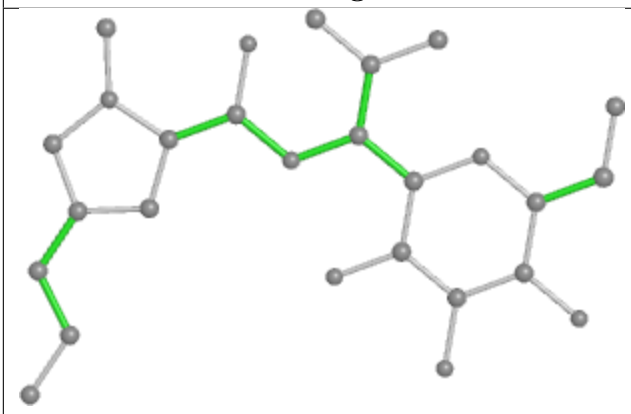
Ligand CLY a 3002



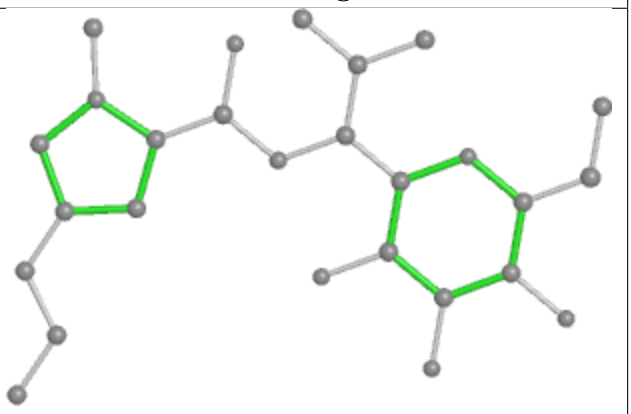
Bond lengths



Bond angles

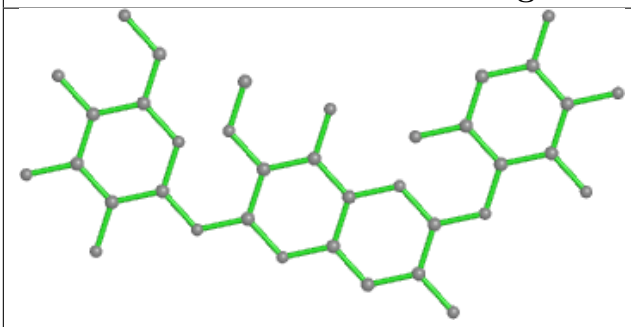


Torsions

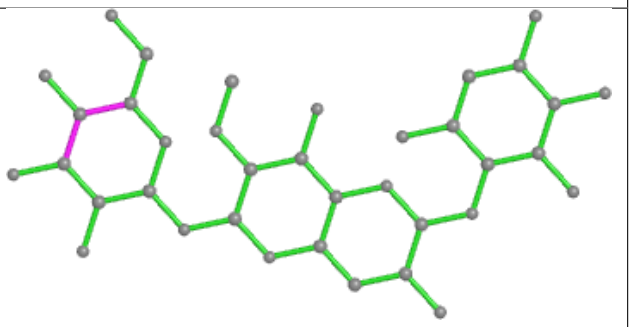


Rings

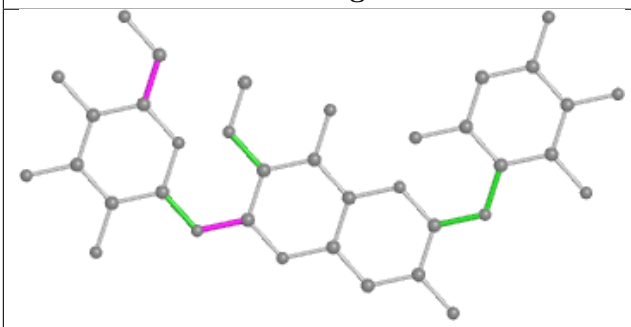
Ligand AM2 a 3003



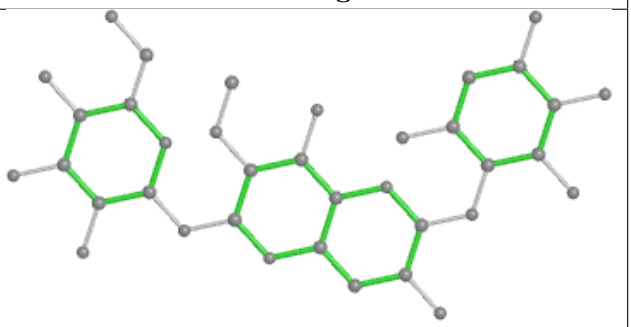
Bond lengths



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.

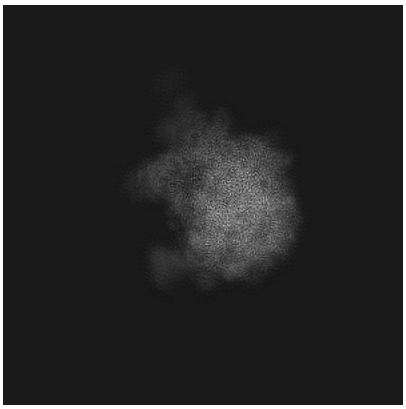
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16641. These allow visual inspection of the internal detail of the map and identification of artifacts.

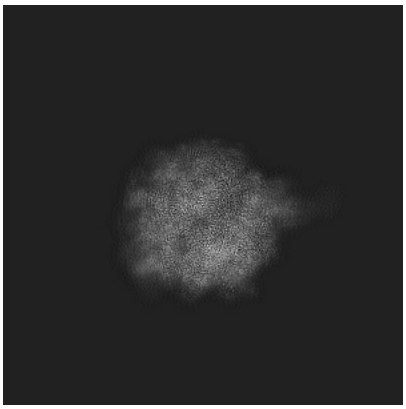
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

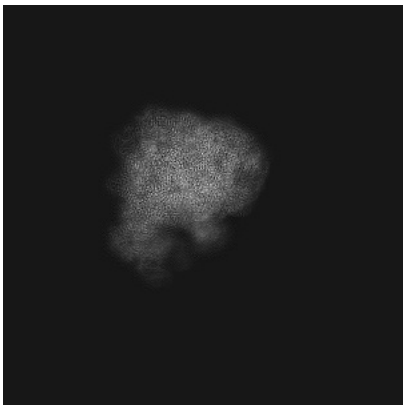
6.1.1 Primary map



X

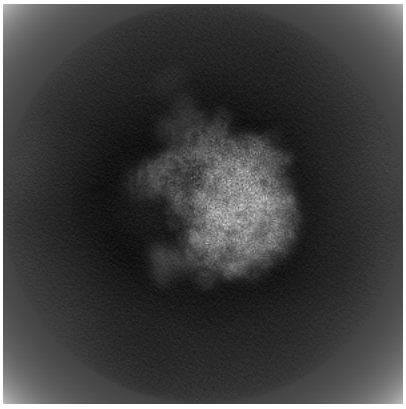


Y

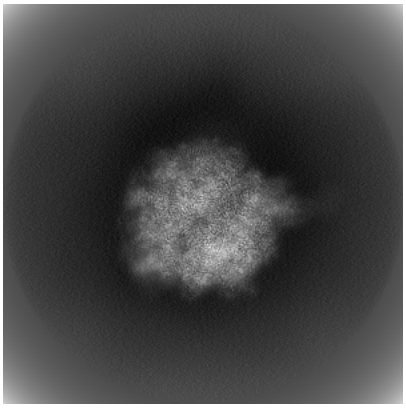


Z

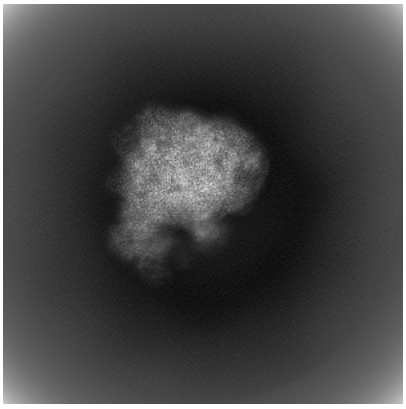
6.1.2 Raw map



X



Y

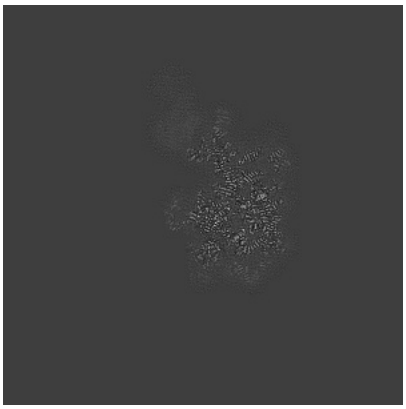


Z

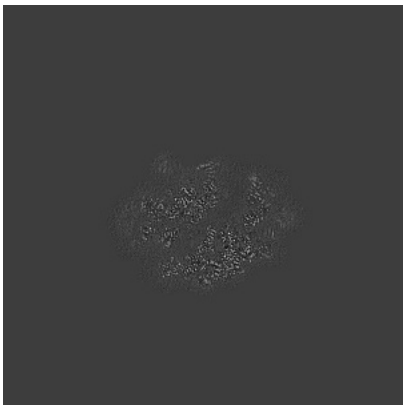
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

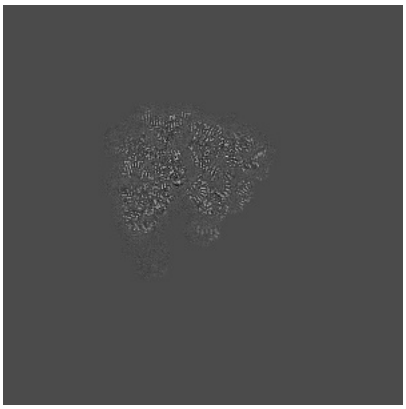
6.2.1 Primary map



X Index: 300

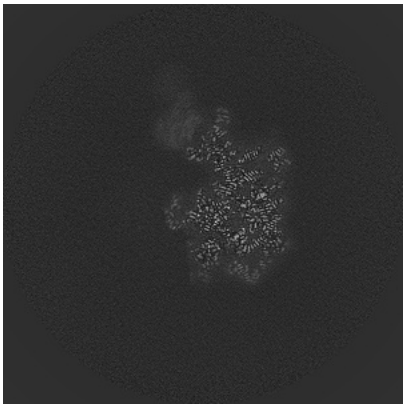


Y Index: 300

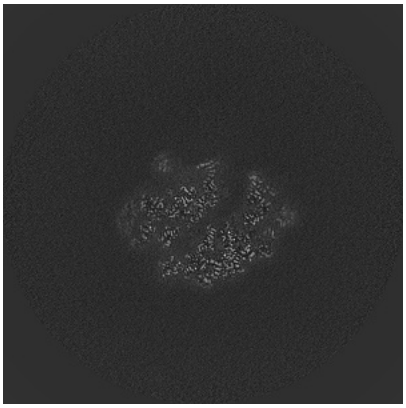


Z Index: 300

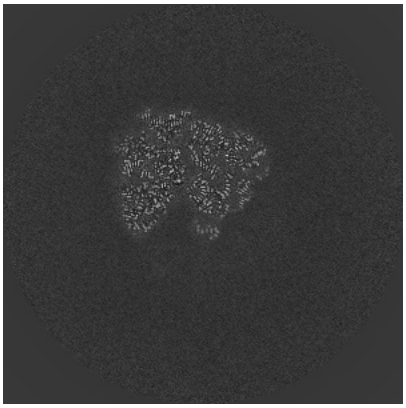
6.2.2 Raw map



X Index: 300



Y Index: 300

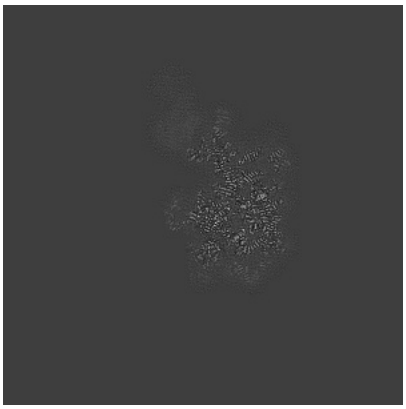


Z Index: 300

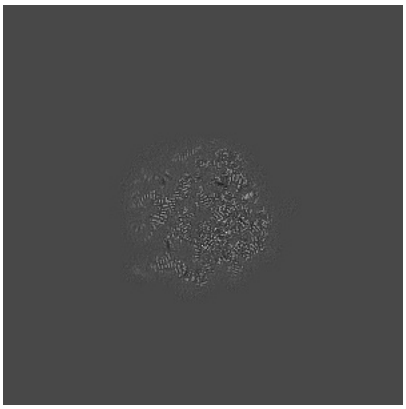
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



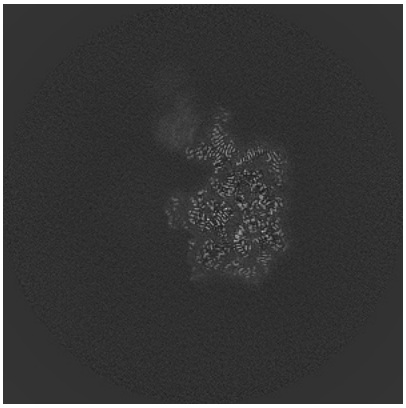
X Index: 300



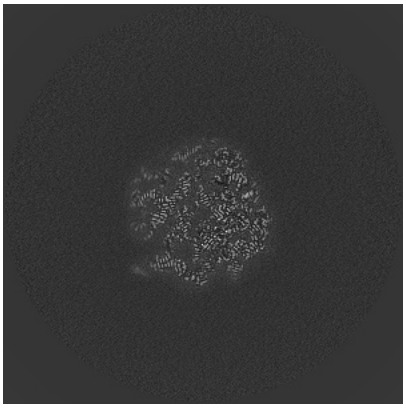
Y Index: 353

Z Index: 309

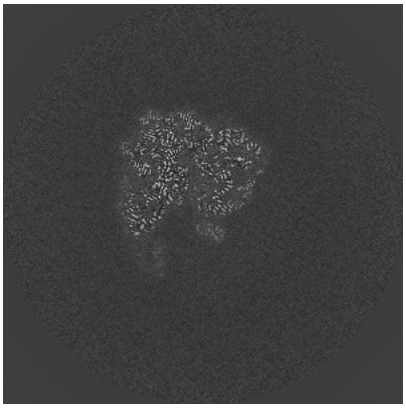
6.3.2 Raw map



X Index: 305



Y Index: 353

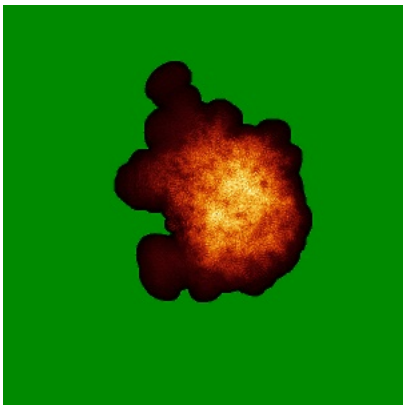


Z Index: 308

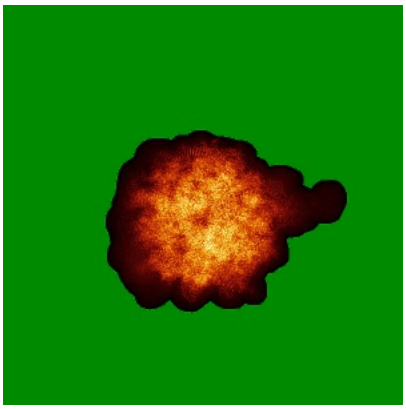
The images above show the largest variance slices of the map in three orthogonal directions.

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

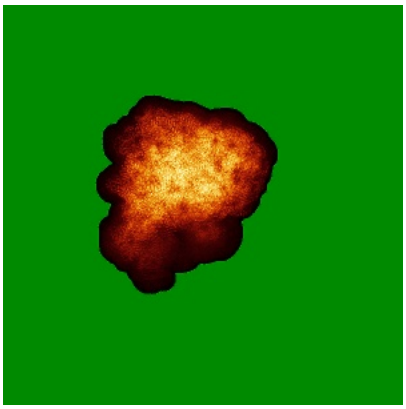
6.4.1 Primary map



X

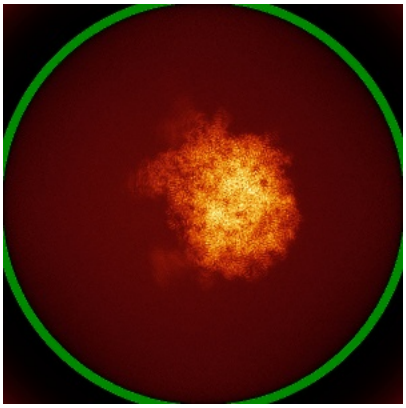


Y

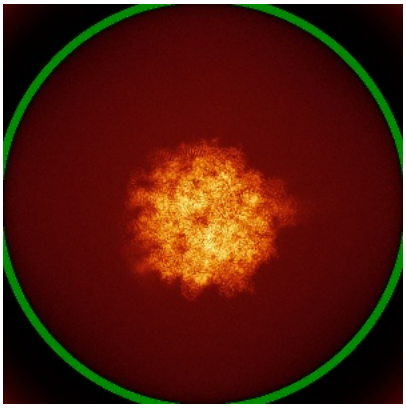


Z

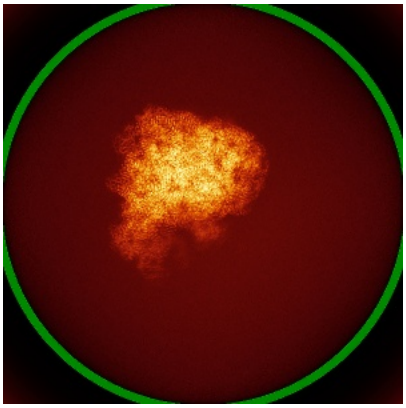
6.4.2 Raw map



X



Y

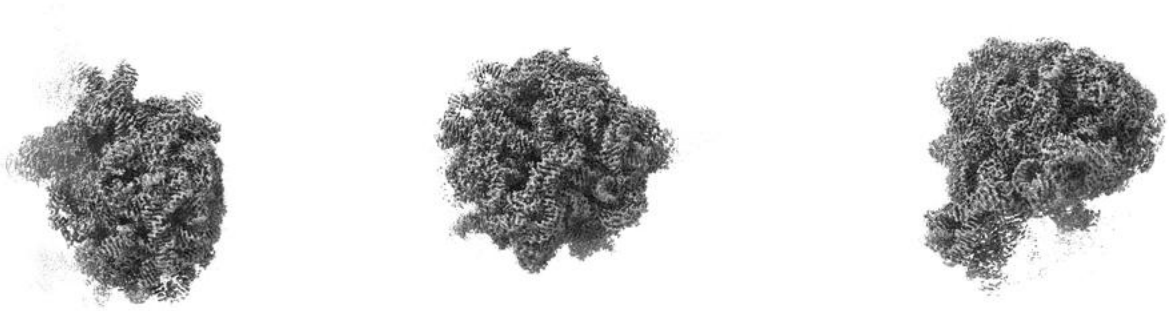


Z

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 0.0147. 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.

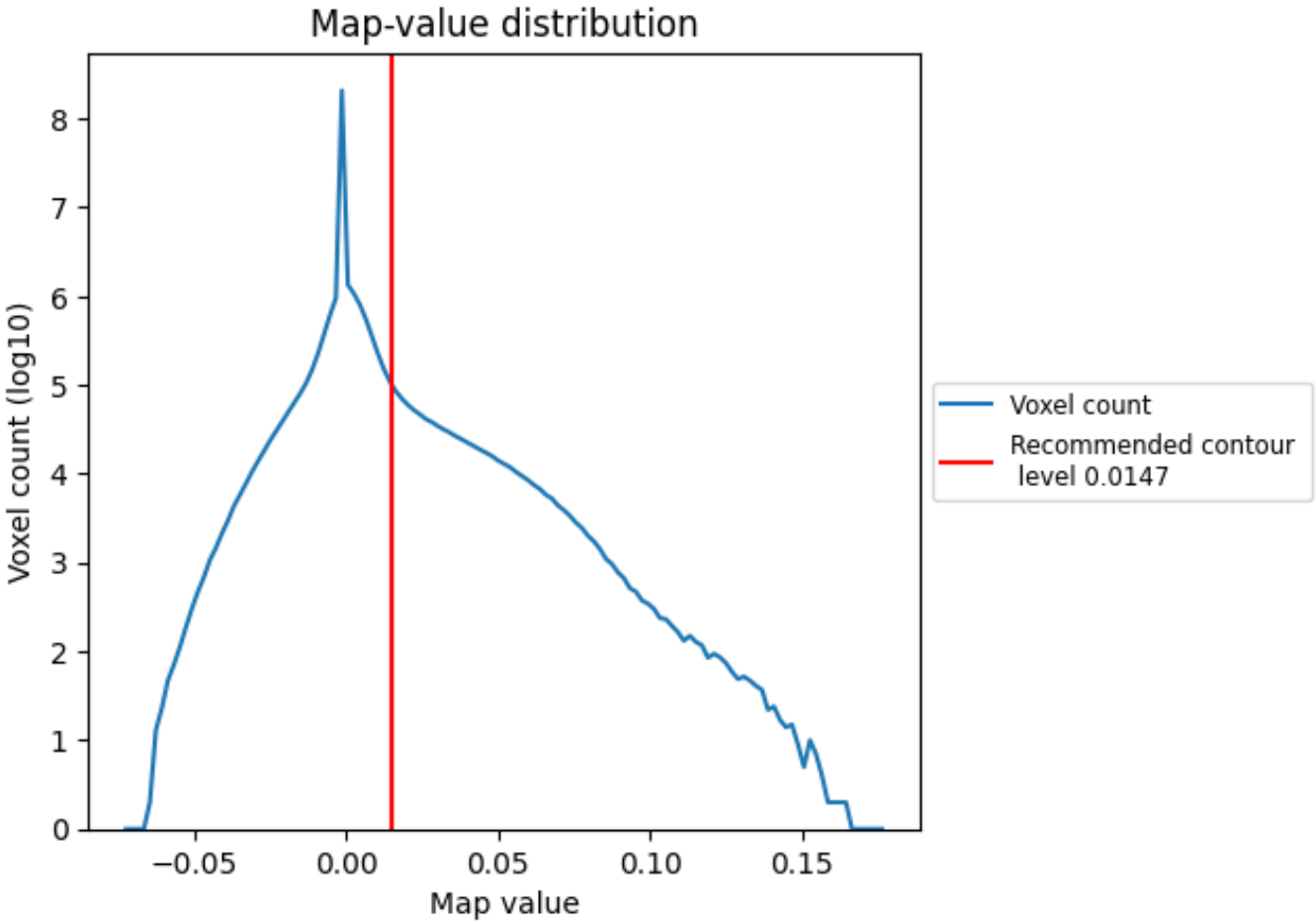
6.6 Mask visualisation (i)

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

7 Map analysis

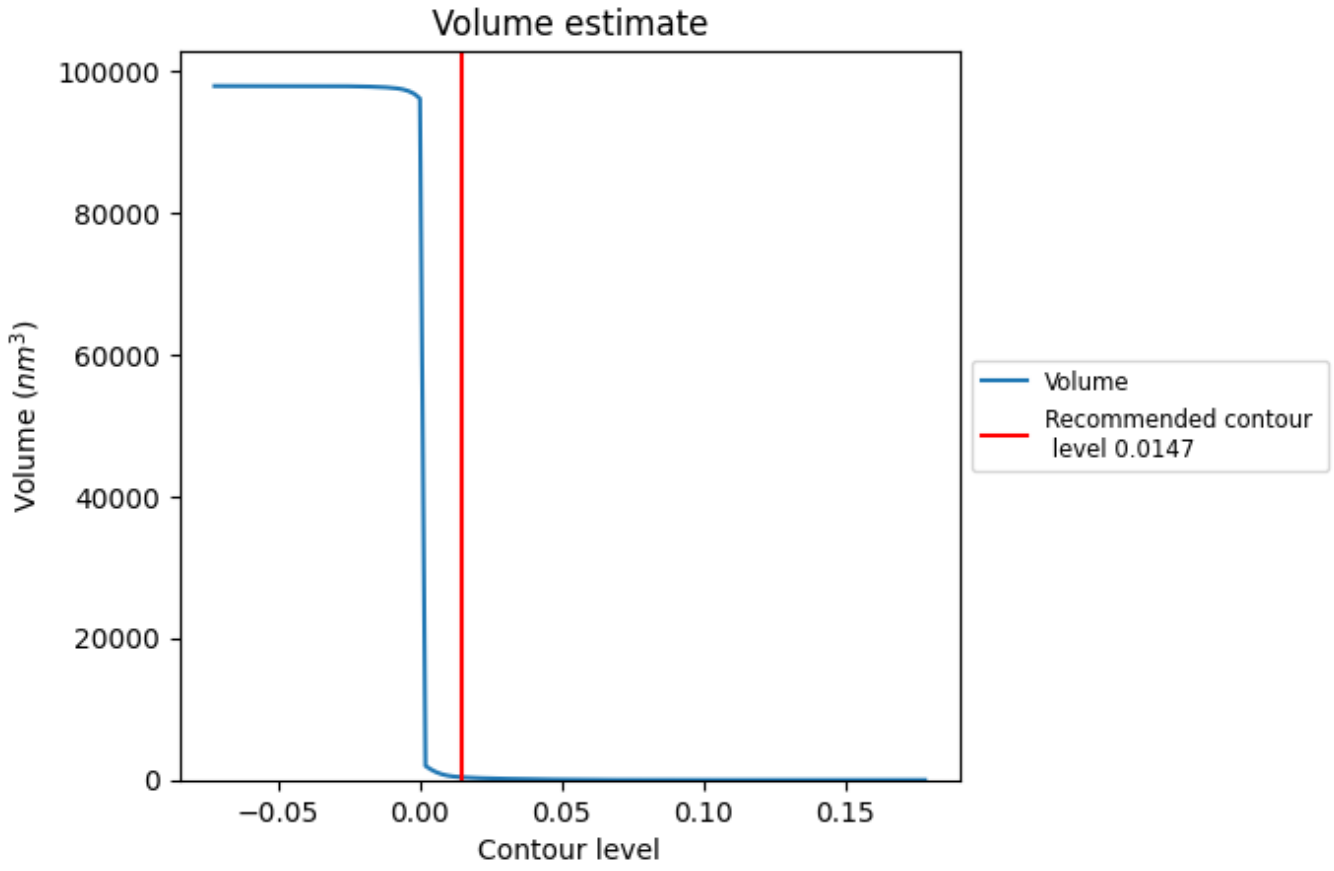
This section contains the results of statistical analysis of the map.

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.

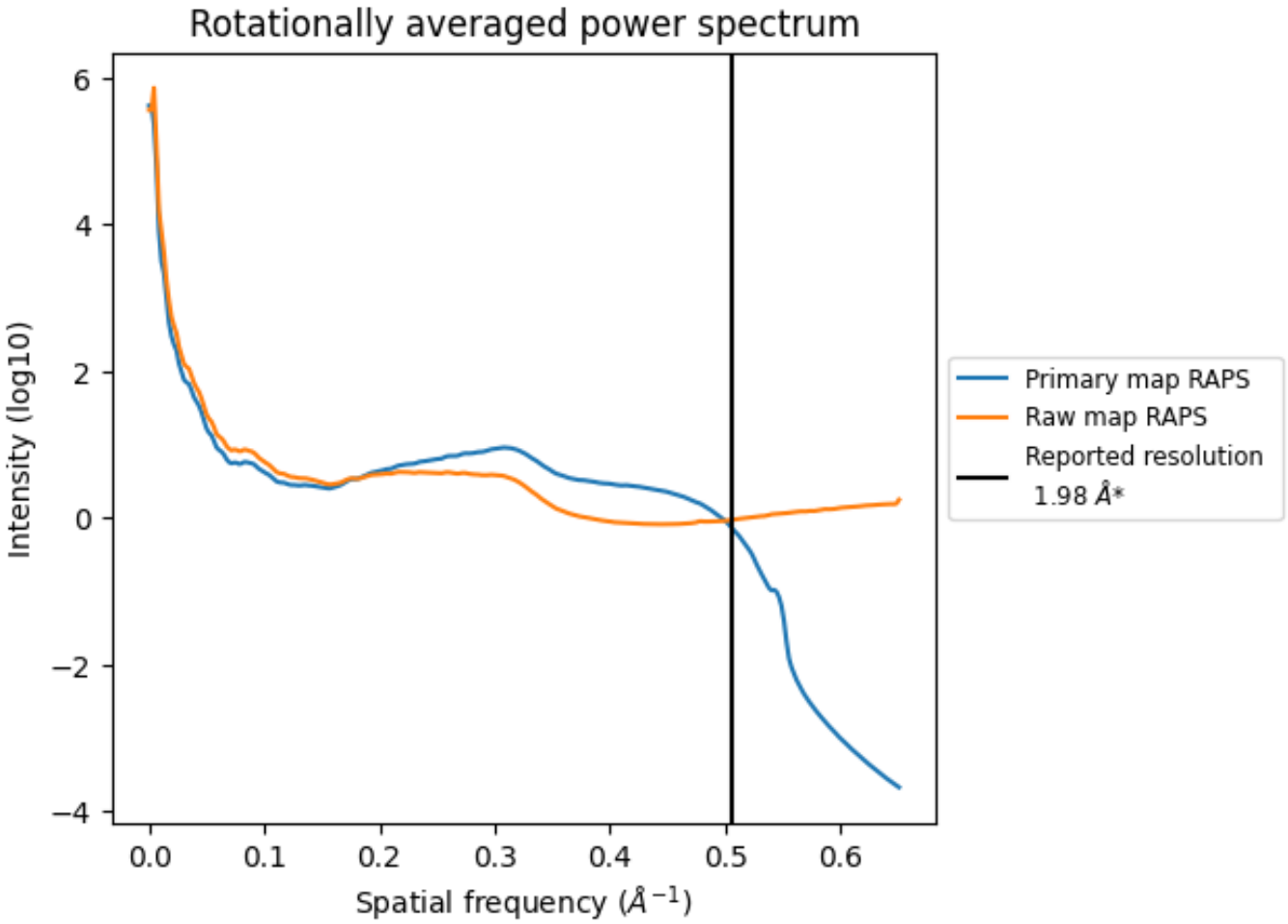
7.2 Volume estimate (i)



The volume at the recommended contour level is 384 nm^3; this corresponds to an approximate mass of 347 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)

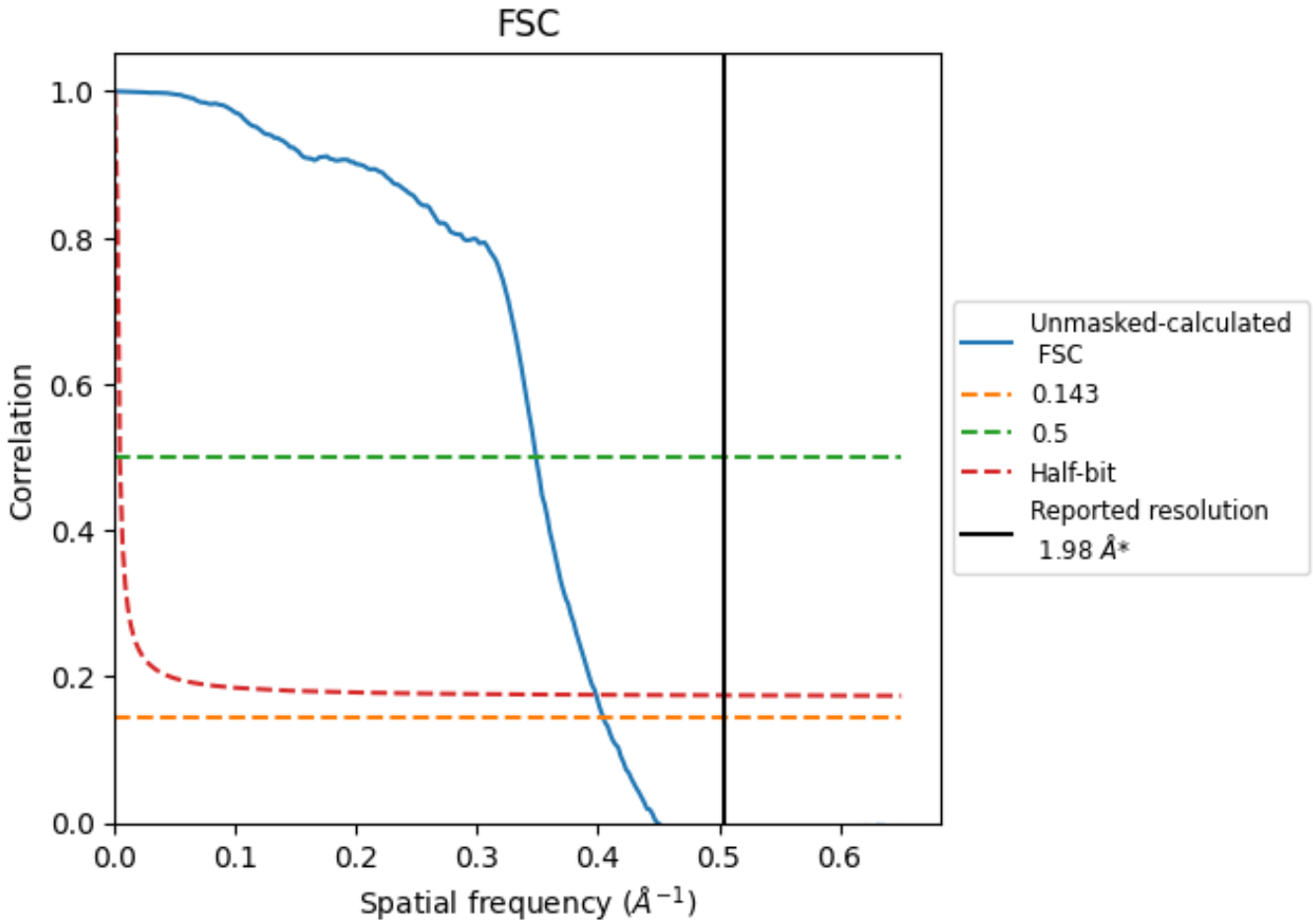


*Reported resolution corresponds to spatial frequency of 0.505 Å^{-1}

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 0.505 Å^{-1}

8.2 Resolution estimates (i)

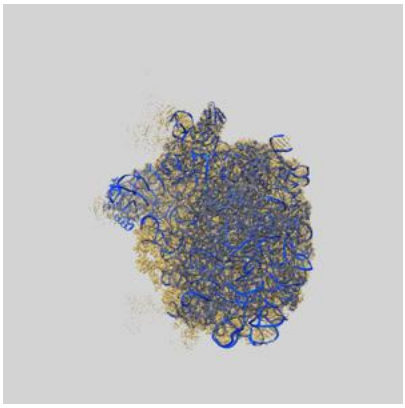
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.98	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.47	2.87	2.51

*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 2.47 differs from the reported value 1.98 by more than 10 %

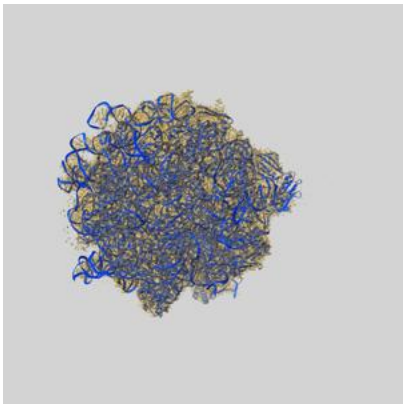
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16641 and PDB model 8CGD. Per-residue inclusion information can be found in section 3 on page 13.

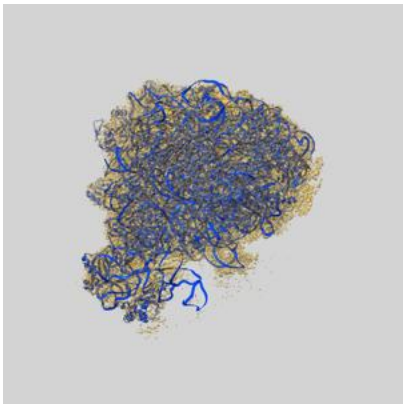
9.1 Map-model overlay



X



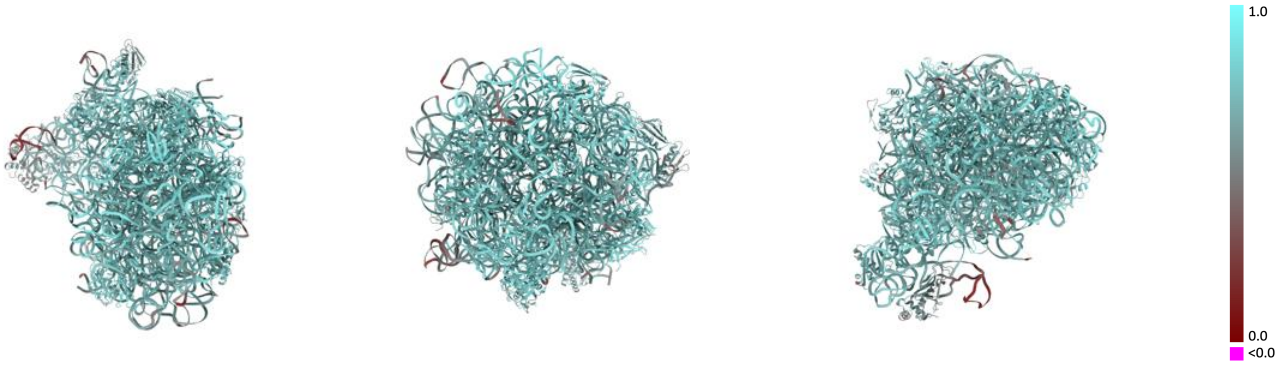
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0147 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.

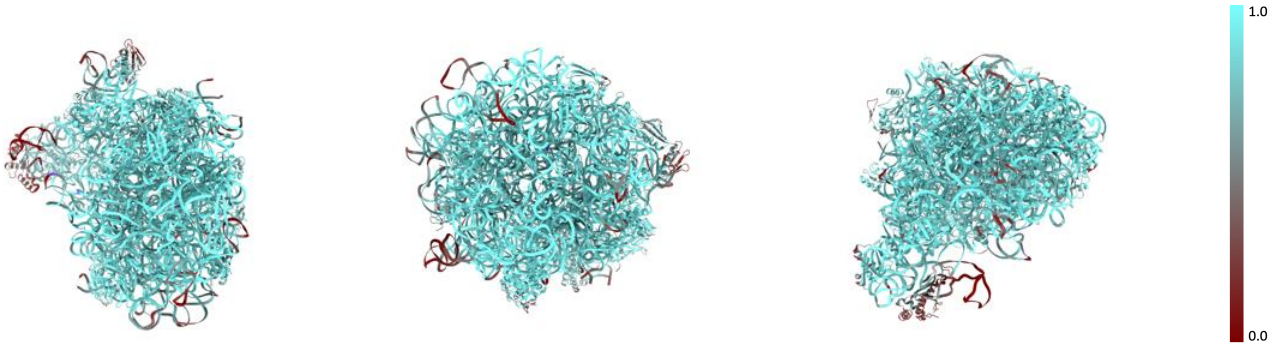
9.2 Q-score mapped to coordinate model (i)



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.

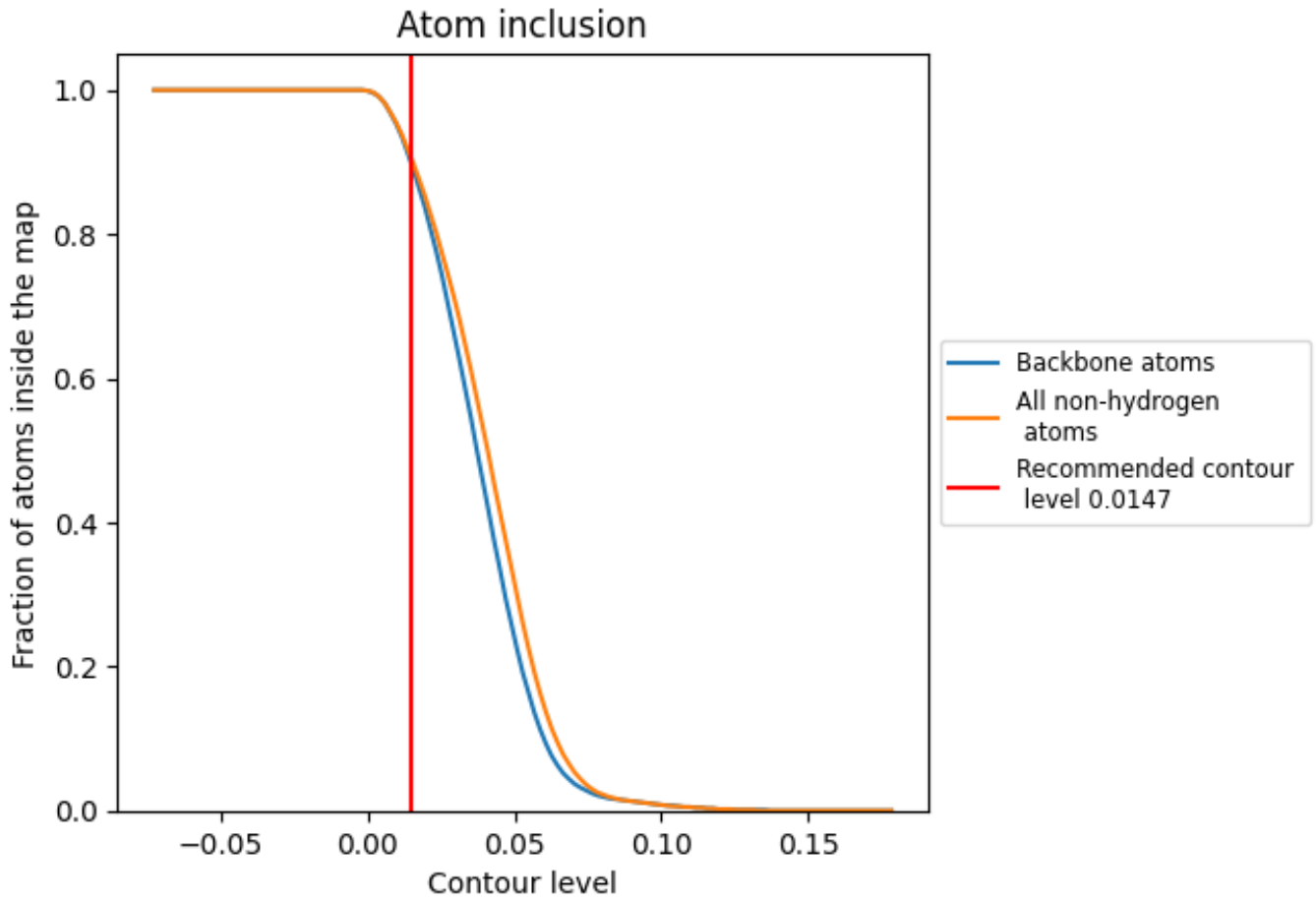
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0147).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 91% 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 (0.0147) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9070	0.7520
0	0.8690	0.7580
1	0.9910	0.8180
2	0.9780	0.8140
3	0.9350	0.7770
a	0.9240	0.7520
b	0.8690	0.7030
c	0.9580	0.7960
d	0.9400	0.7900
e	0.8570	0.7500
f	0.3610	0.5570
g	0.6390	0.6520
h	0.6970	0.6770
i	0.9500	0.7940
j	0.9130	0.7770
k	0.9340	0.7820
l	0.9260	0.7770
m	0.9880	0.8160
n	0.8270	0.7120
o	0.8870	0.7710
p	0.9740	0.8110
q	0.8950	0.7690
r	0.9380	0.7920
s	0.8800	0.7520
t	0.8940	0.7510
u	0.8430	0.7370
v	0.9310	0.7880
w	0.9150	0.7770
x	0.7910	0.7200
y	0.9080	0.7790
z	0.9300	0.7870