wwPDB EM Validation Summary Report

Aug 12, 2024 – 12:49 PM EDT

PDB ID	:	9C4G
EMDB ID	:	EMD-45185
Title	:	Cutibacterium acnes 50S ribosomal subunit with Clindamycin bound
Authors	:	Lomakin, I.B.; Devarkar, S.C.; Bunick, C.G.
Deposited on	:	2024-06-04
Resolution	:	2.53 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:

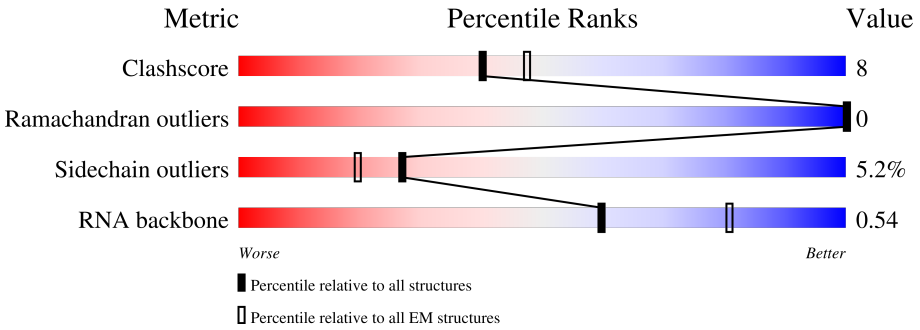
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance

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

The reported resolution of this entry is 2.53 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	c	278	96%
2	d	223	93%
3	e	301	8% 64% 5% 30%
4	f	210	67% 83% 5% 12%
5	g	180	65% 92% 7%
6	i	147	97%
7	j	122	11% 92% 8%

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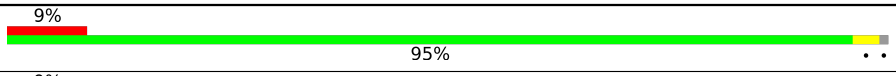
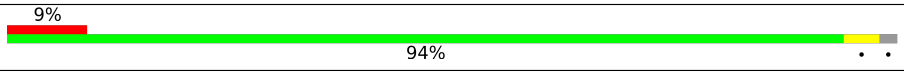
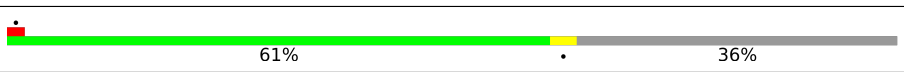
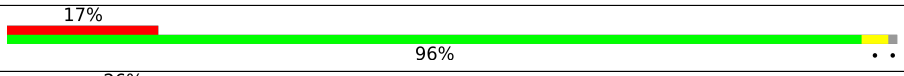
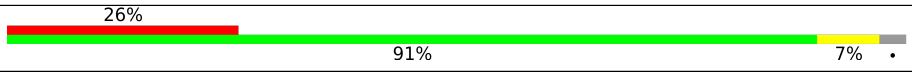
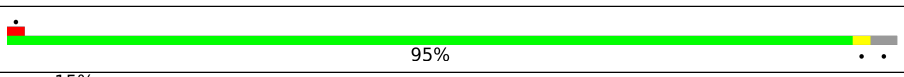
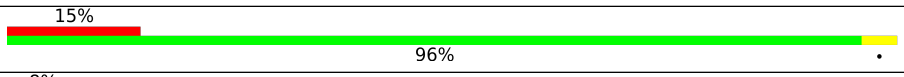
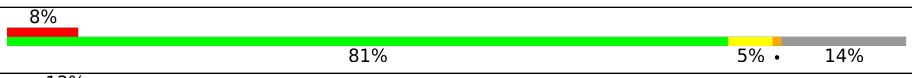
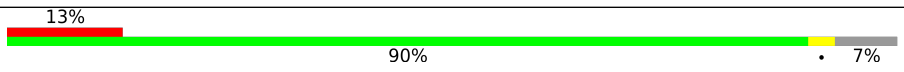
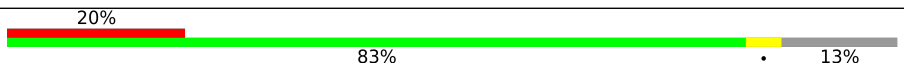
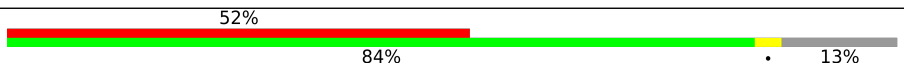
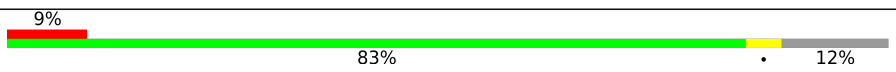
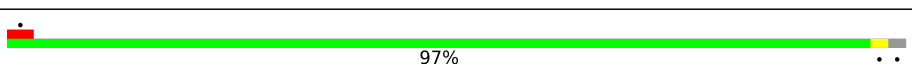
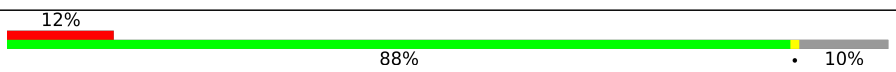
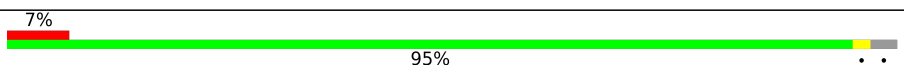
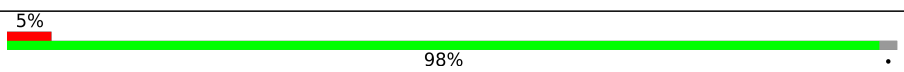
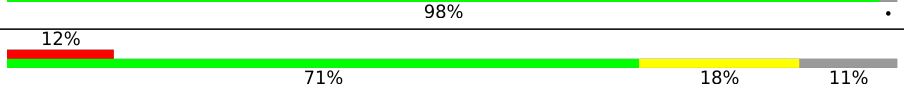
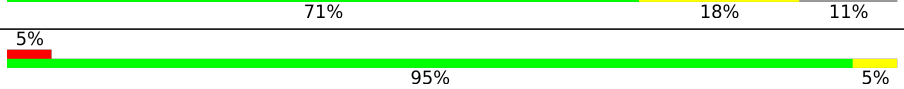
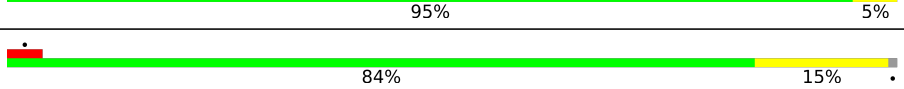
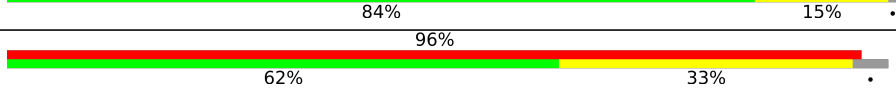
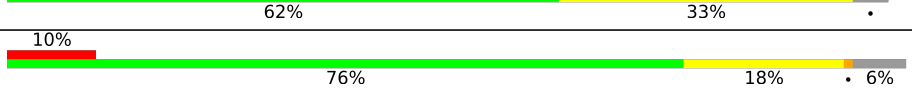
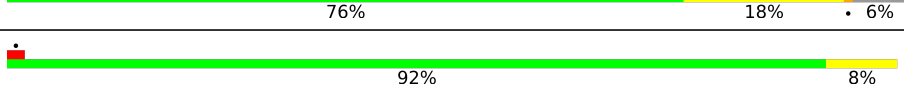
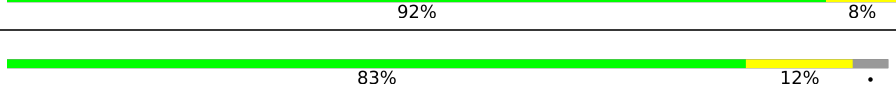
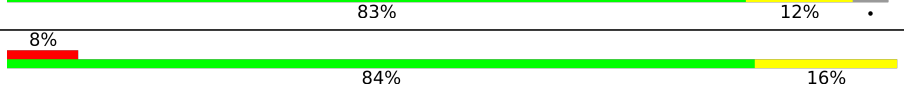
Mol	Chain	Length	Quality of chain
8	k	146	
9	l	139	
10	m	187	
11	n	127	
12	o	117	
13	p	123	
14	q	102	
15	r	153	
16	s	102	
17	t	122	
18	u	205	
19	v	89	
20	w	61	
21	x	77	
22	y	60	
23	z	63	
24	0	56	
25	1	44	
26	2	68	
27	4	69	
28	a	3086	
29	b	120	
30	V	24	
31	3	37	

2 Entry composition (i)

There are 35 unique types of molecules in this entry. The entry contains 91105 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 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	c	274	2091	1289	425	372	5	0	0

- Molecule 2 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	d	214	1586	984	304	291	7	0	0

- Molecule 3 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	e	210	1577	979	301	295	2	0	0

- Molecule 4 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	f	184	1468	924	269	266	9	0	0

- Molecule 5 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	g	177	1376	867	250	258	1	0	0

- Molecule 6 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	i	146	1139	718	213	205	3	0	0

- Molecule 7 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	j	122	Total	C	N	O	S	0	0
			946	596	177	169	4		

- Molecule 8 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	k	144	Total	C	N	O	S	0	0
			1072	675	196	199	2		

- Molecule 9 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	l	136	Total	C	N	O	S	0	0
			1082	685	210	181	6		

- Molecule 10 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	m	120	Total	C	N	O	S	0	0
			936	583	188	163	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
m	124	ALA	THR	conflict	UNP A0A8B2VJI7
m	185	PRO	SER	conflict	UNP A0A8B2VJI7

- Molecule 11 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	n	126	Total	C	N	O	S	0	0
			952	583	190	176	3		

- Molecule 12 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	o	114	Total	C	N	O	S	0	0
			896	559	174	162	1		

- Molecule 13 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	p	119	Total	C	N	O	S	0	0
			958	589	196	171	2		

- Molecule 14 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	q	102	Total	C	N	O	S	0	0
			778	487	140	150	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
q	52	ALA	VAL	conflict	UNP Q6A9I3

- Molecule 15 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	r	132	Total	C	N	O	S	0	0
			1017	624	204	182	7		

- Molecule 16 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	s	95	Total	C	N	O	S	0	0
			751	474	138	138	1		

- Molecule 17 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	t	106	Total	C	N	O	S	0	0
			829	514	162	152	1		

- Molecule 18 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	u	179	Total	C	N	O	S	0	0
			1376	865	240	268	3		

- Molecule 19 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	v	78	Total 591	C 355	N 127	O 109	0	0

- Molecule 20 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	w	60	Total 474	C 290	N 102	O 77	S 5	0	0

- Molecule 21 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	x	69	Total 564	C 348	N 108	O 108	0	0

- Molecule 22 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	y	58	Total 467	C 290	N 91	O 83	S 3	0	0

- Molecule 23 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	z	62	Total 477	C 287	N 102	O 83	S 5	0	0

- Molecule 24 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	0	50	Total 423	C 253	N 91	O 73	S 6	0	0

- Molecule 25 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	1	44	Total 362	C 213	N 91	O 56	S 2	0	0

- Molecule 26 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	2	67	Total	C	N	O	S	0	0
			513	315	110	87	1		

- Molecule 27 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	4	66	Total	C	N	O	S	0	0
			512	313	97	97	5		

- Molecule 28 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	2903	Total	C	N	O	P	0	0
			62406	27794	11385	20324	2903		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	63	A	G	conflict	GB CP012350
a	524	C	G	conflict	GB CP012350
a	1038	PSU	G	conflict	GB CP012350

- Molecule 29 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	120	Total	C	N	O	P	0	0
			2567	1145	466	836	120		

- Molecule 30 is a protein called 50S ribosomal protein bL37.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	V	23	Total	C	N	O	0	0
			183	106	50	27		

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	3	37	Total	C	N	O	S	0	0
			302	184	66	47	5		

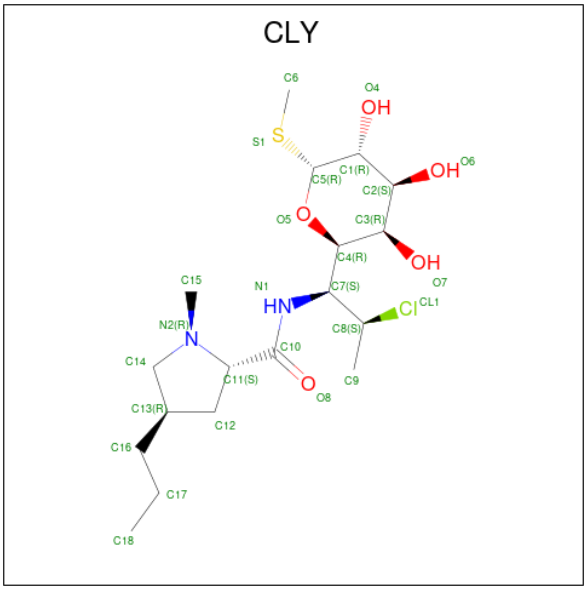
- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
32	c	1	Total Mg 1 1	0
32	d	1	Total Mg 1 1	0
32	k	1	Total Mg 1 1	0
32	a	241	Total Mg 241 241	0
32	b	3	Total Mg 3 3	0

- Molecule 33 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
33	w	1	Total Zn 1 1	0
33	z	1	Total Zn 1 1	0
33	0	1	Total Zn 1 1	0
33	4	1	Total Zn 1 1	0

- Molecule 34 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
34	a	1	Total	C	Cl	N	O	S	0
			27	18	1	2	5	1	

- Molecule 35 is water.

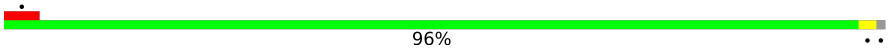
Mol	Chain	Residues	Atoms		AltConf
35	c	1	Total	O	0
			1	1	
35	d	1	Total	O	0
			1	1	
35	e	2	Total	O	0
			2	2	
35	i	1	Total	O	0
			1	1	
35	m	1	Total	O	0
			1	1	
35	o	1	Total	O	0
			1	1	
35	p	1	Total	O	0
			1	1	
35	r	2	Total	O	0
			2	2	
35	z	1	Total	O	0
			1	1	
35	a	141	Total	O	0
			141	141	
35	b	4	Total	O	0
			4	4	

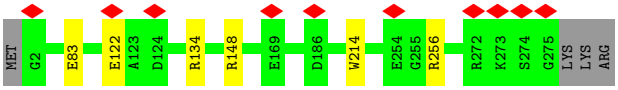
3 Residue-property plots (i)

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

• Molecule 1: 50S ribosomal protein L2

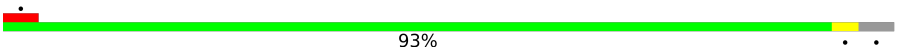
Chain c:

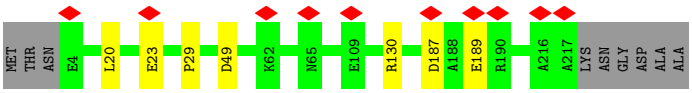




• Molecule 2: 50S ribosomal protein L3

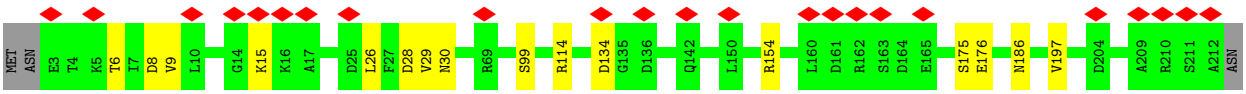
Chain d:





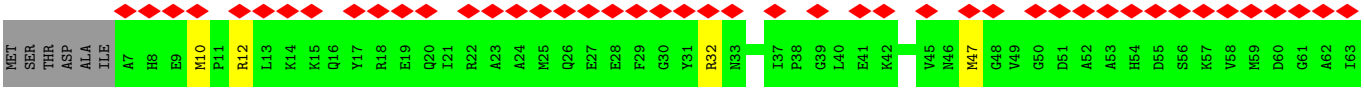
• Molecule 3: 50S ribosomal protein L4

Chain e:

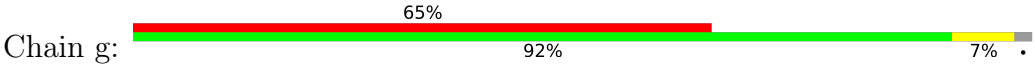


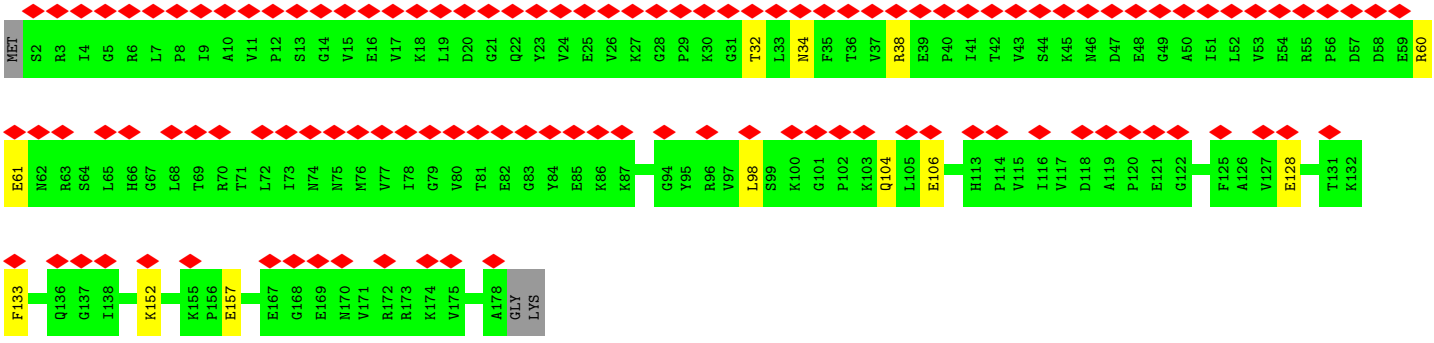
• Molecule 4: 50S ribosomal protein L5

Chain f:

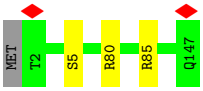


• Molecule 5: 50S ribosomal protein L6

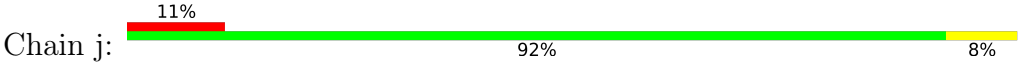


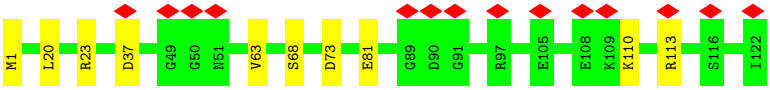


• Molecule 6: 50S ribosomal protein L13

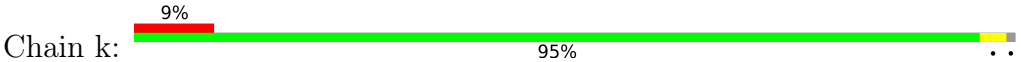


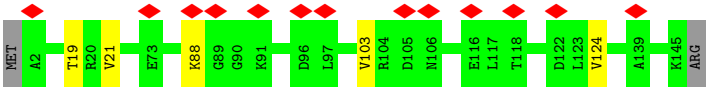
• Molecule 7: 50S ribosomal protein L14



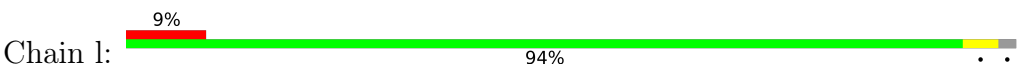


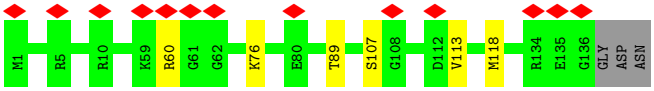
• Molecule 8: 50S ribosomal protein L15





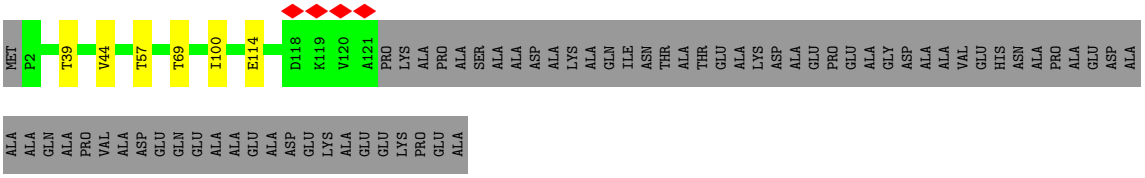
• Molecule 9: 50S ribosomal protein L16





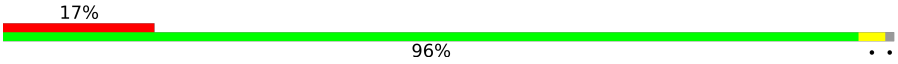
• Molecule 10: Large ribosomal subunit protein bL17

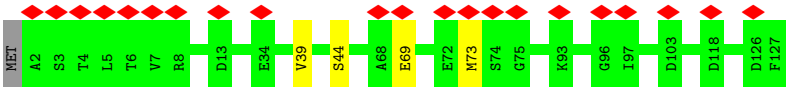
Chain m:



• Molecule 11: 50S ribosomal protein L18

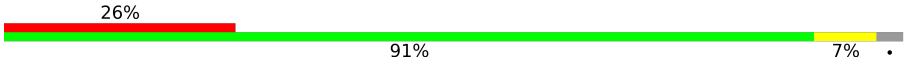
Chain n:





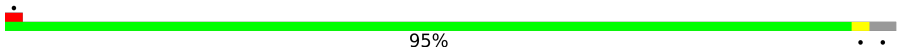
• Molecule 12: 50S ribosomal protein L19

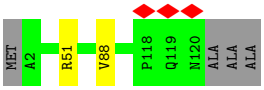
Chain o:



• Molecule 13: 50S ribosomal protein L20

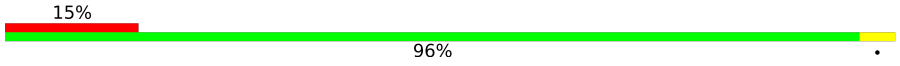
Chain p:

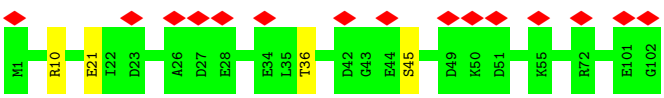




• Molecule 14: Large ribosomal subunit protein bL21

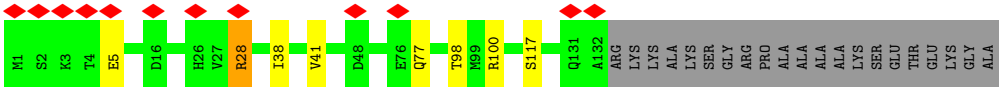
Chain q:



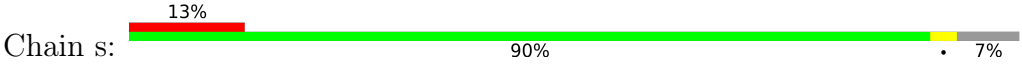


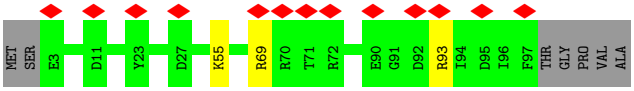
• Molecule 15: 50S ribosomal protein L22

Chain r:

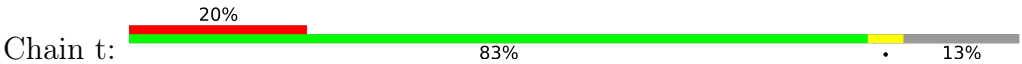


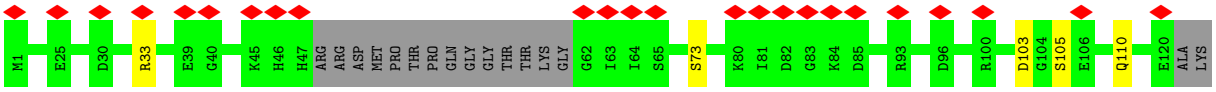
• Molecule 16: 50S ribosomal protein L23



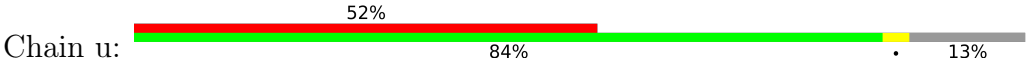


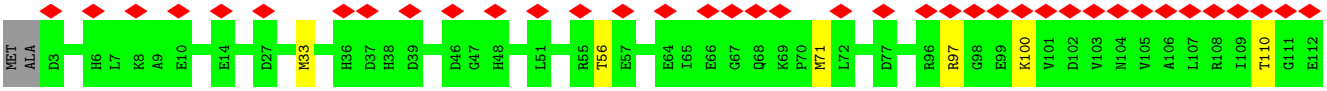
• Molecule 17: Large ribosomal subunit protein uL24

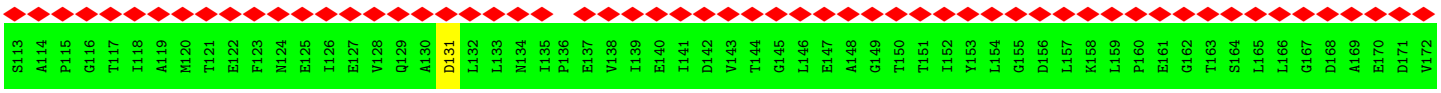


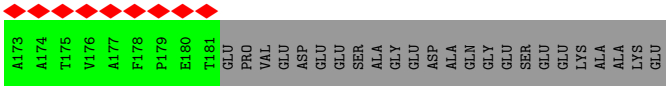


• Molecule 18: 50S ribosomal protein L25

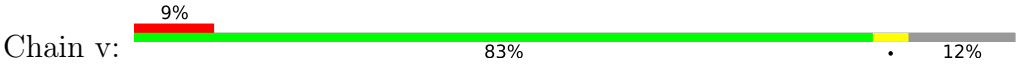


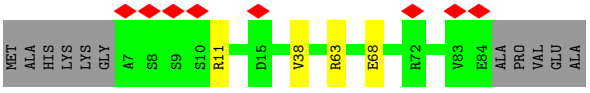




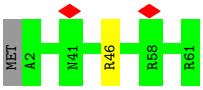


• Molecule 19: 50S ribosomal protein L27



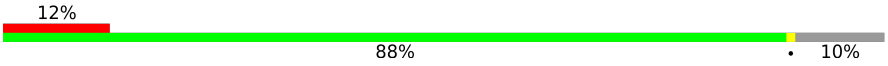


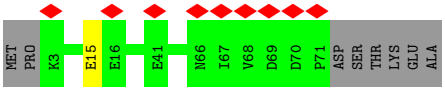
• Molecule 20: 50S ribosomal protein L28



• Molecule 21: 50S ribosomal protein L29

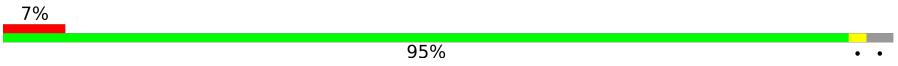
Chain x:

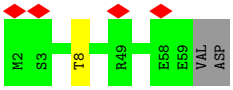




• Molecule 22: 50S ribosomal protein L30

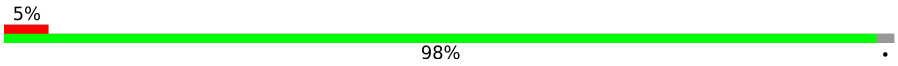
Chain y:

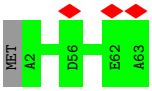




• Molecule 23: 50S ribosomal protein L32

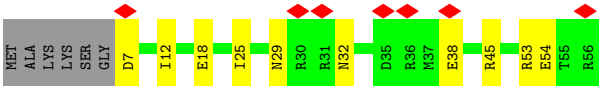
Chain z:





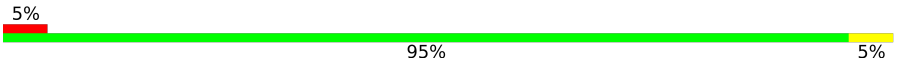
• Molecule 24: 50S ribosomal protein L33

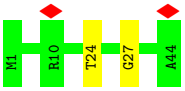
Chain 0:



• Molecule 25: 50S ribosomal protein L34

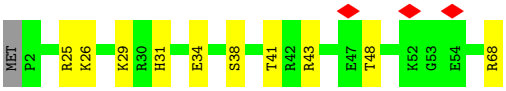
Chain 1:





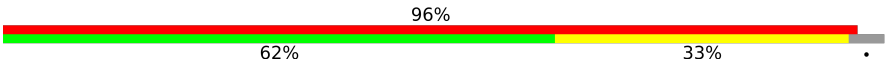
• Molecule 26: Large ribosomal subunit protein bL35

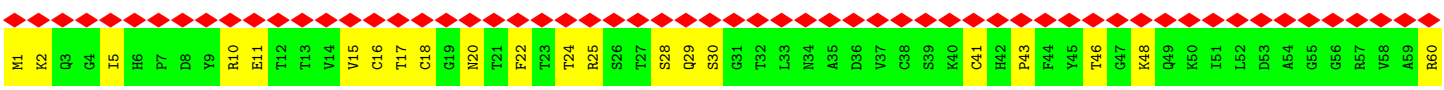
Chain 2:

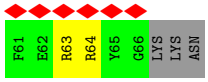


• Molecule 27: 50S ribosomal protein L31

Chain 4:

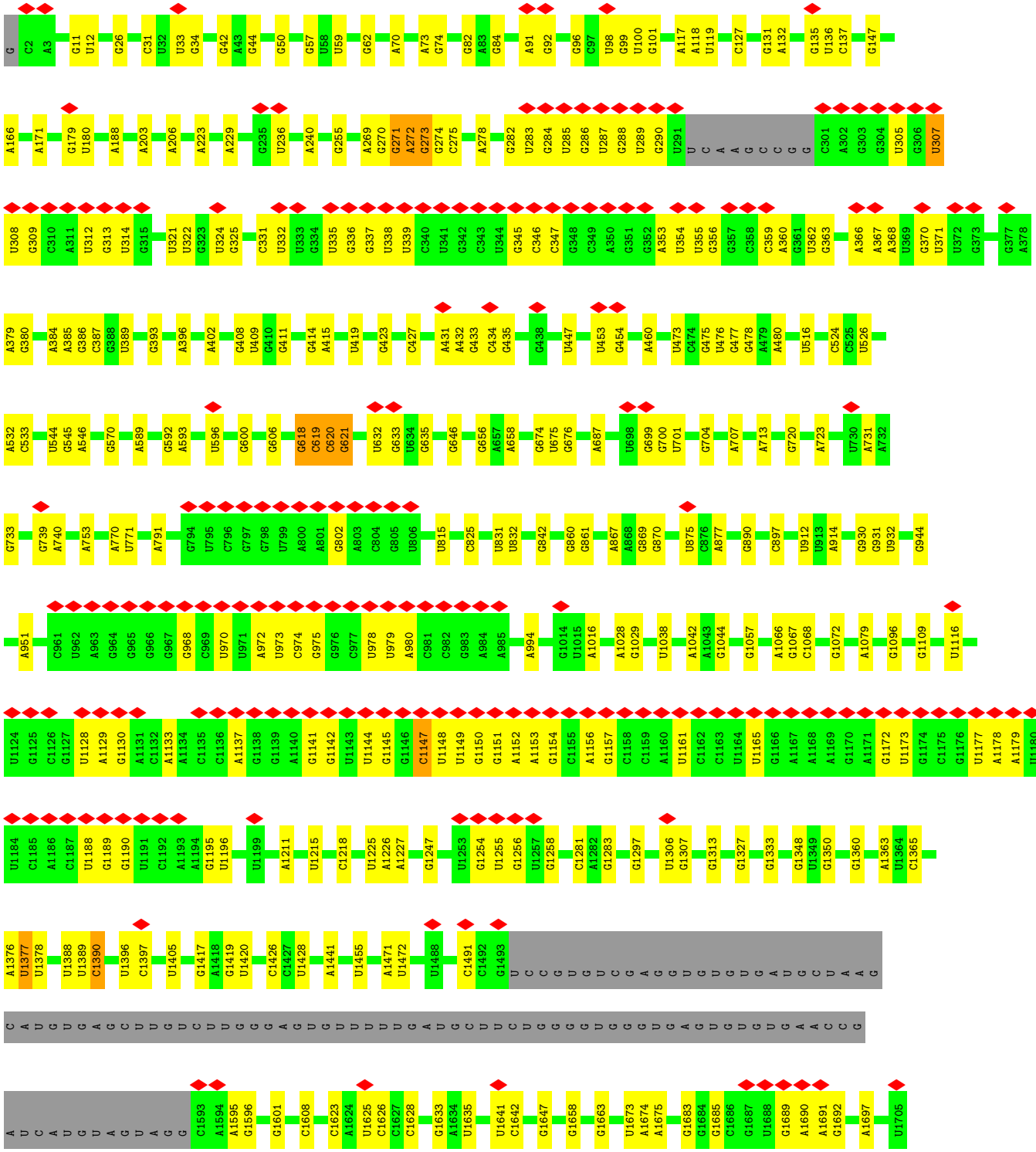


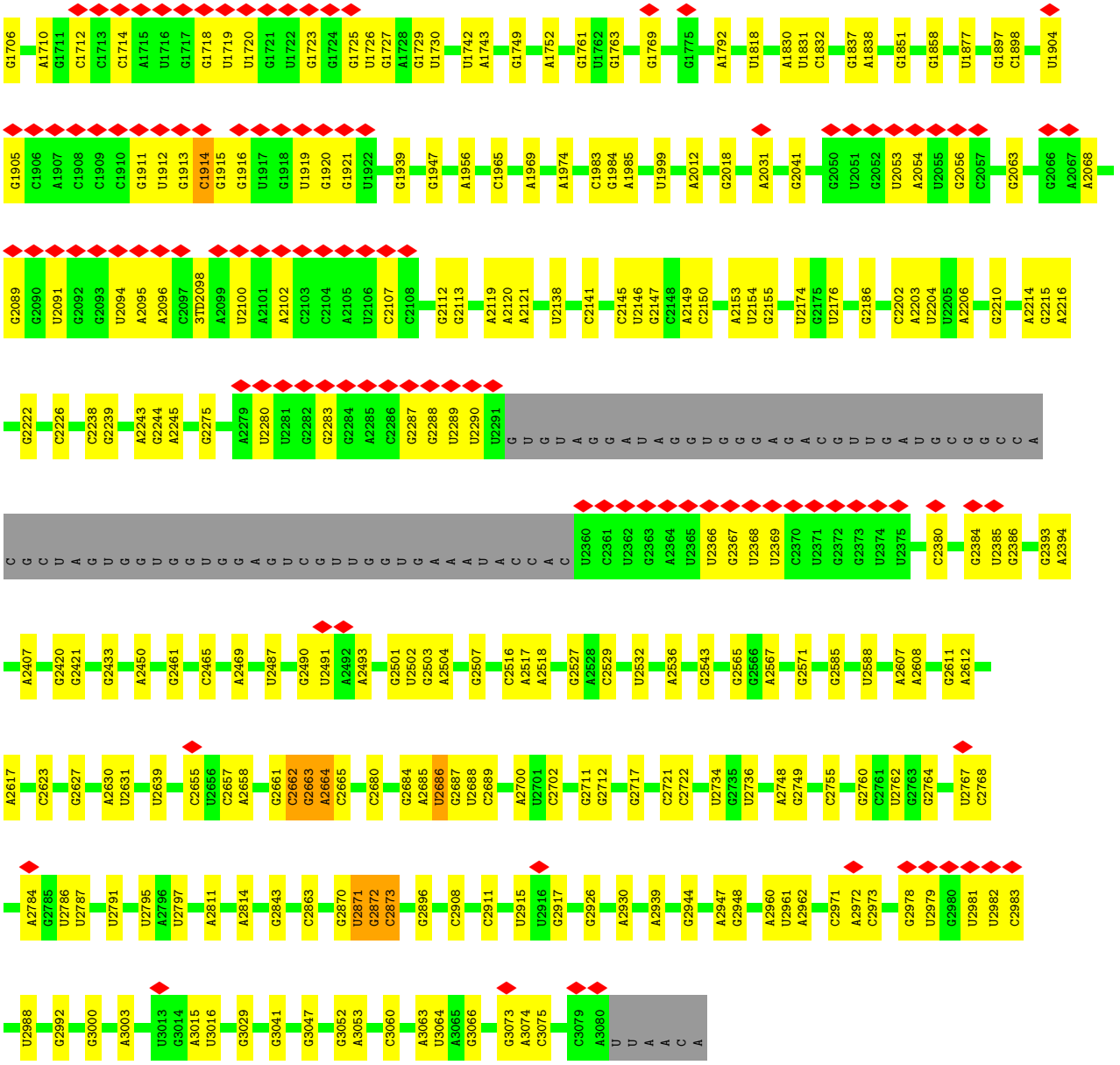




• Molecule 28: 23S rRNA

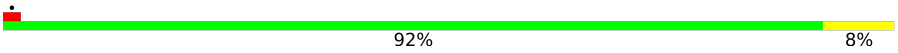
Chain a:

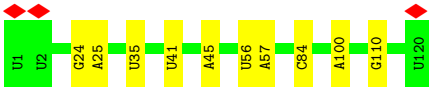




• Molecule 29: 5S rRNA

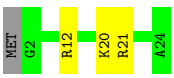
Chain b:





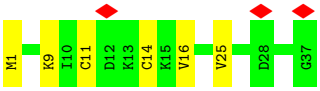
• Molecule 30: 50S ribosomal protein bL37

Chain V:



• Molecule 31: 50S ribosomal protein L36

Chain 3:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	283291	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	38.58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.109	Depositor
Minimum map value	-0.351	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	347.19998, 347.19998, 347.19998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.868, 0.868, 0.868	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: 3TD, CLY, 5MU, 2MA, H2U, MG, OMC, 5MC, OMU, 2MG, OMG, PSU, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	c	0.29	0/2132	0.60	0/2871
2	d	0.28	0/1611	0.56	0/2172
3	e	0.29	0/1600	0.56	0/2165
4	f	0.26	0/1493	0.58	0/2001
5	g	0.28	0/1398	0.56	0/1884
6	i	0.27	0/1164	0.51	0/1574
7	j	0.28	0/957	0.58	0/1282
8	k	0.27	0/1090	0.54	0/1465
9	l	0.27	0/1108	0.56	0/1488
10	m	0.28	0/949	0.59	0/1277
11	n	0.25	0/959	0.57	0/1281
12	o	0.27	0/909	0.58	0/1216
13	p	0.28	0/969	0.53	0/1292
14	q	0.29	0/785	0.54	0/1050
15	r	0.29	0/1028	0.59	0/1379
16	s	0.27	0/759	0.58	0/1022
17	t	0.28	0/836	0.56	0/1118
18	u	0.25	0/1396	0.55	0/1896
19	v	0.27	0/598	0.63	0/800
20	w	0.29	0/483	0.59	0/648
21	x	0.25	0/567	0.54	0/759
22	y	0.25	0/471	0.57	0/627
23	z	0.27	0/487	0.57	0/654
24	0	0.24	0/429	0.60	0/569
25	1	0.25	0/365	0.70	0/478
26	2	0.26	0/519	0.56	0/682
27	4	0.24	0/521	0.58	0/700
28	a	0.41	0/69440	0.84	63/108351 (0.1%)
29	b	0.30	0/2871	0.79	0/4475
30	V	0.24	0/184	0.68	0/236
31	3	0.28	0/305	0.59	0/401
All	All	0.37	0/98383	0.78	63/147813 (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
15	r	0	1

There are no bond length outliers.

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	127	C	C5-C6-N1	14.30	128.15	121.00
28	a	127	C	C5-C4-N4	11.17	128.02	120.20
28	a	2961	U	O4'-C1'-N1	10.85	116.88	108.20
28	a	274	G	P-O3'-C3'	-9.80	107.94	119.70
28	a	270	G	P-O3'-C3'	-9.72	108.03	119.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	r	28	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	c	2091	0	2150	0	0
2	d	1586	0	1634	0	0
3	e	1577	0	1619	0	0
4	f	1468	0	1487	0	0
5	g	1376	0	1421	0	0
6	i	1139	0	1163	0	0
7	j	946	0	1011	0	0
8	k	1072	0	1106	0	0
9	l	1082	0	1117	0	0
10	m	936	0	997	0	0
11	n	952	0	995	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	o	896	0	928	0	0
13	p	958	0	986	0	0
14	q	778	0	824	0	0
15	r	1017	0	1070	0	0
16	s	751	0	803	0	0
17	t	829	0	880	0	0
18	u	1376	0	1397	0	0
19	v	591	0	581	0	0
20	w	474	0	487	0	0
21	x	564	0	582	0	0
22	y	467	0	504	0	0
23	z	477	0	479	0	0
24	0	423	0	429	5	0
25	1	362	0	388	1	0
26	2	513	0	565	3	0
27	4	512	0	498	14	0
28	a	62406	0	31295	0	0
29	b	2567	0	1297	0	0
30	V	183	0	202	1	0
31	3	302	0	330	4	0
32	a	241	0	0	0	0
32	b	3	0	0	0	0
32	c	1	0	0	0	0
32	d	1	0	0	0	0
32	k	1	0	0	0	0
33	0	1	0	0	0	0
33	4	1	0	0	0	0
33	w	1	0	0	0	0
33	z	1	0	0	0	0
34	a	27	0	32	0	0
35	a	141	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	e	2	0	0	0	0
35	i	1	0	0	0	0
35	m	1	0	0	0	0
35	o	1	0	0	0	0
35	p	1	0	0	0	0
35	r	2	0	0	0	0
35	z	1	0	0	0	0
All	All	91105	0	59257	27	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 8.

The worst 5 of 27 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)
31:3:11:CYS:N	31:3:14:CYS:SG	2.51	0.82
27:4:11:GLU:HA	27:4:25:ARG:HG2	1.71	0.73
27:4:43:PRO:HB3	27:4:48:LYS:HB3	1.72	0.71
31:3:16:VAL:HG22	31:3:25:VAL:HG22	1.73	0.71
24:0:29:ASN:ND2	24:0:32:ASN:OD1	2.25	0.68

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	c	272/278 (98%)	255 (94%)	17 (6%)	0	100	100
2	d	212/223 (95%)	200 (94%)	12 (6%)	0	100	100
3	e	208/301 (69%)	190 (91%)	18 (9%)	0	100	100
4	f	182/210 (87%)	169 (93%)	13 (7%)	0	100	100
5	g	175/180 (97%)	162 (93%)	13 (7%)	0	100	100
6	i	144/147 (98%)	143 (99%)	1 (1%)	0	100	100
7	j	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
8	k	142/146 (97%)	120 (84%)	22 (16%)	0	100	100
9	l	134/139 (96%)	131 (98%)	3 (2%)	0	100	100
10	m	118/187 (63%)	114 (97%)	4 (3%)	0	100	100
11	n	124/127 (98%)	119 (96%)	5 (4%)	0	100	100
12	o	112/117 (96%)	110 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	p	117/123 (95%)	114 (97%)	3 (3%)	0	100	100
14	q	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
15	r	130/153 (85%)	126 (97%)	4 (3%)	0	100	100
16	s	93/102 (91%)	86 (92%)	7 (8%)	0	100	100
17	t	102/122 (84%)	99 (97%)	3 (3%)	0	100	100
18	u	177/205 (86%)	167 (94%)	10 (6%)	0	100	100
19	v	76/89 (85%)	73 (96%)	3 (4%)	0	100	100
20	w	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
21	x	67/77 (87%)	65 (97%)	2 (3%)	0	100	100
22	y	56/60 (93%)	54 (96%)	2 (4%)	0	100	100
23	z	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
24	0	48/56 (86%)	45 (94%)	3 (6%)	0	100	100
25	1	42/44 (96%)	42 (100%)	0	0	100	100
26	2	65/68 (96%)	63 (97%)	2 (3%)	0	100	100
27	4	64/69 (93%)	61 (95%)	3 (5%)	0	100	100
30	V	21/24 (88%)	21 (100%)	0	0	100	100
31	3	35/37 (95%)	35 (100%)	0	0	100	100
All	All	3254/3632 (90%)	3087 (95%)	167 (5%)	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	
1	c	216/220 (98%)	210 (97%)	6 (3%)	43	68
2	d	166/172 (96%)	159 (96%)	7 (4%)	30	51
3	e	165/237 (70%)	149 (90%)	16 (10%)	8	15
4	f	154/175 (88%)	144 (94%)	10 (6%)	17	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	g	150/152 (99%)	138 (92%)	12 (8%)	12 22
6	i	118/120 (98%)	115 (98%)	3 (2%)	47 72
7	j	101/101 (100%)	91 (90%)	10 (10%)	8 14
8	k	111/113 (98%)	106 (96%)	5 (4%)	27 48
9	l	108/110 (98%)	102 (94%)	6 (6%)	21 38
10	m	100/142 (70%)	94 (94%)	6 (6%)	19 34
11	n	95/96 (99%)	91 (96%)	4 (4%)	30 51
12	o	97/99 (98%)	89 (92%)	8 (8%)	11 21
13	p	98/99 (99%)	96 (98%)	2 (2%)	55 78
14	q	84/84 (100%)	80 (95%)	4 (5%)	25 45
15	r	105/118 (89%)	97 (92%)	8 (8%)	13 24
16	s	84/89 (94%)	81 (96%)	3 (4%)	35 59
17	t	91/103 (88%)	86 (94%)	5 (6%)	21 39
18	u	149/168 (89%)	142 (95%)	7 (5%)	26 46
19	v	60/67 (90%)	56 (93%)	4 (7%)	16 29
20	w	52/53 (98%)	51 (98%)	1 (2%)	57 79
21	x	61/68 (90%)	60 (98%)	1 (2%)	62 82
22	y	53/55 (96%)	52 (98%)	1 (2%)	57 79
23	z	51/52 (98%)	51 (100%)	0	100 100
24	0	47/51 (92%)	45 (96%)	2 (4%)	29 50
25	1	36/36 (100%)	36 (100%)	0	100 100
26	2	54/55 (98%)	49 (91%)	5 (9%)	9 16
27	4	56/59 (95%)	55 (98%)	1 (2%)	59 80
30	V	16/17 (94%)	14 (88%)	2 (12%)	4 8
31	3	35/35 (100%)	34 (97%)	1 (3%)	42 67
All	All	2713/2946 (92%)	2573 (95%)	140 (5%)	27 41

5 of 140 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	u	33	MET
18	u	100	LYS
24	0	45	ARG

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Mol	Chain	Res	Type
5	g	133	PHE
5	g	128	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
5	g	74	ASN
10	m	107	ASN
17	t	110	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	a	2891/3086 (93%)	531 (18%)	0
29	b	118/120 (98%)	10 (8%)	0
All	All	3009/3206 (93%)	541 (17%)	0

5 of 541 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
28	a	11	G
28	a	12	U
28	a	26	G
28	a	31	C
28	a	33	U

There are no RNA pucker outliers to report.

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

18 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	$\#\|Z\|>2$
28	OMC	a	2680	28,32	19,22,23	0.56	0	26,31,34	0.72	0
28	PSU	a	2787	28	18,21,22	1.07	1 (5%)	22,30,33	1.75	4 (18%)
28	PSU	a	2762	28	18,21,22	1.09	1 (5%)	22,30,33	1.80	5 (22%)
28	PSU	a	1038	28	18,21,22	0.98	1 (5%)	22,30,33	1.82	3 (13%)
28	PSU	a	2094	28	18,21,22	1.10	1 (5%)	22,30,33	1.76	4 (18%)
28	H2U	a	2631	28	18,21,22	0.65	1 (5%)	21,30,33	0.88	1 (4%)
28	PSU	a	2686	28	18,21,22	0.87	1 (5%)	22,30,33	0.67	0
28	2MG	a	2627	28	18,26,27	1.20	3 (16%)	16,38,41	0.96	1 (6%)
28	OMU	a	2734	28	19,22,23	2.88	7 (36%)	26,31,34	1.74	4 (15%)
28	2MG	a	2018	28	18,26,27	1.16	2 (11%)	16,38,41	0.86	1 (6%)
28	2MA	a	2685	28,32	17,25,26	0.99	2 (11%)	17,37,40	0.83	1 (5%)
28	5MC	a	2145	28	18,22,23	0.58	0	26,32,35	1.02	2 (7%)
28	PSU	a	2786	28	18,21,22	1.03	1 (5%)	22,30,33	1.72	4 (18%)
28	3TD	a	2098	28	18,22,23	4.16	6 (33%)	22,32,35	1.63	2 (9%)
28	PSU	a	2100	28	18,21,22	1.09	1 (5%)	22,30,33	1.79	5 (22%)
28	PSU	a	2639	28	18,21,22	1.03	1 (5%)	22,30,33	1.86	6 (27%)
28	5MU	a	2122	28	19,22,23	0.50	0	28,32,35	0.51	0
28	OMG	a	2433	28,32	18,26,27	1.19	2 (11%)	19,38,41	0.87	1 (5%)

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
28	OMC	a	2680	28,32	-	1/9/27/28	0/2/2/2
28	PSU	a	2787	28	-	0/7/25/26	0/2/2/2
28	PSU	a	2762	28	-	0/7/25/26	0/2/2/2
28	PSU	a	1038	28	-	0/7/25/26	0/2/2/2
28	PSU	a	2094	28	-	2/7/25/26	0/2/2/2
28	H2U	a	2631	28	-	0/7/38/39	0/2/2/2
28	PSU	a	2686	28	-	2/7/25/26	0/2/2/2
28	2MG	a	2627	28	-	2/5/27/28	0/3/3/3
28	OMU	a	2734	28	-	0/9/27/28	0/2/2/2
28	2MG	a	2018	28	-	0/5/27/28	0/3/3/3
28	2MA	a	2685	28,32	-	3/3/25/26	0/3/3/3
28	5MC	a	2145	28	-	0/7/25/26	0/2/2/2
28	PSU	a	2786	28	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	3TD	a	2098	28	-	2/7/25/26	0/2/2/2
28	PSU	a	2100	28	-	0/7/25/26	0/2/2/2
28	PSU	a	2639	28	-	0/7/25/26	0/2/2/2
28	5MU	a	2122	28	-	0/7/25/26	0/2/2/2
28	OMG	a	2433	28,32	-	1/5/27/28	0/3/3/3

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	2098	3TD	C6-C5	12.30	1.49	1.35
28	a	2098	3TD	C2-N1	9.08	1.49	1.37
28	a	2734	OMU	C2-N1	6.91	1.49	1.38
28	a	2734	OMU	C2-N3	6.39	1.49	1.38
28	a	2098	3TD	C6-N1	6.03	1.46	1.36

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	2734	OMU	C4-N3-C2	-5.28	119.61	126.58
28	a	1038	PSU	C4-N3-C2	-5.07	119.03	126.34
28	a	2098	3TD	N1-C2-N3	4.99	120.08	116.14
28	a	2639	PSU	N1-C2-N3	4.86	120.64	115.13
28	a	2639	PSU	C4-N3-C2	-4.73	119.53	126.34

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	a	2433	OMG	C1'-C2'-O2'-CM2
28	a	2685	2MA	O4'-C4'-C5'-O5'
28	a	2685	2MA	C3'-C4'-C5'-O5'
28	a	2098	3TD	C3'-C4'-C5'-O5'
28	a	2627	2MG	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 252 ligands modelled in this entry, 251 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	$\#\|Z\| > 2$
34	CLY	a	3342	-	25,28,28	0.29	0	29,40,40	0.72	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
34	CLY	a	3342	-	-	2/21/53/53	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	a	3342	CLY	C14-C13-C16-C17
34	a	3342	CLY	C12-C13-C16-C17

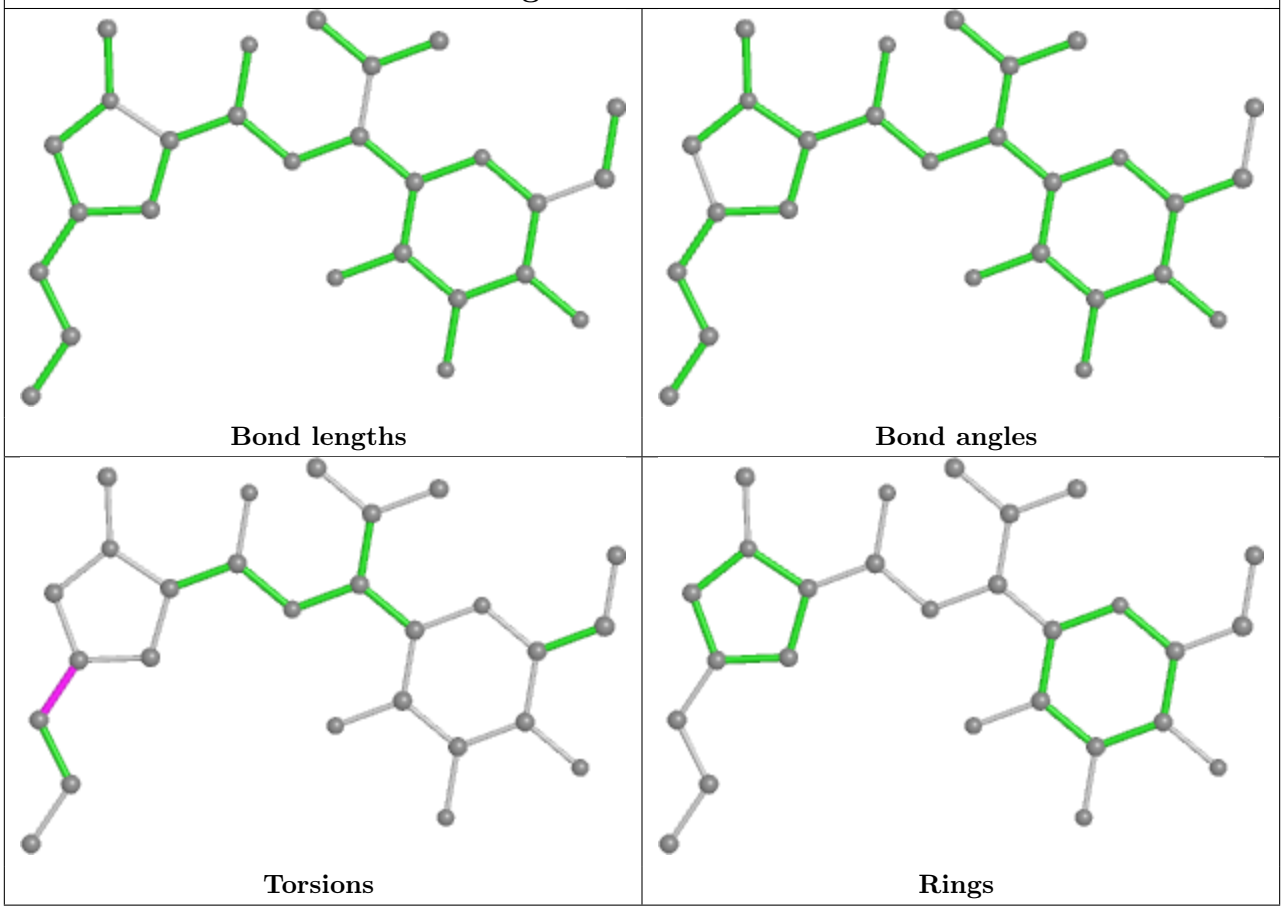
There are no ring outliers.

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 3342



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.

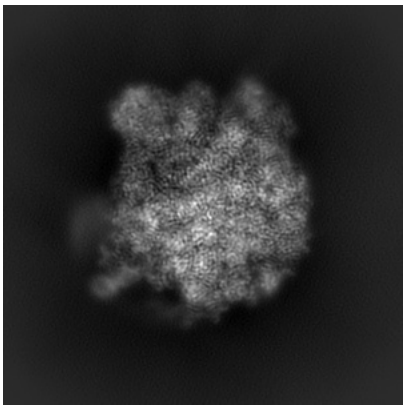
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-45185. 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



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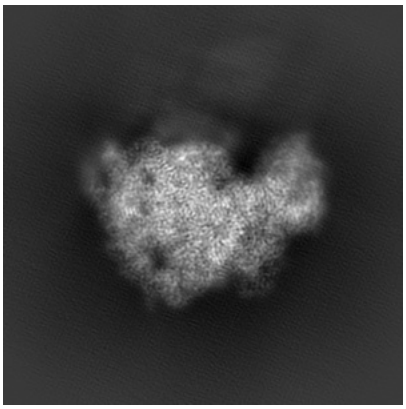
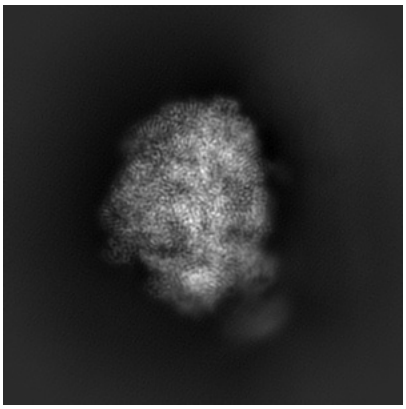
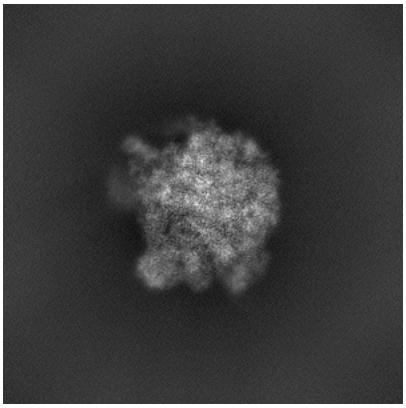


Y

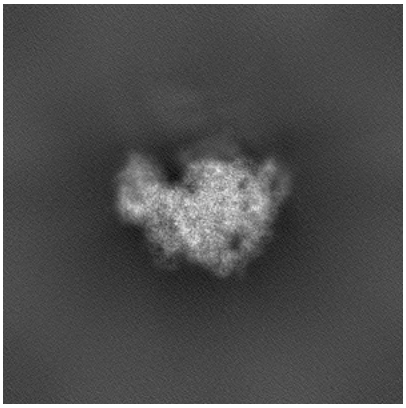


Z

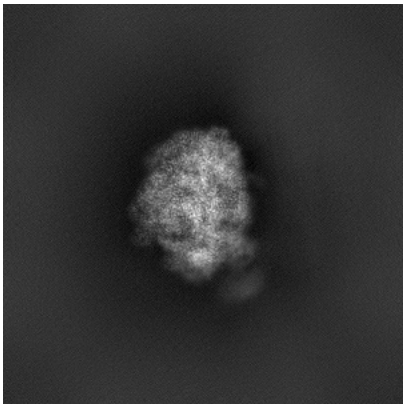
6.1.2 Raw map



X



Y

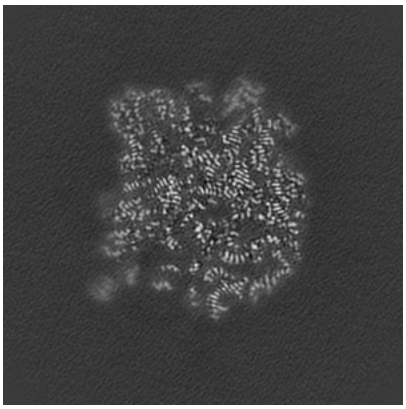


Z

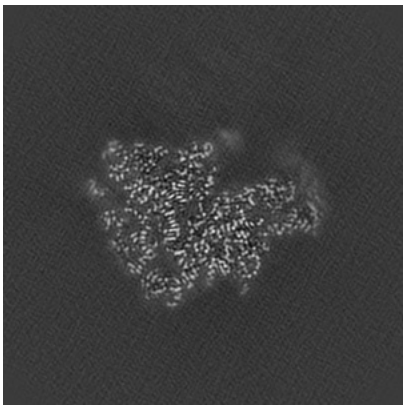
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

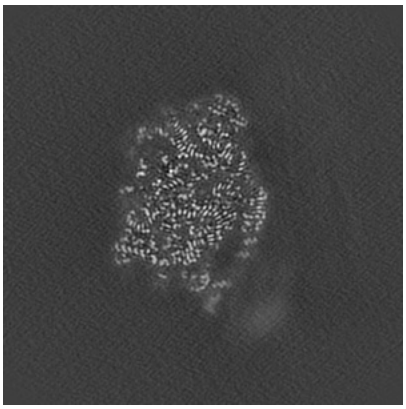
6.2.1 Primary map



X Index: 200

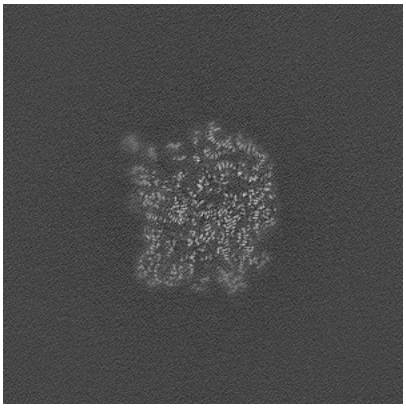


Y Index: 200

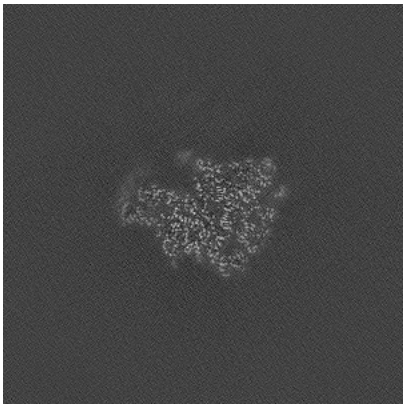


Z Index: 200

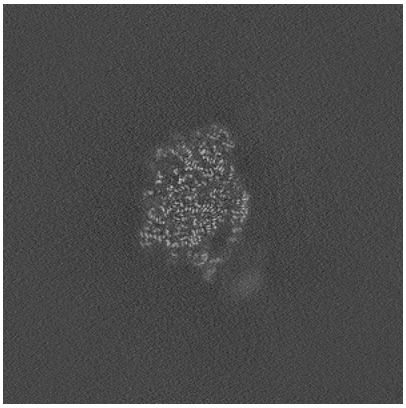
6.2.2 Raw map



X Index: 280



Y Index: 280

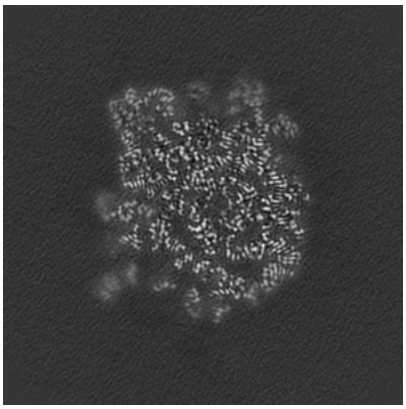


Z Index: 280

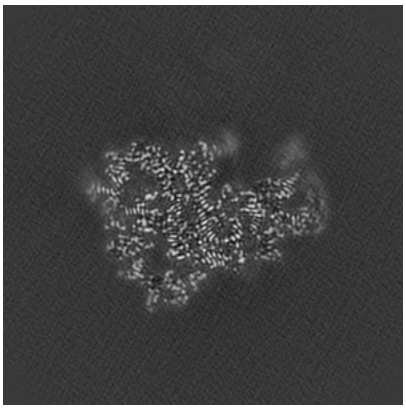
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

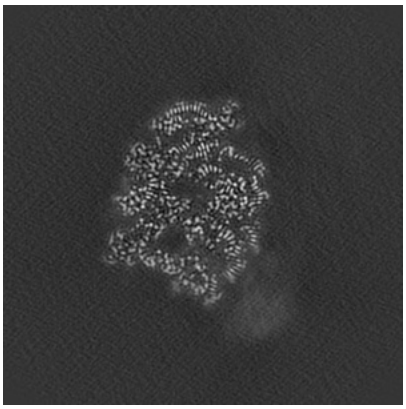
6.3.1 Primary map



X Index: 204

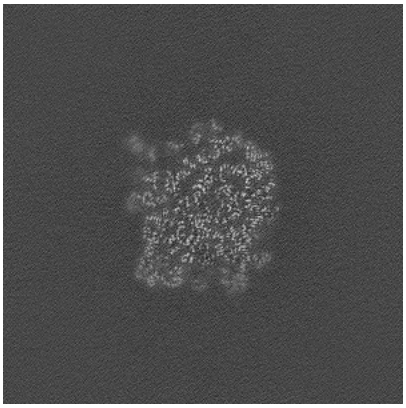


Y Index: 192

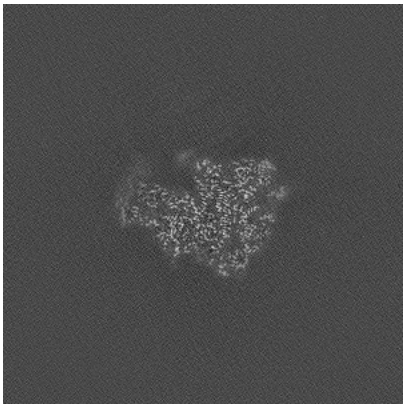


Z Index: 187

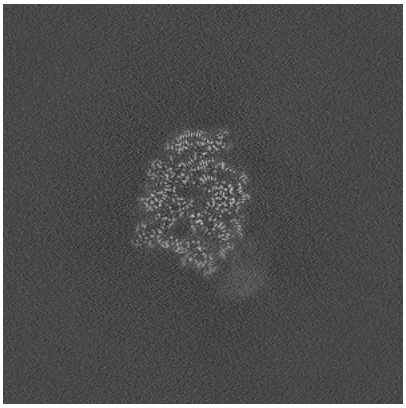
6.3.2 Raw map



X Index: 284



Y Index: 278

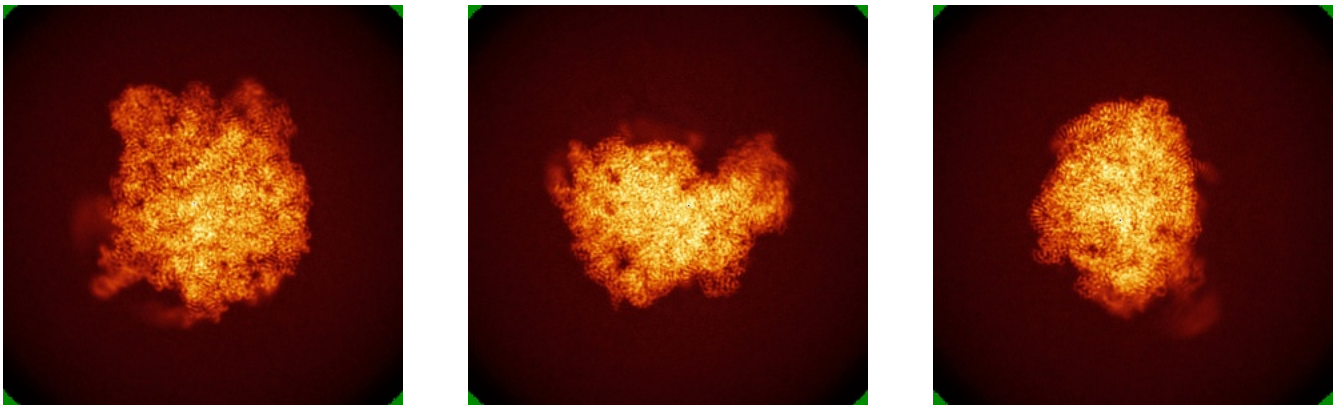


Z Index: 293

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

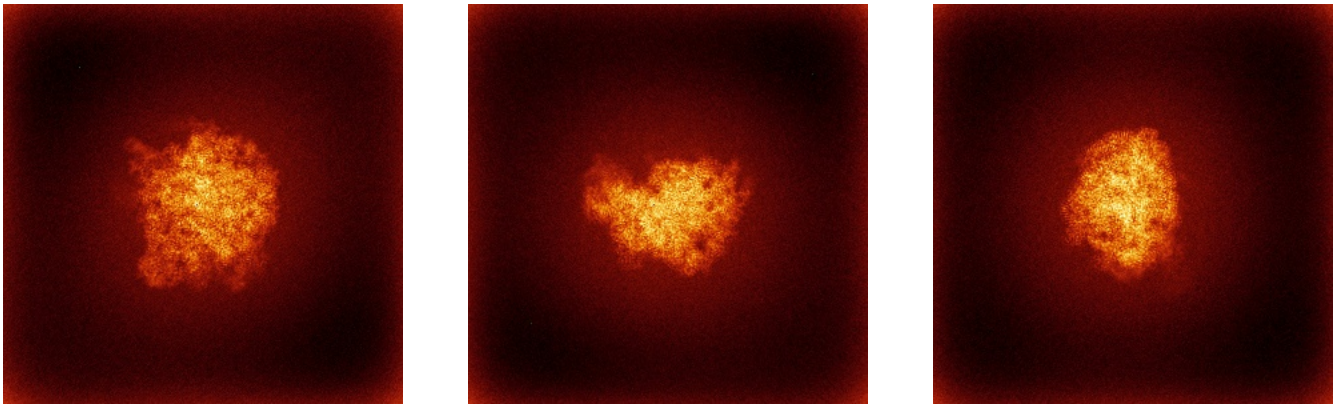
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map

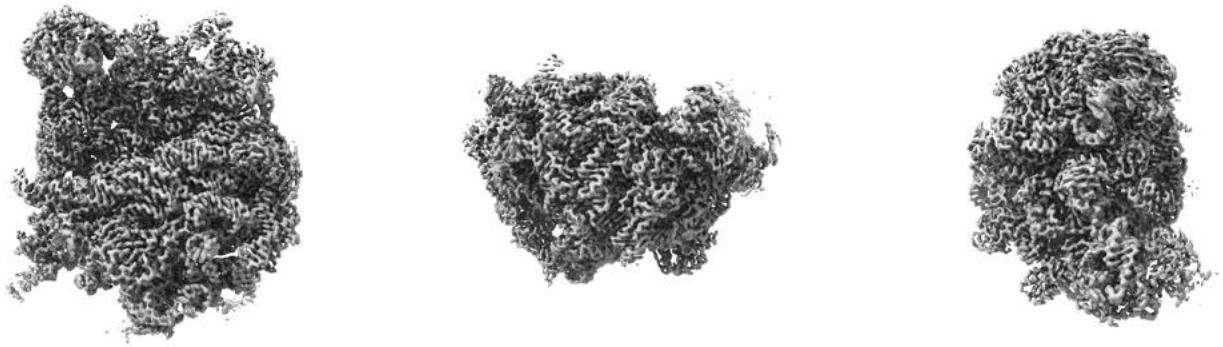


X Y Z

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 0.25. 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.

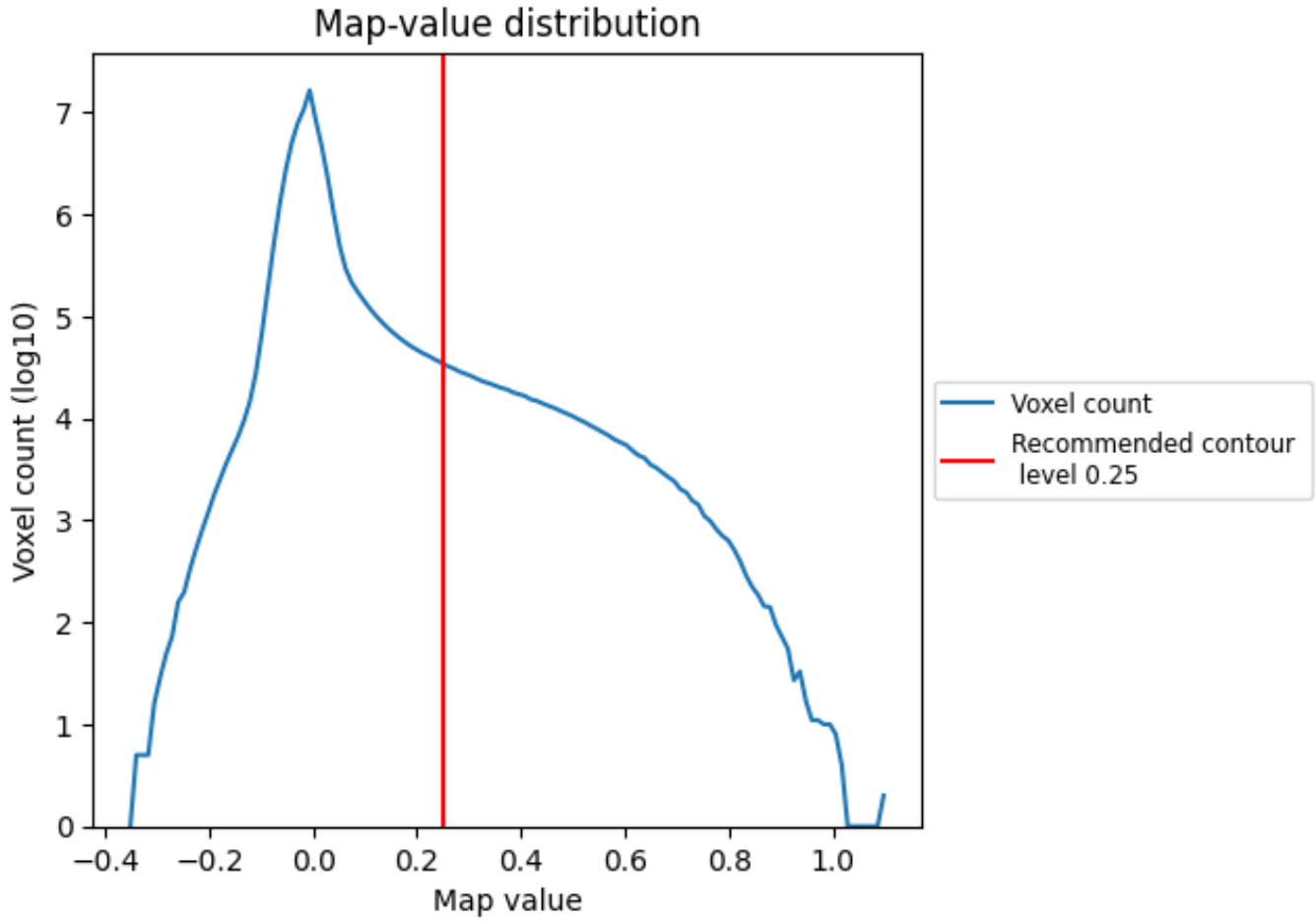
6.6 Mask visualisation (i)

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

7 Map analysis

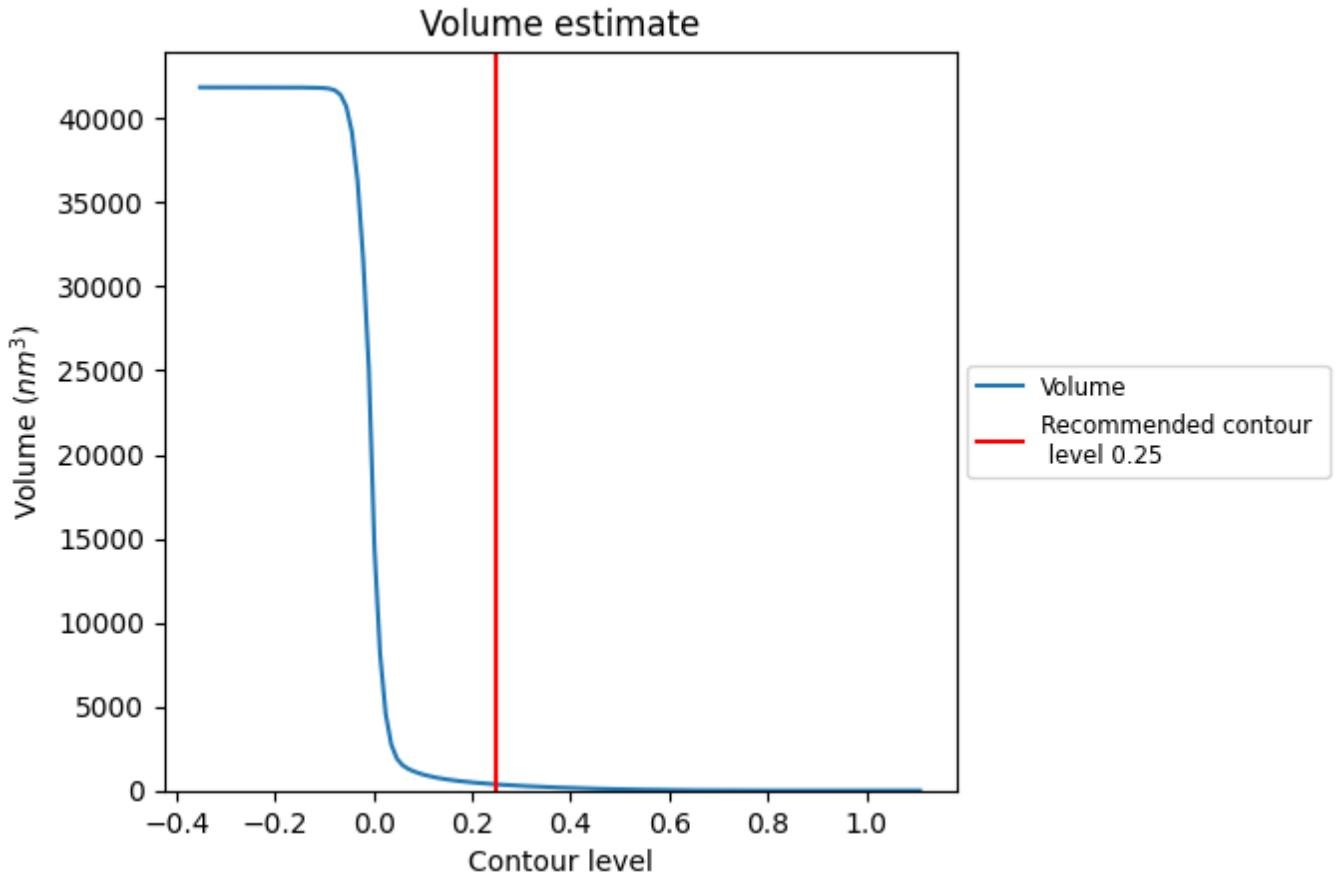
This section contains the results of statistical analysis of the map.

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.

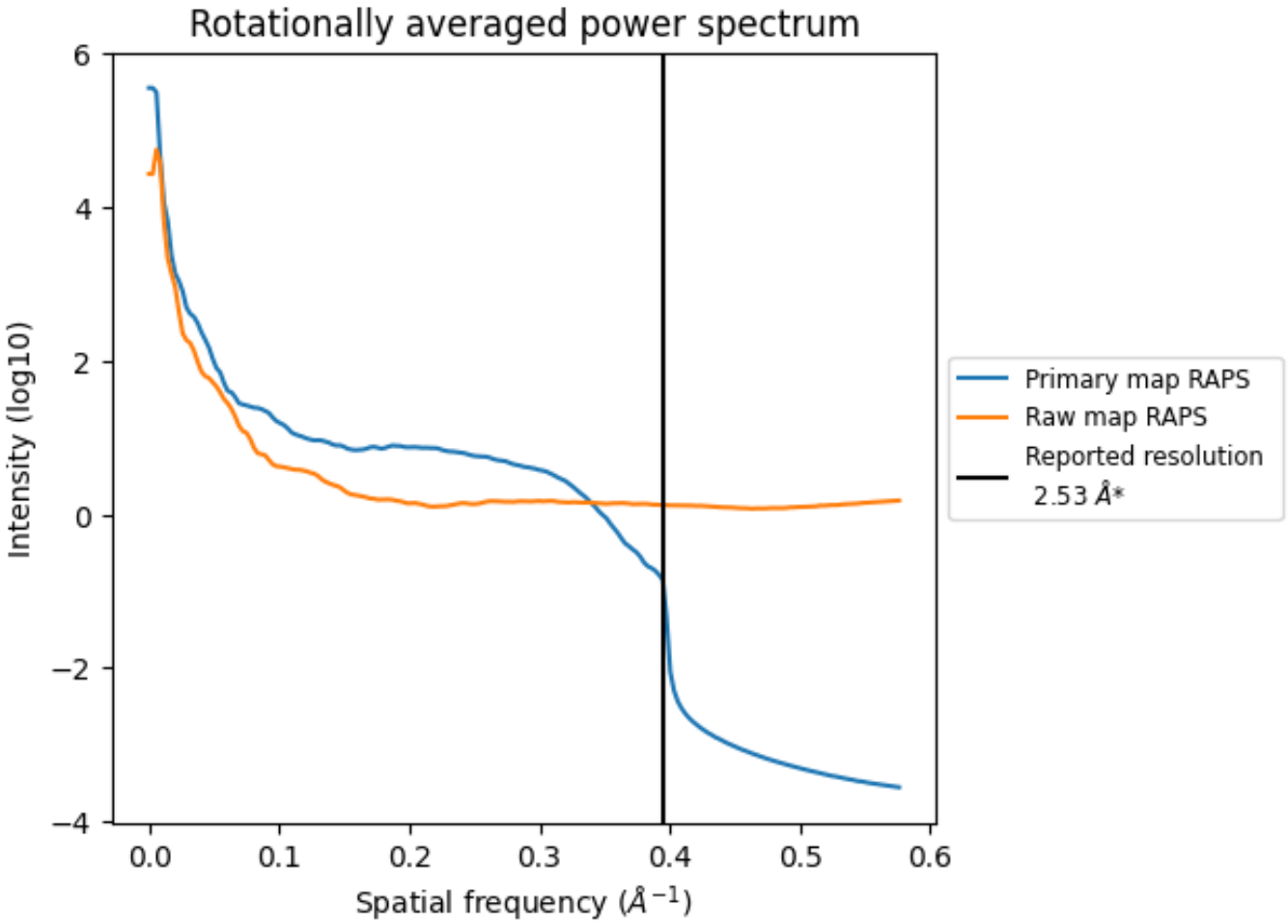
7.2 Volume estimate (i)



The volume at the recommended contour level is 369 nm^3; this corresponds to an approximate mass of 333 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)

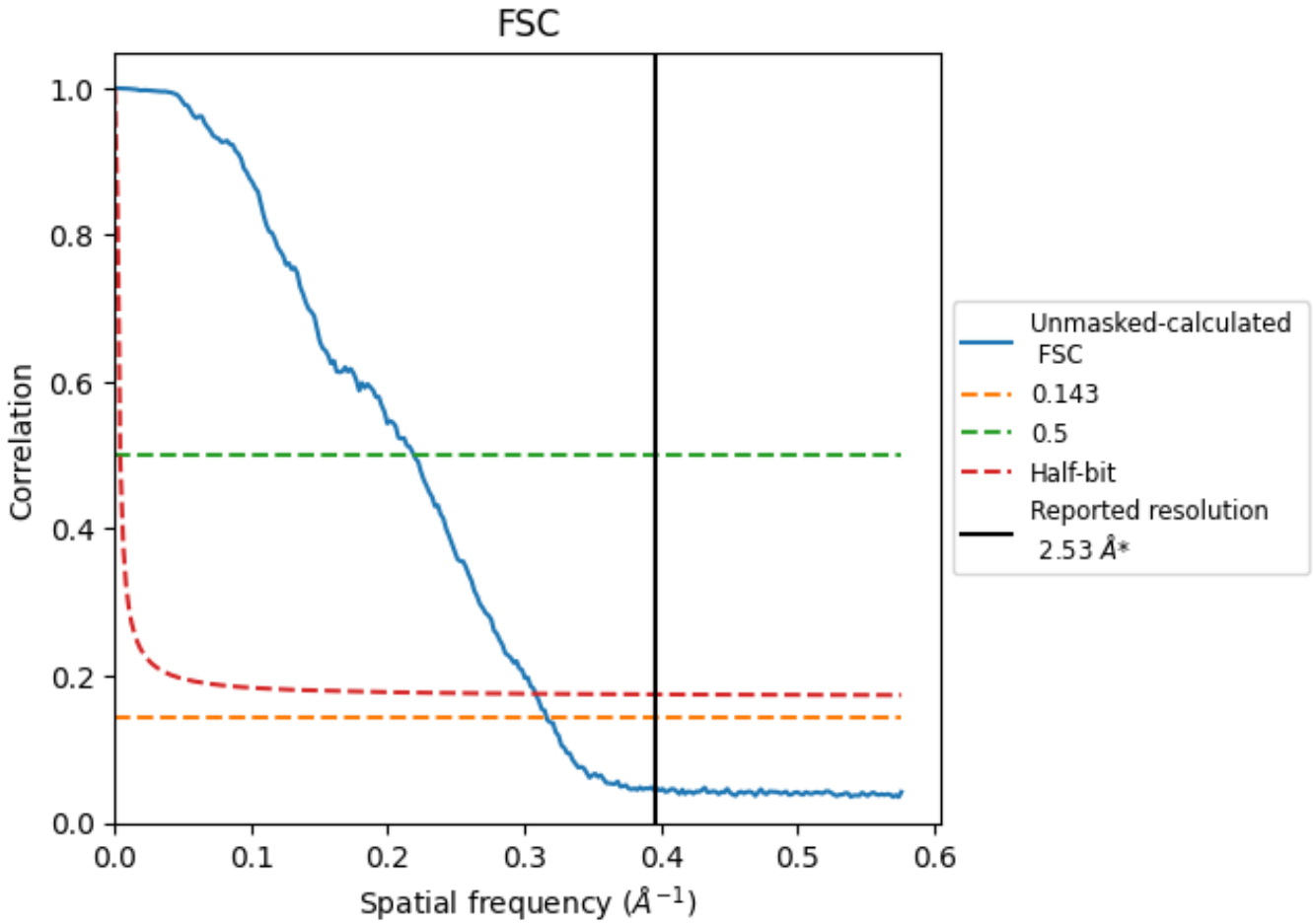


*Reported resolution corresponds to spatial frequency of 0.395 Å^{-1}

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 0.395 Å^{-1}

8.2 Resolution estimates (i)

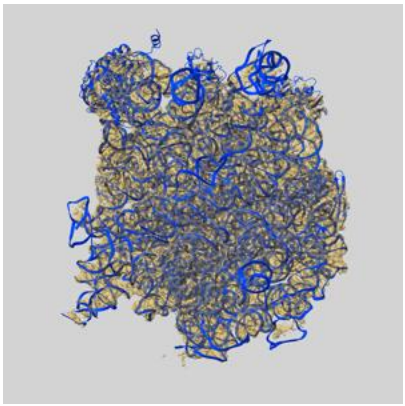
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.53	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.16	4.56	3.24

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.16 differs from the reported value 2.53 by more than 10 %

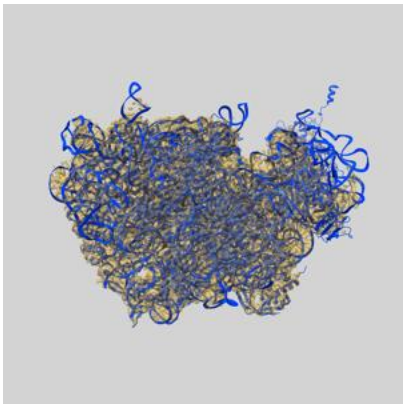
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-45185 and PDB model 9C4G. Per-residue inclusion information can be found in section 3 on page 11.

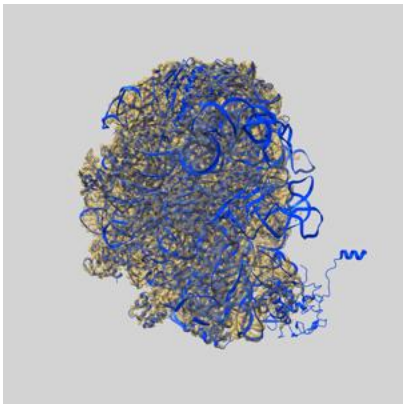
9.1 Map-model overlay



X



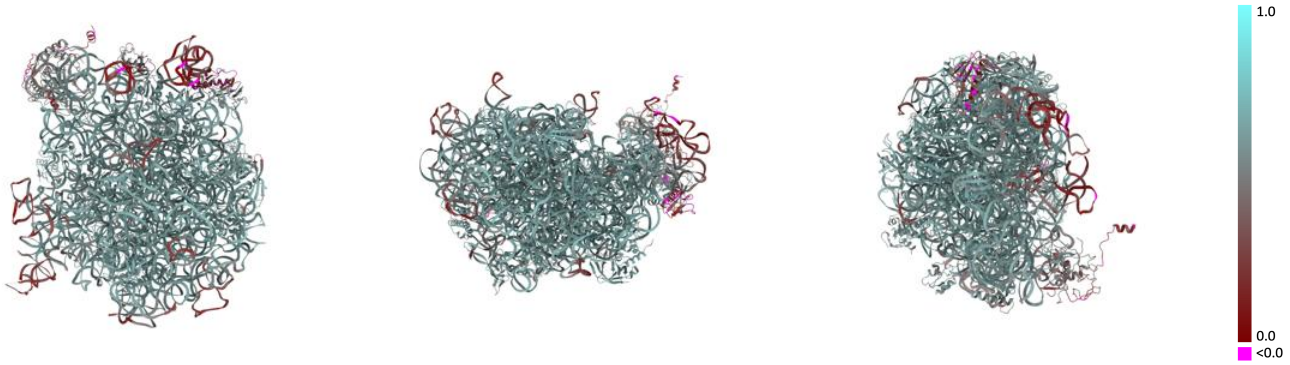
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25 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.

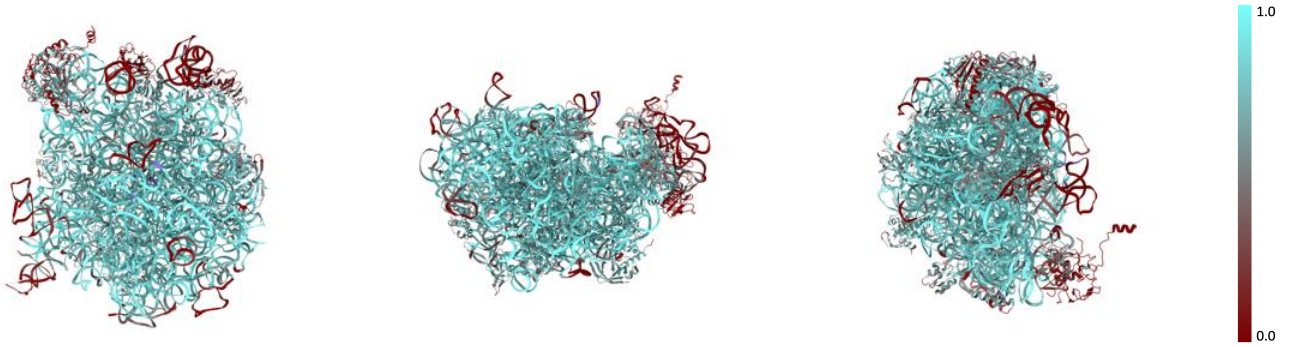
9.2 Q-score mapped to coordinate model (i)



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.

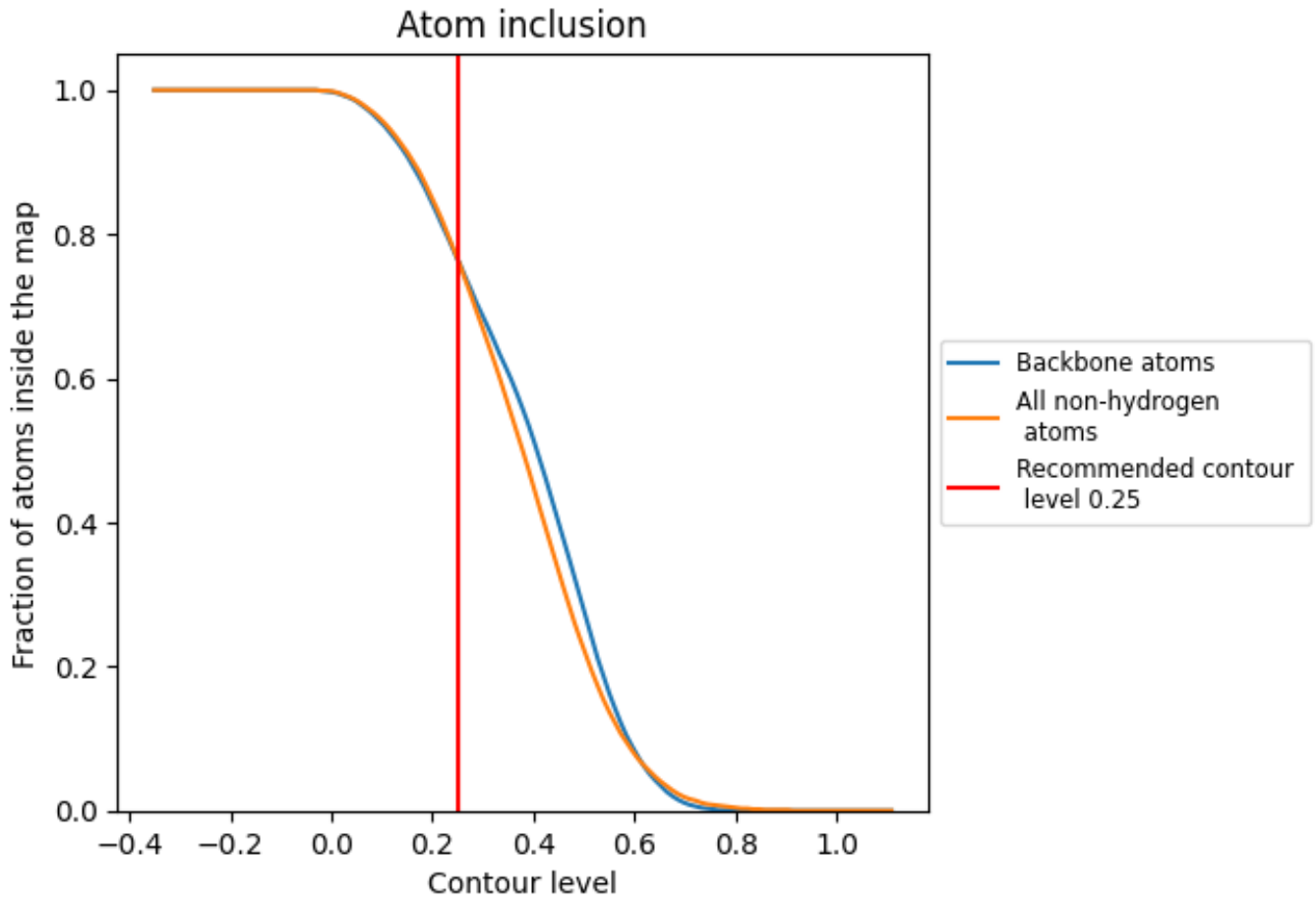
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.25).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 76% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7650	0.5760
0	0.6620	0.6030
1	0.8010	0.6370
2	0.7300	0.6290
3	0.6920	0.6130
4	0.0040	0.2200
V	0.8190	0.6400
a	0.8220	0.5780
b	0.8380	0.5750
c	0.7890	0.6250
d	0.7610	0.6200
e	0.6990	0.5830
f	0.2360	0.4560
g	0.2840	0.3450
i	0.7730	0.6300
j	0.6570	0.6030
k	0.6850	0.5980
l	0.6870	0.6100
m	0.7720	0.6160
n	0.6140	0.5610
o	0.5920	0.5670
p	0.7900	0.6210
q	0.6670	0.6100
r	0.7110	0.6060
s	0.6580	0.5970
t	0.5810	0.5710
u	0.3150	0.4740
v	0.7550	0.6210
w	0.7990	0.6300
x	0.6130	0.5870
y	0.7110	0.6150
z	0.7720	0.6280