wwPDB EM Validation Summary Report (i)

Jun 3, 2024 – 04:57 pm BST

PDB ID	:	8S1P
EMDB ID	:	EMD-19638
Title	:	YlmH bound to PtRNA-50S
Authors	:	Paternoga, H.; Dimitrova-Paternoga, L.; Wilson, D.N.
Deposited on	:	2024-02-15
Resolution	:	1.96 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

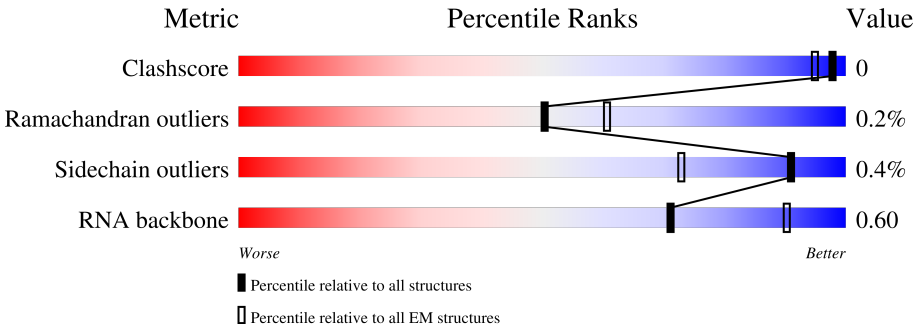
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.96 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	3	66	92% 5% ·
2	4	37	14% 100%
3	6	66	70% 62% 8% 30%
4	A	2928	12% 79% 14% · 7%
5	B	112	71% 80% 16% ·
6	C	277	6% 98% ··
7	D	209	7% 99% ·

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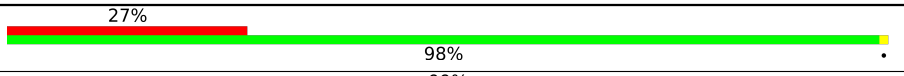
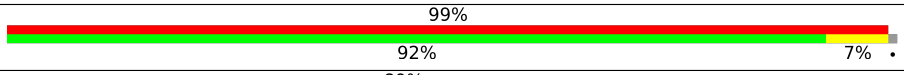
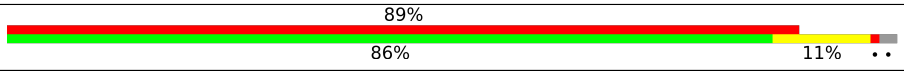
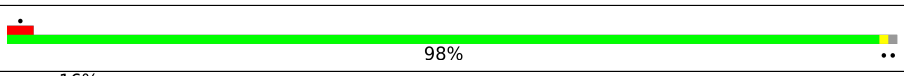
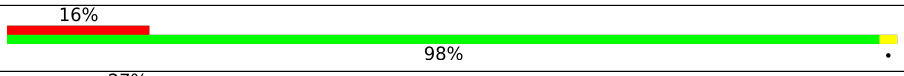
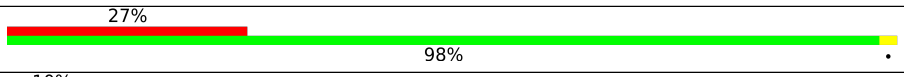
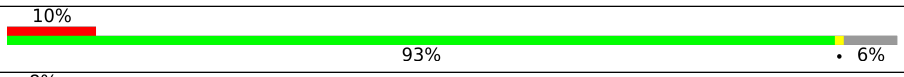
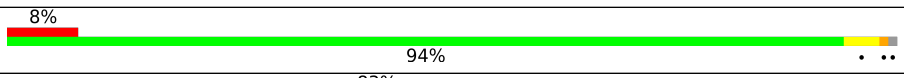
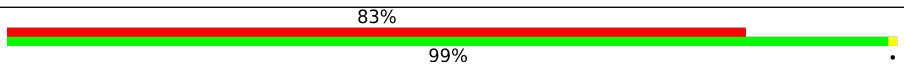
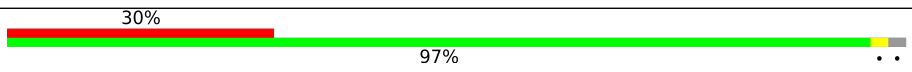
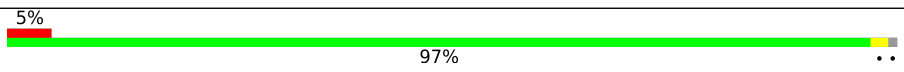
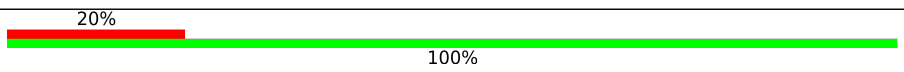
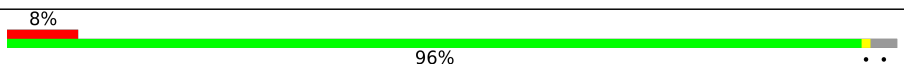
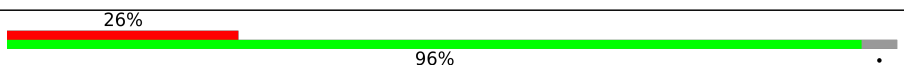
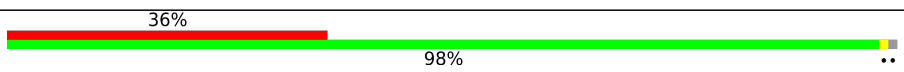
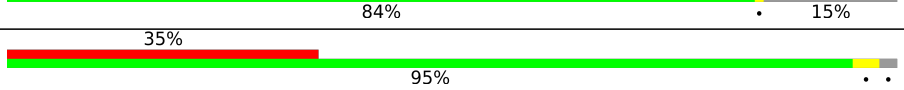
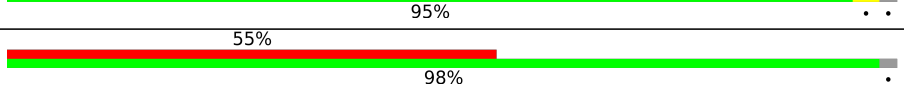
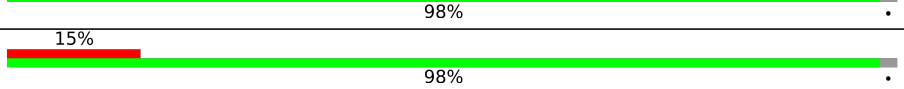
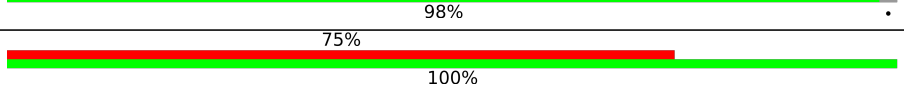
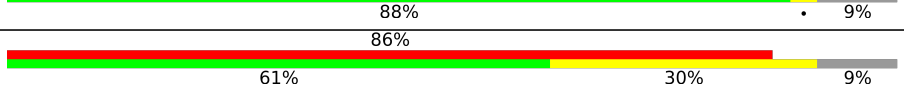
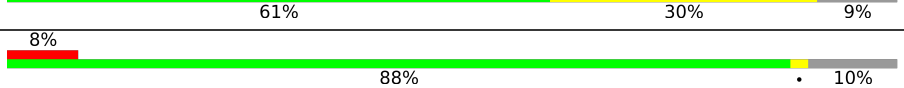
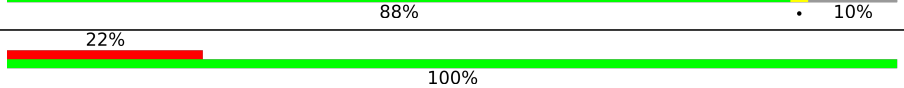
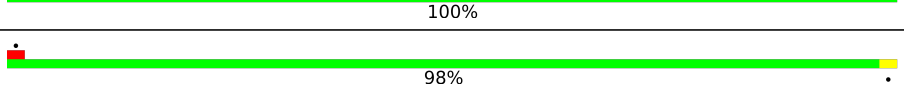
Mol	Chain	Length	Quality of chain
8	E	207	
9	F	179	
10	G	179	
11	J	145	
12	K	122	
13	L	146	
14	M	144	
15	N	120	
16	O	120	
17	P	115	
18	Q	119	
19	R	102	
20	S	113	
21	T	95	
22	U	103	
23	W	94	
24	X	62	
25	Y	66	
26	Z	59	
27	b	4	
28	V	275	
29	a	76	
30	0	59	
31	1	49	
32	2	44	

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 91097 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 L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3	64	Total	C	N	O	S	0	0
			512	321	107	82	2		

- Molecule 2 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	4	37	Total	C	N	O	S	0	0
			297	186	60	46	5		

- Molecule 3 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	6	46	Total	C	N	O	S	0	0
			356	222	63	66	5		

- Molecule 4 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	2733	Total	C	N	O	P	0	0
			58713	26198	10859	18924	2732		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	112	Total	C	N	O	P	0	0
			2392	1068	435	778	111		

- Molecule 6 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	273	Total	C	N	O	S	0	0
			2094	1302	412	374	6		

- Molecule 7 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	207	Total	C	N	O	S	0	0
			1575	988	290	292	5		

- Molecule 8 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	206	Total	C	N	O	S	0	0
			1567	983	290	292	2		

- Molecule 9 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	178	Total	C	N	O	S	0	0
			1405	893	245	260	7		

- Molecule 10 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	175	Total	C	N	O	S	0	0
			1342	835	248	257	2		

- Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	143	Total	C	N	O	S	0	0
			1131	714	207	205	5		

- Molecule 12 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	122	Total	C	N	O	S	0	0
			921	571	173	173	4		

- Molecule 13 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	146	Total	C	N	O	S	0	0
			1082	671	207	202	2		

- Molecule 14 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	135	Total	C	N	O	S	0	0
			1076	690	205	176	5		

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	119	Total	C	N	O	S	0	0
			954	583	186	181	4		

- Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	120	Total	C	N	O	S	0	0
			913	564	176	172	1		

- Molecule 17 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	113	Total	C	N	O	S	0	0
			922	588	177	156	1		

- Molecule 18 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	118	Total	C	N	O	S	0	0
			950	597	191	158	4		

- Molecule 19 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	102	Total	C	N	O	S	0	0
			795	506	140	148	1		

- Molecule 20 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	110	Total	C	N	O	S	0	0
			850	530	165	151	4		

- Molecule 21 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	91	Total	C	N	O	S	0	0
			733	458	135	137	3		

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	102	Total	C	N	O	S	0	0
			770	482	143	141	4		

- Molecule 23 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	W	80	Total	C	N	O	0	0
			611	378	119	114		

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	61	Total	C	N	O	S	0	0
			468	289	98	79	2		

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	65	Total	C	N	O	S	0	0
			530	328	102	98	2		

- Molecule 26 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	58	Total	C	N	O	S	0	0
			456	281	89	85	1		

- Molecule 27 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	b	4	Total	C	N	O	0	0
			20	12	4	4		

- Molecule 28 is a protein called Putative RNA-binding protein YlmH.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	249	Total	C	N	O	S	0	0
			1988	1256	350	376	6		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	258	GLY	-	expression tag	UNP P71020
V	259	SER	-	expression tag	UNP P71020
V	260	GLY	-	expression tag	UNP P71020
V	261	SER	-	expression tag	UNP P71020
V	262	GLY	-	expression tag	UNP P71020
V	263	SER	-	expression tag	UNP P71020
V	264	GLY	-	expression tag	UNP P71020
V	265	SER	-	expression tag	UNP P71020
V	266	GLY	-	expression tag	UNP P71020
V	267	SER	-	expression tag	UNP P71020
V	268	ASP	-	expression tag	UNP P71020
V	269	TYR	-	expression tag	UNP P71020
V	270	LYS	-	expression tag	UNP P71020
V	271	ASP	-	expression tag	UNP P71020
V	272	ASP	-	expression tag	UNP P71020
V	273	ASP	-	expression tag	UNP P71020
V	274	ASP	-	expression tag	UNP P71020
V	275	LYS	-	expression tag	UNP P71020

- Molecule 29 is a RNA chain called P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	69	Total	C	N	O	P	0	0
			1477	657	268	483	69		

- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	0	53	Total	C	N	O	S	0	0
			418	258	84	69	7		

- Molecule 31 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	1	49	Total	C	N	O	S	0	0
			411	250	82	75	4		

- Molecule 32 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	2	44	Total	C	N	O	S	0	0
			368	222	89	55	2		

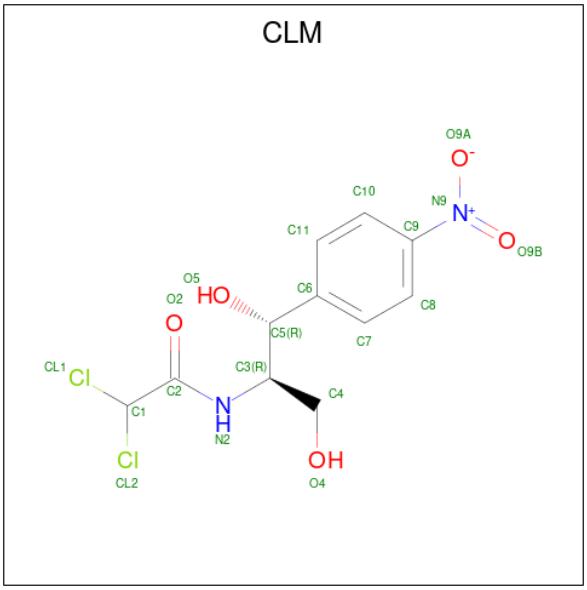
- Molecule 33 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
33	4	1	Total	Zn	0
			1	1	
33	6	1	Total	Zn	0
			1	1	
33	0	1	Total	Zn	0
			1	1	
33	1	1	Total	Zn	0
			1	1	

- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
34	A	45	Total	K	0
			45	45	
34	C	2	Total	K	0
			2	2	

- Molecule 35 is CHLORAMPHENICOL (three-letter code: CLM) (formula: $C_{11}H_{12}Cl_2N_2O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
35	A	1	Total	C	Cl	N	O	0
			20	11	2	2	5	

- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
36	A	154	Total	Mg	0
			154	154	
36	C	1	Total	Mg	0
			1	1	
36	D	1	Total	Mg	0
			1	1	
36	N	1	Total	Mg	0
			1	1	
36	a	1	Total	Mg	0
			1	1	

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		AltConf
37	3	15	Total	O	0
			15	15	
37	4	3	Total	O	0
			3	3	
37	A	2422	Total	O	0
			2422	2422	
37	B	10	Total	O	0
			10	10	
37	C	55	Total	O	0
			55	55	
37	D	28	Total	O	0
			28	28	
37	E	28	Total	O	0
			28	28	
37	J	13	Total	O	0
			13	13	
37	K	15	Total	O	0
			15	15	
37	L	25	Total	O	0
			25	25	
37	M	12	Total	O	0
			12	12	
37	N	20	Total	O	0
			20	20	

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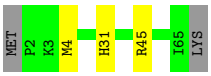
Mol	Chain	Residues	Atoms	AltConf
37	P	15	Total O 15 15	0
37	Q	24	Total O 24 24	0
37	R	16	Total O 16 16	0
37	S	13	Total O 13 13	0
37	T	8	Total O 8 8	0
37	U	3	Total O 3 3	0
37	W	7	Total O 7 7	0
37	X	6	Total O 6 6	0
37	Z	4	Total O 4 4	0
37	a	2	Total O 2 2	0
37	0	14	Total O 14 14	0
37	2	13	Total O 13 13	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.

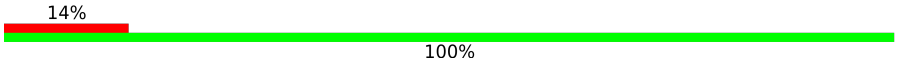
• Molecule 1: 50S ribosomal protein L35

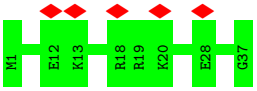
Chain 3:



• Molecule 2: 50S ribosomal protein L36

Chain 4:



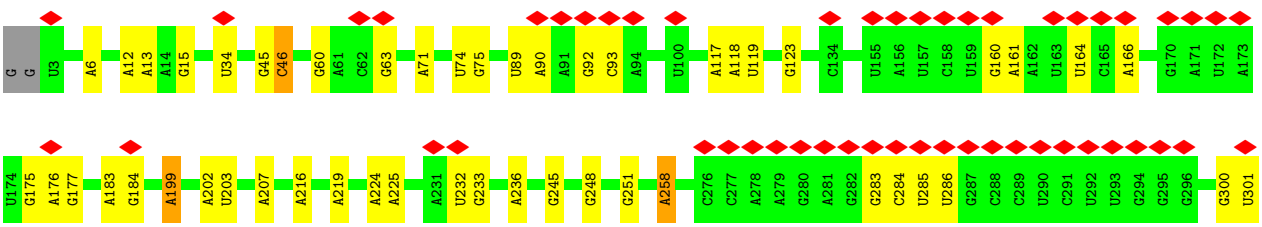


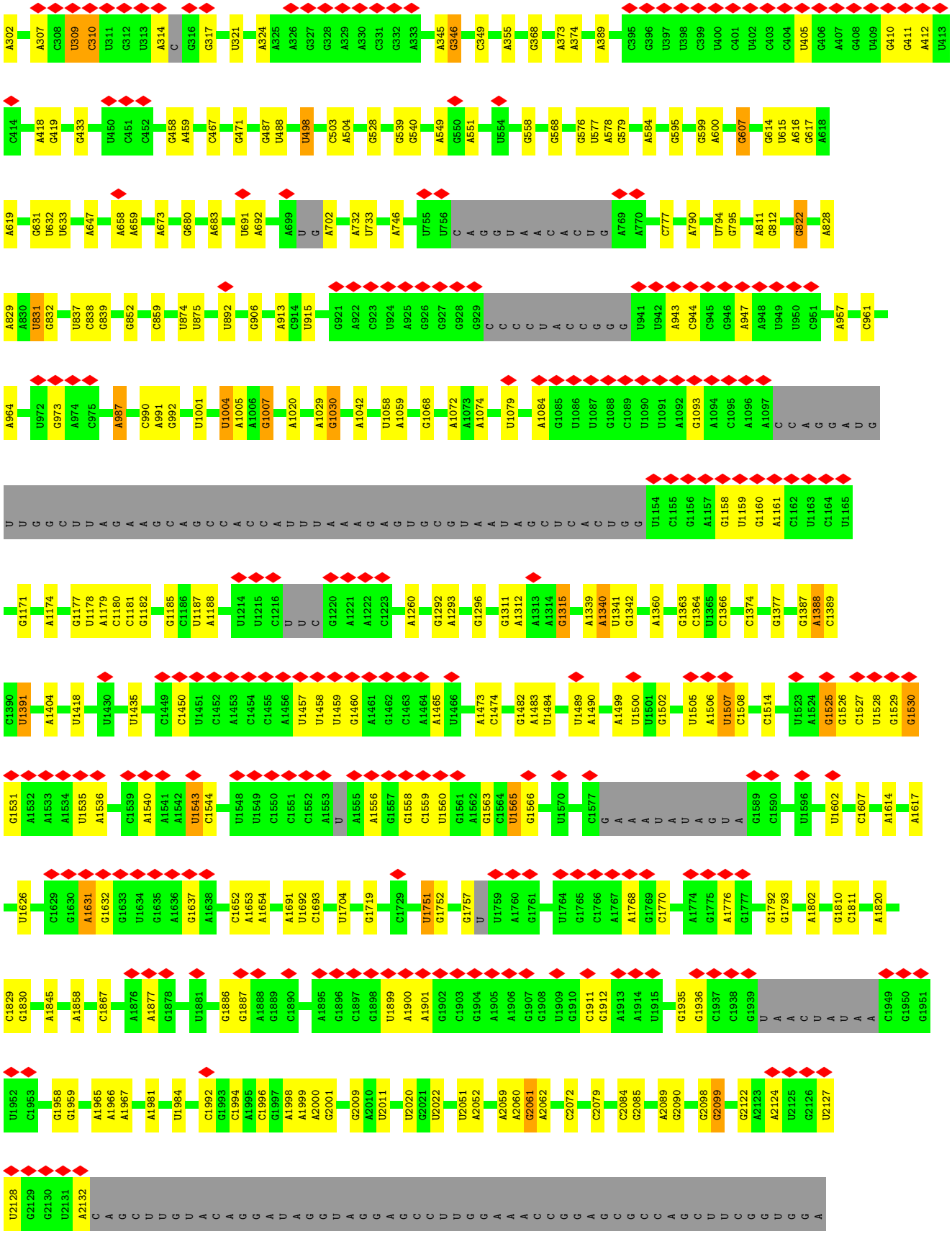
• Molecule 3: 50S ribosomal protein L31

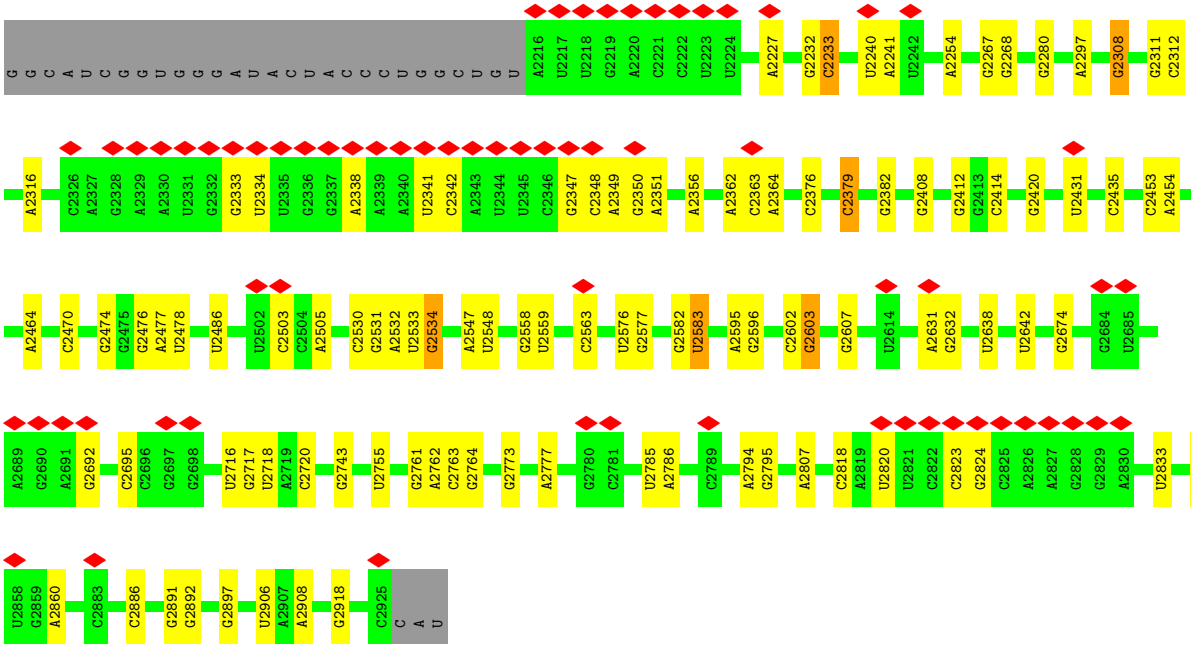
Chain 6:

• Molecule 4: 23S rRNA

Chain A:

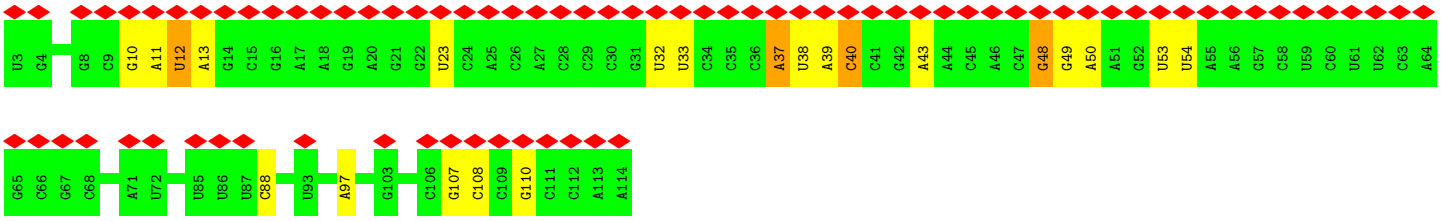






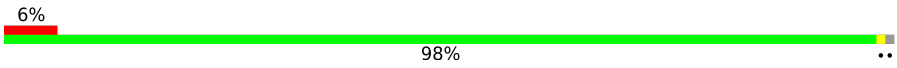
• Molecule 5: 5S rRNA

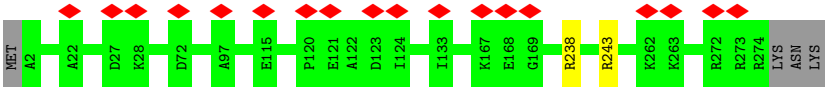
Chain B:



• Molecule 6: 50S ribosomal protein L2

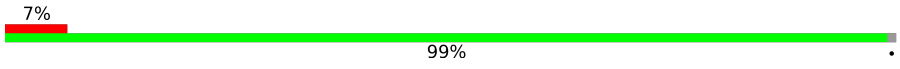
Chain C:

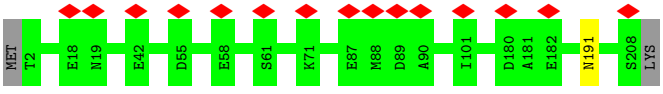




• Molecule 7: 50S ribosomal protein L3

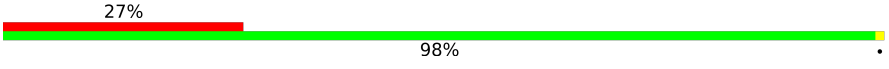
Chain D:

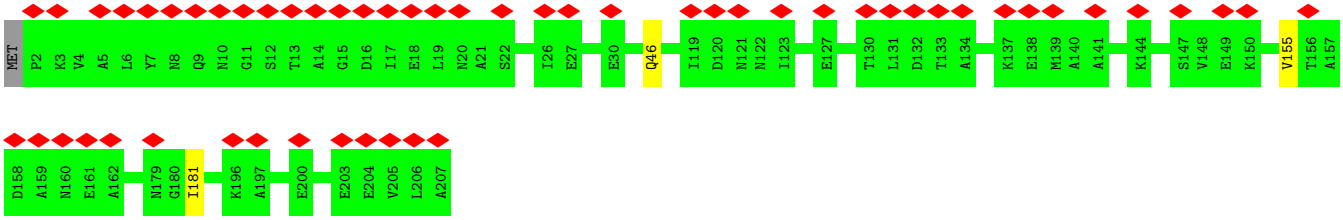




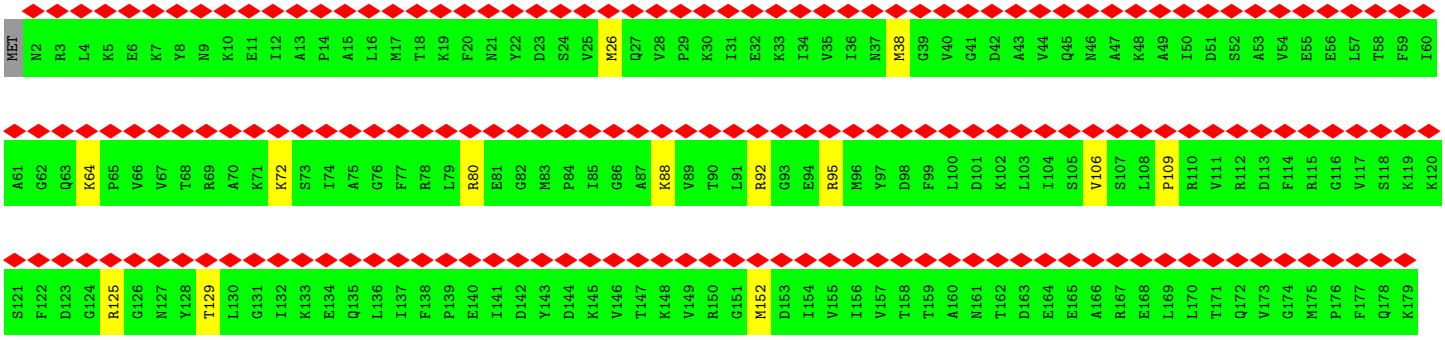
• Molecule 8: 50S ribosomal protein L4

Chain E:

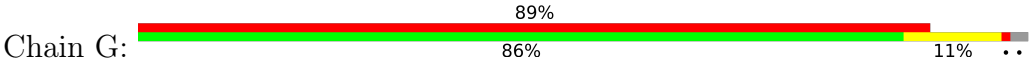


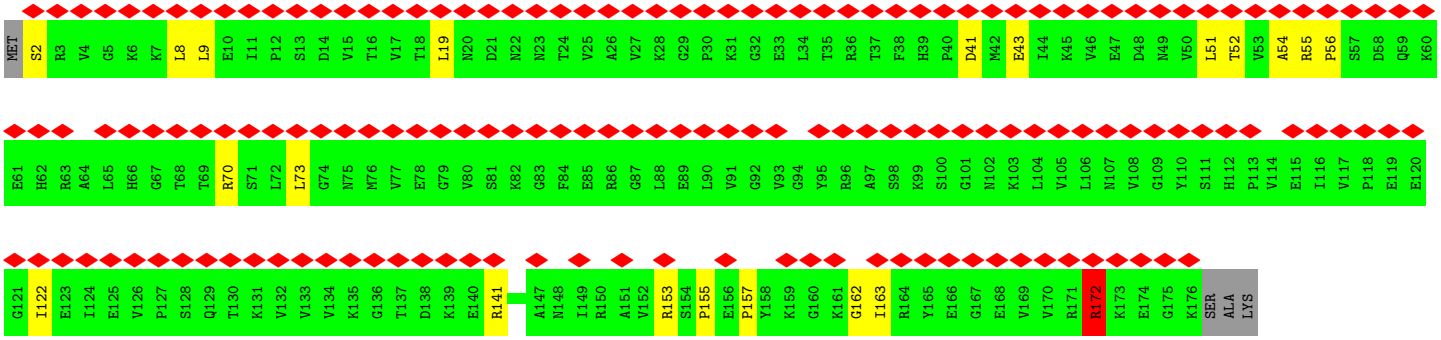


• Molecule 9: 50S ribosomal protein L5

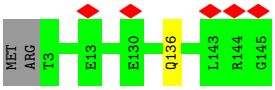


• Molecule 10: Large ribosomal subunit protein uL6

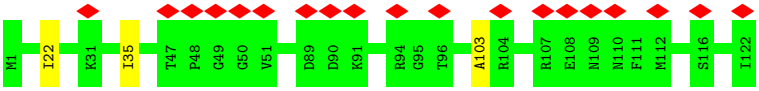




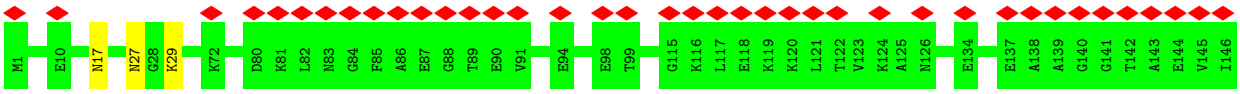
• Molecule 11: 50S ribosomal protein L13



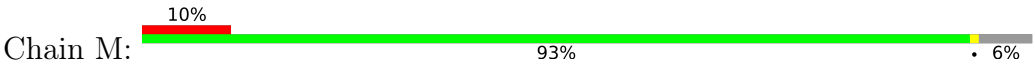
• Molecule 12: 50S ribosomal protein L14

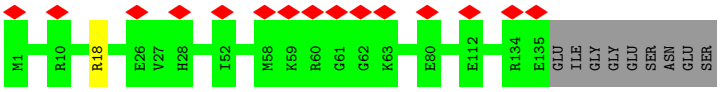


• Molecule 13: 50S ribosomal protein L15

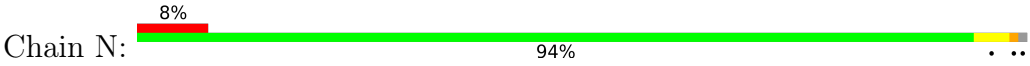


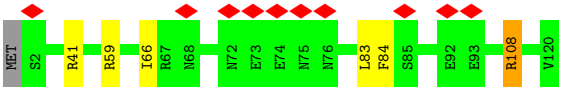
• Molecule 14: 50S ribosomal protein L16



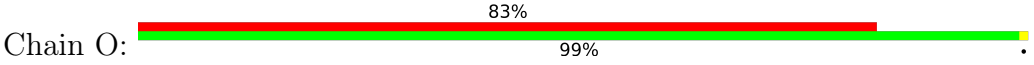


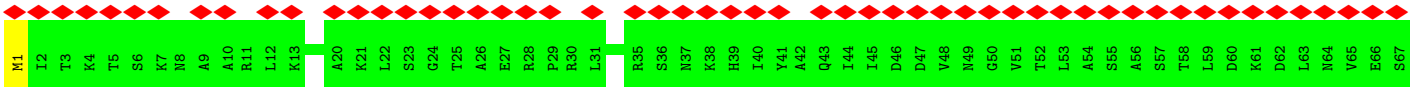
• Molecule 15: 50S ribosomal protein L17

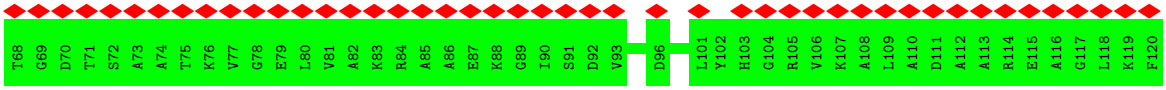




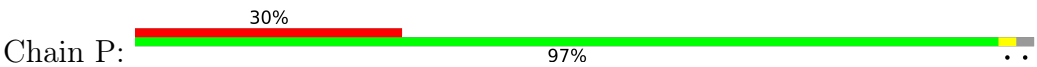
• Molecule 16: 50S ribosomal protein L18

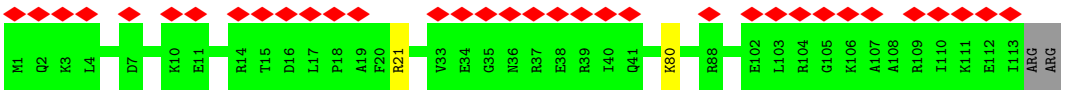




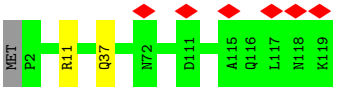


• Molecule 17: 50S ribosomal protein L19



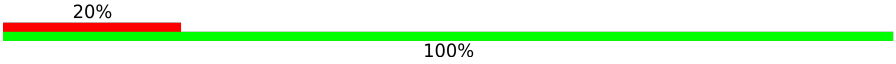


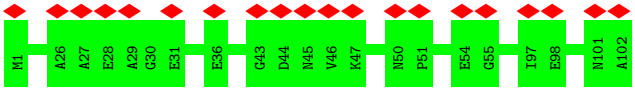
• Molecule 18: Large ribosomal subunit protein bL20



• Molecule 19: 50S ribosomal protein L21

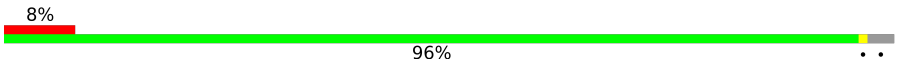
Chain R:

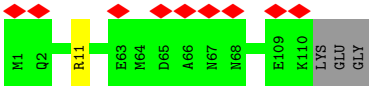




• Molecule 20: 50S ribosomal protein L22

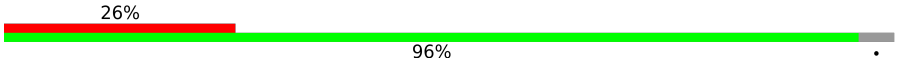
Chain S:

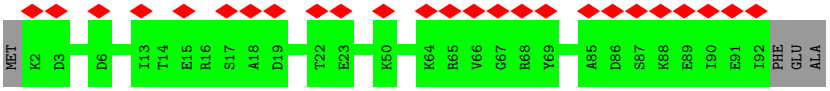




• Molecule 21: Large ribosomal subunit protein uL23

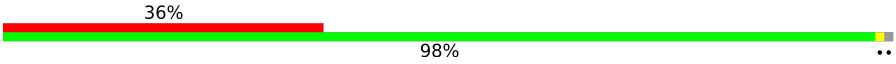
Chain T:

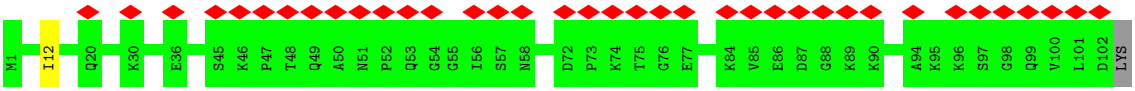




• Molecule 22: 50S ribosomal protein L24

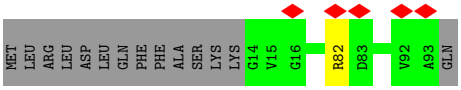
Chain U:





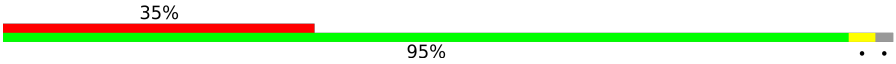
• Molecule 23: Large ribosomal subunit protein bL27

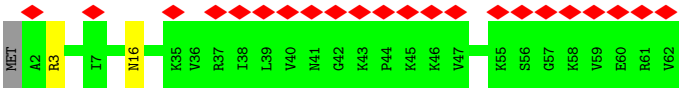
Chain W:



• Molecule 24: 50S ribosomal protein L28

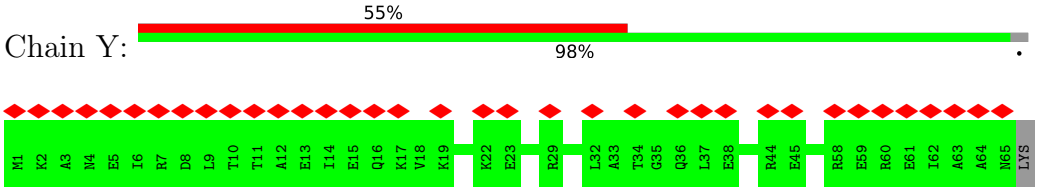
Chain X:





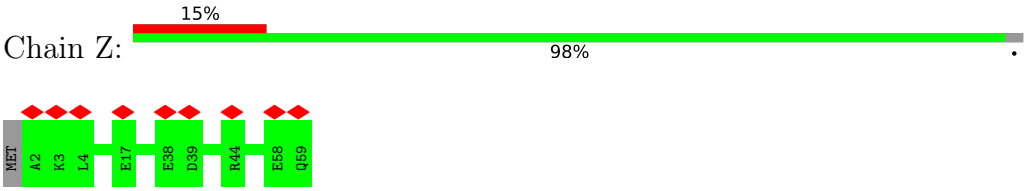
• Molecule 25: 50S ribosomal protein L29

Chain Y:



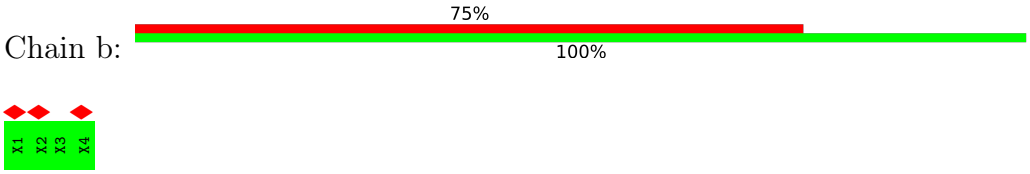
• Molecule 26: Large ribosomal subunit protein uL30

Chain Z:



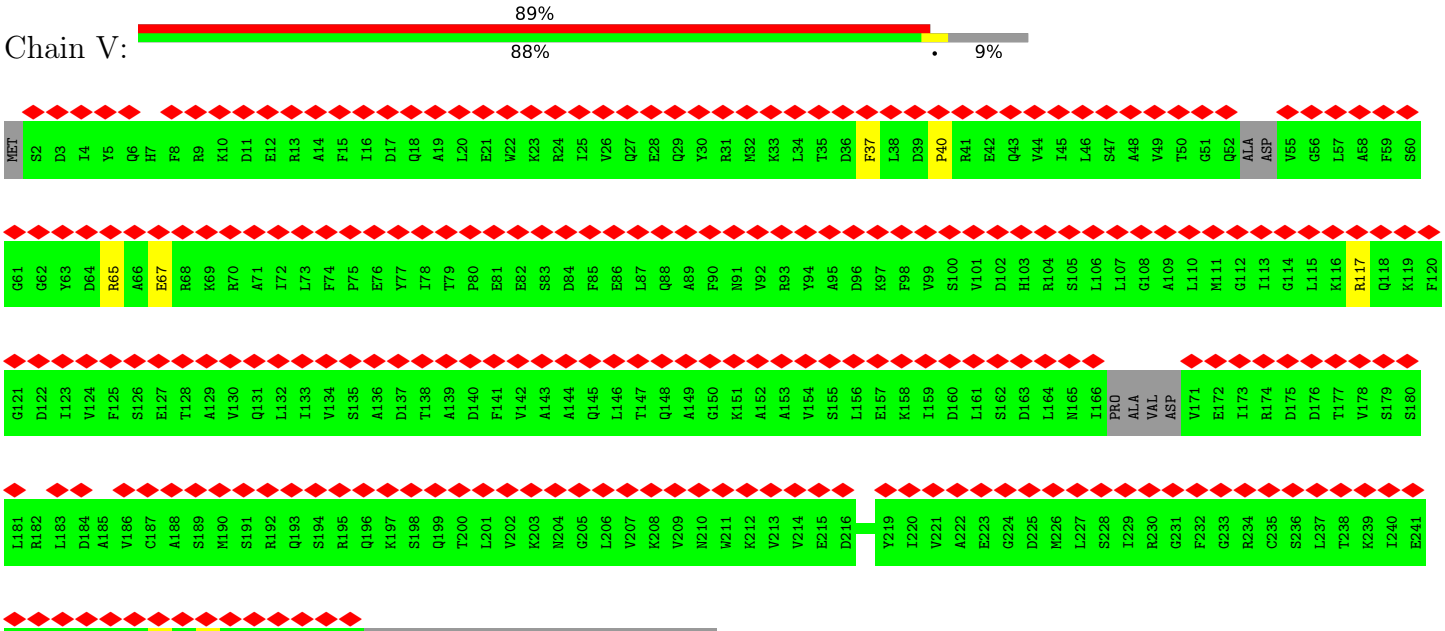
• Molecule 27: Nascent chain

Chain b:



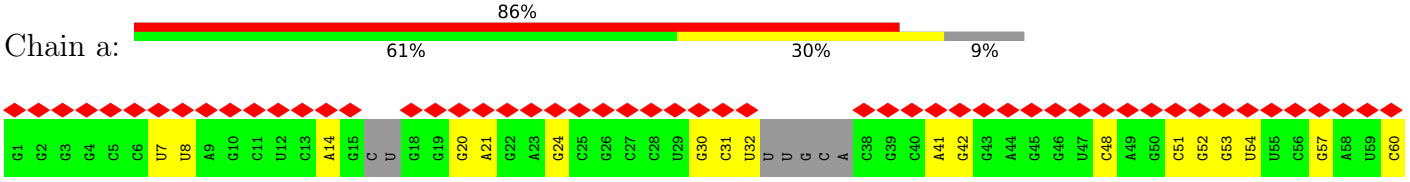
• Molecule 28: Putative RNA-binding protein YlmH

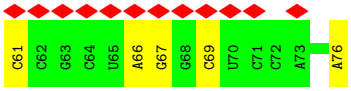
Chain V:



• Molecule 29: P-tRNA

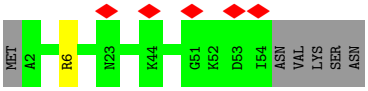
Chain a:





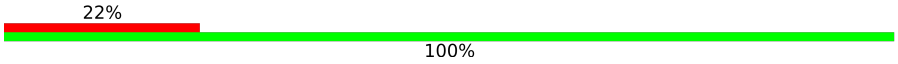
• Molecule 30: 50S ribosomal protein L32

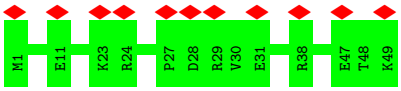
Chain 0:



• Molecule 31: 50S ribosomal protein L33 1

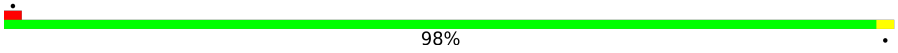
Chain 1:

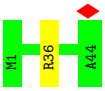




• Molecule 32: 50S ribosomal protein L34

Chain 2:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	66113	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	900	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.352	Depositor
Minimum map value	-0.119	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0445	Depositor
Map size (Å)	307.2, 307.2, 307.2	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8, 0.8, 0.8	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: G7M, K, OMG, MG, 5MU, ZN, CLM, PSU, H2U, 2MA, 2MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	3	0.40	0/519	0.78	1/680 (0.1%)
2	4	0.34	0/300	0.77	0/393
3	6	0.37	0/363	0.67	1/485 (0.2%)
4	A	0.48	0/65469	1.12	58/102117 (0.1%)
5	B	0.55	0/2675	1.13	3/4170 (0.1%)
6	C	0.34	0/2131	0.73	1/2859 (0.0%)
7	D	0.33	0/1597	0.72	0/2140
8	E	0.32	0/1586	0.69	0/2139
9	F	0.35	0/1424	0.69	1/1910 (0.1%)
10	G	0.33	0/1360	0.65	0/1832
11	J	0.33	0/1154	0.69	0/1552
12	K	0.33	0/928	0.73	0/1245
13	L	0.35	0/1094	0.74	0/1457
14	M	0.34	0/1099	0.71	0/1468
15	N	0.31	0/961	0.74	1/1284 (0.1%)
16	O	0.33	0/922	0.70	0/1236
17	P	0.32	0/935	0.79	0/1251
18	Q	0.33	0/962	0.77	1/1277 (0.1%)
19	R	0.32	0/806	0.67	0/1080
20	S	0.33	0/859	0.76	0/1156
21	T	0.33	0/739	0.74	0/985
22	U	0.34	0/780	0.69	0/1043
23	W	0.37	0/619	0.79	0/824
24	X	0.33	0/472	0.71	0/627
25	Y	0.30	0/531	0.71	0/707
26	Z	0.32	0/458	0.72	0/613
28	V	0.35	0/2016	0.71	0/2709
29	a	0.62	0/1648	1.19	2/2564 (0.1%)
30	0	0.35	0/425	0.80	0/563
31	1	0.34	0/416	0.75	0/551
32	2	0.36	0/371	0.81	0/483
All	All	0.45	0/95619	1.04	69/143400 (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
6	C	0	1
9	F	0	3
10	G	0	1
14	M	0	1
17	P	0	1
24	X	0	1
28	V	0	1
30	0	0	1
32	2	0	1
All	All	0	11

There are no bond length outliers.

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	558	G	O4'-C1'-N9	8.72	115.18	108.20
4	A	2583	U	O5'-P-OP1	-8.25	98.27	105.70
4	A	46	C	O5'-P-OP2	-8.07	98.44	105.70
4	A	987	A	O5'-P-OP1	-8.03	98.47	105.70
4	A	2061	G	O5'-P-OP1	-7.95	98.55	105.70

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	C	238	ARG	Sidechain
9	F	80	ARG	Sidechain
9	F	92	ARG	Sidechain
9	F	95	ARG	Sidechain
10	G	172	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	3	512	0	564	1	0
2	4	297	0	339	0	0
3	6	356	0	346	3	0
4	A	58713	0	29543	27	0
5	B	2392	0	1213	2	0
6	C	2094	0	2181	0	0
7	D	1575	0	1642	0	0
8	E	1567	0	1652	2	0
9	F	1405	0	1467	6	0
10	G	1342	0	1388	10	0
11	J	1131	0	1169	1	0
12	K	921	0	977	2	0
13	L	1082	0	1132	1	0
14	M	1076	0	1145	0	0
15	N	954	0	983	5	0
16	O	913	0	947	1	0
17	P	922	0	994	0	0
18	Q	950	0	1018	3	0
19	R	795	0	838	0	0
20	S	850	0	911	0	0
21	T	733	0	781	0	0
22	U	770	0	824	1	0
23	W	611	0	618	1	0
24	X	468	0	514	0	0
25	Y	530	0	568	0	0
26	Z	456	0	491	0	0
27	b	20	0	7	0	0
28	V	1988	0	2006	0	0
29	a	1477	0	750	0	0
30	0	418	0	435	0	0
31	1	411	0	423	0	0
32	2	368	0	410	0	0
33	0	1	0	0	0	0
33	1	1	0	0	0	0
33	4	1	0	0	0	0
33	6	1	0	0	0	0
34	A	45	0	0	0	0
34	C	2	0	0	0	0
35	A	20	0	11	1	0
36	A	154	0	0	0	0
36	C	1	0	0	0	0
36	D	1	0	0	0	0
36	N	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	a	1	0	0	0	0
37	0	14	0	0	0	0
37	2	13	0	0	0	0
37	3	15	0	0	0	0
37	4	3	0	0	0	0
37	A	2422	0	0	0	0
37	B	10	0	0	0	0
37	C	55	0	0	0	0
37	D	28	0	0	0	0
37	E	28	0	0	0	0
37	J	13	0	0	0	0
37	K	15	0	0	0	0
37	L	25	0	0	0	0
37	M	12	0	0	0	0
37	N	20	0	0	0	0
37	P	15	0	0	0	0
37	Q	24	0	0	0	0
37	R	16	0	0	0	0
37	S	13	0	0	0	0
37	T	8	0	0	0	0
37	U	3	0	0	0	0
37	W	7	0	0	0	0
37	X	6	0	0	0	0
37	Z	4	0	0	0	0
37	a	2	0	0	0	0
All	All	91097	0	58287	50	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

The worst 5 of 50 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:A:607:G:H21	18:Q:37:GLN:HE22	1.33	0.77
10:G:122:ILE:HD11	10:G:141:ARG:HB3	1.68	0.76
4:A:1292:G:H1	18:Q:37:GLN:HE21	1.32	0.75
4:A:2534:G:O4'	35:A:3032:CLM:CL1	2.48	0.68
4:A:790:A:O2'	4:A:1704:U:OP1	2.11	0.67

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	3	62/66 (94%)	62 (100%)	0	0	100 100
2	4	35/37 (95%)	35 (100%)	0	0	100 100
3	6	44/66 (67%)	44 (100%)	0	0	100 100
6	C	271/277 (98%)	263 (97%)	8 (3%)	0	100 100
7	D	205/209 (98%)	199 (97%)	6 (3%)	0	100 100
8	E	204/207 (99%)	197 (97%)	7 (3%)	0	100 100
9	F	176/179 (98%)	173 (98%)	3 (2%)	0	100 100
10	G	173/179 (97%)	167 (96%)	6 (4%)	0	100 100
11	J	141/145 (97%)	139 (99%)	2 (1%)	0	100 100
12	K	120/122 (98%)	113 (94%)	7 (6%)	0	100 100
13	L	144/146 (99%)	138 (96%)	5 (4%)	1 (1%)	22 11
14	M	133/144 (92%)	130 (98%)	3 (2%)	0	100 100
15	N	117/120 (98%)	115 (98%)	2 (2%)	0	100 100
16	O	118/120 (98%)	112 (95%)	6 (5%)	0	100 100
17	P	111/115 (96%)	109 (98%)	2 (2%)	0	100 100
18	Q	116/119 (98%)	115 (99%)	1 (1%)	0	100 100
19	R	100/102 (98%)	97 (97%)	3 (3%)	0	100 100
20	S	108/113 (96%)	108 (100%)	0	0	100 100
21	T	89/95 (94%)	87 (98%)	2 (2%)	0	100 100
22	U	100/103 (97%)	94 (94%)	6 (6%)	0	100 100
23	W	78/94 (83%)	75 (96%)	3 (4%)	0	100 100
24	X	59/62 (95%)	55 (93%)	3 (5%)	1 (2%)	9 2
25	Y	63/66 (96%)	62 (98%)	1 (2%)	0	100 100
26	Z	56/59 (95%)	55 (98%)	1 (2%)	0	100 100
28	V	243/275 (88%)	220 (90%)	19 (8%)	4 (2%)	9 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
30	0	51/59 (86%)	49 (96%)	2 (4%)	0	100 100
31	1	47/49 (96%)	45 (96%)	2 (4%)	0	100 100
32	2	42/44 (96%)	41 (98%)	1 (2%)	0	100 100
All	All	3206/3372 (95%)	3099 (97%)	101 (3%)	6 (0%)	50 38

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
24	X	3	ARG
28	V	65	ARG
28	V	37	PHE
13	L	29	LYS
28	V	67	GLU

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	3	54/56 (96%)	53 (98%)	1 (2%)	57 50
2	4	35/35 (100%)	35 (100%)	0	100 100
3	6	39/55 (71%)	38 (97%)	1 (3%)	46 36
6	C	221/225 (98%)	221 (100%)	0	100 100
7	D	168/170 (99%)	167 (99%)	1 (1%)	86 85
8	E	169/170 (99%)	169 (100%)	0	100 100
9	F	153/154 (99%)	151 (99%)	2 (1%)	69 65
10	G	148/151 (98%)	146 (99%)	2 (1%)	67 62
11	J	121/123 (98%)	121 (100%)	0	100 100
12	K	101/101 (100%)	101 (100%)	0	100 100
13	L	110/110 (100%)	110 (100%)	0	100 100
14	M	109/116 (94%)	109 (100%)	0	100 100
15	N	99/100 (99%)	99 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
16	O	93/93 (100%)	93 (100%)	0	100 100
17	P	98/100 (98%)	97 (99%)	1 (1%)	76 74
18	Q	97/98 (99%)	97 (100%)	0	100 100
19	R	84/84 (100%)	84 (100%)	0	100 100
20	S	91/93 (98%)	90 (99%)	1 (1%)	73 71
21	T	82/85 (96%)	82 (100%)	0	100 100
22	U	86/87 (99%)	86 (100%)	0	100 100
23	W	61/74 (82%)	61 (100%)	0	100 100
24	X	49/50 (98%)	49 (100%)	0	100 100
25	Y	56/57 (98%)	56 (100%)	0	100 100
26	Z	52/53 (98%)	52 (100%)	0	100 100
28	V	215/234 (92%)	213 (99%)	2 (1%)	78 77
30	0	47/53 (89%)	47 (100%)	0	100 100
31	1	47/47 (100%)	47 (100%)	0	100 100
32	2	39/39 (100%)	39 (100%)	0	100 100
All	All	2724/2813 (97%)	2713 (100%)	11 (0%)	91 90

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

Mol	Chain	Res	Type
17	P	80	LYS
20	S	11	ARG
28	V	250	ARG
28	V	40	PRO
9	F	88	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
28	V	52	GLN
24	X	23	ASN
13	L	27	ASN
22	U	20	GLN
12	K	3	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	a	66/76 (86%)	21 (31%)	0
4	A	2721/2928 (92%)	341 (12%)	53 (1%)
5	B	111/112 (99%)	18 (16%)	4 (3%)
All	All	2898/3116 (93%)	380 (13%)	57 (1%)

5 of 380 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	A	12	A
4	A	13	A
4	A	15	G
4	A	34	U
4	A	45	G

5 of 57 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	A	1527	C
5	B	48	G
4	A	1602	U
5	B	37	A
4	A	2631	A

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

12 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	$\#\|Z\| > 2$
4	PSU	A	1001	4	18,21,22	1.03	1 (5%)	22,30,33	0.65	0
4	OMG	A	2280	4,29,34	18,26,27	0.99	2 (11%)	19,38,41	0.81	0
4	5MU	A	1968	4	19,22,23	0.34	0	28,32,35	0.42	0
4	2MG	A	2474	4	18,26,27	1.02	1 (5%)	16,38,41	0.84	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	OMG	A	2582	4	18,26,27	0.98	2 (11%)	19,38,41	0.70	0
4	G7M	A	2603	4,36	20,26,27	1.11	2 (10%)	17,39,42	0.32	0
4	5MU	A	794	4	19,22,23	0.34	0	28,32,35	0.44	0
4	H2U	A	2478	4	18,21,22	0.59	0	21,30,33	0.71	1 (4%)
4	PSU	A	2486	4	18,21,22	1.00	1 (5%)	22,30,33	0.62	0
4	PSU	A	2533	4,34	18,21,22	0.92	1 (5%)	22,30,33	0.77	0
4	2MA	A	2532	4,36,34	17,25,26	0.96	2 (11%)	17,37,40	1.15	1 (5%)
4	5MU	A	620	4,36,34	19,22,23	0.30	0	28,32,35	0.52	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
4	PSU	A	1001	4	-	0/7/25/26	0/2/2/2
4	OMG	A	2280	4,29,34	-	0/5/27/28	0/3/3/3
4	5MU	A	1968	4	-	0/7/25/26	0/2/2/2
4	2MG	A	2474	4	-	0/5/27/28	0/3/3/3
4	OMG	A	2582	4	-	1/5/27/28	0/3/3/3
4	G7M	A	2603	4,36	-	0/3/25/26	0/3/3/3
4	5MU	A	794	4	-	0/7/25/26	0/2/2/2
4	H2U	A	2478	4	-	0/7/38/39	0/2/2/2
4	PSU	A	2486	4	-	0/7/25/26	0/2/2/2
4	PSU	A	2533	4,34	-	0/7/25/26	0/2/2/2
4	2MA	A	2532	4,36,34	-	2/3/25/26	0/3/3/3
4	5MU	A	620	4,36,34	-	0/7/25/26	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2486	PSU	C6-C5	3.97	1.39	1.35
4	A	1001	PSU	C6-C5	3.97	1.39	1.35
4	A	2533	PSU	C6-C5	3.68	1.39	1.35
4	A	2603	G7M	C8-N9	3.50	1.39	1.33
4	A	2280	OMG	C5-C6	-2.62	1.42	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2532	2MA	CM2-C2-N1	3.62	124.28	116.23
4	A	2474	2MG	O6-C6-C5	2.03	128.34	124.37
4	A	2478	H2U	O2-C2-N1	-2.01	120.58	123.11

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2582	OMG	C3'-C2'-O2'-CM2
4	A	2532	2MA	O4'-C4'-C5'-O5'
4	A	2532	2MA	C4'-C5'-O5'-P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2603	G7M	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 210 ligands modelled in this entry, 209 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	$\#\|Z\| > 2$
35	CLM	A	3032	-	19,20,20	0.65	0	23,27,27	0.90	1 (4%)

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
35	CLM	A	3032	-	-	4/20/22/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	A	3032	CLM	C5-C3-N2	3.02	115.77	110.05

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	A	3032	CLM	O2-C2-N2-C3
35	A	3032	CLM	C1-C2-N2-C3
35	A	3032	CLM	CL1-C1-C2-O2
35	A	3032	CLM	CL1-C1-C2-N2

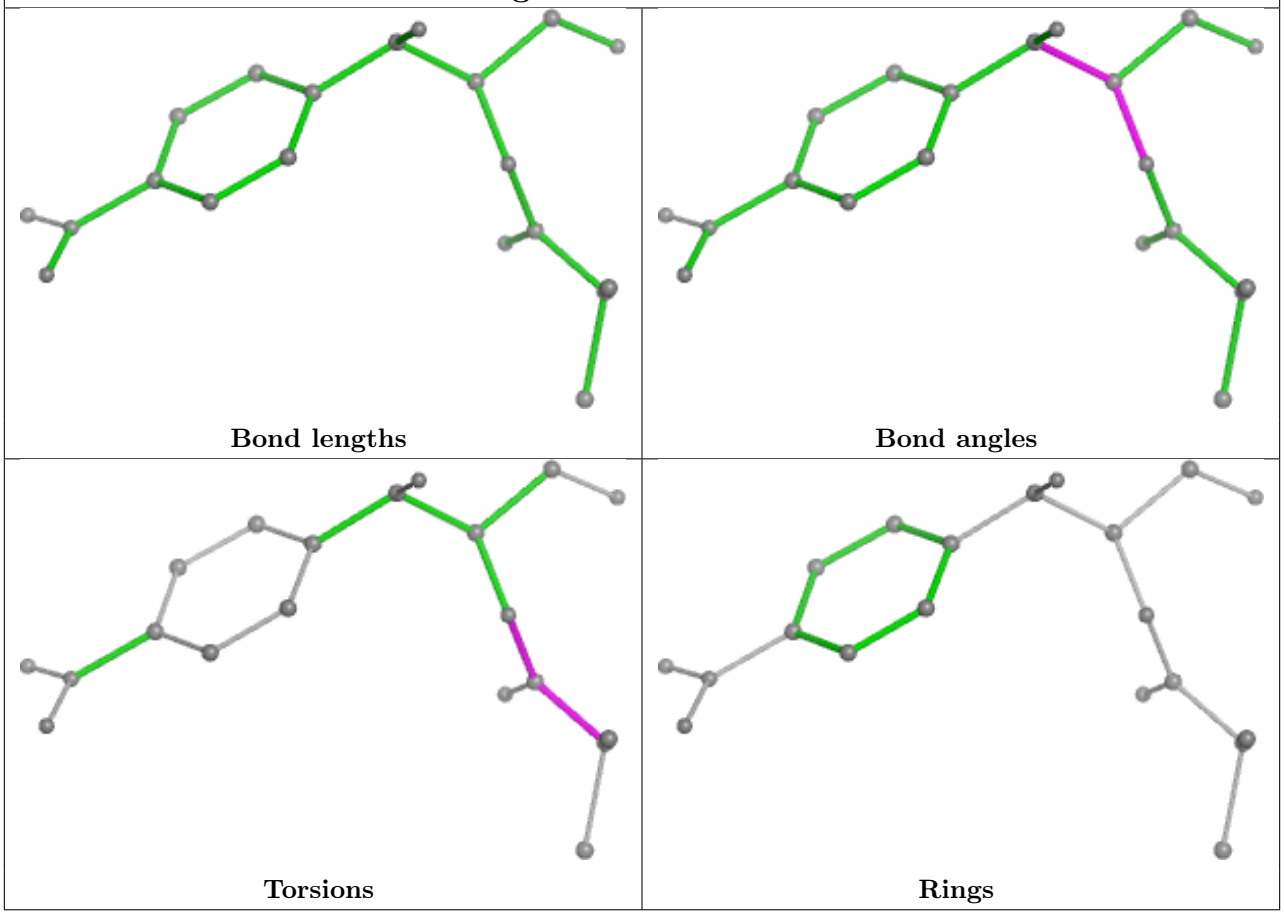
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	A	3032	CLM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand CLM A 3032



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.

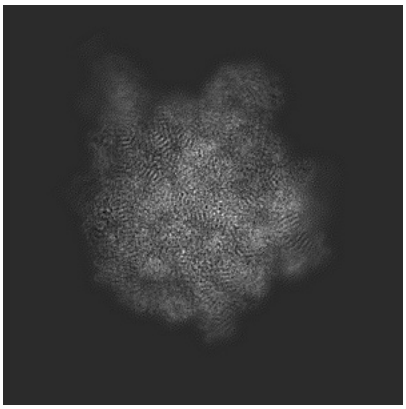
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19638. 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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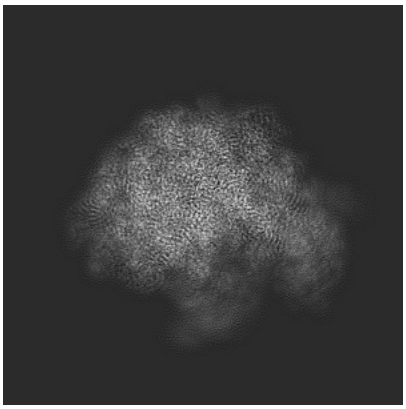
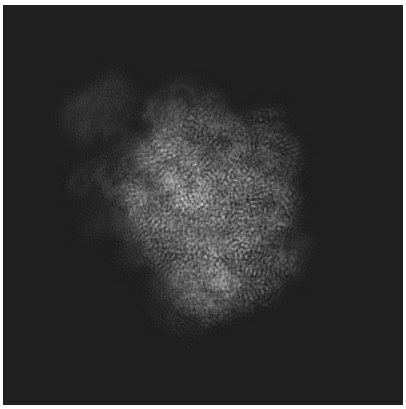
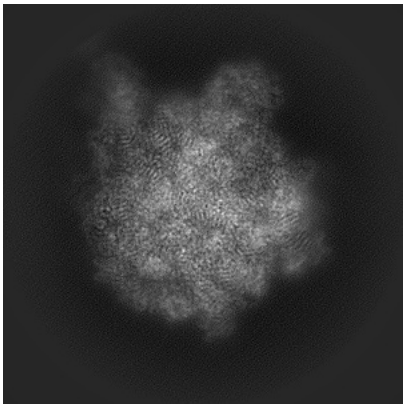


Y

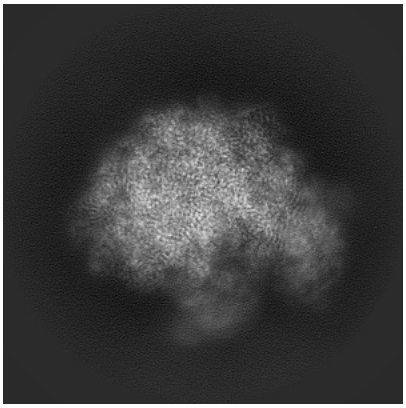


Z

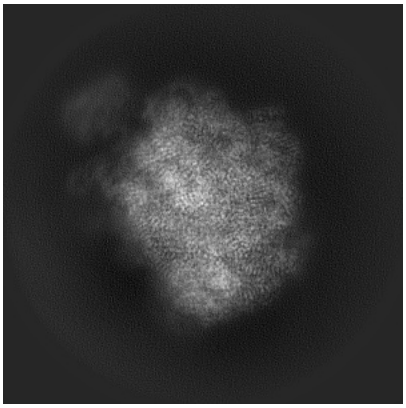
6.1.2 Raw map



X



Y

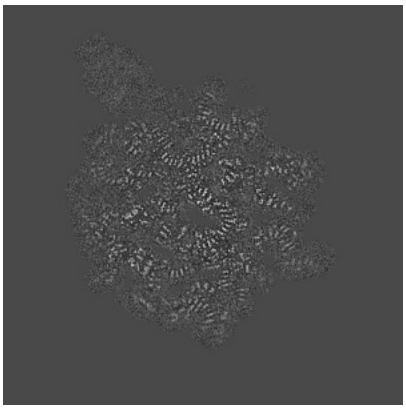


Z

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

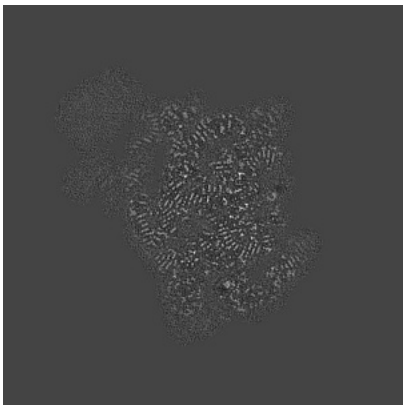
6.2 Central slices (i)

6.2.1 Primary map



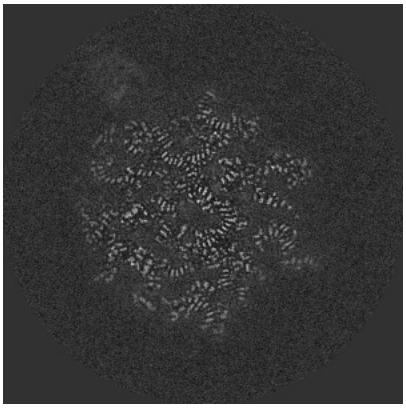
X Index: 192

Y Index: 192

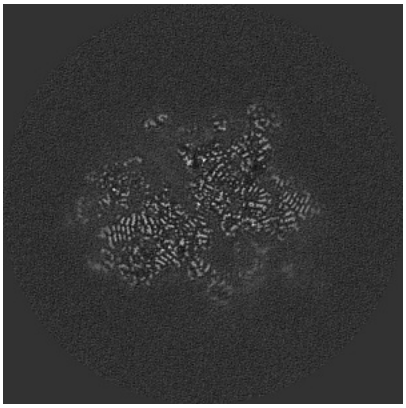


Z Index: 192

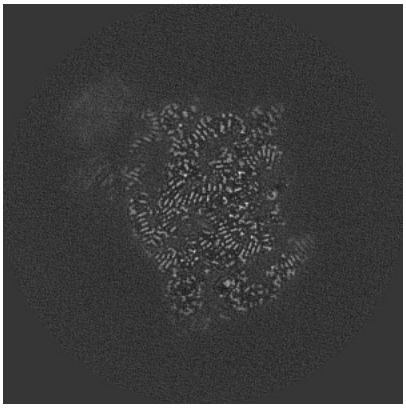
6.2.2 Raw map



X Index: 192



Y Index: 192

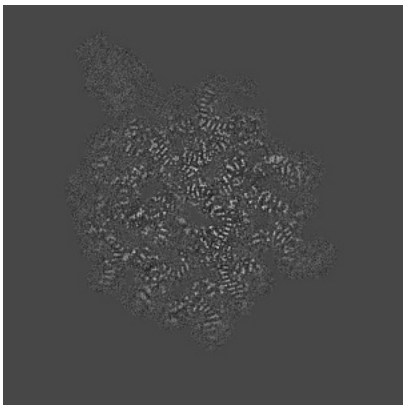


Z Index: 192

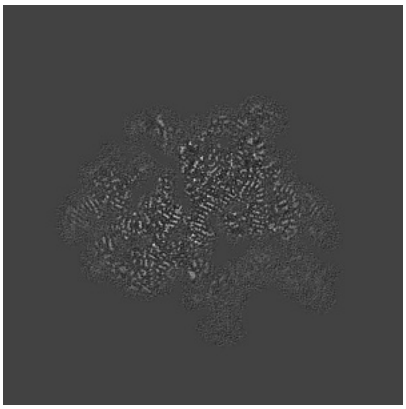
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

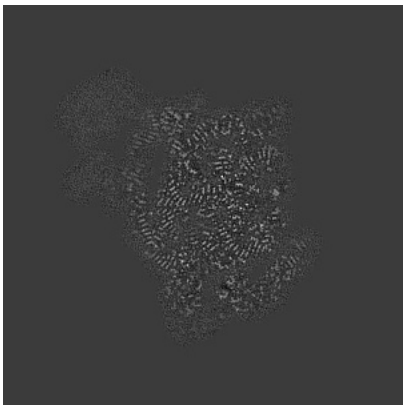
6.3.1 Primary map



X Index: 189

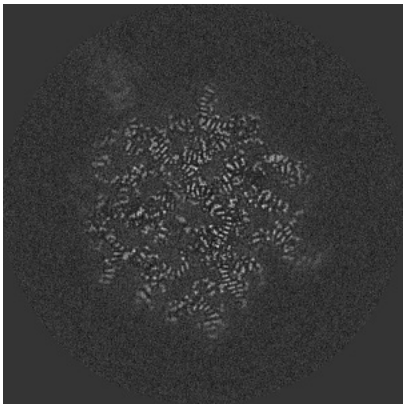


Y Index: 198

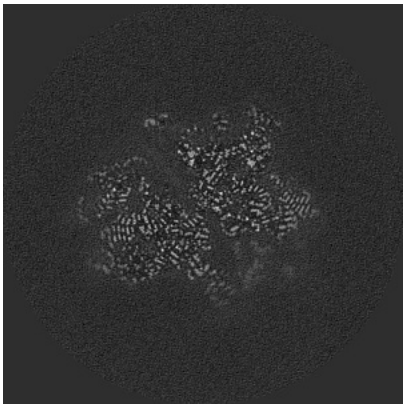


Z Index: 193

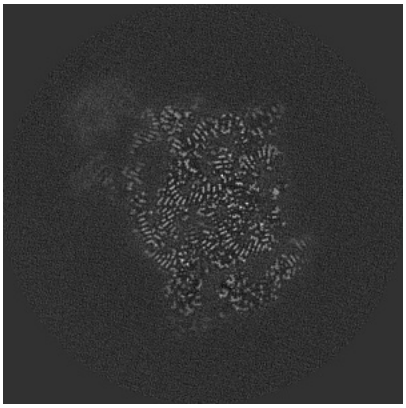
6.3.2 Raw map



X Index: 189



Y Index: 191

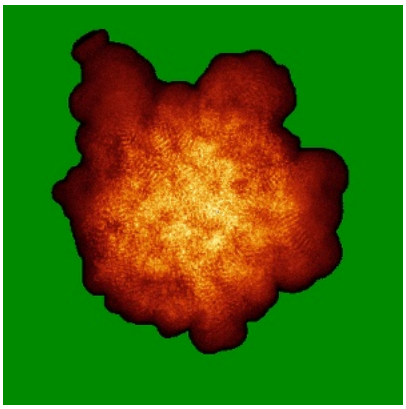


Z Index: 193

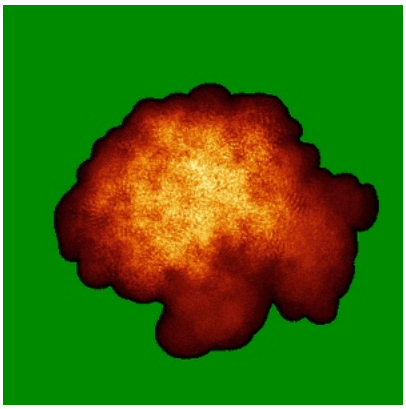
The images above show the largest variance slices of the map in three orthogonal directions.

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

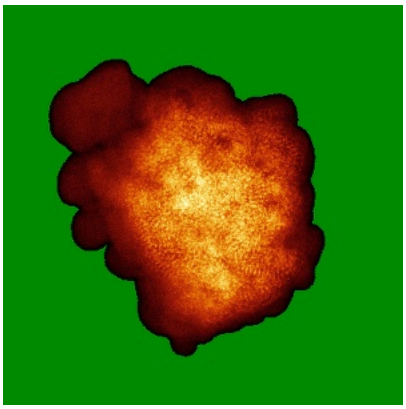
6.4.1 Primary map



X

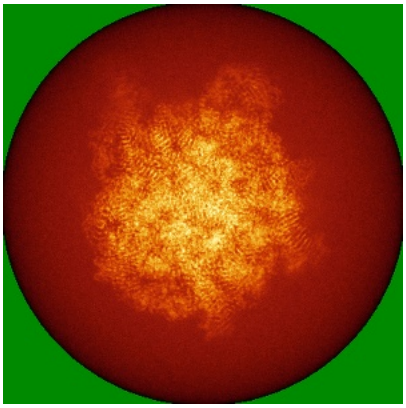


Y

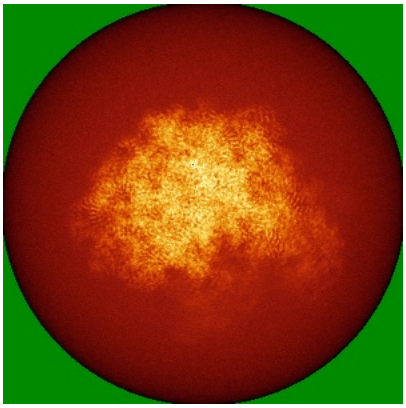


Z

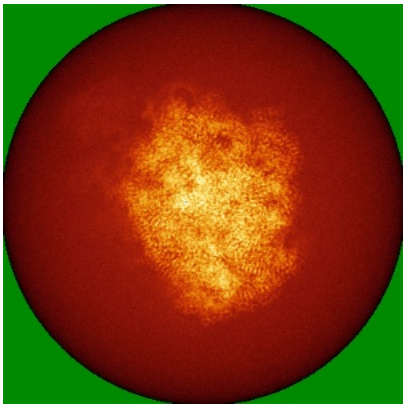
6.4.2 Raw map



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 0.0445. 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.

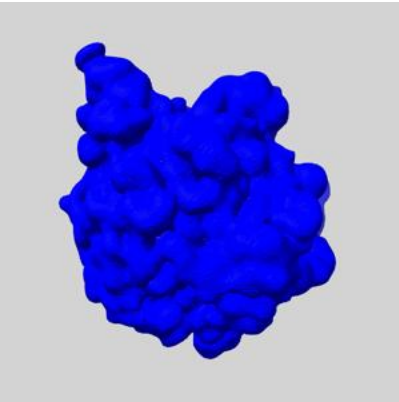
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

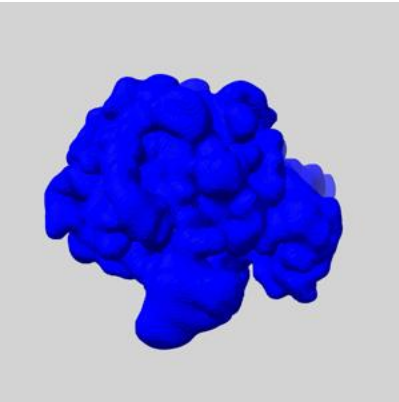
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

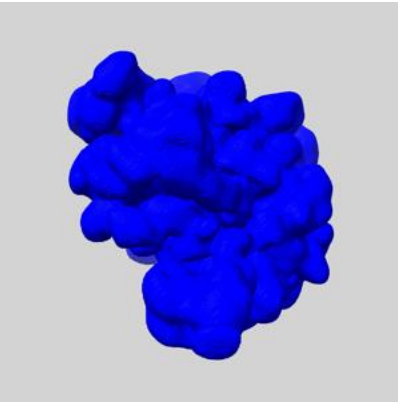
6.6.1 emd_19638_msk_1.map (i)



X



Y

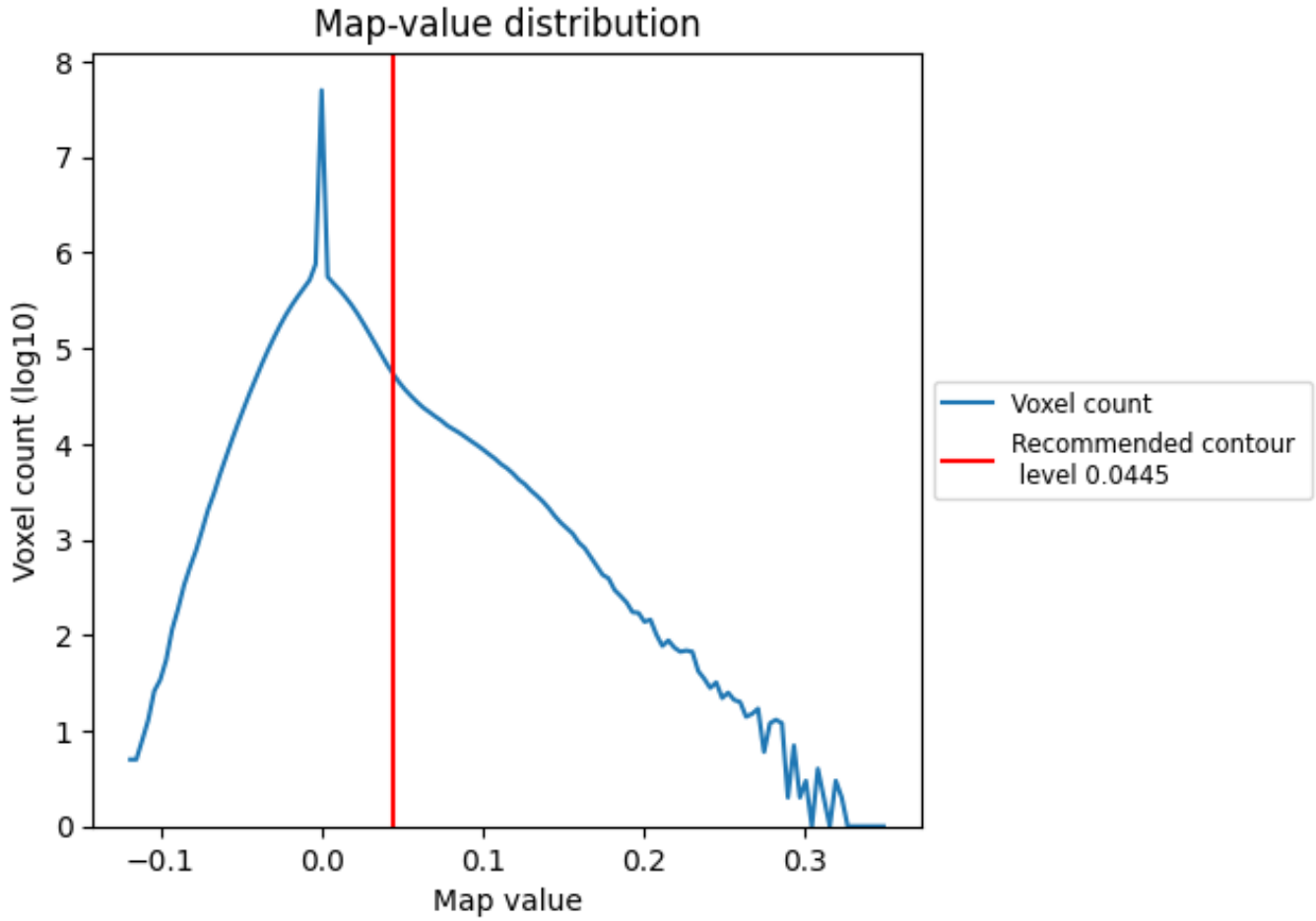


Z

7 Map analysis

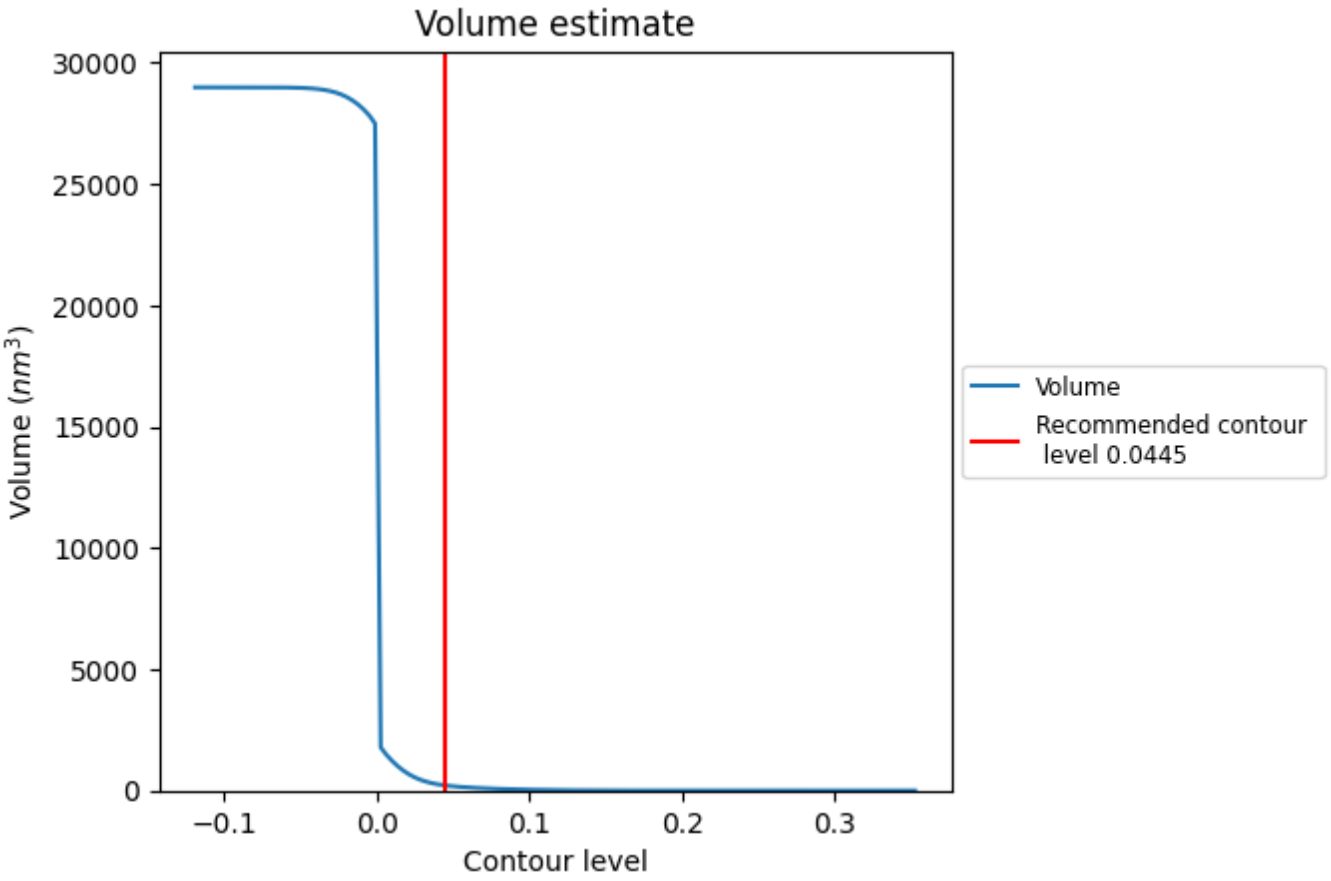
This section contains the results of statistical analysis of the map.

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.

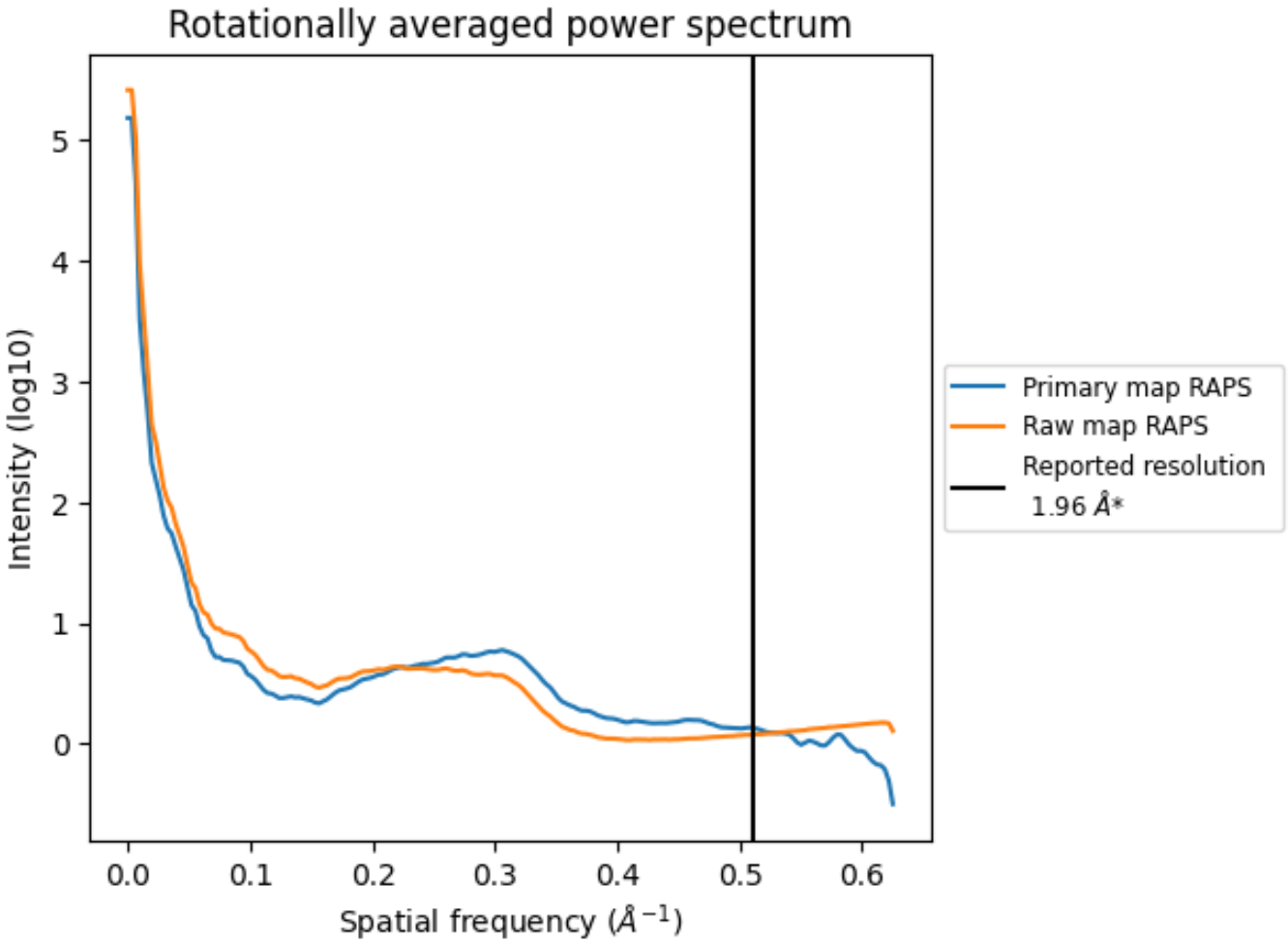
7.2 Volume estimate (i)



The volume at the recommended contour level is 215 nm^3; this corresponds to an approximate mass of 195 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)

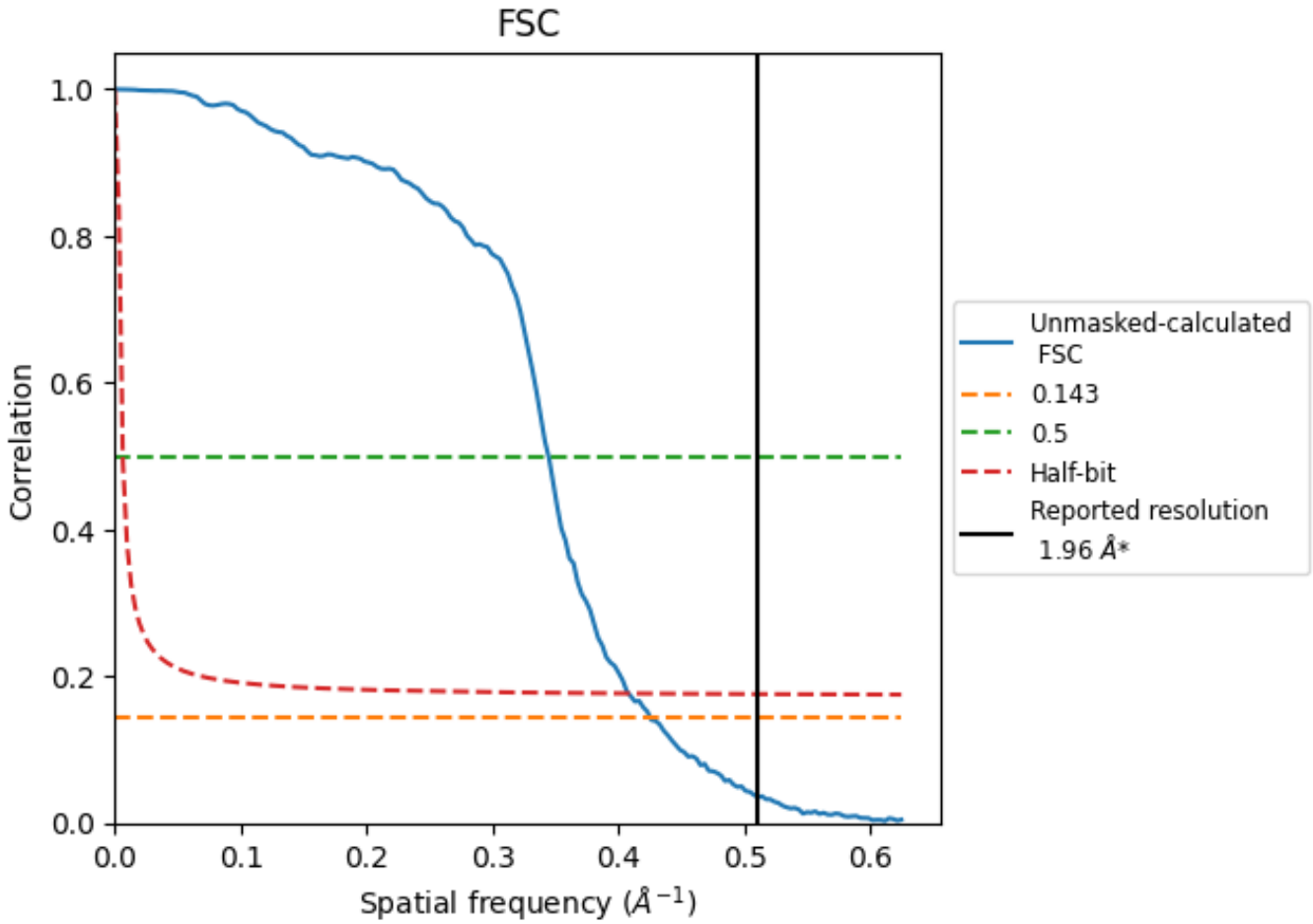


*Reported resolution corresponds to spatial frequency of 0.510 Å^{-1}

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 0.510 Å^{-1}

8.2 Resolution estimates (i)

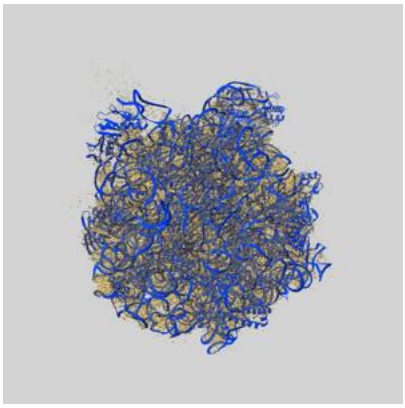
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.96	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.35	2.90	2.45

*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 2.35 differs from the reported value 1.96 by more than 10 %

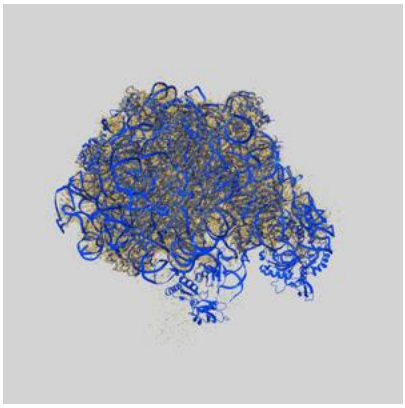
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19638 and PDB model 8S1P. Per-residue inclusion information can be found in section 3 on page 12.

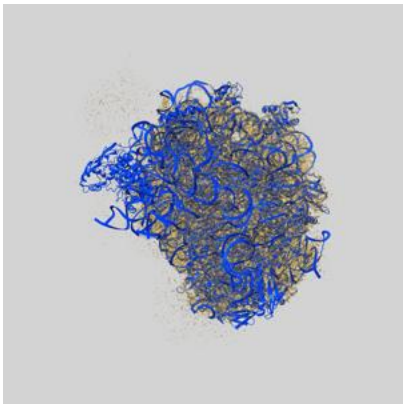
9.1 Map-model overlay



X



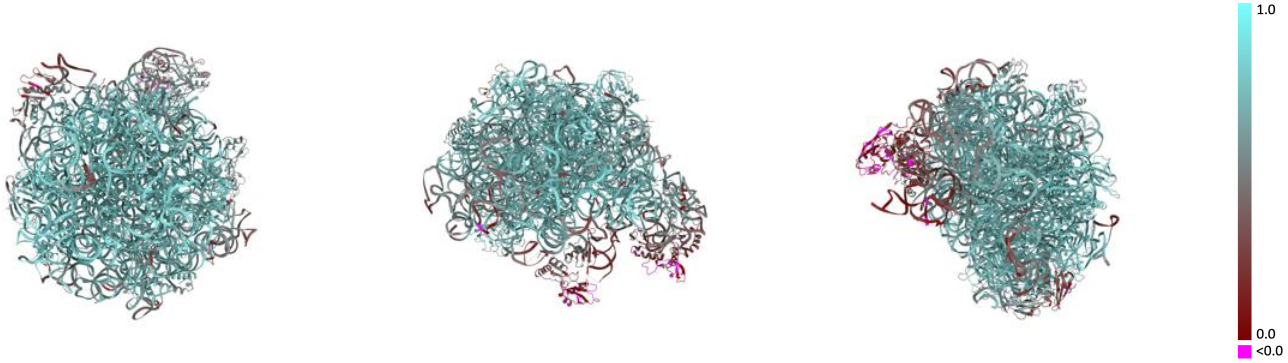
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0445 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

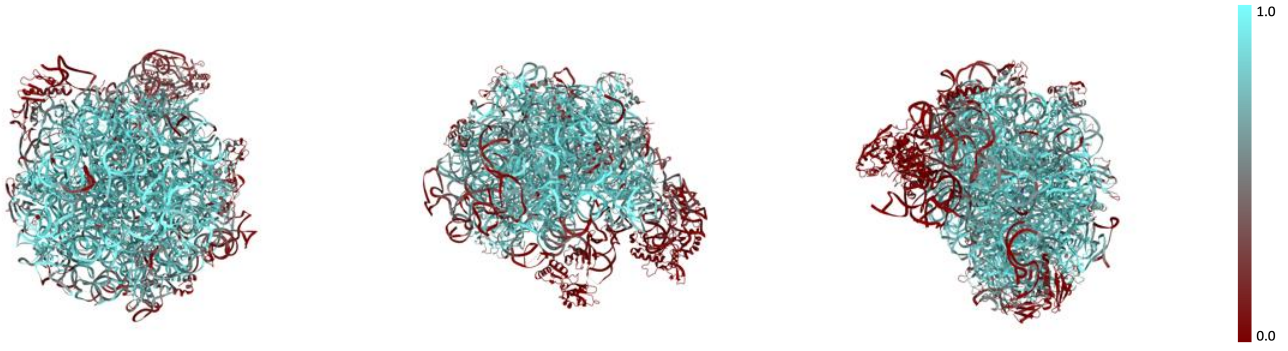
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

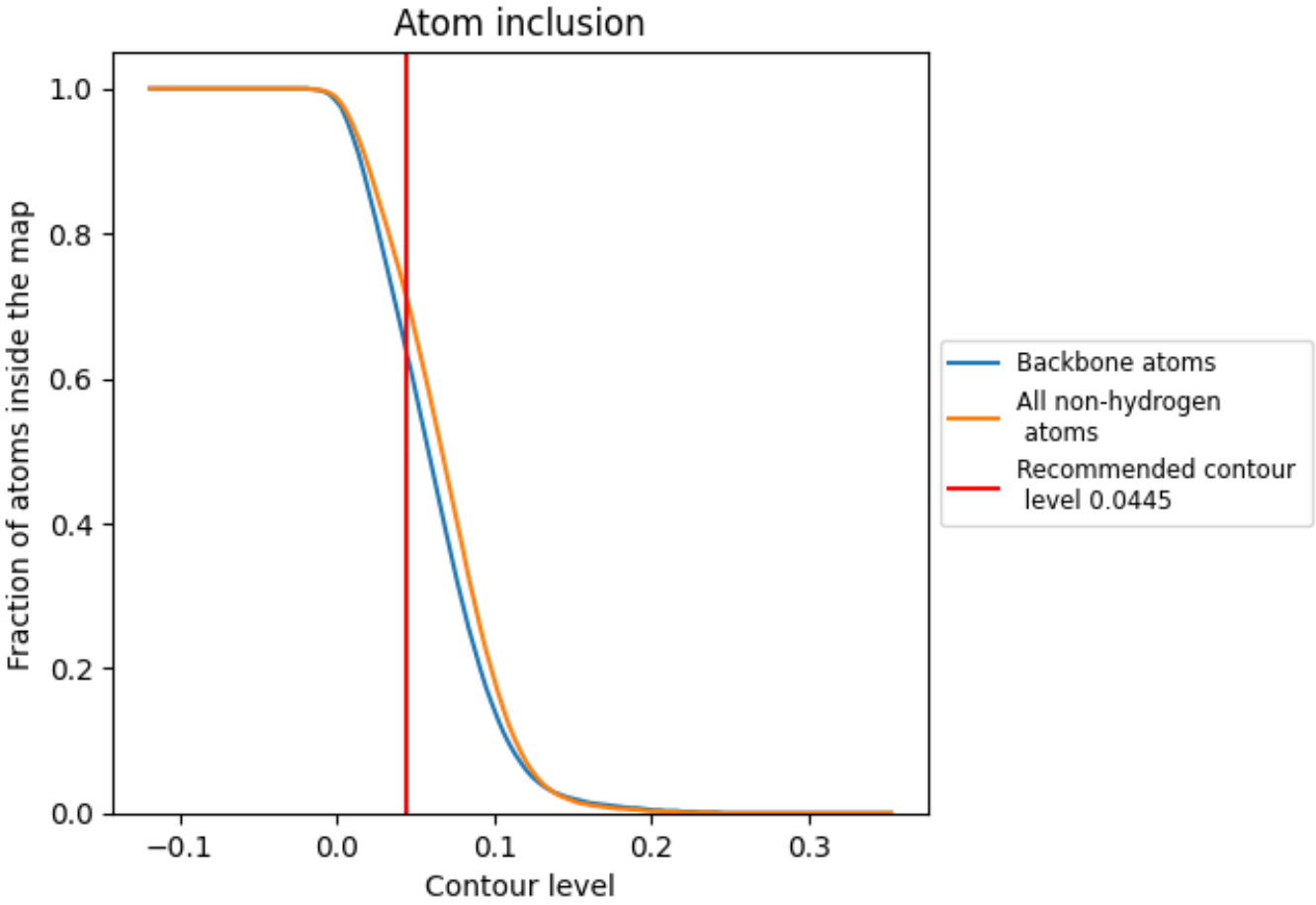
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0445).

9.4 Atom inclusion (i)



At the recommended contour level, 63% of all backbone atoms, 71% 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 (0.0445) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7080	0.6880
0	0.8080	0.7640
1	0.5880	0.6680
2	0.9100	0.8090
3	0.8800	0.7880
4	0.7530	0.7130
6	0.0000	0.0780
A	0.7970	0.7270
B	0.3260	0.5440
C	0.8170	0.7620
D	0.8060	0.7610
E	0.6630	0.7110
F	0.0090	0.2330
G	0.1260	0.4350
J	0.8430	0.7700
K	0.6950	0.7140
L	0.6260	0.6940
M	0.7220	0.7190
N	0.8250	0.7590
O	0.2070	0.5130
P	0.6120	0.6670
Q	0.8510	0.7900
R	0.6880	0.7250
S	0.8100	0.7600
T	0.6040	0.6760
U	0.5190	0.6220
V	0.0400	0.2750
W	0.8170	0.7500
X	0.5660	0.6610
Y	0.4340	0.6240
Z	0.7040	0.7250
a	0.0930	0.3040
b	0.3500	0.6970