wwPDB EM Validation Summary Report (i)

Nov 10, 2022 – 10:45 pm GMT

PDB ID	:	8A57
EMDB ID	:	EMD-15161
Title	:	Cryo-EM structure of HflXr bound to the Listeria monocytogenes 50S ribosomal subunit.
Authors	:	Koller, T.O.; Crowe-McAuliffe, C.; Wilson, D.N.
Deposited on	:	2022-06-14
Resolution	:	2.30 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:

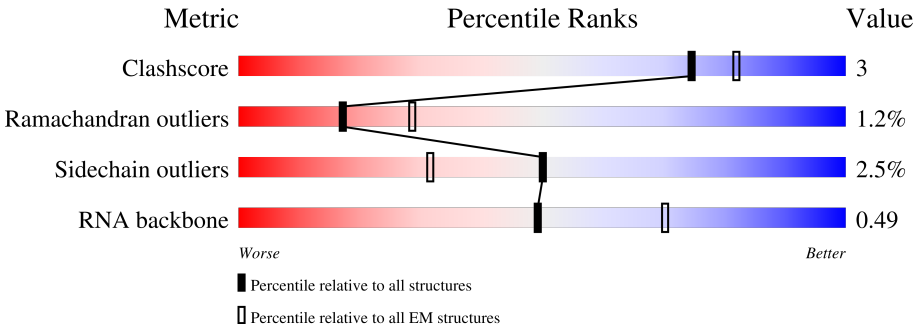
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 2.30 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	1	62	19% 81% 10% · 6%
2	2	63	21% 87% 6% 6%
3	3	59	5% 88% 7% 5%
4	4	81	73% 69% · 27%
5	5	57	33% 70% 23% 7%
6	6	49	47% 80% 14% · ·
7	7	44	91% 5% 5%

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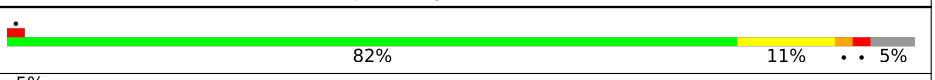
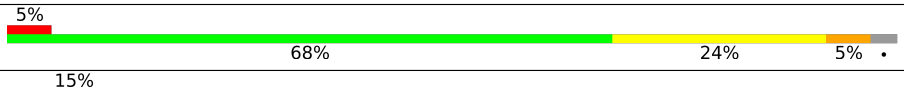
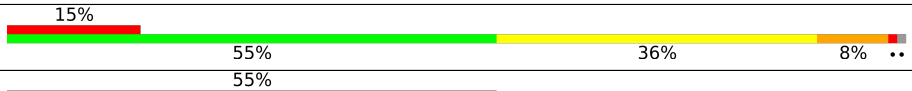
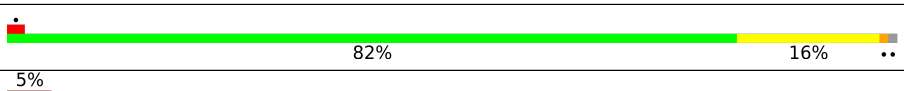
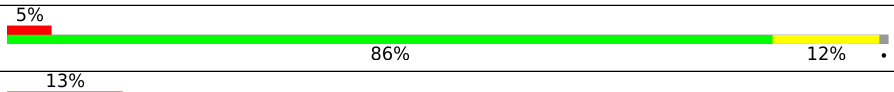
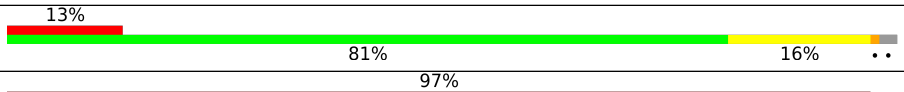
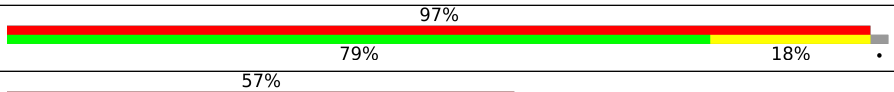
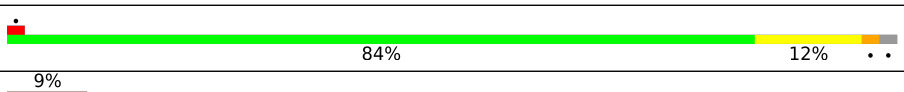
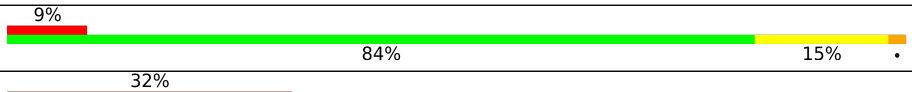
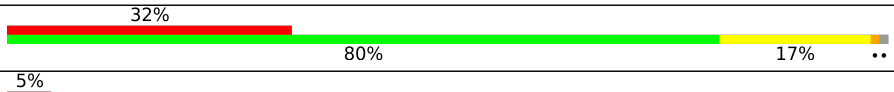
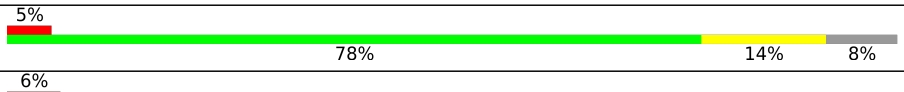
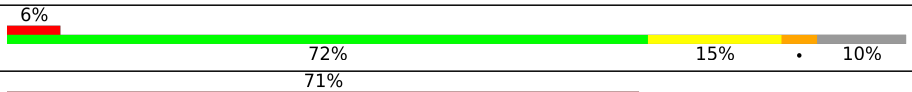
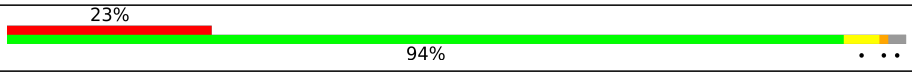
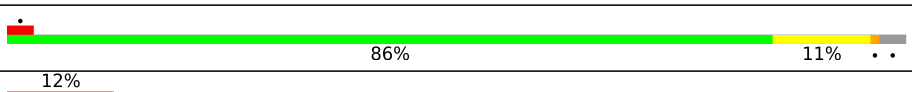
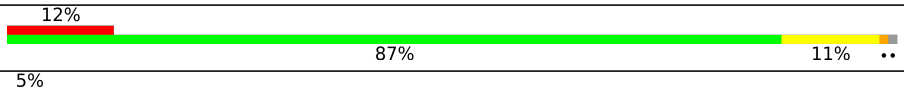
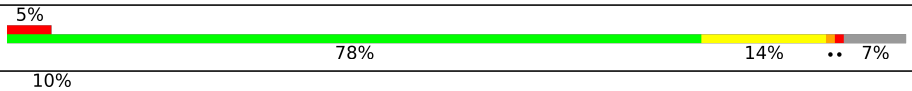
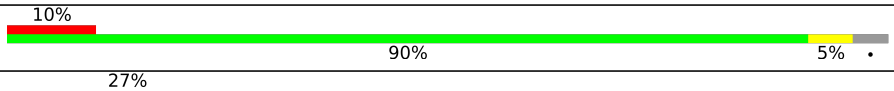
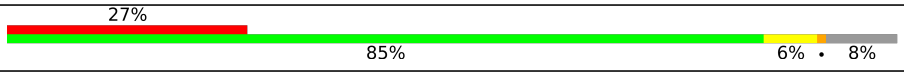
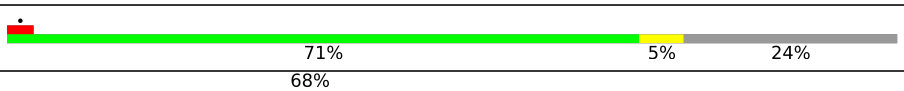
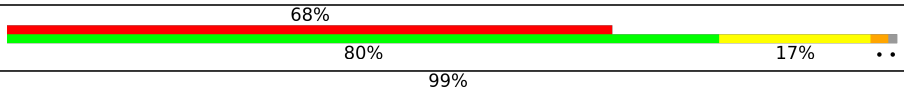
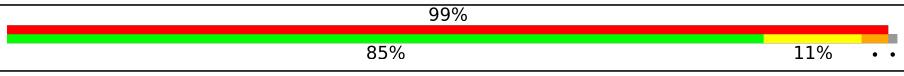
Mol	Chain	Length	Quality of chain
8	8	66	
9	9	37	
10	A	2931	
11	B	114	
12	G	277	
13	H	209	
14	I	207	
15	J	179	
16	K	178	
17	M	145	
18	N	122	
19	O	146	
20	P	144	
21	Q	135	
22	R	119	
23	S	114	
24	T	119	
25	U	102	
26	V	118	
27	W	94	
28	X	103	
29	Z	96	
30	D	418	
31	E	141	

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 92760 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 L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	58	457	283	96	76	2	0	0

- Molecule 2 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	59	487	298	94	94	1	0	0

- Molecule 3 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	56	433	272	82	78	1	0	0

- Molecule 4 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4	59	477	305	75	96	1	0	0

- Molecule 5 is a protein called 50S ribosomal protein L32-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	5	53	425	259	87	74	5	0	0

- Molecule 6 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	6	47	400	243	81	73	3	0	0

- Molecule 7 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	42	Total	C	N	O	S	0	0
			357	217	87	52	1		

- Molecule 8 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	63	Total	C	N	O	S	0	0
			512	317	113	78	4		

- Molecule 9 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	36	Total	C	N	O	S	0	0
			292	183	59	44	6		

- Molecule 10 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	2908	Total	C	N	O	P	0	0
			62459	27874	11544	20133	2908		

- Molecule 11 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	114	Total	C	N	O	P	0	0
			2430	1083	430	803	114		

- Molecule 12 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	273	Total	C	N	O	S	0	0
			2108	1307	415	379	7		

- Molecule 13 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	206	Total	C	N	O	S	0	0
			1582	995	291	292	4		

- Molecule 14 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	I	203	Total 1563	C 987	N 286	O 290	0	0

- Molecule 15 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	175	Total 1365	C 865	N 236	O 258	S 6	0	0

- Molecule 16 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	165	Total 1271	C 801	N 232	O 237	S 1	0	0

- Molecule 17 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	142	Total 1117	C 708	N 201	O 205	S 3	0	0

- Molecule 18 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	122	Total 925	C 573	N 175	O 172	S 5	0	0

- Molecule 19 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	O	144	Total 1094	C 675	N 214	O 205	0	0

- Molecule 20 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	133	Total 1055	C 675	N 205	O 170	S 5	0	0

- Molecule 21 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	122	Total	C	N	O	S	0	0
			983	619	191	172	1		

- Molecule 22 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	R	118	Total	C	N	O	0	0
			914	564	176	174		

- Molecule 23 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	S	112	Total	C	N	O	0	0
			905	570	181	154		

- Molecule 24 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	116	Total	C	N	O	S	0	0
			939	596	185	154	4		

- Molecule 25 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	101	Total	C	N	O	S	0	0
			786	507	134	144	1		

- Molecule 26 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	V	110	Total	C	N	O	0	0
			848	534	160	154		

- Molecule 27 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	90	Total	C	N	O	S	0	0
			731	462	129	138	2		

- Molecule 28 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	95	Total	C	N	O	S	0	0
			723	459	134	127	3		

- Molecule 29 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	73	Total	C	N	O	S	0	0
			563	345	111	106	1		

- Molecule 30 is a protein called GTPase HflX.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	D	414	Total	C	N	O	S	0	0
			3310	2081	565	652	12		

- Molecule 31 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	E	140	Total	C	N	O	S	0	0
			1032	655	178	193	6		

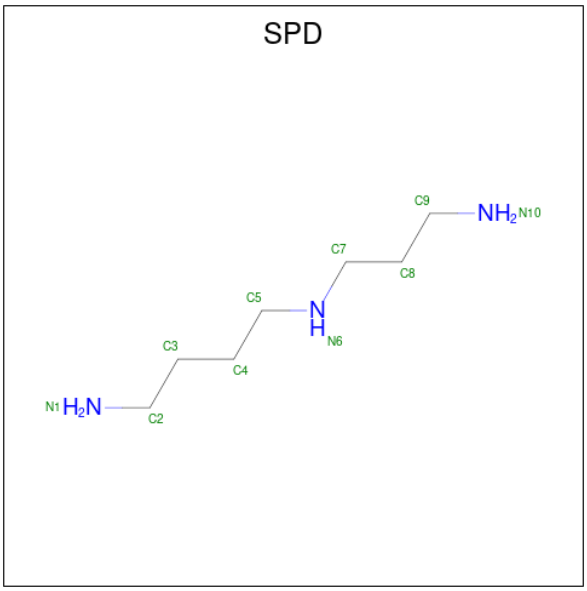
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	137	ILE	THR	conflict	UNP P66054

- Molecule 32 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
32	5	1	Total	Zn	0
			1	1	
32	9	1	Total	Zn	0
			1	1	

- Molecule 33 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).

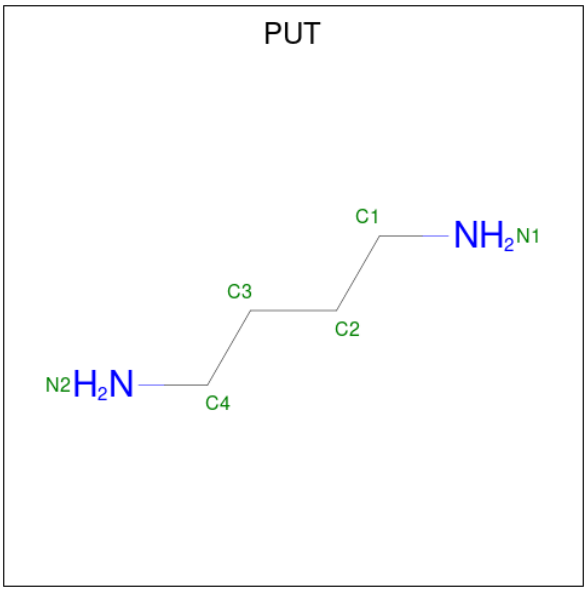


Mol	Chain	Residues	Atoms	AltConf
33	A	1	Total C N 10 7 3	0

- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
34	A	156	Total Mg 156 156	0
34	G	1	Total Mg 1 1	0
34	H	1	Total Mg 1 1	0
34	O	1	Total Mg 1 1	0
34	D	1	Total Mg 1 1	0

- Molecule 35 is 1,4-DIAMINOBUTANE (three-letter code: PUT) (formula: $C_4H_{12}N_2$).

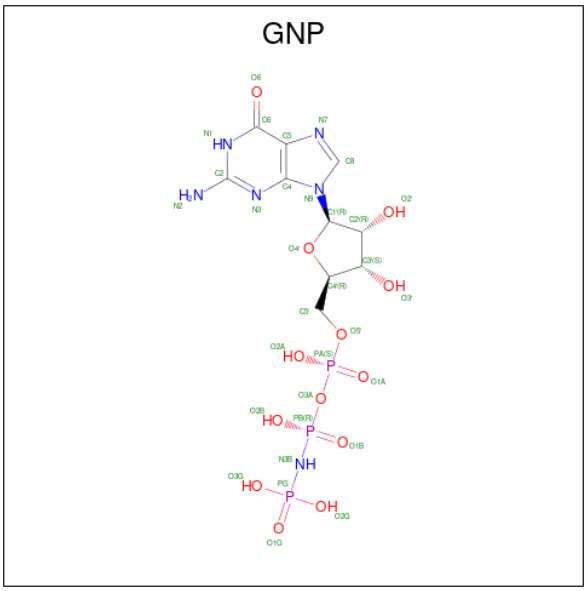


Mol	Chain	Residues	Atoms	AltConf
35	A	1	Total C N 12 8 4	0
35	A	1	Total C N 12 8 4	0

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

Mol	Chain	Residues	Atoms	AltConf
36	P	1	Total K 1 1	0

- Molecule 37 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



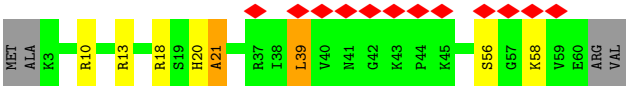
Mol	Chain	Residues	Atoms					AltConf
37	D	1	Total	C	N	O	P	0
			32	10	6	13	3	

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.

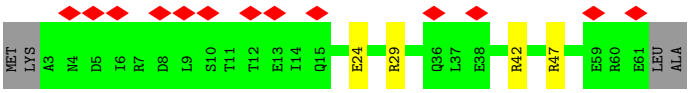
• Molecule 1: 50S ribosomal protein L28

Chain 1:



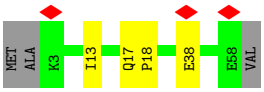
• Molecule 2: 50S ribosomal protein L29

Chain 2:



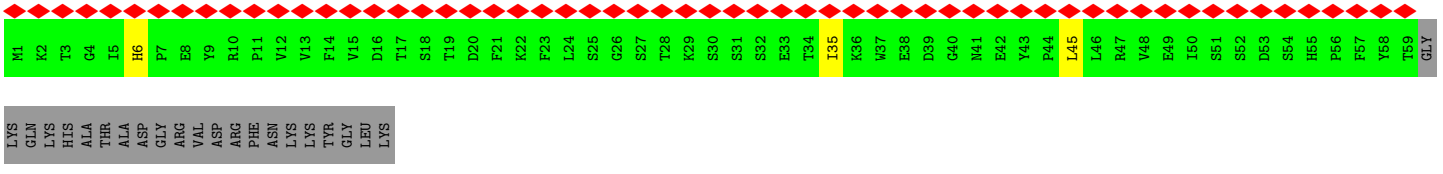
• Molecule 3: 50S ribosomal protein L30

Chain 3:



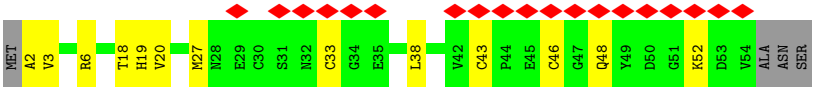
• Molecule 4: 50S ribosomal protein L31 type B

Chain 4:

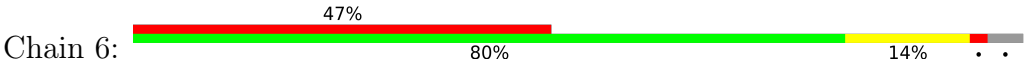


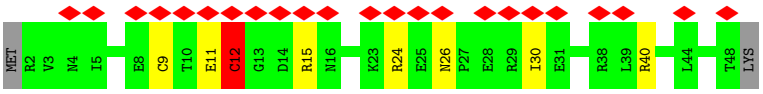
• Molecule 5: 50S ribosomal protein L32-2

Chain 5:

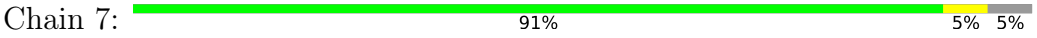


• Molecule 6: 50S ribosomal protein L33 1

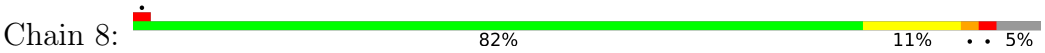




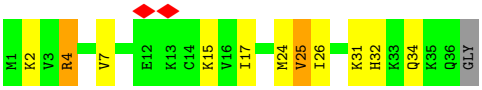
• Molecule 7: 50S ribosomal protein L34



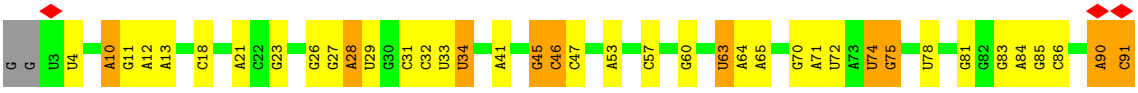
• Molecule 8: 50S ribosomal protein L35

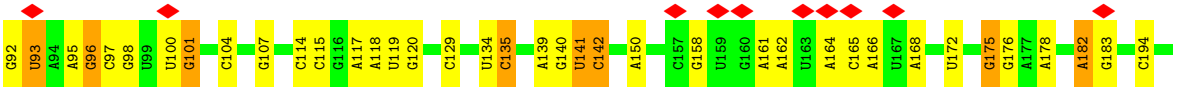


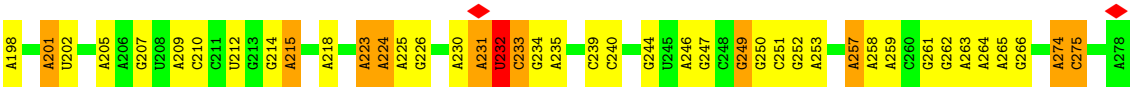
• Molecule 9: 50S ribosomal protein L36

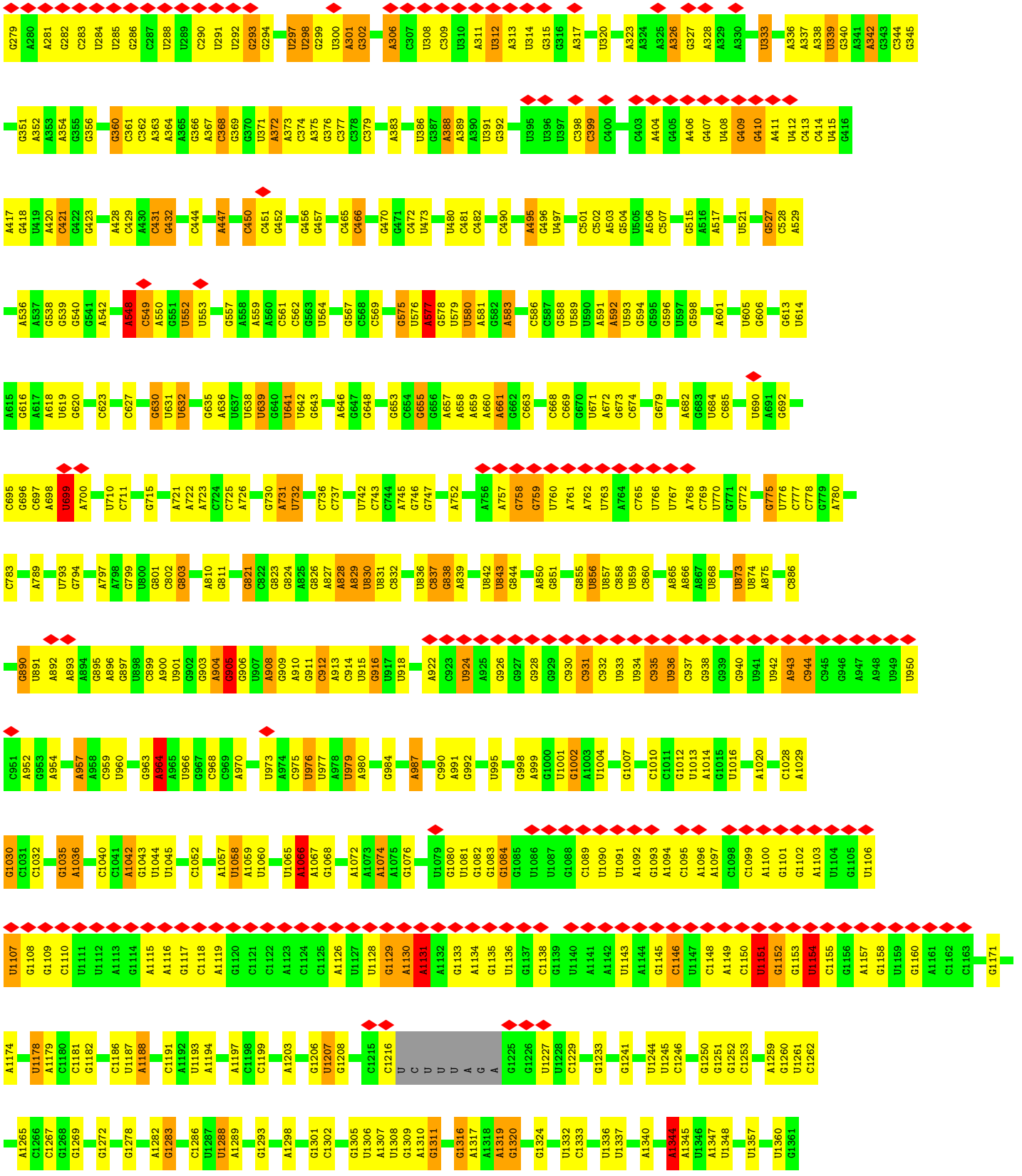


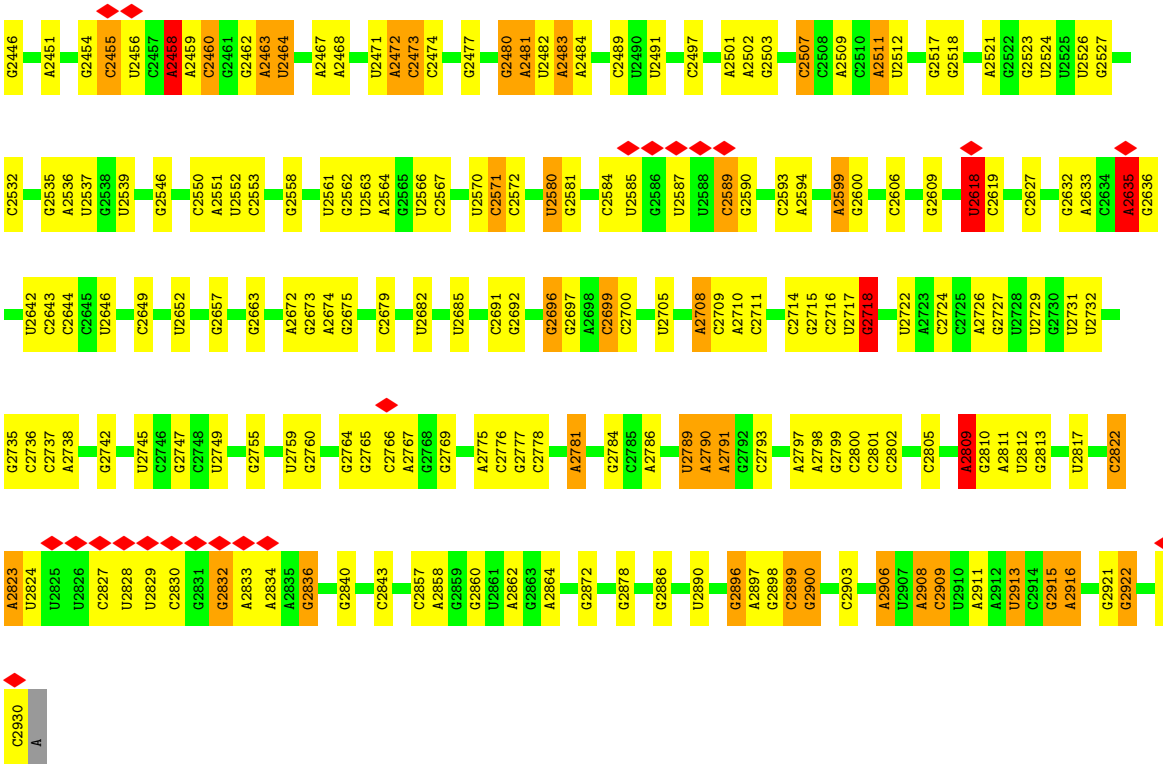
• Molecule 10: 23S ribosomal RNA





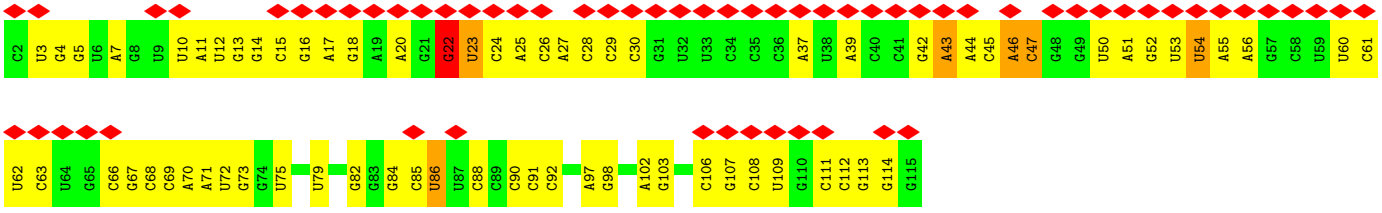






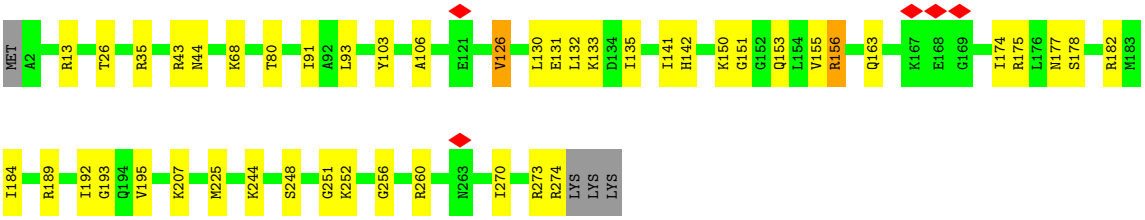
• Molecule 11: 5S ribosomal RNA

Chain B:



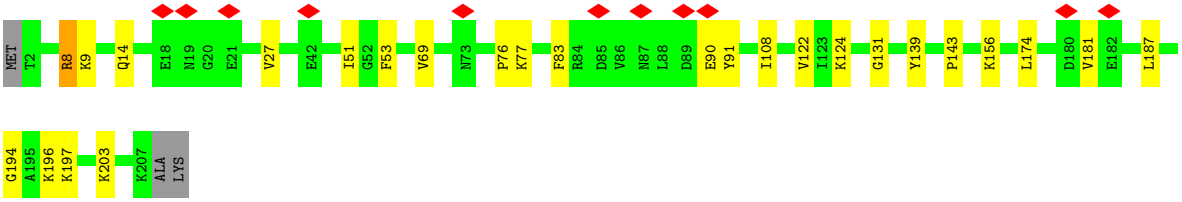
• Molecule 12: 50S ribosomal protein L2

Chain G:

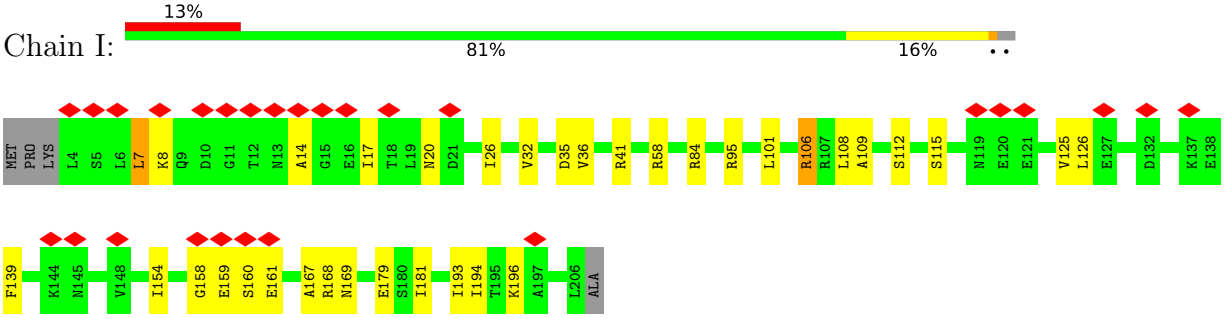


• Molecule 13: 50S ribosomal protein L3

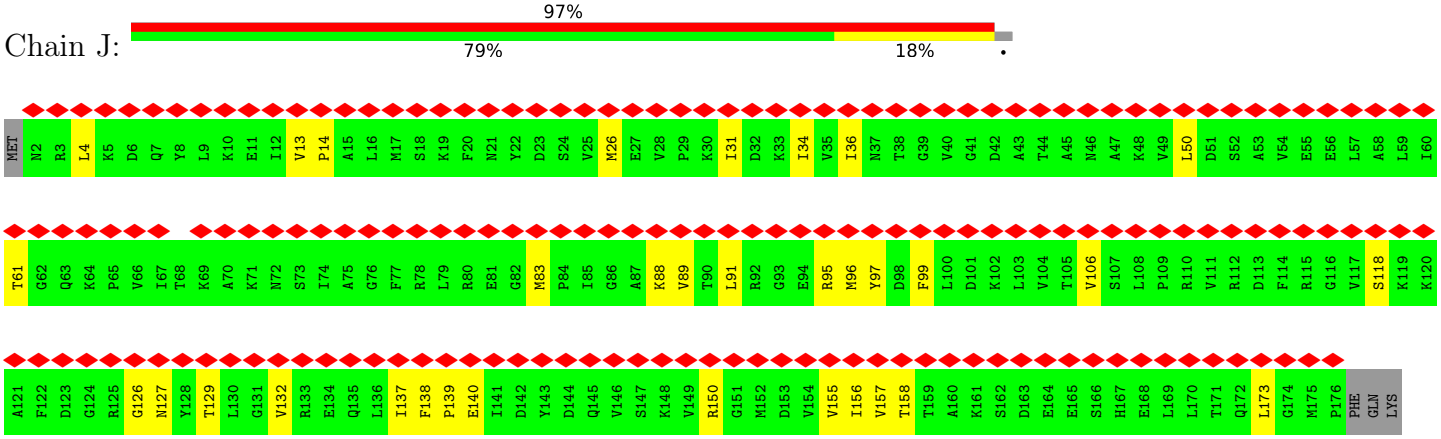
Chain H:



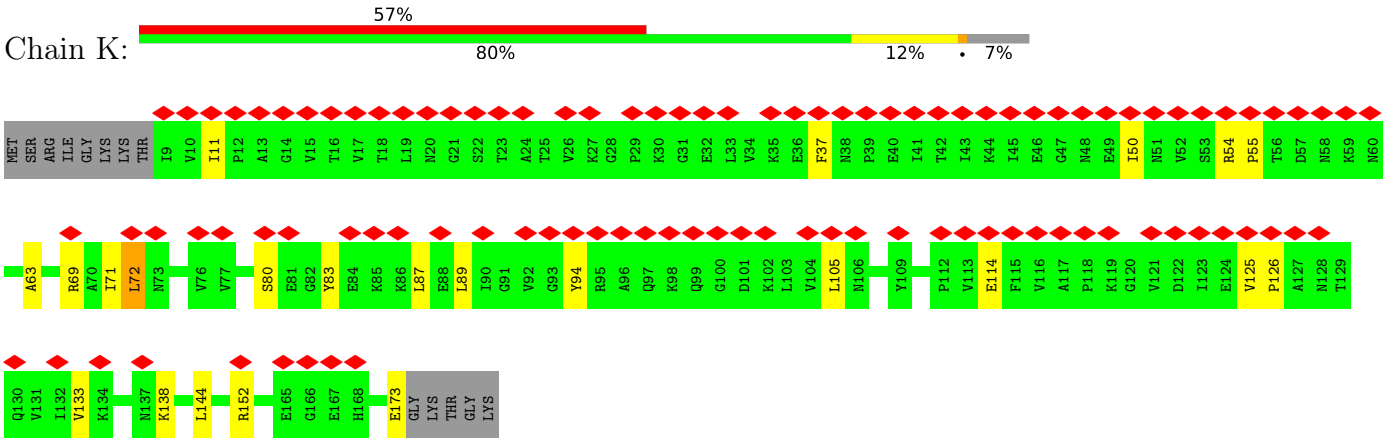
• Molecule 14: 50S ribosomal protein L4



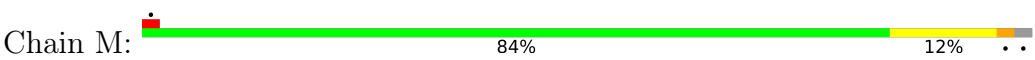
• Molecule 15: 50S ribosomal protein L5

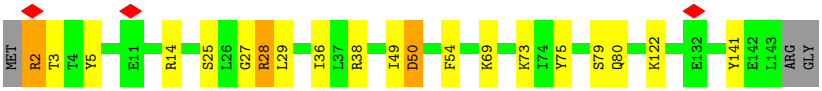


• Molecule 16: 50S ribosomal protein L6

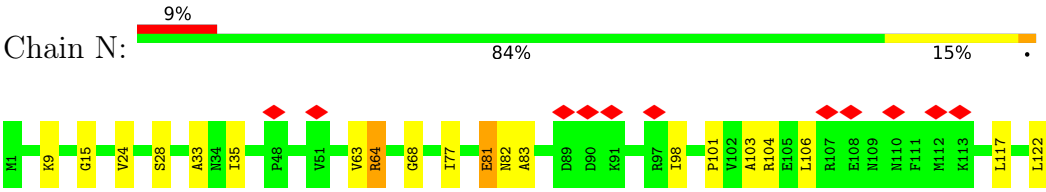


• Molecule 17: 50S ribosomal protein L13

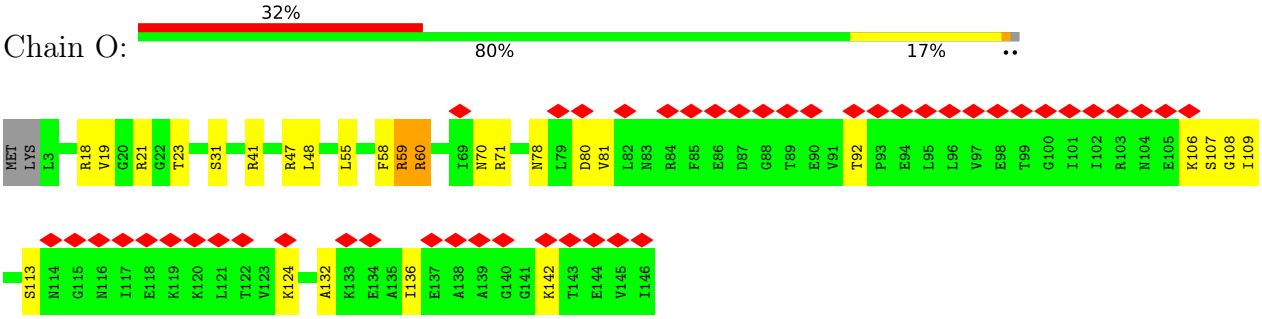




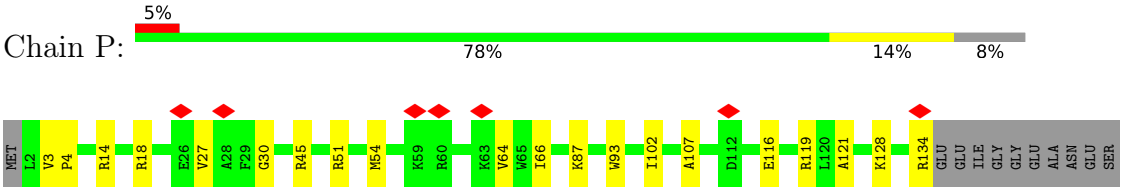
• Molecule 18: 50S ribosomal protein L14



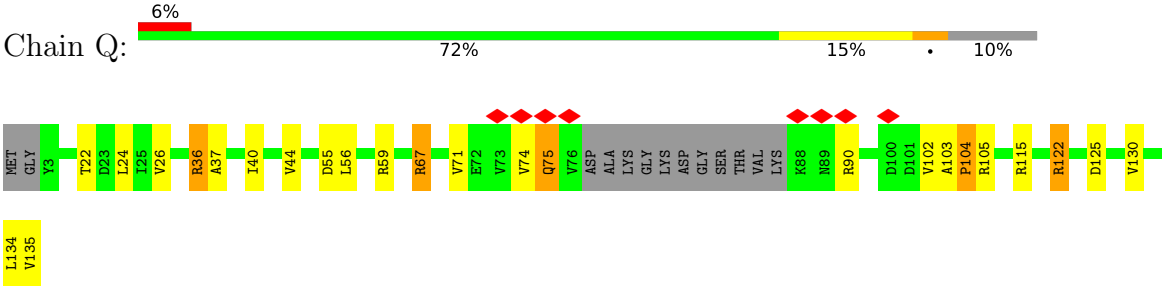
• Molecule 19: 50S ribosomal protein L15



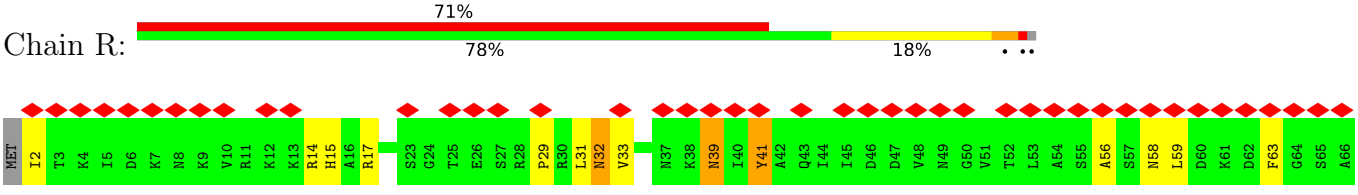
• Molecule 20: 50S ribosomal protein L16



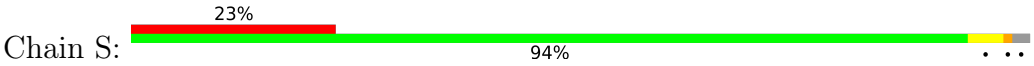
• Molecule 21: 50S ribosomal protein L17



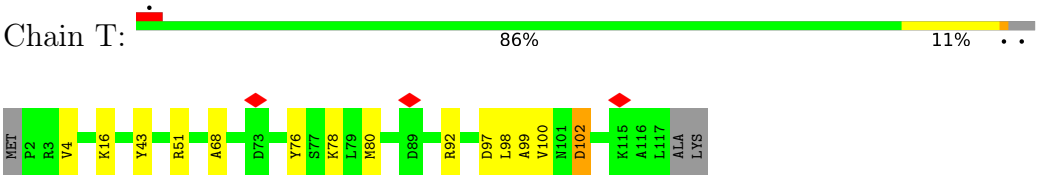
• Molecule 22: 50S ribosomal protein L18



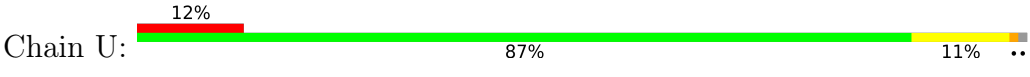
• Molecule 23: 50S ribosomal protein L19



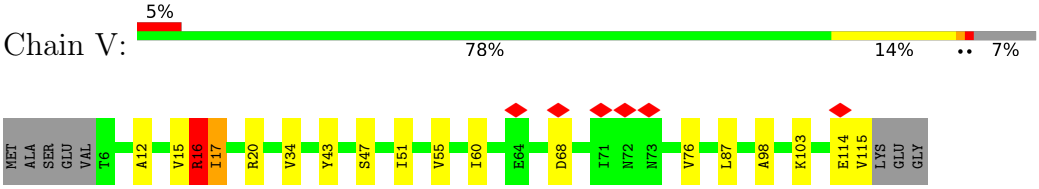
• Molecule 24: 50S ribosomal protein L20



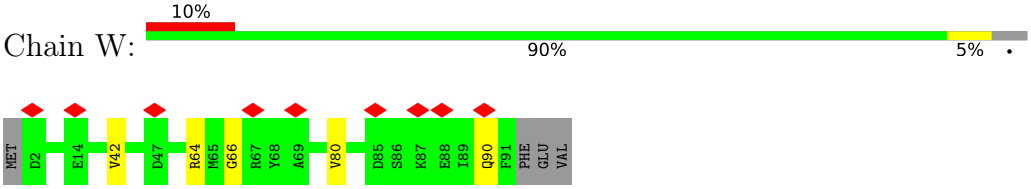
• Molecule 25: 50S ribosomal protein L21



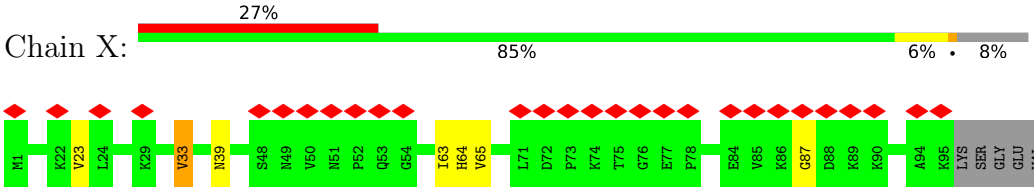
• Molecule 26: 50S ribosomal protein L22



• Molecule 27: 50S ribosomal protein L23

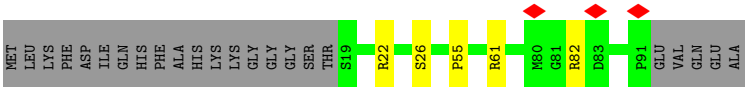


• Molecule 28: 50S ribosomal protein L24



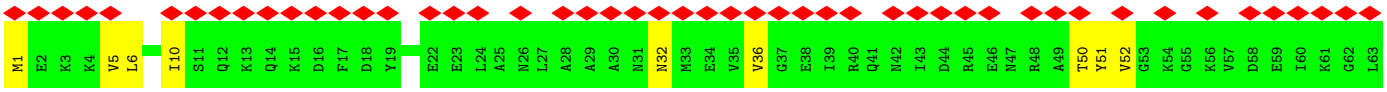
• Molecule 29: 50S ribosomal protein L27

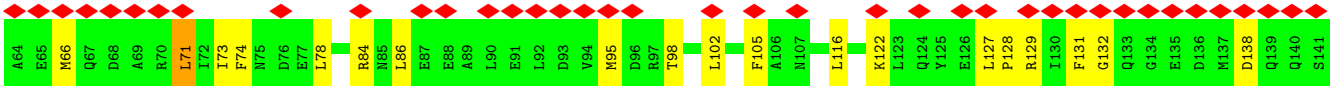
Chain Z:

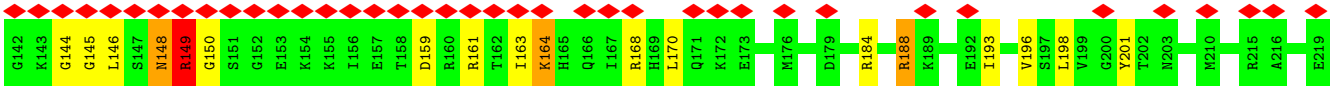


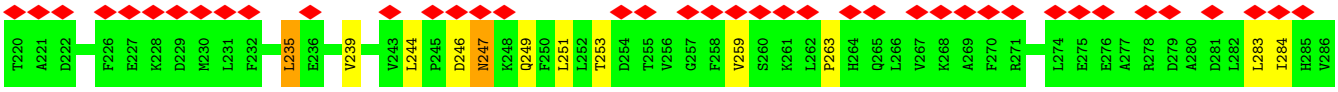
• Molecule 30: GTPase HflX

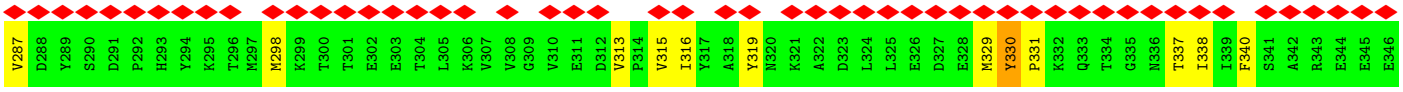
Chain D:

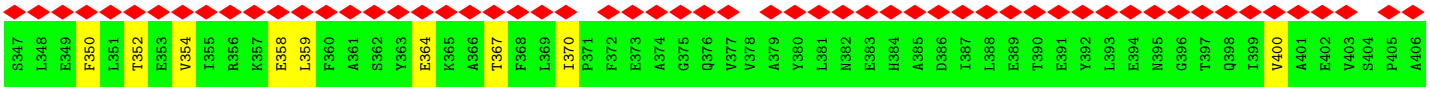


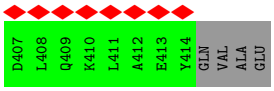






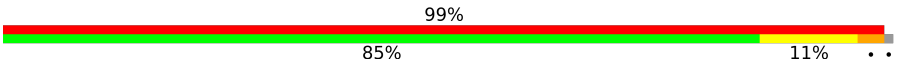


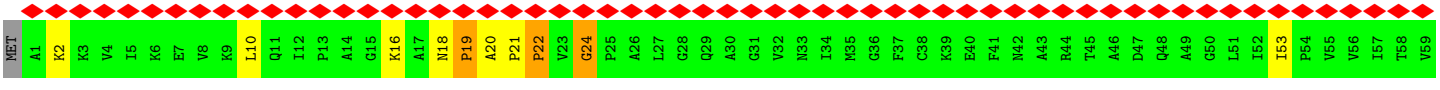


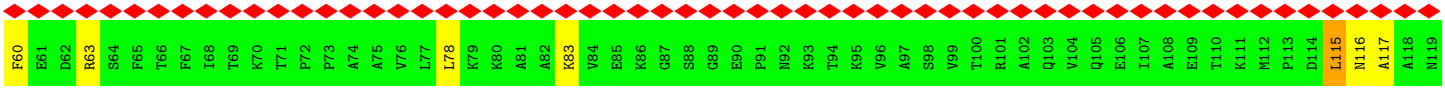


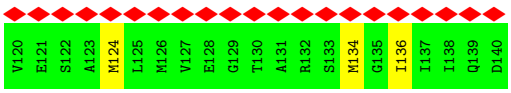
• Molecule 31: 50S ribosomal protein L11

Chain E:









4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	204545	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 ($e^-/Å^2$)	35.022	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	165000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.318	Depositor
Minimum map value	-0.158	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	295.2, 295.2, 295.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82000005, 0.82000005, 0.82000005	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: MG, ZN, SPD, GNP, K, PUT

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	1	0.36	0/462	0.55	0/612
2	2	0.25	0/488	0.42	0/651
3	3	0.29	0/436	0.51	0/585
4	4	0.29	0/491	0.46	0/666
5	5	0.35	0/433	0.59	0/577
6	6	0.25	0/404	0.52	0/541
7	7	0.37	0/360	0.69	0/469
8	8	0.35	0/519	0.58	0/675
9	9	0.30	0/295	0.62	0/387
10	A	0.67	14/69974 (0.0%)	1.20	738/109160 (0.7%)
11	B	0.91	0/2714	1.30	47/4229 (1.1%)
12	G	0.62	0/2144	0.80	0/2875
13	H	0.61	0/1604	0.79	0/2156
14	I	0.64	0/1583	0.76	0/2133
15	J	0.71	0/1383	0.75	0/1863
16	K	0.69	0/1293	0.76	0/1749
17	M	0.61	0/1140	0.73	0/1533
18	N	0.63	0/932	0.78	0/1248
19	O	0.64	0/1105	0.78	0/1470
20	P	0.60	0/1077	0.74	0/1439
21	Q	0.61	0/994	0.77	0/1329
22	R	0.68	0/923	0.74	0/1232
23	S	0.63	0/917	0.77	0/1230
24	T	0.60	0/952	0.75	0/1266
25	U	0.60	0/799	0.80	0/1072
26	V	0.63	0/858	0.76	0/1160
27	W	0.61	0/739	0.75	0/990
28	X	0.66	0/733	0.77	0/980
29	Z	0.60	0/570	0.79	0/758
30	D	0.67	0/3353	0.74	0/4516
31	E	0.73	0/1046	0.77	0/1413
All	All	0.66	14/100721 (0.0%)	1.10	785/150964 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	3
2	2	0	1
5	5	0	1
7	7	0	2
8	8	0	2
9	9	0	1
12	G	0	6
13	H	0	1
14	I	0	3
16	K	0	2
17	M	0	2
19	O	0	6
20	P	0	3
21	Q	0	4
22	R	0	4
23	S	0	3
24	T	0	2
25	U	0	1
26	V	0	1
27	W	0	1
29	Z	0	1
30	D	0	5
All	All	0	55

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	205	A	N9-C4	11.65	1.44	1.37
10	A	2726	A	N9-C4	9.63	1.43	1.37
10	A	726	A	N9-C4	7.51	1.42	1.37
10	A	723	A	N9-C4	7.47	1.42	1.37
10	A	844	G	C8-N7	7.17	1.35	1.30

The worst 5 of 785 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	2366	A	P-O3'-C3'	-11.19	106.27	119.70
10	A	605	U	P-O3'-C3'	-11.12	106.36	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	548	A	P-O3'-C3'	10.54	132.35	119.70
10	A	85	G	P-O3'-C3'	-9.27	108.57	119.70
10	A	502	C	P-O3'-C3'	-9.18	108.69	119.70

There are no chirality outliers.

5 of 55 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	10	ARG	Sidechain
1	1	13	ARG	Sidechain
1	1	18	ARG	Sidechain
2	2	47	ARG	Sidechain
5	5	6	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	1	457	0	502	2	0
2	2	487	0	504	2	0
3	3	433	0	479	2	0
4	4	477	0	454	1	0
5	5	425	0	421	12	0
6	6	400	0	411	10	0
7	7	357	0	405	0	0
8	8	512	0	562	6	0
9	9	292	0	334	5	0
10	A	62459	0	31403	223	0
11	B	2430	0	1229	5	0
12	G	2108	0	2184	29	0
13	H	1582	0	1646	14	0
14	I	1563	0	1655	25	0
15	J	1365	0	1417	18	0
16	K	1271	0	1308	9	0
17	M	1117	0	1140	12	0
18	N	925	0	982	16	0
19	O	1094	0	1137	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	P	1055	0	1125	12	0
21	Q	983	0	1045	17	0
22	R	914	0	941	13	0
23	S	905	0	973	6	0
24	T	939	0	1011	8	0
25	U	786	0	825	7	0
26	V	848	0	905	12	0
27	W	731	0	763	2	0
28	X	723	0	794	3	0
29	Z	563	0	568	3	0
30	D	3310	0	3336	46	0
31	E	1032	0	1097	10	0
32	5	1	0	0	0	0
32	9	1	0	0	0	0
33	A	10	0	19	1	0
34	A	156	0	0	0	0
34	D	1	0	0	0	0
34	G	1	0	0	0	0
34	H	1	0	0	0	0
34	O	1	0	0	0	0
35	A	12	0	24	0	0
36	P	1	0	0	0	0
37	D	32	0	13	0	0
All	All	92760	0	61612	475	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 475 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)
6:6:9:CYS:SG	6:6:12:CYS:HB2	1.79	1.22
10:A:1489:A:H2	10:A:1604:G:H21	1.12	0.96
10:A:655:G:H21	10:A:661:A:H62	1.07	0.92
10:A:655:G:N2	10:A:661:A:H62	1.66	0.91
10:A:1713:A:H61	10:A:2029:C:H5	1.17	0.88

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	1	56/62 (90%)	48 (86%)	6 (11%)	2 (4%)	3 2
2	2	57/63 (90%)	56 (98%)	1 (2%)	0	100 100
3	3	54/59 (92%)	51 (94%)	3 (6%)	0	100 100
4	4	57/81 (70%)	48 (84%)	9 (16%)	0	100 100
5	5	51/57 (90%)	47 (92%)	4 (8%)	0	100 100
6	6	45/49 (92%)	42 (93%)	2 (4%)	1 (2%)	6 5
7	7	40/44 (91%)	40 (100%)	0	0	100 100
8	8	61/66 (92%)	58 (95%)	1 (2%)	2 (3%)	4 2
9	9	34/37 (92%)	33 (97%)	1 (3%)	0	100 100
12	G	271/277 (98%)	252 (93%)	17 (6%)	2 (1%)	22 26
13	H	204/209 (98%)	191 (94%)	13 (6%)	0	100 100
14	I	201/207 (97%)	189 (94%)	11 (6%)	1 (0%)	29 35
15	J	173/179 (97%)	138 (80%)	31 (18%)	4 (2%)	6 5
16	K	163/178 (92%)	149 (91%)	11 (7%)	3 (2%)	8 7
17	M	140/145 (97%)	131 (94%)	7 (5%)	2 (1%)	11 11
18	N	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	19 23
19	O	142/146 (97%)	128 (90%)	11 (8%)	3 (2%)	7 5
20	P	131/144 (91%)	123 (94%)	8 (6%)	0	100 100
21	Q	118/135 (87%)	109 (92%)	7 (6%)	2 (2%)	9 8
22	R	116/119 (98%)	103 (89%)	11 (10%)	2 (2%)	9 8
23	S	110/114 (96%)	104 (94%)	6 (6%)	0	100 100
24	T	114/119 (96%)	112 (98%)	2 (2%)	0	100 100
25	U	99/102 (97%)	91 (92%)	6 (6%)	2 (2%)	7 6
26	V	108/118 (92%)	100 (93%)	6 (6%)	2 (2%)	8 7
27	W	88/94 (94%)	82 (93%)	5 (6%)	1 (1%)	14 15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
28	X	93/103 (90%)	85 (91%)	7 (8%)	1 (1%)	14 15
29	Z	71/96 (74%)	66 (93%)	5 (7%)	0	100 100
30	D	412/418 (99%)	376 (91%)	29 (7%)	7 (2%)	9 8
31	E	138/141 (98%)	116 (84%)	18 (13%)	4 (3%)	4 3
All	All	3467/3684 (94%)	3180 (92%)	245 (7%)	42 (1%)	17 14

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	21	ALA
12	G	126	VAL
17	M	50	ASP
26	V	17	ILE
30	D	247	ASN

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	1	50/53 (94%)	48 (96%)	2 (4%)	31 44
2	2	52/55 (94%)	52 (100%)	0	100 100
3	3	50/52 (96%)	49 (98%)	1 (2%)	55 72
4	4	56/73 (77%)	55 (98%)	1 (2%)	59 75
5	5	47/50 (94%)	45 (96%)	2 (4%)	29 40
6	6	46/48 (96%)	42 (91%)	4 (9%)	10 12
7	7	38/39 (97%)	38 (100%)	0	100 100
8	8	53/56 (95%)	52 (98%)	1 (2%)	57 73
9	9	35/35 (100%)	32 (91%)	3 (9%)	10 12
12	G	221/225 (98%)	217 (98%)	4 (2%)	59 75
13	H	169/171 (99%)	167 (99%)	2 (1%)	71 84
14	I	171/174 (98%)	167 (98%)	4 (2%)	50 67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
15	J	151/155 (97%)	145 (96%)	6 (4%)	31 44
16	K	137/147 (93%)	132 (96%)	5 (4%)	35 49
17	M	119/121 (98%)	118 (99%)	1 (1%)	81 91
18	N	101/101 (100%)	99 (98%)	2 (2%)	55 72
19	O	113/115 (98%)	112 (99%)	1 (1%)	78 89
20	P	105/113 (93%)	105 (100%)	0	100 100
21	Q	102/111 (92%)	102 (100%)	0	100 100
22	R	96/97 (99%)	91 (95%)	5 (5%)	23 32
23	S	98/100 (98%)	98 (100%)	0	100 100
24	T	95/97 (98%)	93 (98%)	2 (2%)	53 70
25	U	82/82 (100%)	80 (98%)	2 (2%)	49 66
26	V	91/97 (94%)	89 (98%)	2 (2%)	52 69
27	W	80/84 (95%)	80 (100%)	0	100 100
28	X	81/88 (92%)	79 (98%)	2 (2%)	47 65
29	Z	58/76 (76%)	58 (100%)	0	100 100
30	D	362/365 (99%)	346 (96%)	16 (4%)	28 39
31	E	110/111 (99%)	103 (94%)	7 (6%)	17 23
All	All	2969/3091 (96%)	2894 (98%)	75 (2%)	50 65

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
30	D	138	ASP
31	E	83	LYS
30	D	149	ARG
30	D	329	MET
15	J	4	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
15	J	172	GLN
30	D	249	GLN
18	N	109	ASN
31	E	92	ASN

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Mol	Chain	Res	Type
30	D	47	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	2905/2931 (99%)	556 (19%)	76 (2%)
11	B	113/114 (99%)	24 (21%)	2 (1%)
All	All	3018/3045 (99%)	580 (19%)	78 (2%)

5 of 580 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	A	10	A
10	A	12	A
10	A	13	A
10	A	34	U
10	A	45	G

5 of 78 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	A	1949	A
10	A	2809	A
10	A	2030	A
10	A	2472	A
10	A	2921	G

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 167 ligands modelled in this entry, 163 are monoatomic - leaving 4 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	PUT	A	3151	-	5,5,5	0.20	0	4,4,4	0.21	0
37	GNP	D	501	34	29,34,34	1.46	6 (20%)	33,54,54	2.24	5 (15%)
33	SPD	A	3001	-	9,9,9	0.30	0	8,8,8	0.73	0
35	PUT	A	3152	-	5,5,5	0.20	0	4,4,4	0.20	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
35	PUT	A	3151	-	-	1/3/3/3	-
37	GNP	D	501	34	-	4/14/38/38	0/3/3/3
33	SPD	A	3001	-	-	5/7/7/7	-
35	PUT	A	3152	-	-	0/3/3/3	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	D	501	GNP	C6-N1	4.05	1.40	1.33
37	D	501	GNP	PG-O1G	3.35	1.51	1.46
37	D	501	GNP	PB-O1B	2.84	1.50	1.46
37	D	501	GNP	PG-O3G	-2.31	1.50	1.56
37	D	501	GNP	PG-O2G	-2.31	1.50	1.56

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	D	501	GNP	C5-C6-N1	-8.81	111.38	123.43
37	D	501	GNP	C2-N1-C6	5.93	125.36	115.93
37	D	501	GNP	O2B-PB-O1B	4.06	118.44	109.92
37	D	501	GNP	N3-C2-N1	-2.83	123.45	127.22
37	D	501	GNP	C2-N3-C4	-2.76	112.20	115.36

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

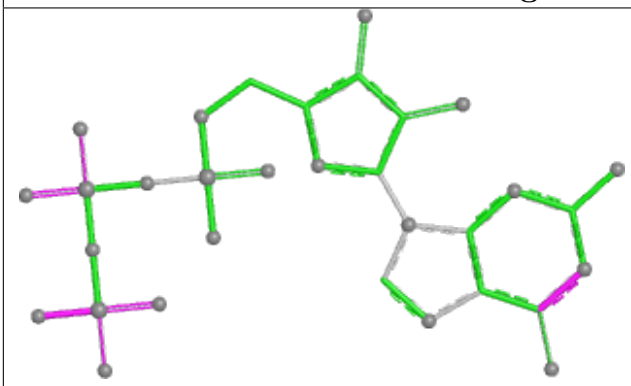
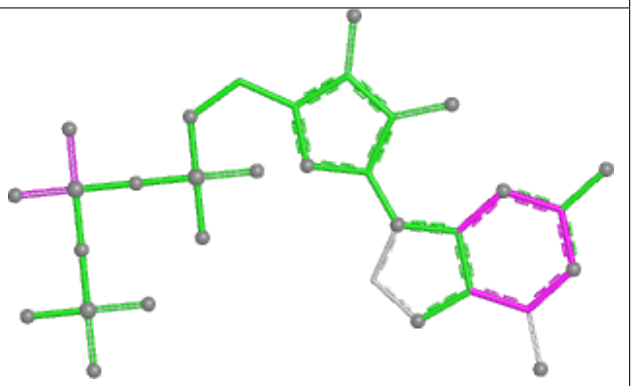
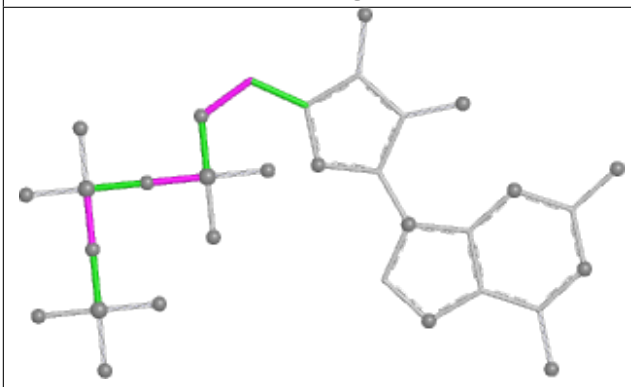
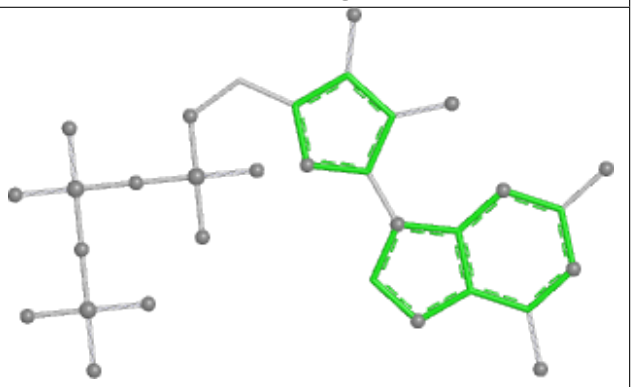
Mol	Chain	Res	Type	Atoms
33	A	3001	SPD	C3-C4-C5-N6
33	A	3001	SPD	C8-C7-N6-C5
33	A	3001	SPD	N6-C7-C8-C9
35	A	3151	PUT	C1-C2-C3-C4
37	D	501	GNP	PB-O3A-PA-O1A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	A	3001	SPD	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 GNP D 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

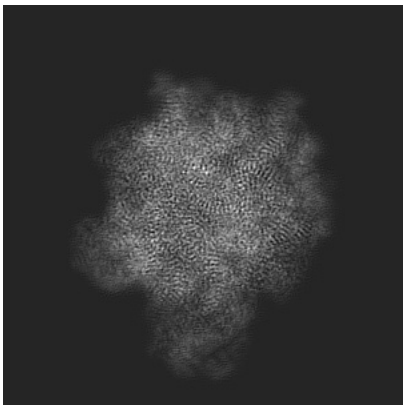
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-15161. These allow visual inspection of the internal detail of the map and identification of artifacts.

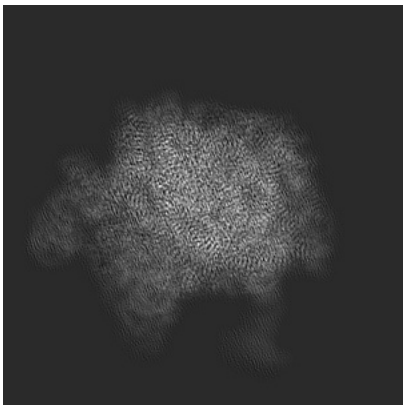
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

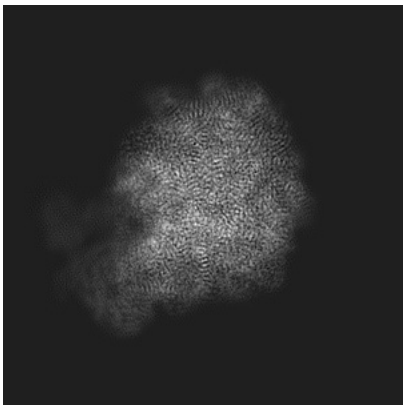
6.1.1 Primary map



X

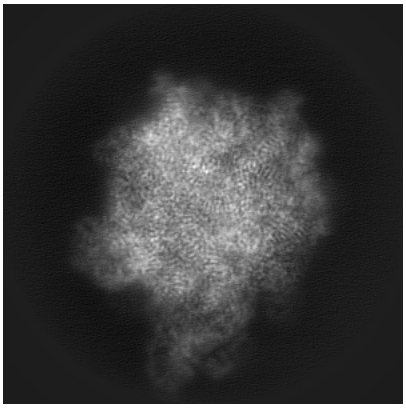


Y

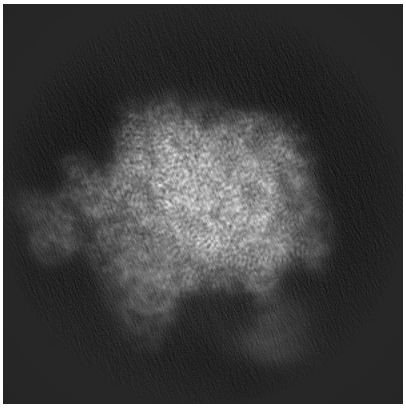


Z

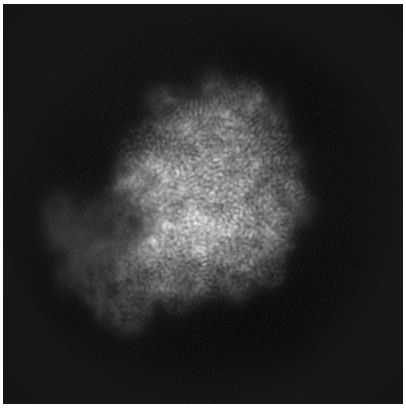
6.1.2 Raw map



X



Y

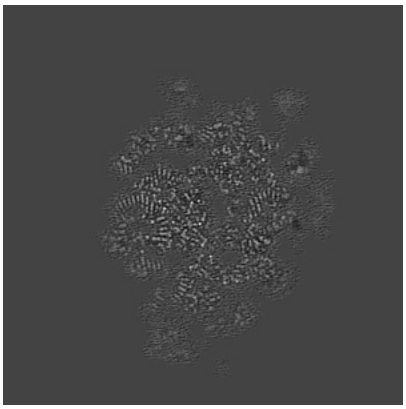


Z

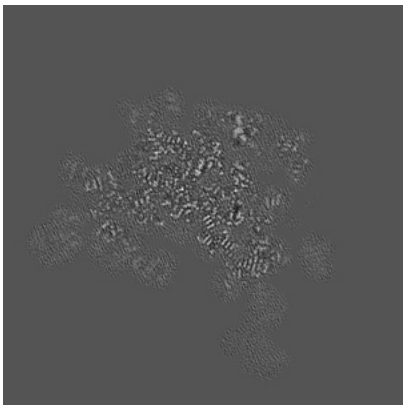
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

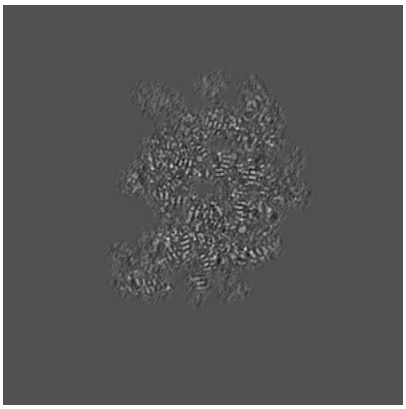
6.2.1 Primary map



X Index: 180

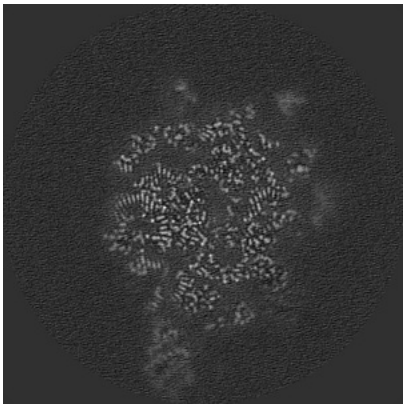


Y Index: 180

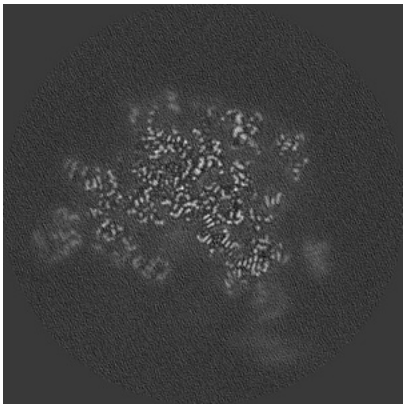


Z Index: 180

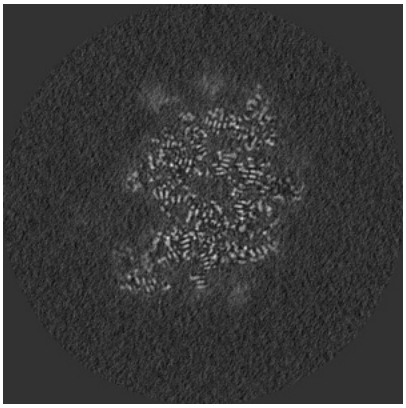
6.2.2 Raw map



X Index: 180



Y Index: 180

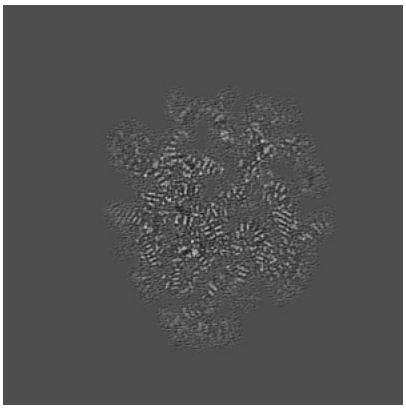


Z Index: 180

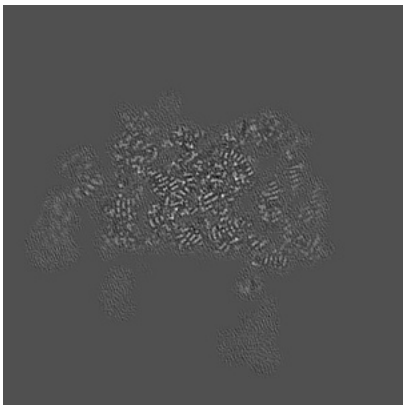
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

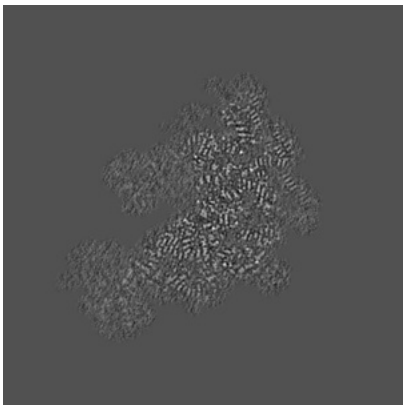
6.3.1 Primary map



X Index: 206

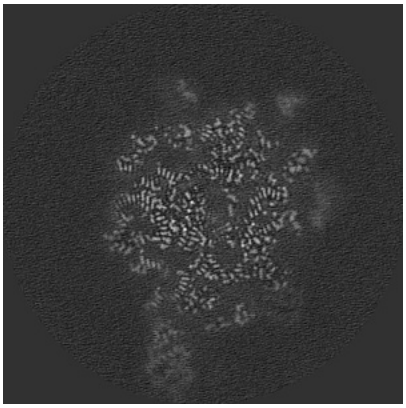


Y Index: 162

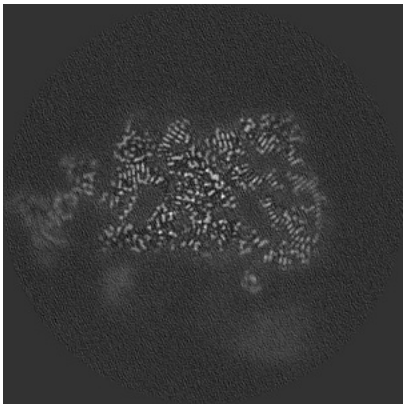


Z Index: 148

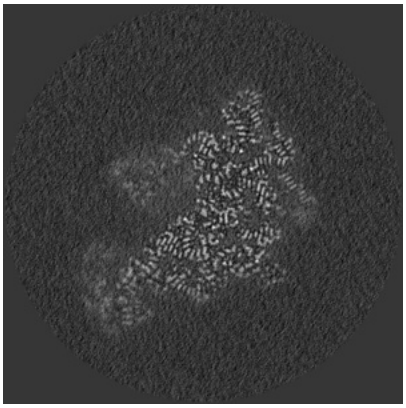
6.3.2 Raw map



X Index: 181



Y Index: 156



Z Index: 148

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

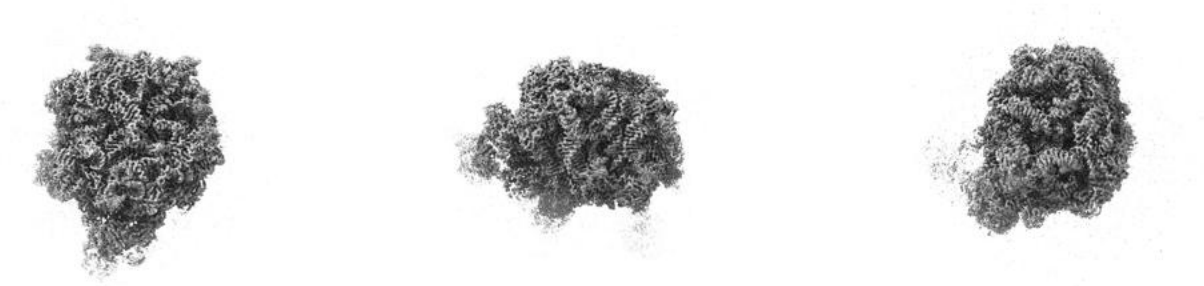
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

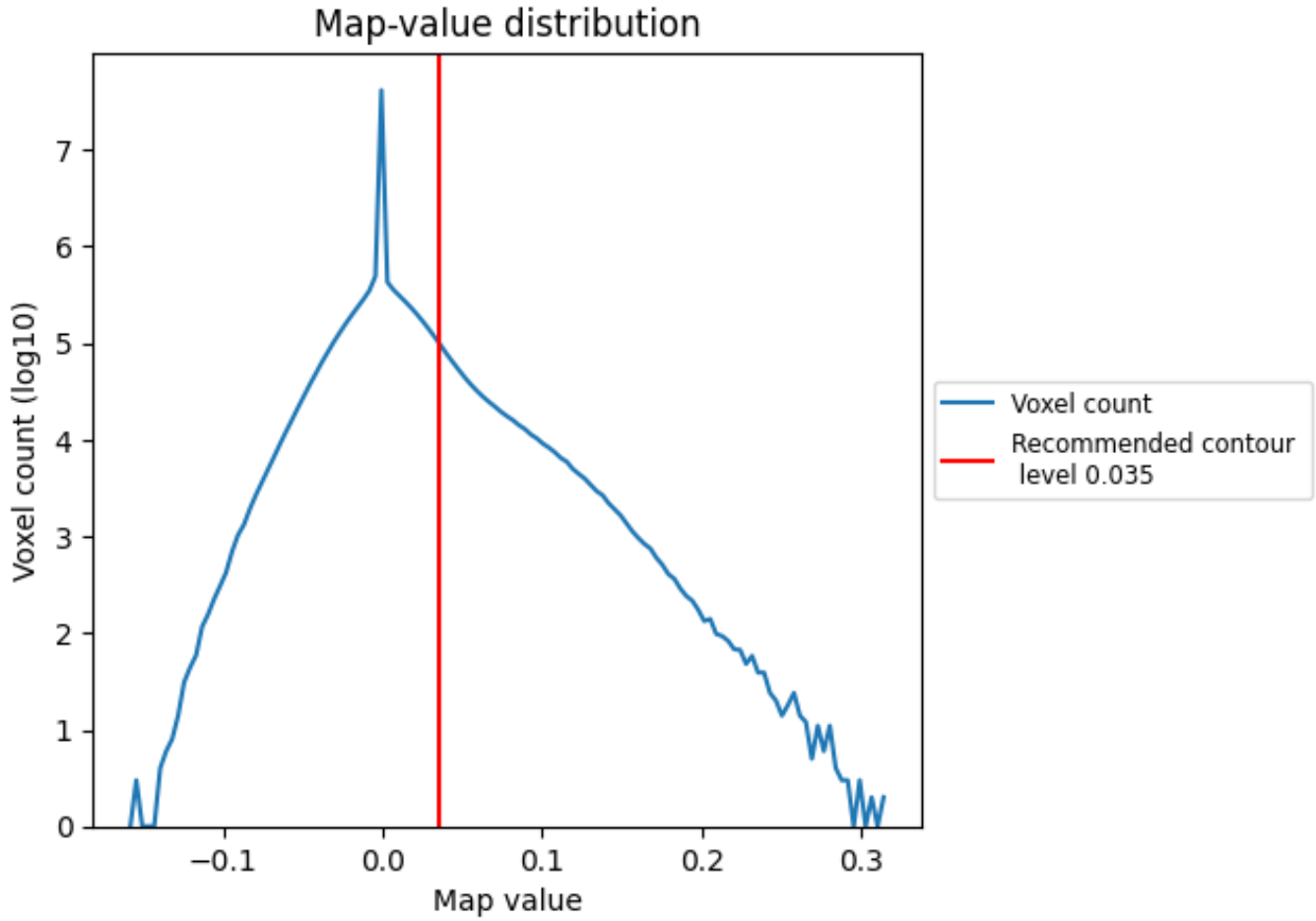
6.5 Mask visualisation (i)

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

7 Map analysis

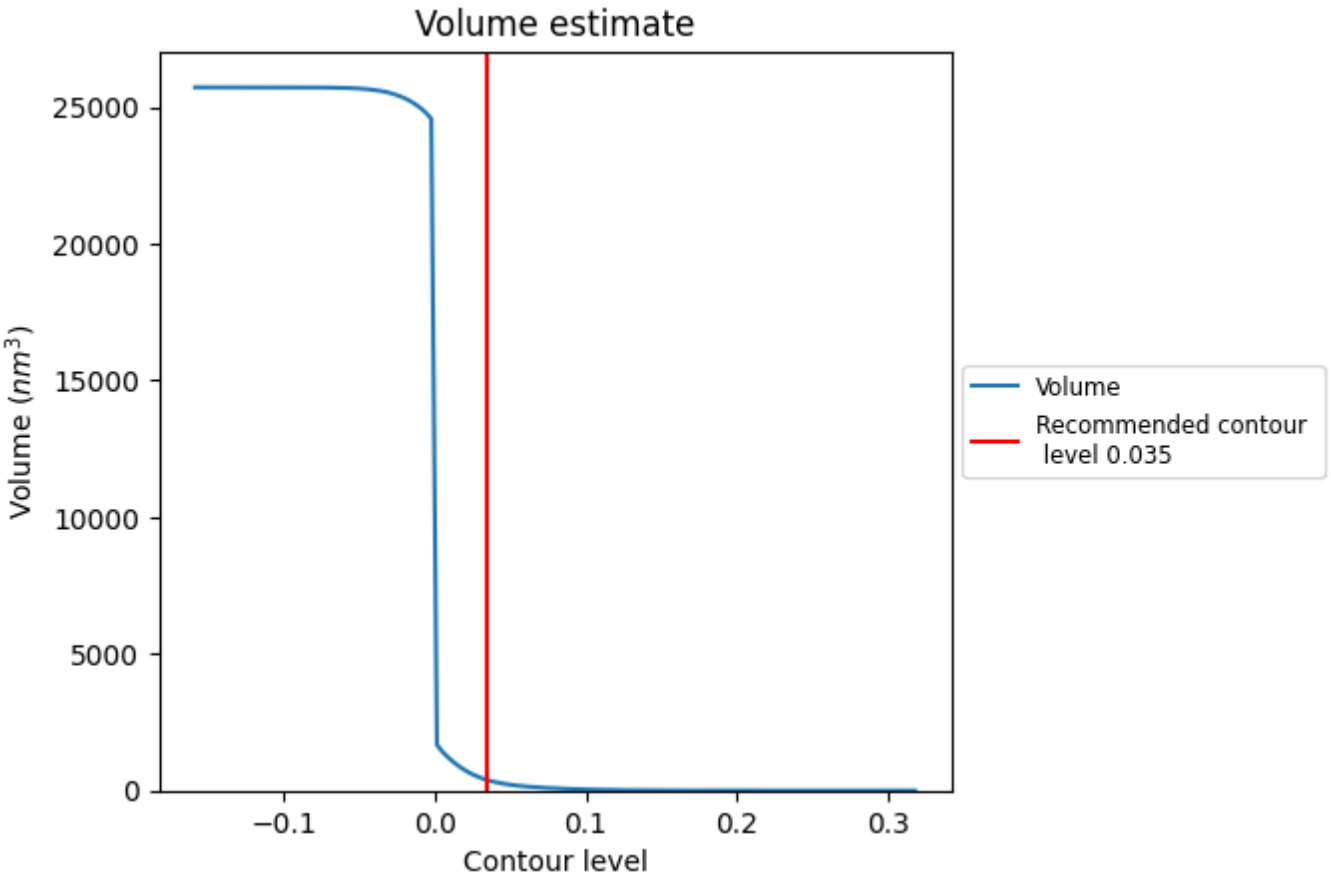
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

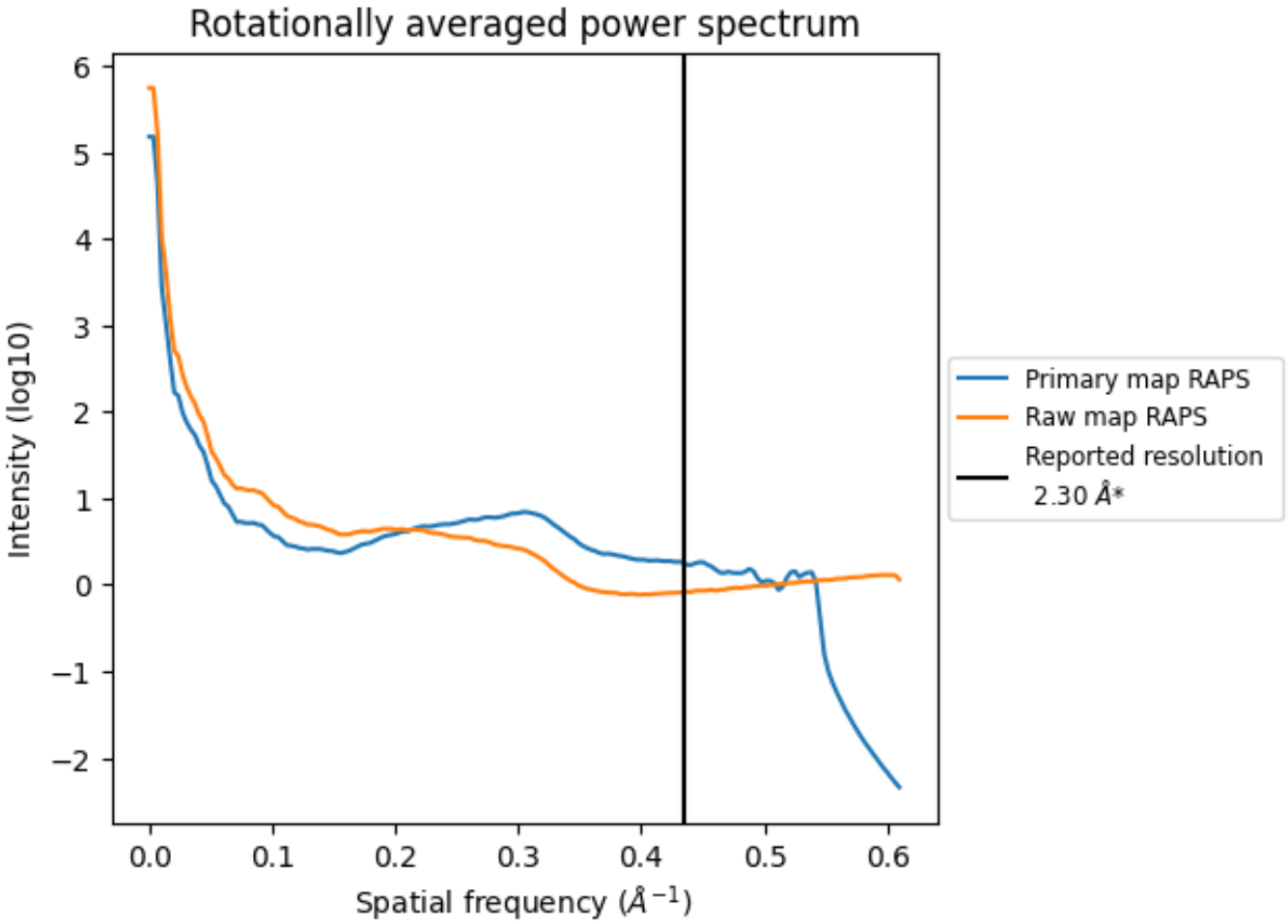
7.2 Volume estimate (i)



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

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

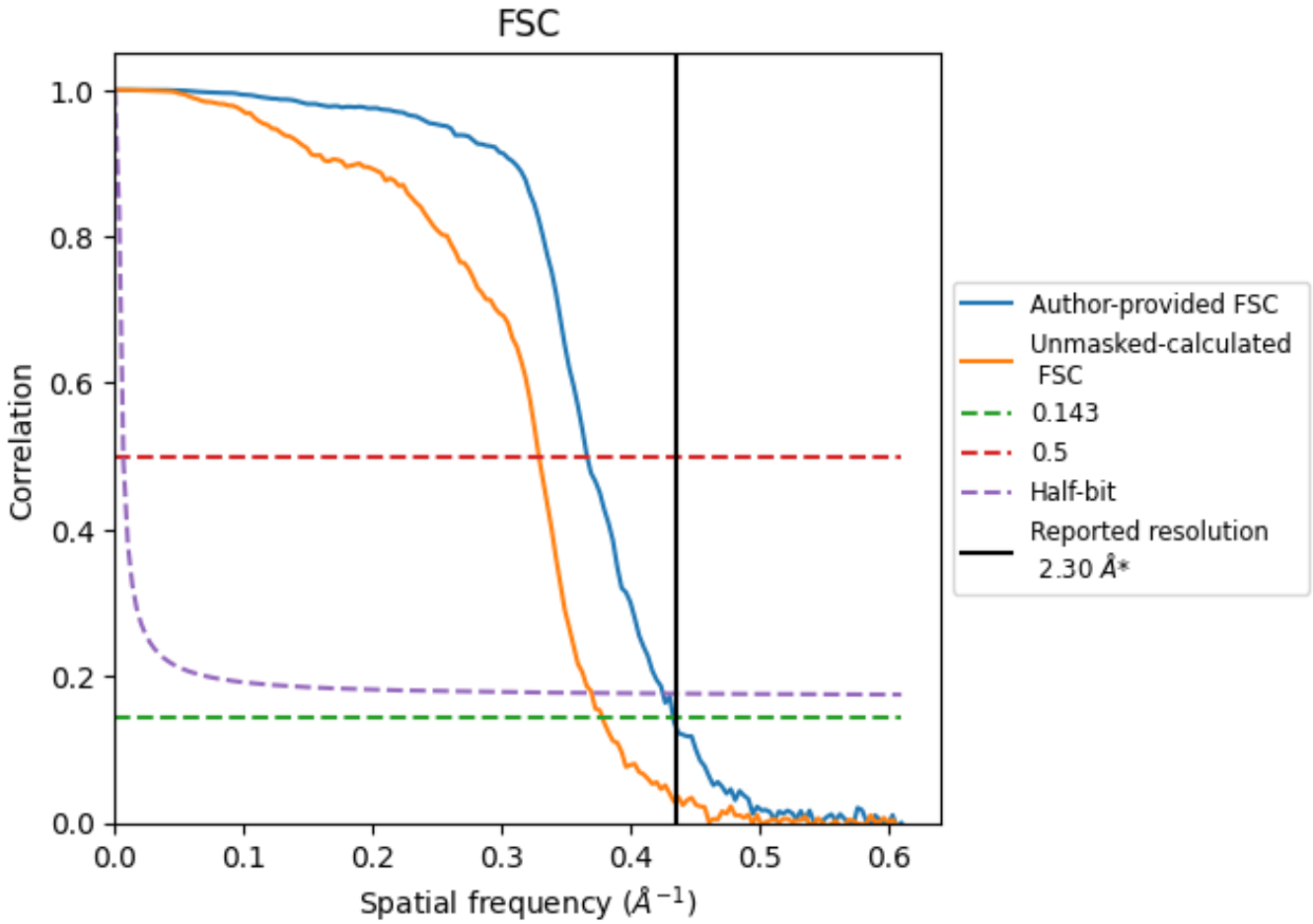


*Reported resolution corresponds to spatial frequency of 0.435 Å^{-1}

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 0.435 Å^{-1}

8.2 Resolution estimates (i)

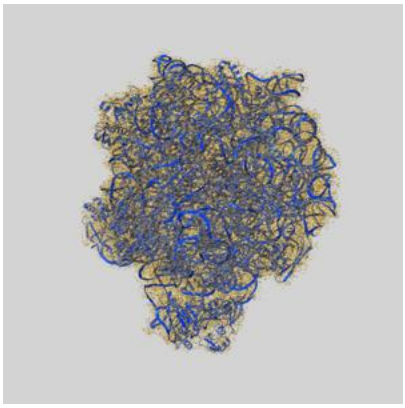
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	2.31	2.73	2.35
Unmasked-calculated*	2.64	3.04	2.71

*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 2.64 differs from the reported value 2.3 by more than 10 %

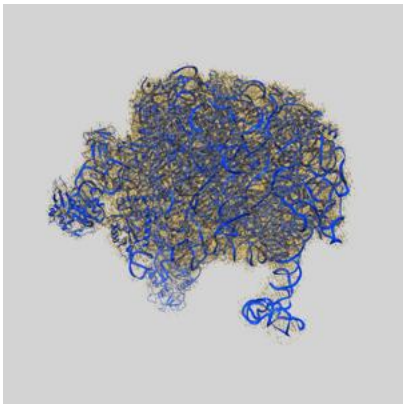
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-15161 and PDB model 8A57. Per-residue inclusion information can be found in section 3 on page 12.

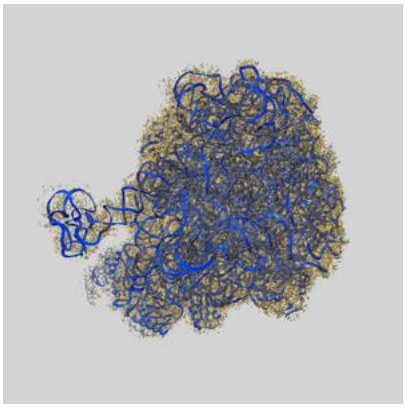
9.1 Map-model overlay



X



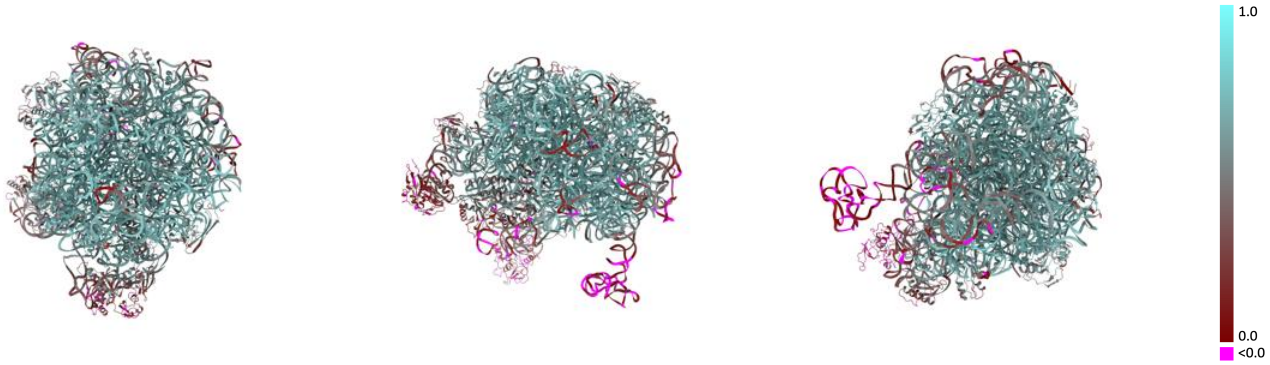
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.035 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.

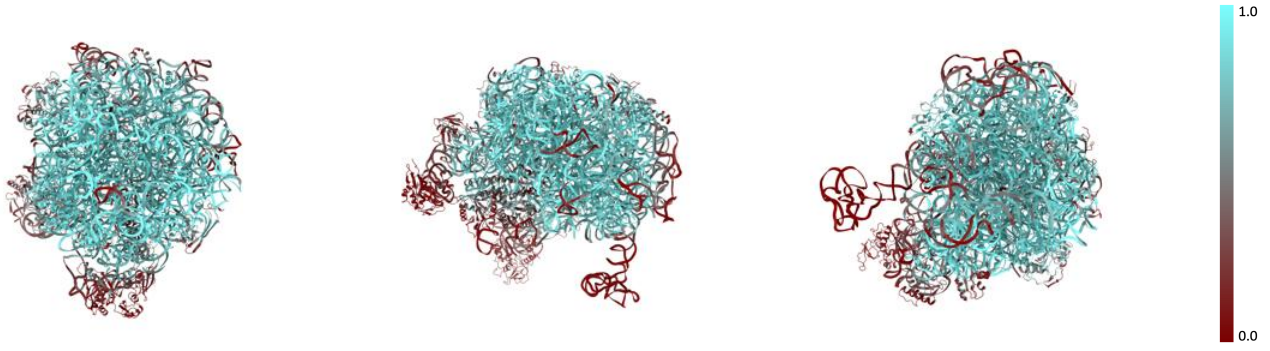
9.2 Q-score mapped to coordinate model (i)



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.

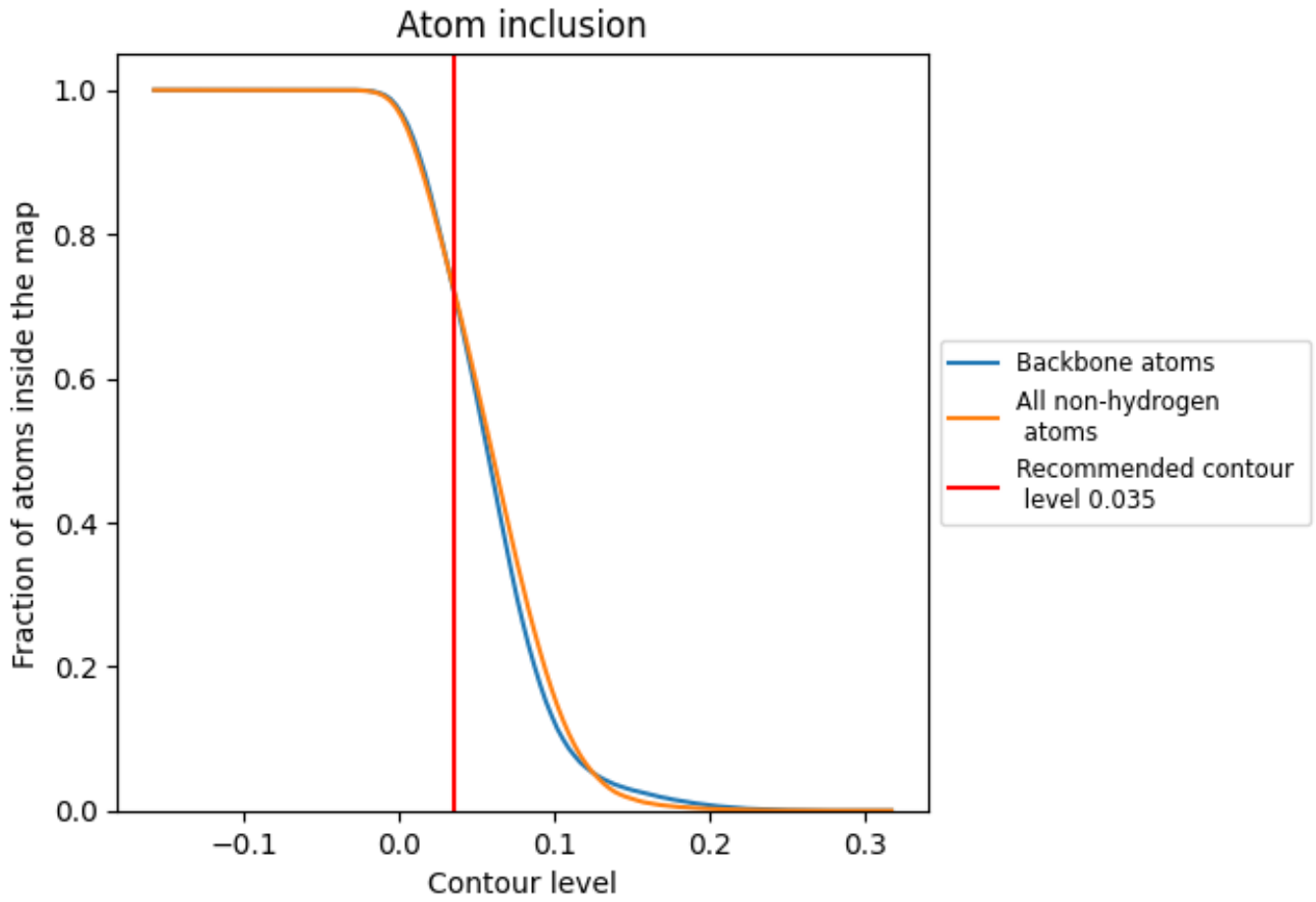
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.035).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 73% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7252	0.5790
1	0.7472	0.5970
2	0.6285	0.5470
3	0.8000	0.6390
4	0.0171	0.0140
5	0.6359	0.5470
6	0.4764	0.4880
7	0.9671	0.7490
8	0.8684	0.6820
9	0.8362	0.6480
A	0.7859	0.6080
B	0.4395	0.4340
D	0.3012	0.3590
E	0.0361	0.0850
G	0.8542	0.6770
H	0.8355	0.6700
I	0.7459	0.6210
J	0.0523	0.1020
K	0.3416	0.3970
M	0.8756	0.6900
N	0.7439	0.6160
O	0.6333	0.5620
P	0.8057	0.6390
Q	0.8342	0.6510
R	0.3037	0.3620
S	0.6774	0.5720
T	0.9128	0.7200
U	0.7706	0.6300
V	0.8717	0.6850
W	0.7654	0.6150
X	0.5796	0.5240
Z	0.8856	0.6870