wwPDB EM Validation Summary Report

Jan 23, 2025 – 02:55 PM EST

PDB ID	:	9BS0
EMDB ID	:	EMD-44849
Title	:	YphC-treated 45SYphC particle. Class 5
Authors	:	Arpin, D.; Ortega, J.
Deposited on	:	2024-05-12
Resolution	:	3.30 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 ⓘ symbol.

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

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

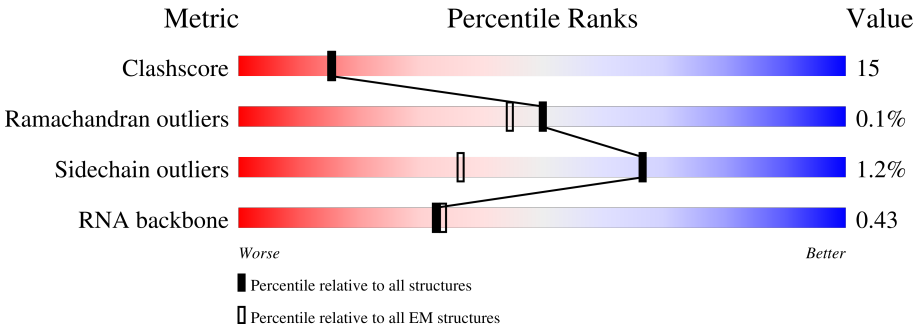
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 3.30 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2927	5% 31% 39% 20% • 9%
2	B	119	• 23% 36% 33% • 7%
3	C	277	6% 93% • •
4	D	209	10% 82% 6% 12%
5	E	207	9% 93% 6% •
6	F	179	21% 26% 10% 64%
7	G	145	• 91% 8% •

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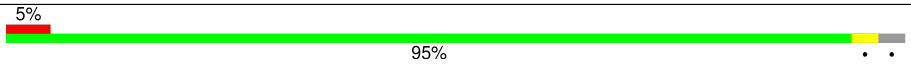
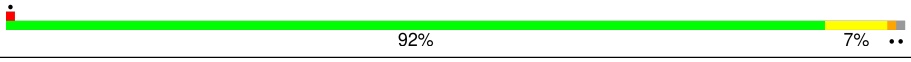
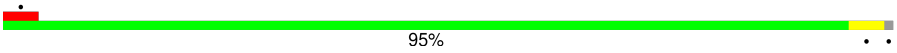
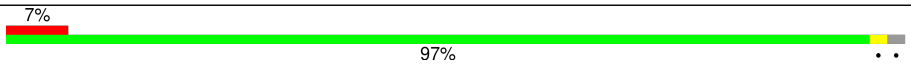
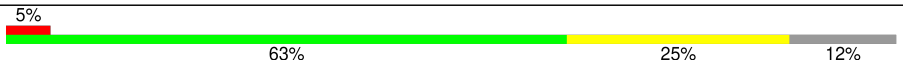
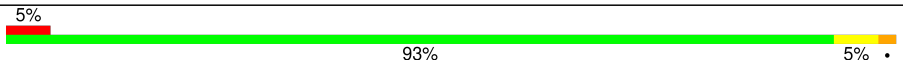
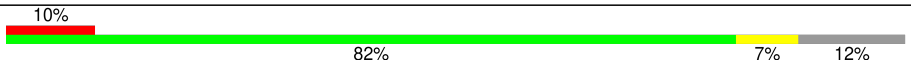
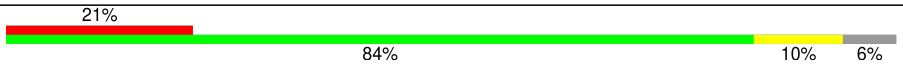
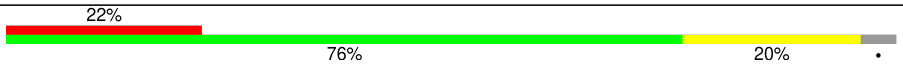
Mol	Chain	Length	Quality of chain
8	H	122	
9	I	146	
10	J	120	
11	K	115	
12	L	118	
13	M	102	
14	N	113	
15	O	95	
16	P	103	
17	Q	94	
18	R	66	
19	S	59	
20	T	59	
21	U	44	
22	V	120	
23	W	436	
24	Z	49	
25	Y	232	

2 Entry composition (i)

There are 26 unique types of molecules in this entry. The entry contains 81446 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2678	57517	25661	10633	18545	2678	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	267	C	U	conflict	GB 1775206404
A	640	U	C	conflict	GB 1775206404
A	1558	C	G	conflict	GB 1775206404

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	111	2375	1059	433	772	111	0	0

- Molecule 3 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	266	1977	1231	381	361	4	0	0

- Molecule 4 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	184	1351	852	238	257	4	0	0

- Molecule 5 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	205	1499	938	275	285	1	0	0

- Molecule 6 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	65	Total	C	N	O	S	0	0
			468	288	87	91	2		

- Molecule 7 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	144	Total	C	N	O	S	0	0
			1121	709	206	202	4		

- Molecule 8 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	121	Total	C	N	O	S	0	0
			880	546	164	167	3		

- Molecule 9 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	117	Total	C	N	O	S	0	0
			854	532	161	160	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	119	Total	C	N	O	S	0	0
			933	572	185	172	4		

- Molecule 11 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	112	Total	C	N	O	0	0
			869	553	168	148		

- Molecule 12 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	117	Total	C	N	O	S	0	0
			904	566	182	153	3		

- Molecule 13 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	101	Total	C	N	O	0	0
			770	491	134	145		

- Molecule 14 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	109	Total	C	N	O	S	0	0
			824	514	158	150	2		

- Molecule 15 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	91	Total	C	N	O	S	0	0
			725	452	133	137	3		

- Molecule 16 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	93	Total	C	N	O	S	0	0
			686	433	127	124	2		

- Molecule 17 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	62	Total	C	N	O	0	0
			398	244	77	77		

- Molecule 18 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	65	Total	C	N	O	S	0	0
			500	305	97	96	2		

- Molecule 19 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	58	Total	C	N	O	S	0	0
			447	275	87	84	1		

- Molecule 20 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	52	Total	C	N	O	S	0	0
			402	246	81	68	7		

- Molecule 21 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	44	Total	C	N	O	S	0	0
			363	219	88	54	2		

- Molecule 22 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	V	106	Total	C	N	O	0	0
			739	455	142	142		

- Molecule 23 is a protein called GTPase Der.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	411	Total	C	N	O	S	0	0
			3064	1942	526	590	6		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	70	THR	ALA	conflict	UNP P50743
W	98	SER	ALA	conflict	UNP P50743
W	159	CYS	VAL	conflict	UNP P50743
W	217	ALA	SER	conflict	UNP P50743
W	262	GLY	ALA	conflict	UNP P50743
W	269	ASN	GLU	conflict	UNP P50743
W	292	ILE	VAL	conflict	UNP P50743
W	311	GLN	GLU	conflict	UNP P50743
W	315	GLU	ASP	conflict	UNP P50743
W	325	VAL	ILE	conflict	UNP P50743

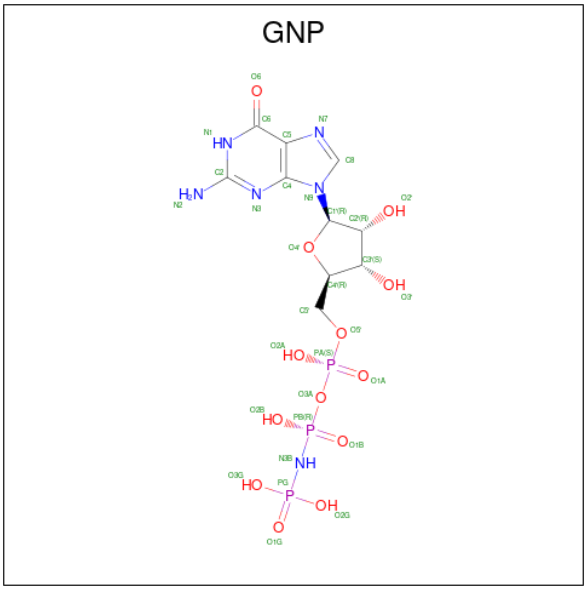
- Molecule 24 is a protein called Large ribosomal subunit protein bL33A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	47	Total	C	N	O	S	0	0
			373	227	71	72	3		

- Molecule 25 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	178	Total	C	N	O	S	0	0
			1343	857	227	255	4		

- Molecule 26 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



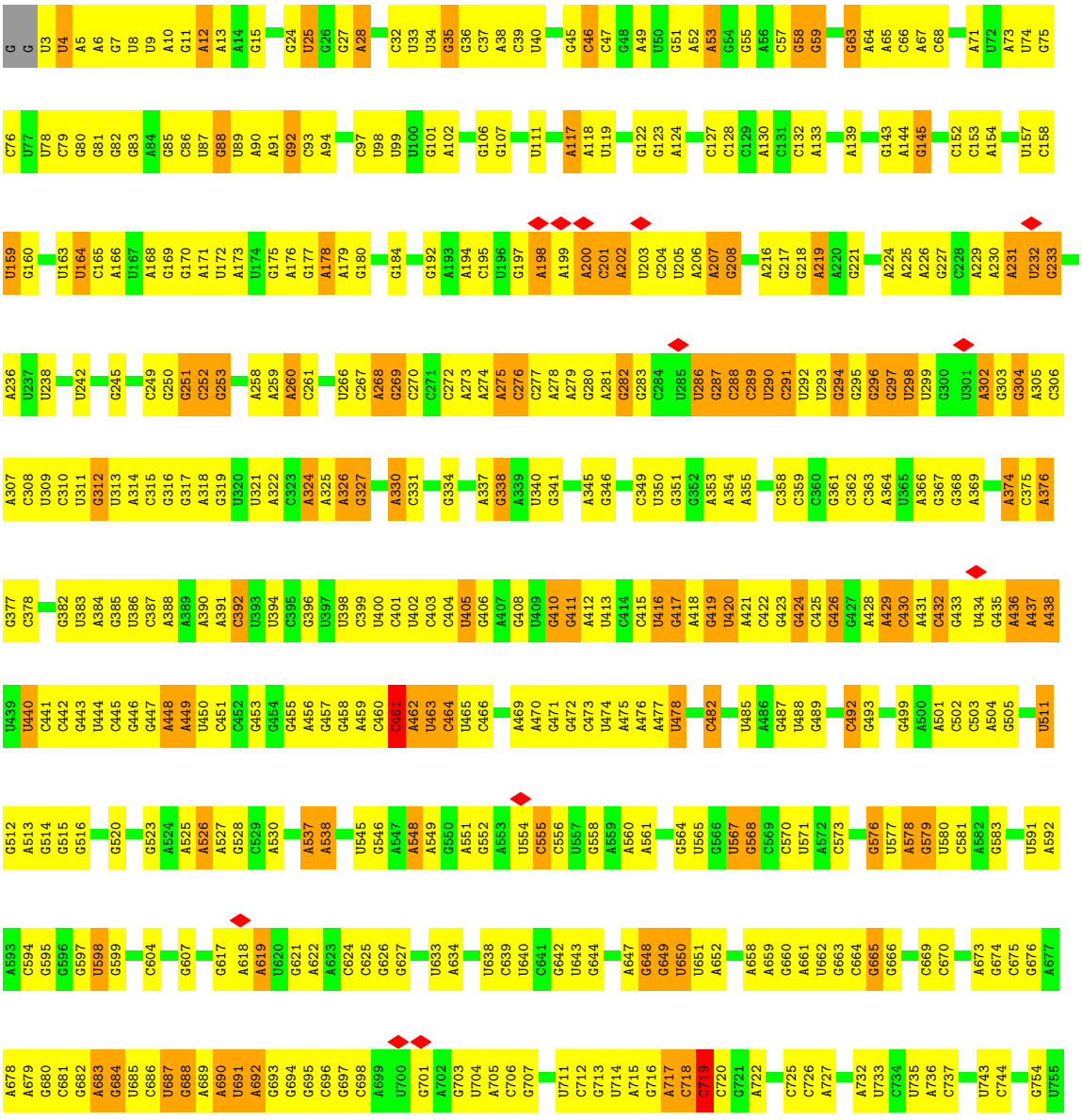
Mol	Chain	Residues	Atoms					AltConf
26	W	1	Total	C	N	O	P	0
			32	10	6	13	3	
26	W	1	Total	C	N	O	P	0
			32	10	6	13	3	

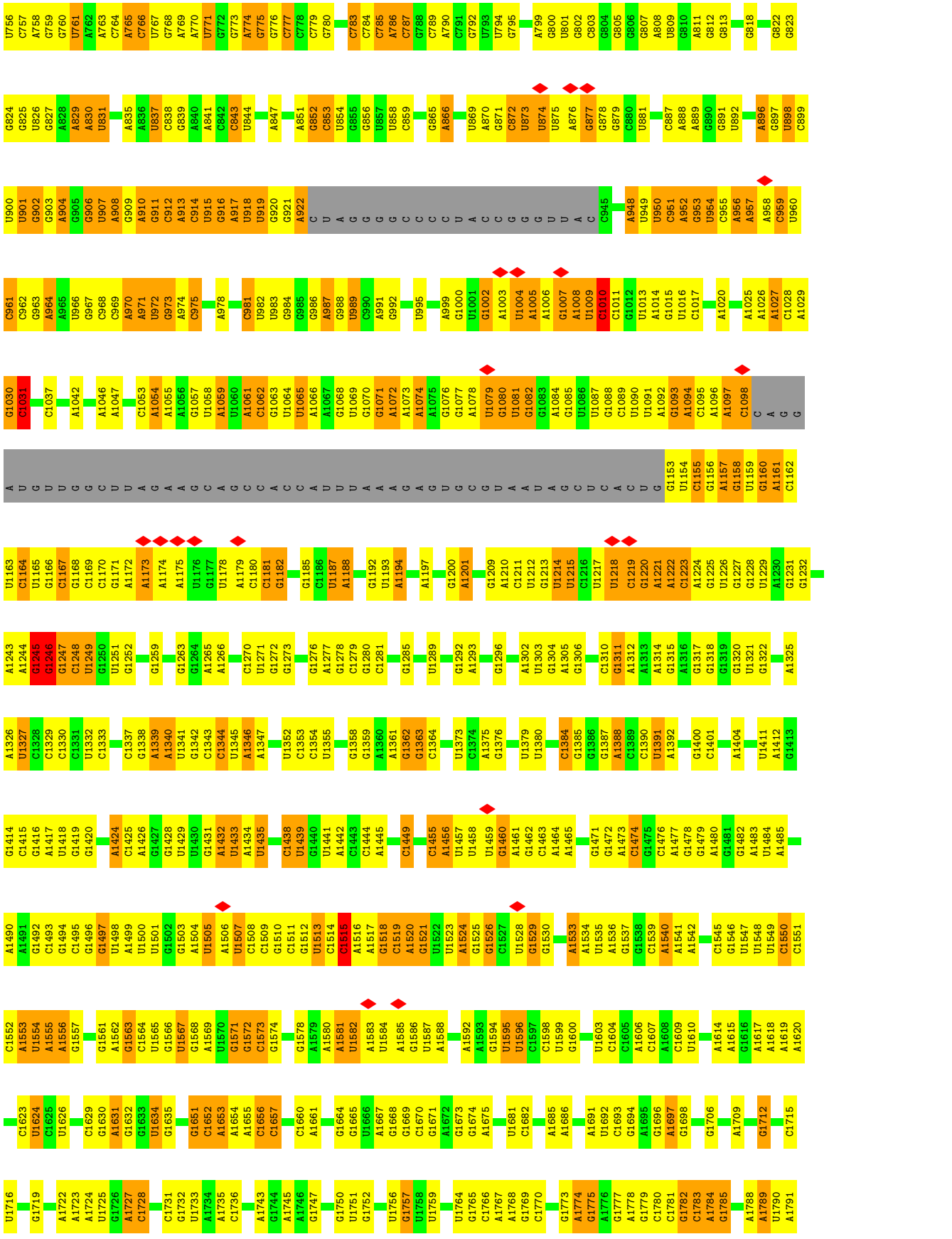
3 Residue-property plots (i)

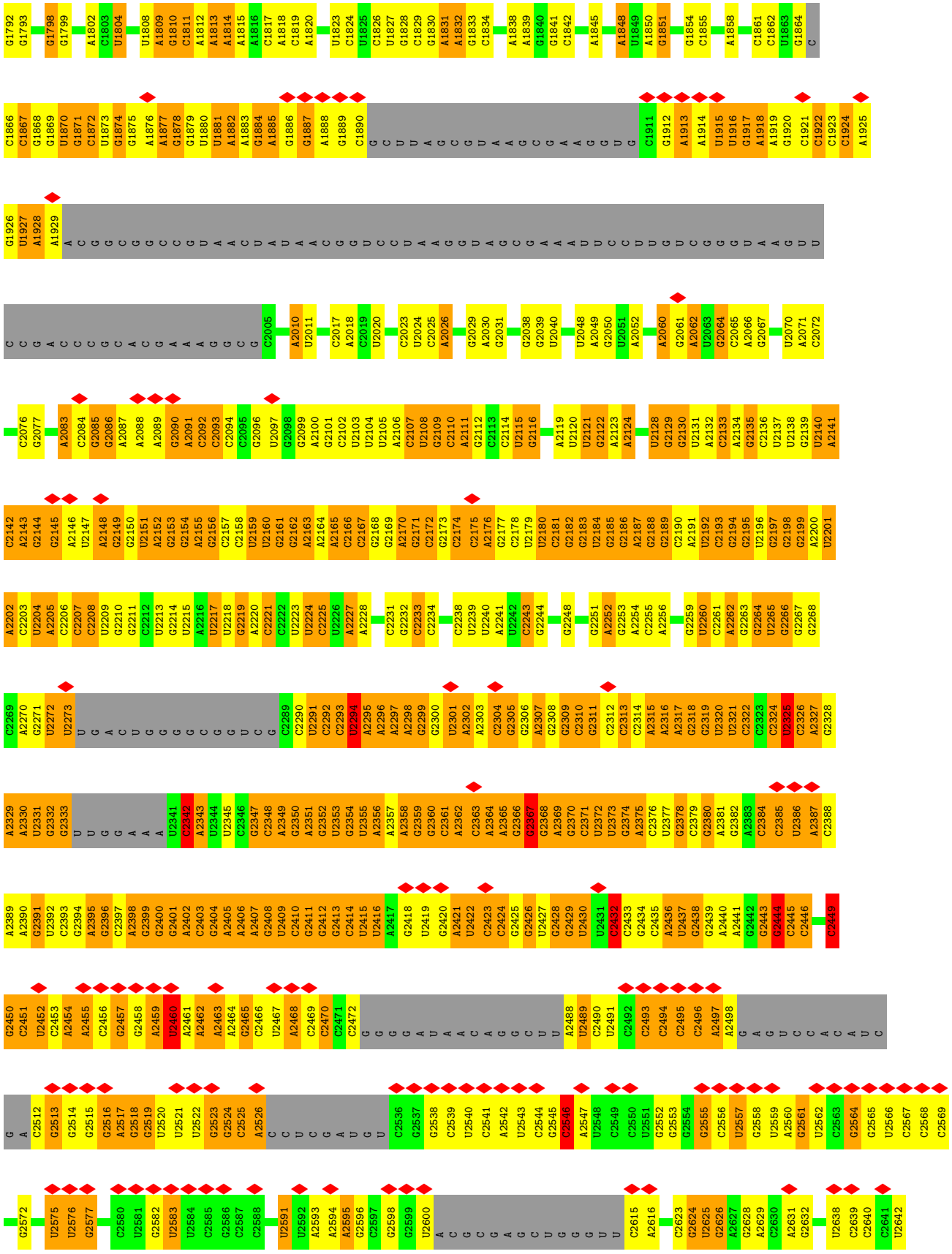
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

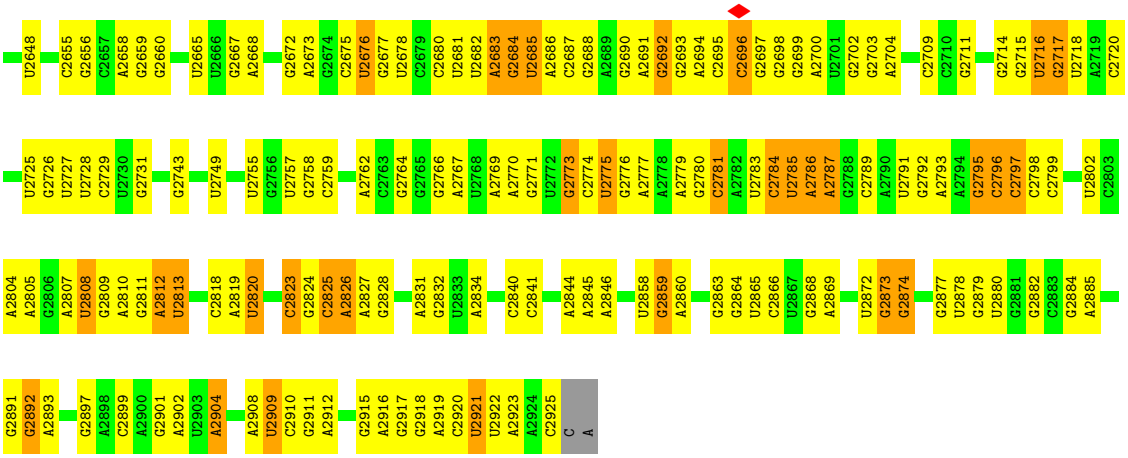
- Molecule 1: 23S rRNA

Chain A:



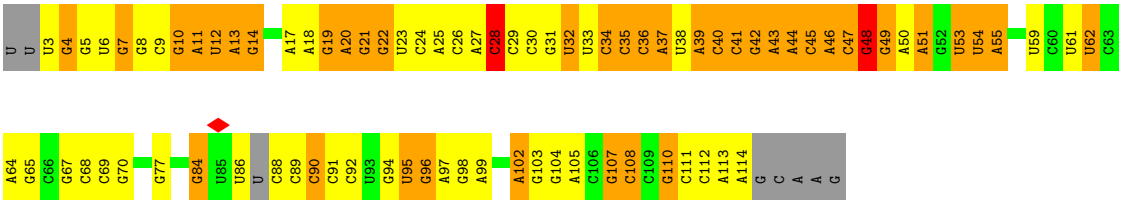






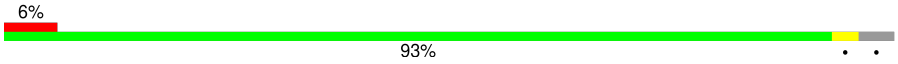
• Molecule 2: 5S rRNA

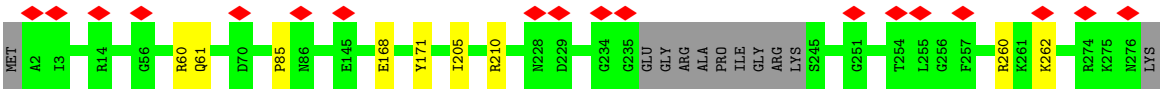
Chain B:



• Molecule 3: Large ribosomal subunit protein uL2

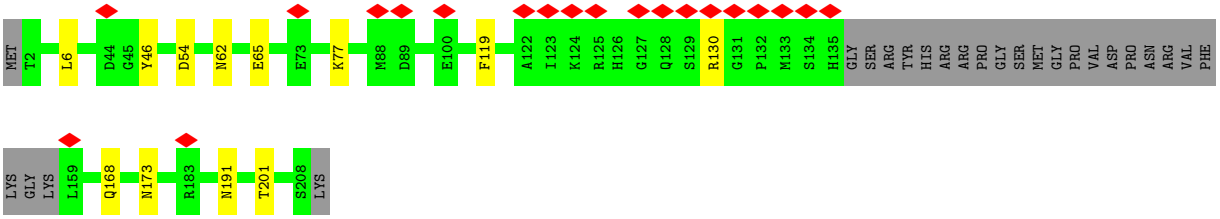
Chain C:





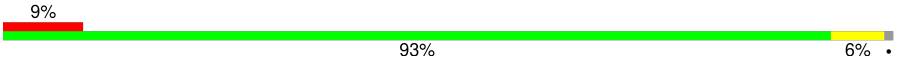
• Molecule 4: Large ribosomal subunit protein uL3

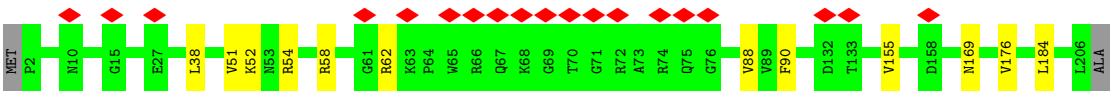
Chain D:



• Molecule 5: Large ribosomal subunit protein uL4

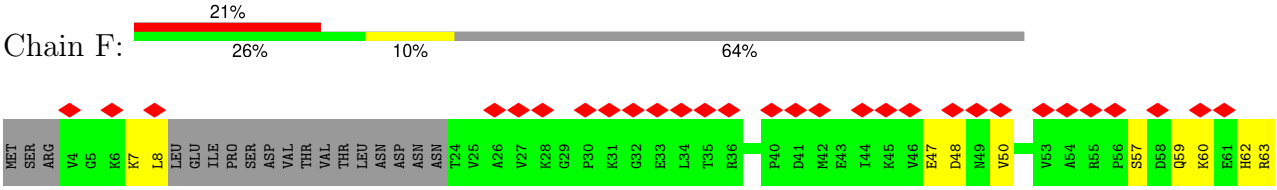
Chain E:





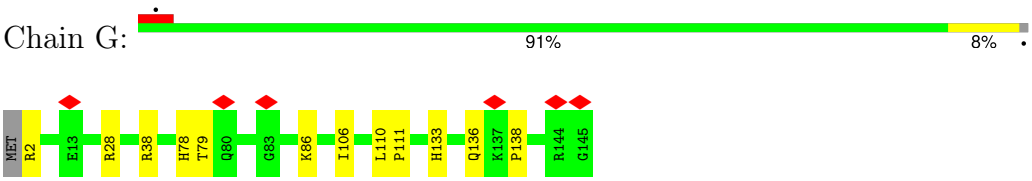
• Molecule 6: Large ribosomal subunit protein uL6

Chain F:



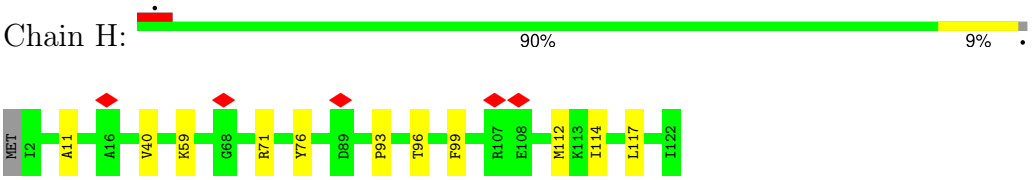
• Molecule 7: Large ribosomal subunit protein uL13

Chain G:



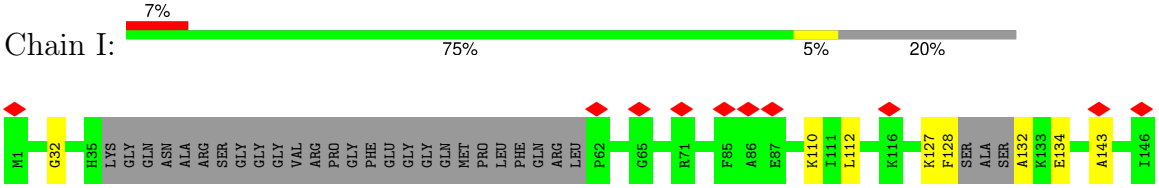
• Molecule 8: Large ribosomal subunit protein uL14

Chain H:



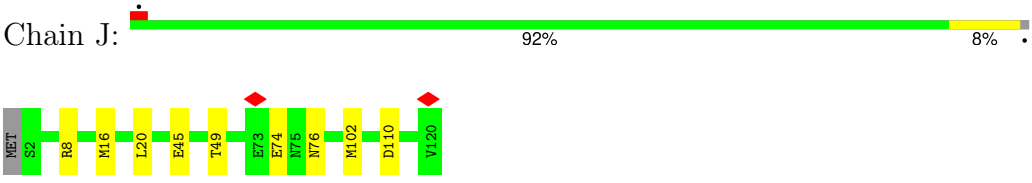
• Molecule 9: Large ribosomal subunit protein uL15

Chain I:



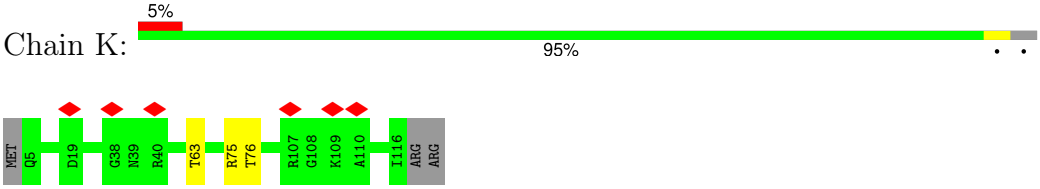
• Molecule 10: Large ribosomal subunit protein bL17

Chain J:



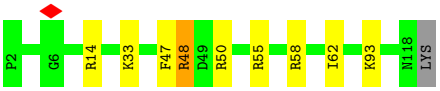
• Molecule 11: Large ribosomal subunit protein bL19

Chain K:



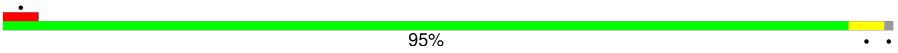
• Molecule 12: Large ribosomal subunit protein bL20

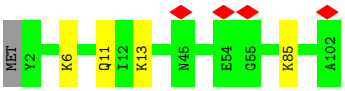
Chain L:



• Molecule 13: Large ribosomal subunit protein bL21

Chain M:



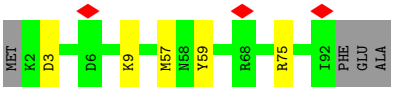


• Molecule 14: Large ribosomal subunit protein uL22

Chain N:

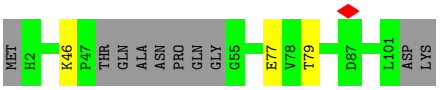
• Molecule 15: Large ribosomal subunit protein uL23

Chain O:



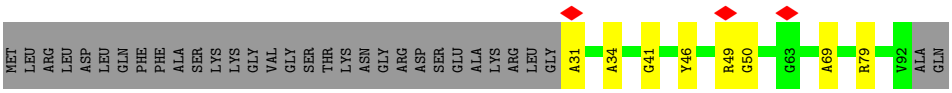
• Molecule 16: Large ribosomal subunit protein uL24

Chain P:



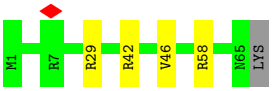
• Molecule 17: Large ribosomal subunit protein bL27

Chain Q:



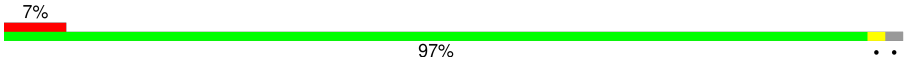
• Molecule 18: Large ribosomal subunit protein uL29

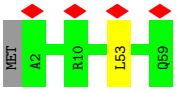
Chain R:



• Molecule 19: Large ribosomal subunit protein uL30

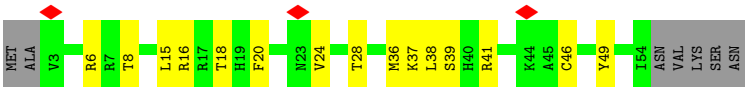
Chain S:





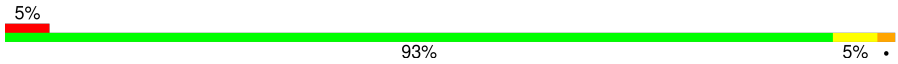
• Molecule 20: Large ribosomal subunit protein bL32

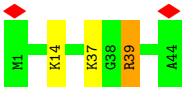
Chain T:



• Molecule 21: Large ribosomal subunit protein bL34

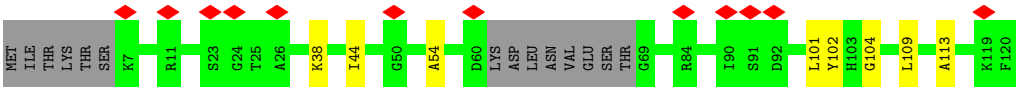
Chain U:





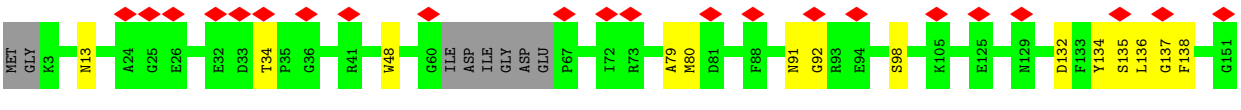
• Molecule 22: Large ribosomal subunit protein uL18

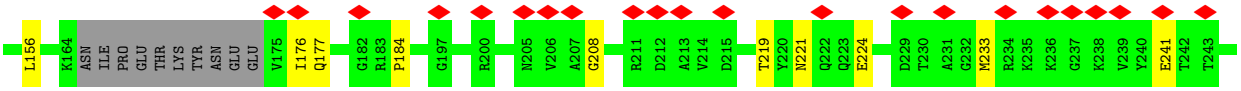
Chain V:

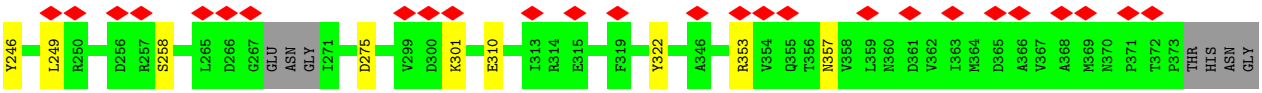


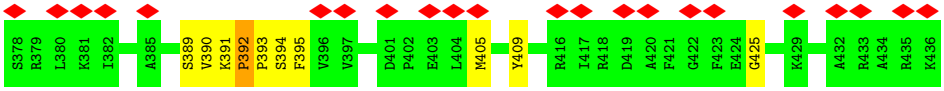
• Molecule 23: GTPase Der

Chain W:



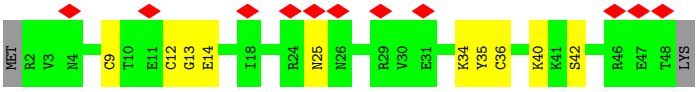






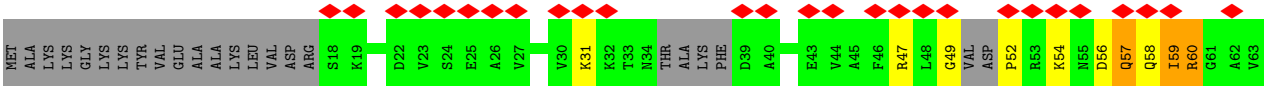
• Molecule 24: Large ribosomal subunit protein bL33A

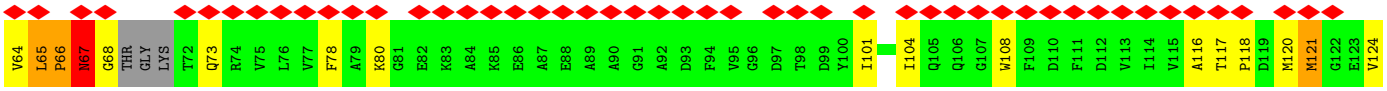
Chain Z:

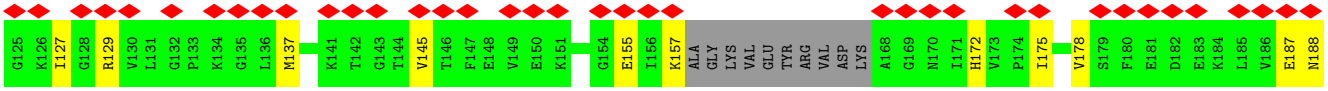


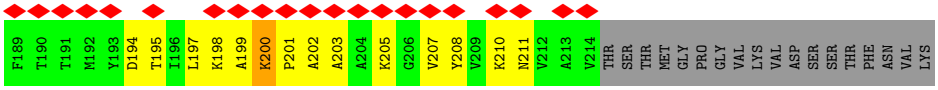
• Molecule 25: Large ribosomal subunit protein uL1

Chain Y:









4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18086	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)	1000	Depositor
Maximum defocus (nm)	2750	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.941	Depositor
Minimum map value	-0.280	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.061	Depositor
Recommended contour level	0.255	Depositor
Map size (Å)	362.52002, 362.52002, 362.52002	wwPDB
Map dimensions	424, 424, 424	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.855, 0.855, 0.855	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: GNP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.54	0/64420	0.88	47/100477 (0.0%)
2	B	0.36	0/2655	0.85	3/4136 (0.1%)
3	C	0.32	0/2011	0.57	0/2710
4	D	0.31	0/1365	0.59	0/1834
5	E	0.33	0/1516	0.55	0/2057
6	F	0.28	0/472	0.57	0/634
7	G	0.32	0/1144	0.57	0/1543
8	H	0.36	0/887	0.66	1/1200 (0.1%)
9	I	0.32	0/860	0.62	0/1146
10	J	0.33	0/940	0.68	0/1260
11	K	0.37	0/882	0.65	0/1189
12	L	0.40	0/916	0.60	0/1224
13	M	0.35	0/781	0.60	0/1051
14	N	0.33	0/833	0.62	0/1125
15	O	0.40	0/731	0.78	1/977 (0.1%)
16	P	0.34	0/694	0.62	0/928
17	Q	0.35	0/404	0.66	0/549
18	R	0.30	0/501	0.61	0/674
19	S	0.34	0/449	0.71	0/605
20	T	0.34	0/409	0.65	0/544
21	U	0.32	0/366	0.72	0/479
22	V	0.27	0/745	0.60	0/1006
23	W	0.31	0/3115	0.58	0/4237
24	Z	0.35	0/378	0.68	0/508
25	Y	0.34	0/1361	0.69	1/1833 (0.1%)
All	All	0.49	0/88835	0.83	53/133926 (0.0%)

There are no bond length outliers.

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1433	U	C2-N1-C1'	7.30	126.46	117.70
1	A	461	C	C2-N1-C1'	7.06	126.57	118.80
1	A	1921	C	N3-C2-O2	-6.89	117.08	121.90
1	A	461	C	N1-C2-O2	6.85	123.01	118.90
25	Y	54	LYS	N-CA-CB	-6.75	98.45	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	57517	0	28951	1602	0
2	B	2375	0	1203	78	0
3	C	1977	0	1995	6	0
4	D	1351	0	1384	12	0
5	E	1499	0	1523	9	0
6	F	468	0	460	12	0
7	G	1121	0	1145	11	0
8	H	880	0	895	6	0
9	I	854	0	886	13	0
10	J	933	0	956	8	0
11	K	869	0	883	3	0
12	L	904	0	921	16	0
13	M	770	0	791	2	0
14	N	824	0	861	7	0
15	O	725	0	759	4	0
16	P	686	0	724	2	0
17	Q	398	0	311	12	0
18	R	500	0	491	4	0
19	S	447	0	469	1	0
20	T	402	0	403	12	0
21	U	363	0	399	3	0
22	V	739	0	700	5	0
23	W	3064	0	2926	66	0
24	Z	373	0	355	9	0
25	Y	1343	0	1366	118	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	W	64	0	26	1	0
All	All	81446	0	51783	1886	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 15.

The worst 5 of 1886 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)
23:W:132:ASP:HA	25:Y:137:MET:CE	1.33	1.55
23:W:132:ASP:CA	25:Y:137:MET:HE1	1.35	1.52
23:W:389:SER:OG	23:W:394:SER:HB2	1.21	1.36
23:W:134:TYR:O	25:Y:129:ARG:CD	1.83	1.26
1:A:2351:A:H2	1:A:2361:C:N4	1.31	1.26

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	
3	C	262/277 (95%)	238 (91%)	24 (9%)	0	100	100
4	D	180/209 (86%)	170 (94%)	10 (6%)	0	100	100
5	E	203/207 (98%)	189 (93%)	14 (7%)	0	100	100
6	F	61/179 (34%)	59 (97%)	2 (3%)	0	100	100
7	G	142/145 (98%)	130 (92%)	12 (8%)	0	100	100
8	H	119/122 (98%)	106 (89%)	13 (11%)	0	100	100
9	I	111/146 (76%)	105 (95%)	6 (5%)	0	100	100
10	J	117/120 (98%)	108 (92%)	9 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	110/115 (96%)	103 (94%)	7 (6%)	0	100	100
12	L	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
13	M	99/102 (97%)	89 (90%)	10 (10%)	0	100	100
14	N	107/113 (95%)	100 (94%)	7 (6%)	0	100	100
15	O	89/95 (94%)	81 (91%)	8 (9%)	0	100	100
16	P	89/103 (86%)	80 (90%)	9 (10%)	0	100	100
17	Q	60/94 (64%)	56 (93%)	4 (7%)	0	100	100
18	R	63/66 (96%)	58 (92%)	5 (8%)	0	100	100
19	S	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
20	T	50/59 (85%)	46 (92%)	4 (8%)	0	100	100
21	U	42/44 (96%)	40 (95%)	2 (5%)	0	100	100
22	V	102/120 (85%)	94 (92%)	8 (8%)	0	100	100
23	W	401/436 (92%)	367 (92%)	33 (8%)	1 (0%)	44	71
24	Z	45/49 (92%)	43 (96%)	2 (4%)	0	100	100
25	Y	168/232 (72%)	148 (88%)	18 (11%)	2 (1%)	11	38
All	All	2791/3210 (87%)	2572 (92%)	216 (8%)	3 (0%)	50	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	Y	66	PRO
25	Y	67	ASN
23	W	392	PRO

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	
3	C	202/225 (90%)	202 (100%)	0	100	100
4	D	139/170 (82%)	138 (99%)	1 (1%)	81	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	E	155/170 (91%)	154 (99%)	1 (1%)	84 90
6	F	48/151 (32%)	47 (98%)	1 (2%)	48 70
7	G	117/123 (95%)	117 (100%)	0	100 100
8	H	92/101 (91%)	92 (100%)	0	100 100
9	I	85/110 (77%)	85 (100%)	0	100 100
10	J	94/100 (94%)	94 (100%)	0	100 100
11	K	85/100 (85%)	85 (100%)	0	100 100
12	L	86/97 (89%)	85 (99%)	1 (1%)	67 80
13	M	79/84 (94%)	78 (99%)	1 (1%)	65 79
14	N	86/93 (92%)	85 (99%)	1 (1%)	67 80
15	O	80/85 (94%)	79 (99%)	1 (1%)	65 79
16	P	74/87 (85%)	74 (100%)	0	100 100
17	Q	27/74 (36%)	27 (100%)	0	100 100
18	R	48/57 (84%)	48 (100%)	0	100 100
19	S	50/53 (94%)	50 (100%)	0	100 100
20	T	44/53 (83%)	43 (98%)	1 (2%)	45 68
21	U	38/39 (97%)	37 (97%)	1 (3%)	41 66
22	V	64/93 (69%)	63 (98%)	1 (2%)	58 76
23	W	309/372 (83%)	302 (98%)	7 (2%)	45 68
24	Z	41/47 (87%)	41 (100%)	0	100 100
25	Y	140/185 (76%)	130 (93%)	10 (7%)	12 37
All	All	2183/2669 (82%)	2156 (99%)	27 (1%)	66 80

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	W	395	PHE
25	Y	56	ASP
25	Y	200	LYS
23	W	409	TYR
25	Y	57	GLN

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

Mol	Chain	Res	Type
25	Y	188	ASN
25	Y	106	GLN
23	W	13	ASN
25	Y	67	ASN
21	U	6	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2666/2927 (91%)	919 (34%)	75 (2%)
2	B	109/119 (91%)	55 (50%)	5 (4%)
All	All	2775/3046 (91%)	974 (35%)	80 (2%)

5 of 974 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	12	A
1	A	13	A
1	A	15	G
1	A	25	U

5 of 80 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2374	G
1	A	2784	C
1	A	2400	G
1	A	2450	G
2	B	13	A

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands 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	$\#\|Z\| > 2$
26	GNP	W	502	-	29,34,34	1.58	6 (20%)	33,54,54	2.22	5 (15%)
26	GNP	W	501	-	29,34,34	1.52	7 (24%)	33,54,54	2.18	4 (12%)

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
26	GNP	W	502	-	-	5/14/38/38	0/3/3/3
26	GNP	W	501	-	-	6/14/38/38	0/3/3/3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	W	502	GNP	PB-O3A	4.36	1.64	1.59
26	W	501	GNP	PB-O3A	3.24	1.63	1.59
26	W	501	GNP	C6-N1	3.11	1.38	1.33
26	W	501	GNP	PB-O1B	3.10	1.50	1.46
26	W	502	GNP	C6-N1	2.98	1.38	1.33

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	W	502	GNP	C5-C6-N1	-8.64	111.87	123.42
26	W	501	GNP	C5-C6-N1	-8.64	111.87	123.42
26	W	501	GNP	C2-N1-C6	6.65	125.21	115.96
26	W	502	GNP	C2-N1-C6	6.62	125.16	115.96
26	W	501	GNP	N3-C2-N1	-2.87	123.56	127.21

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	W	501	GNP	PG-N3B-PB-O1B
26	W	501	GNP	C5'-O5'-PA-O3A
26	W	501	GNP	C5'-O5'-PA-O2A
26	W	501	GNP	O4'-C4'-C5'-O5'
26	W	502	GNP	PB-N3B-PG-O1G

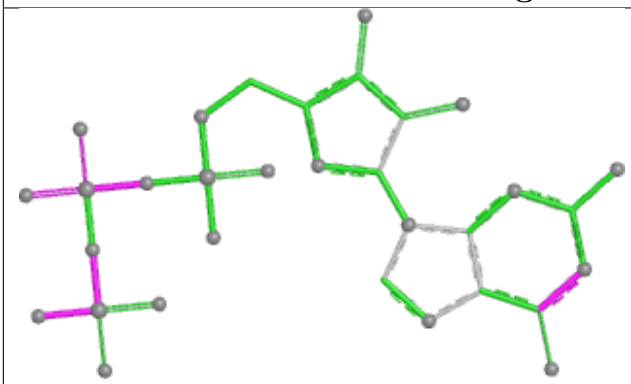
There are no ring outliers.

1 monomer is involved in 1 short contact:

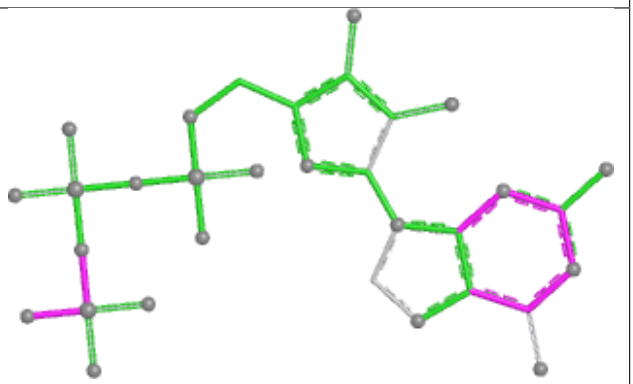
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	W	502	GNP	1	0

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.

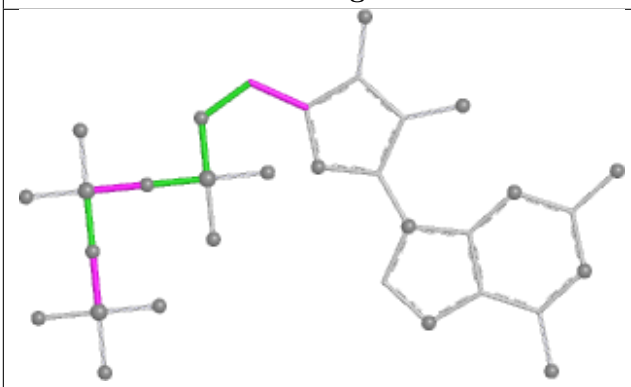
Ligand GNP W 502



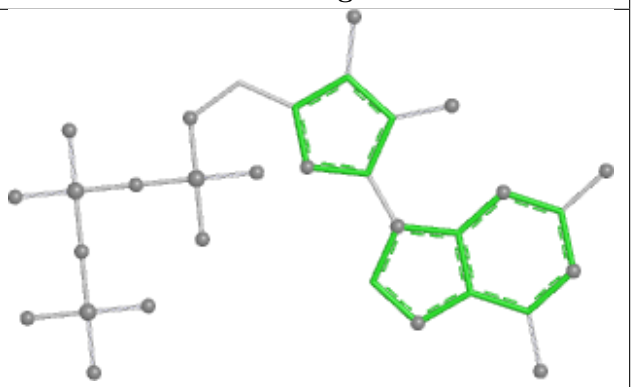
Bond lengths



Bond angles

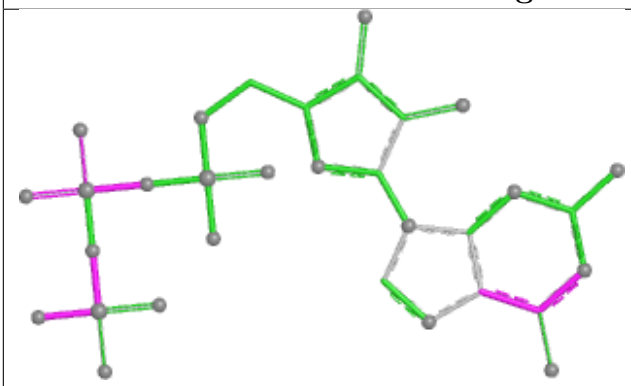


Torsions

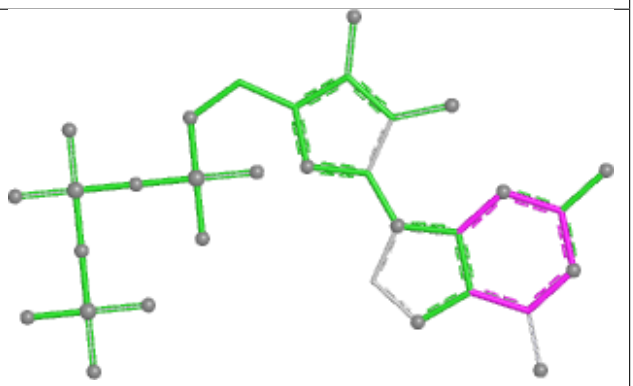


Rings

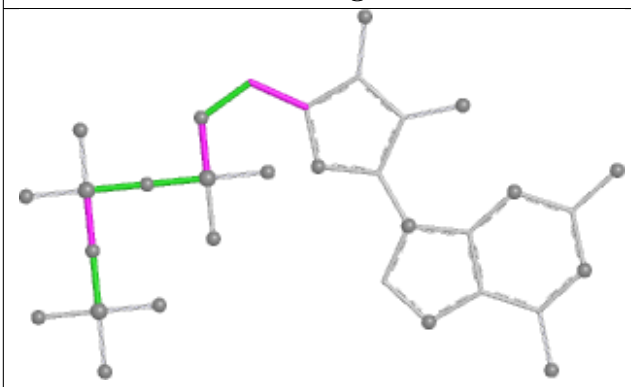
Ligand GNP W 501



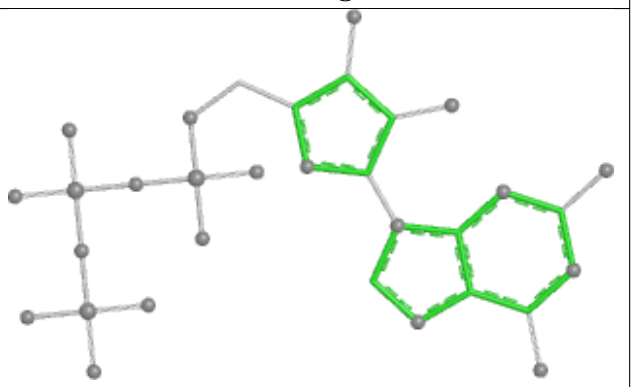
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

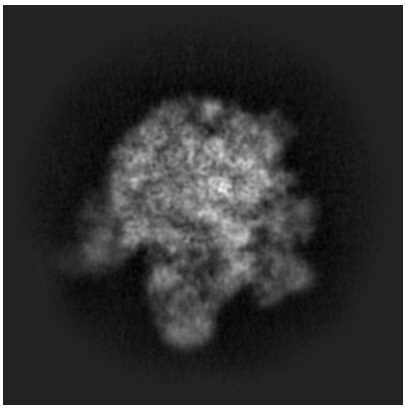
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-44849. These allow visual inspection of the internal detail of the map and identification of artifacts.

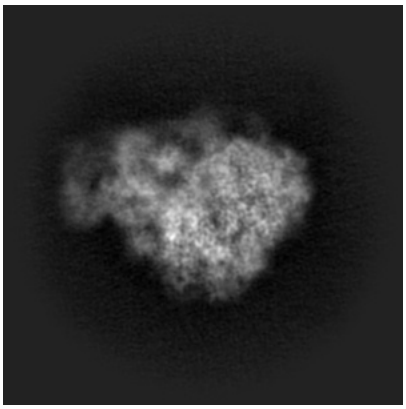
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

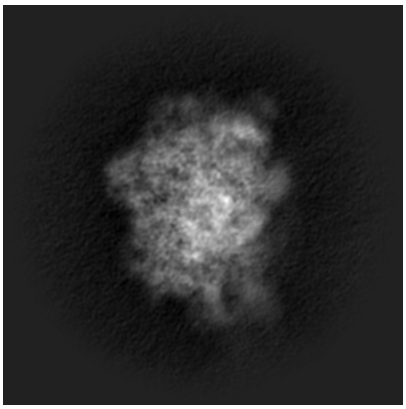
6.1.1 Primary map



X

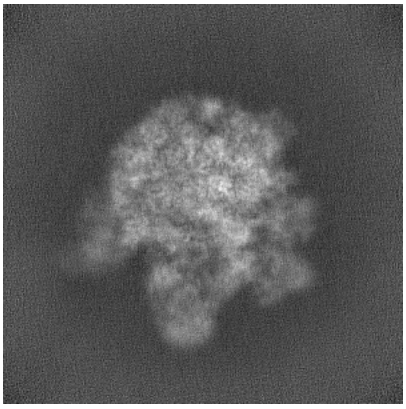


Y

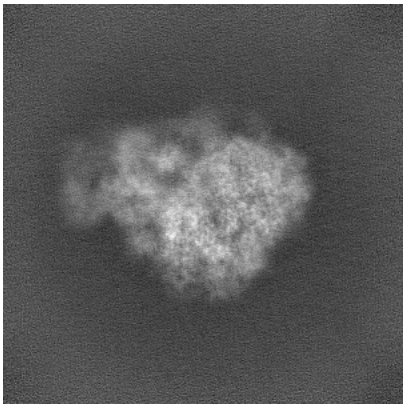


Z

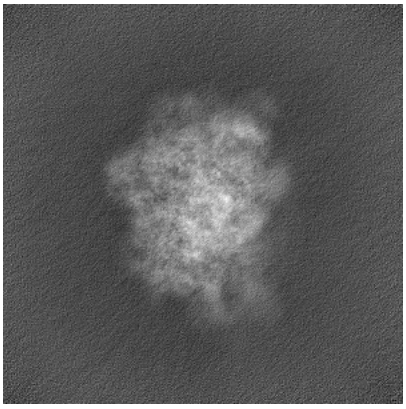
6.1.2 Raw map



X



Y

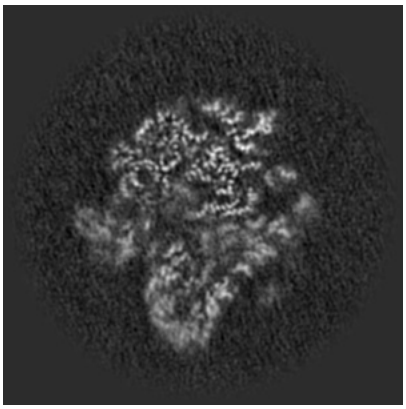


Z

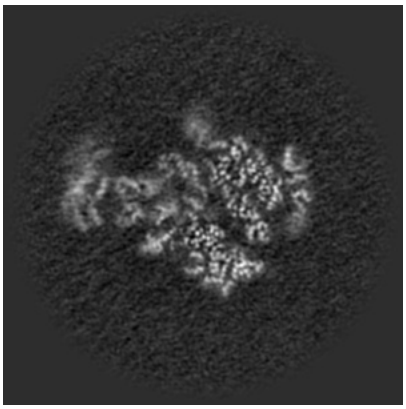
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

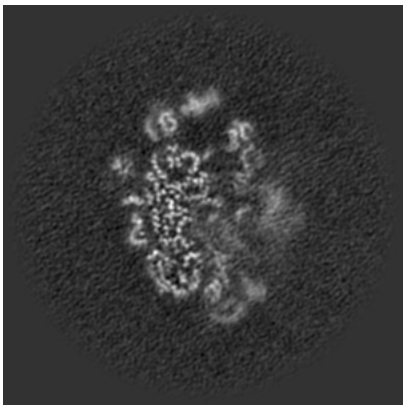
6.2.1 Primary map



X Index: 212

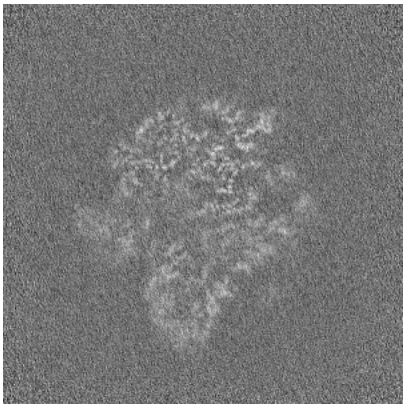


Y Index: 212

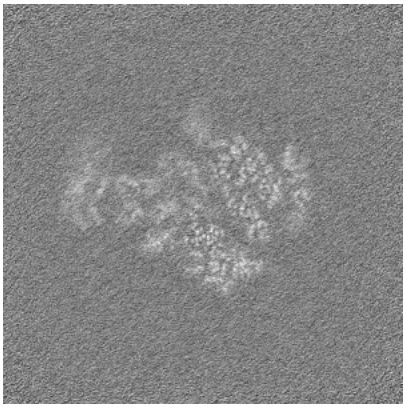


Z Index: 212

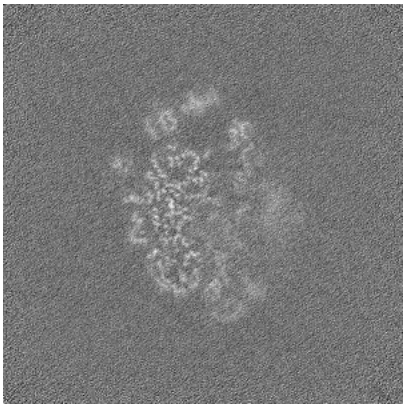
6.2.2 Raw map



X Index: 212



Y Index: 212

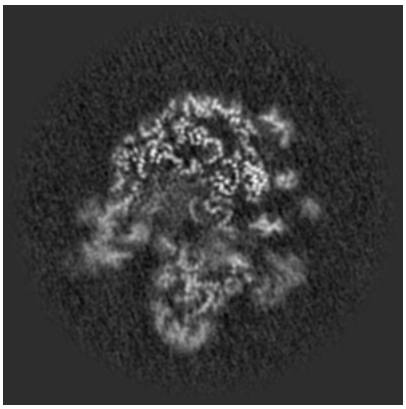


Z Index: 212

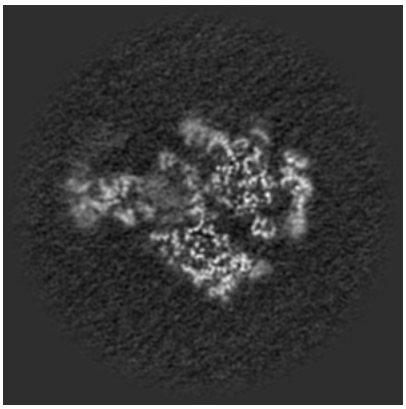
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

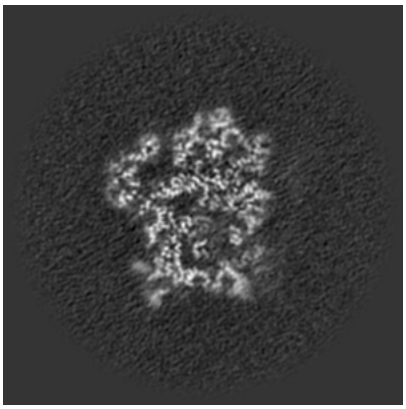
6.3.1 Primary map



X Index: 224

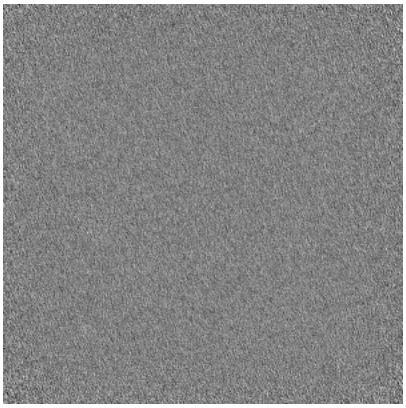


Y Index: 219

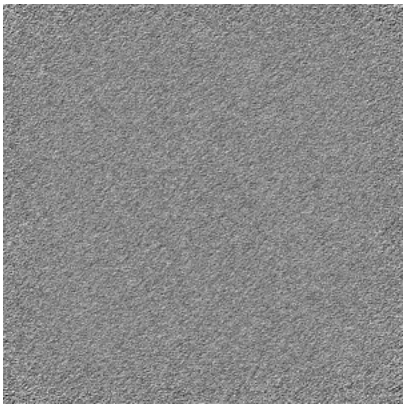


Z Index: 238

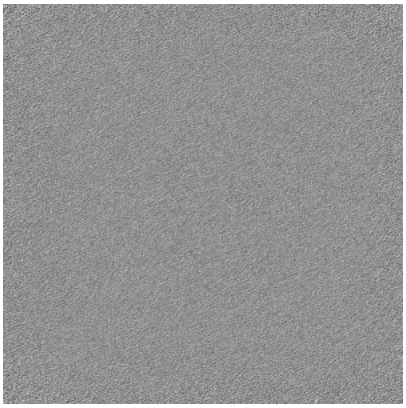
6.3.2 Raw map



X Index: 0



Y Index: 0

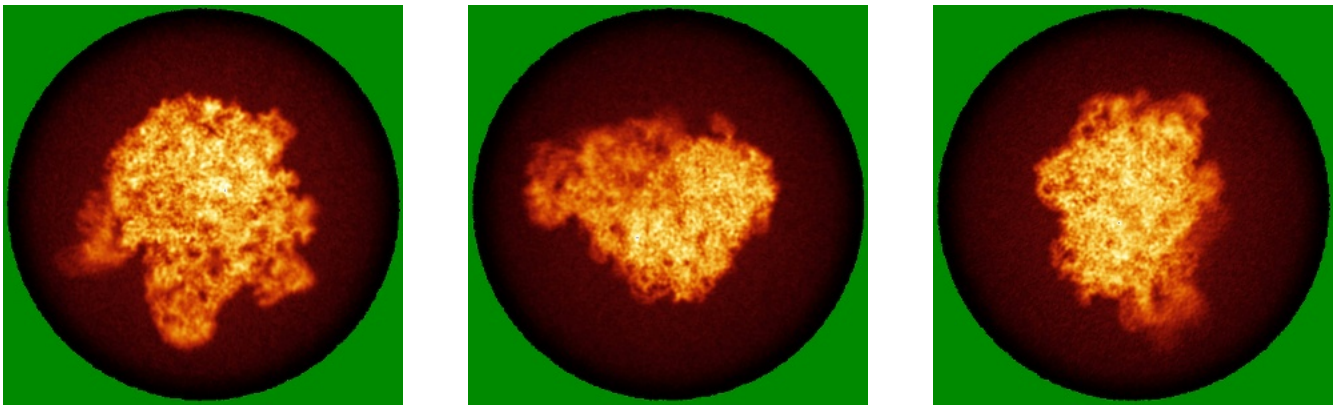


Z Index: 0

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

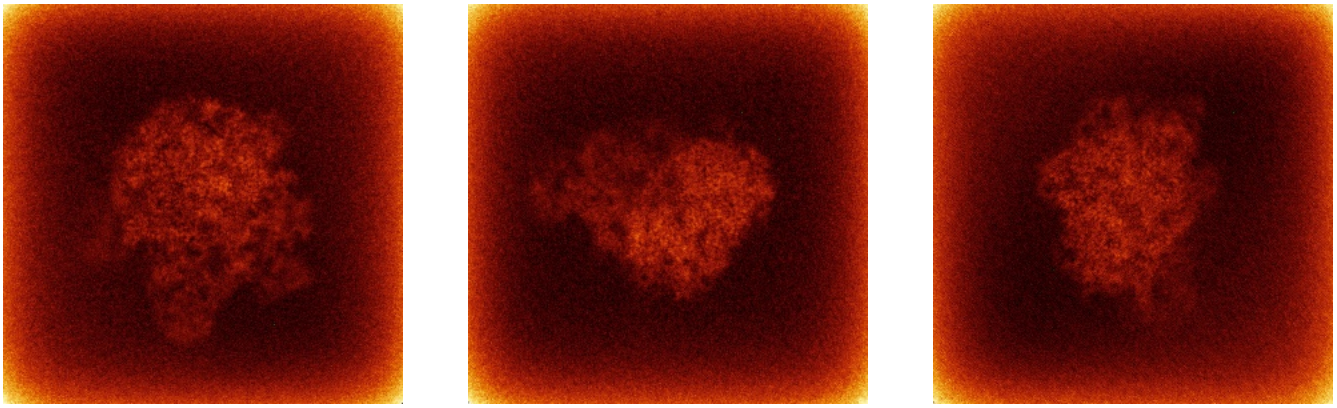
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map



X Y Z

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

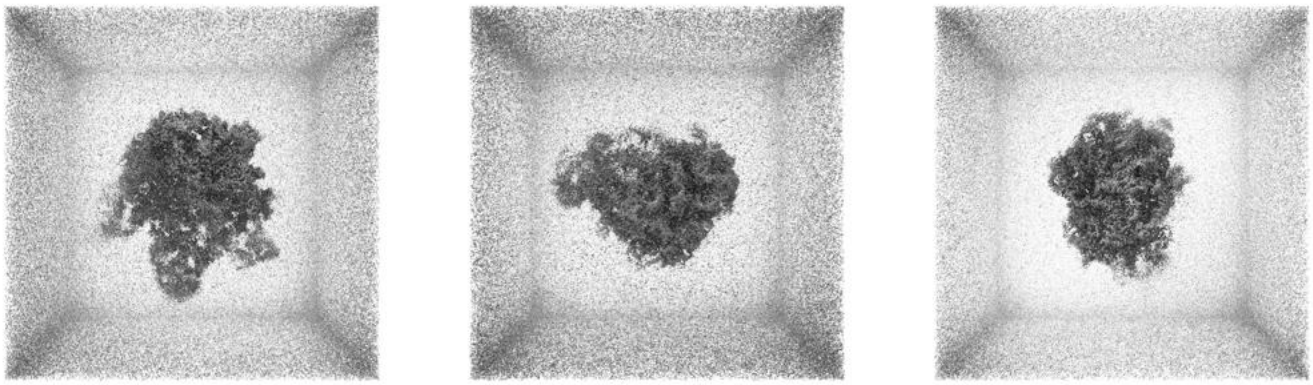
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.255. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

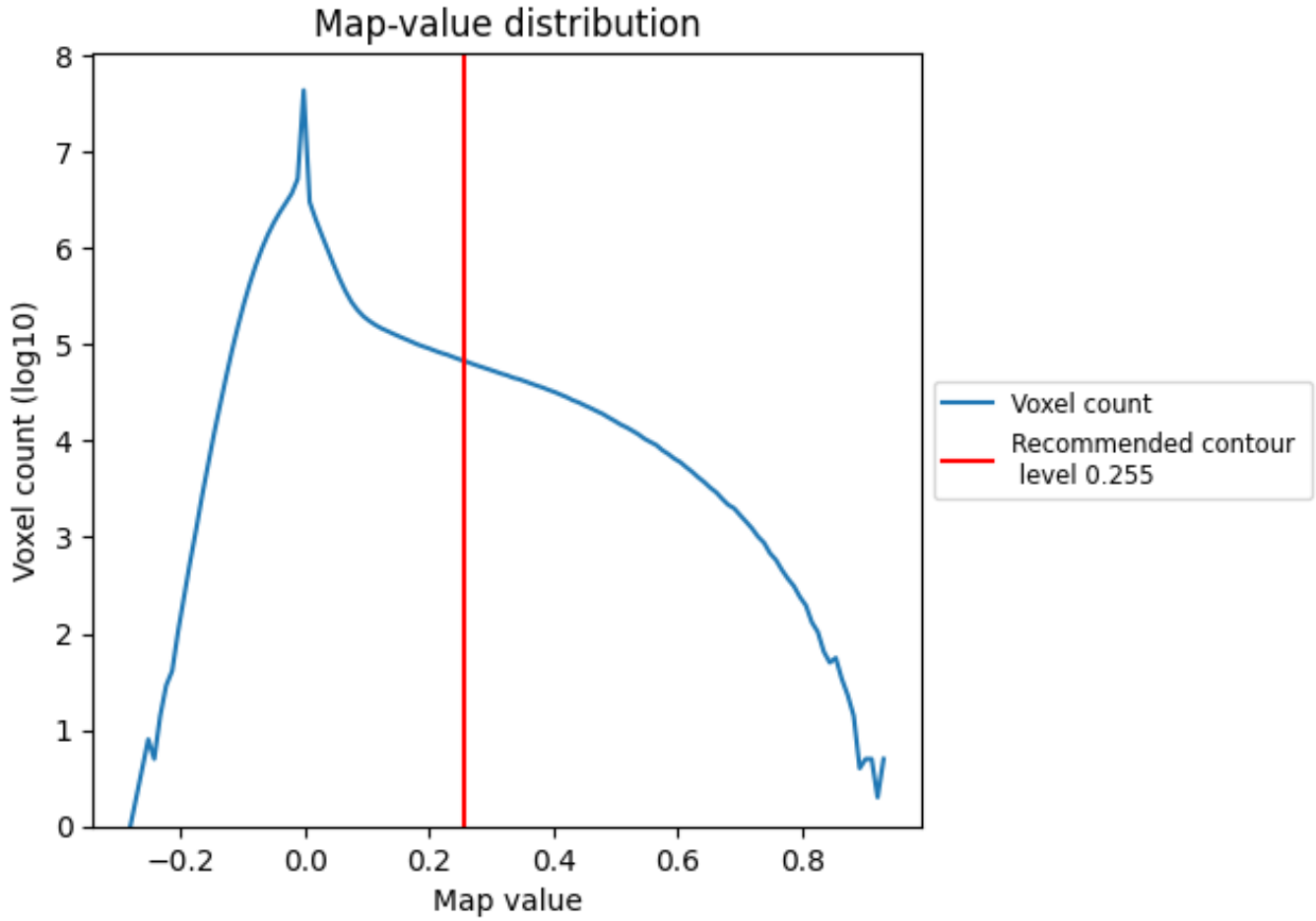
6.6 Mask visualisation (i)

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

7 Map analysis

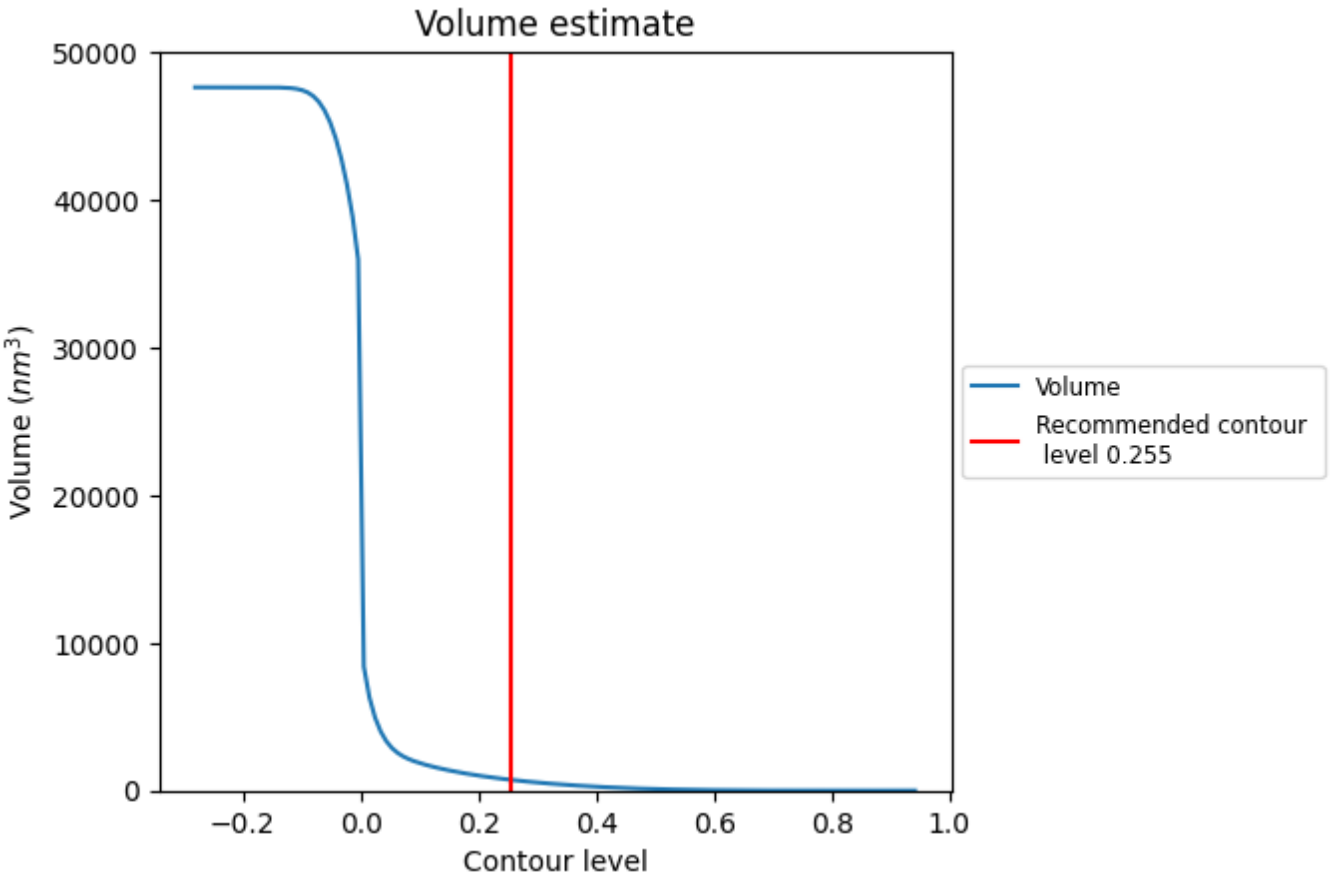
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

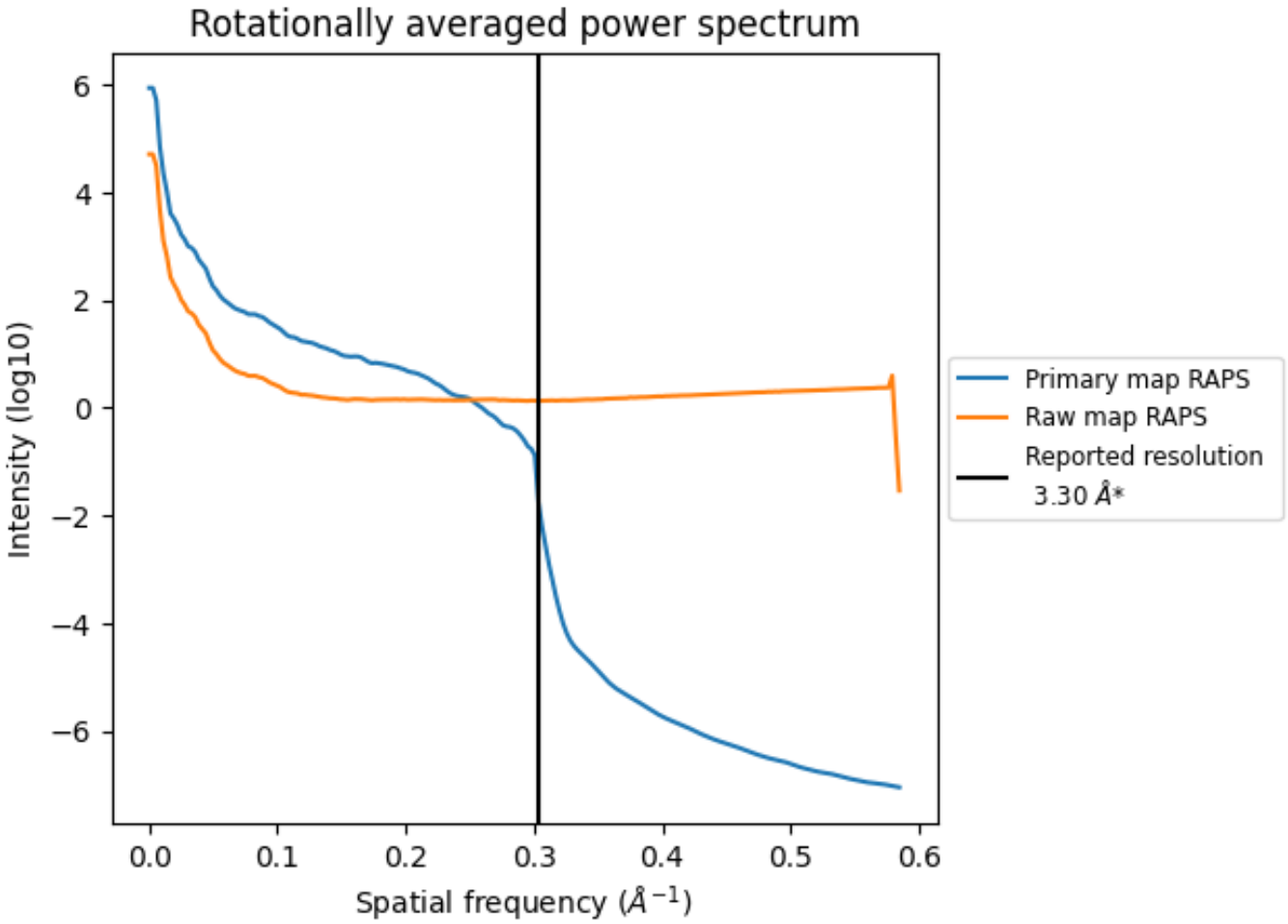
7.2 Volume estimate (i)



The volume at the recommended contour level is 729 nm^3; this corresponds to an approximate mass of 658 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)

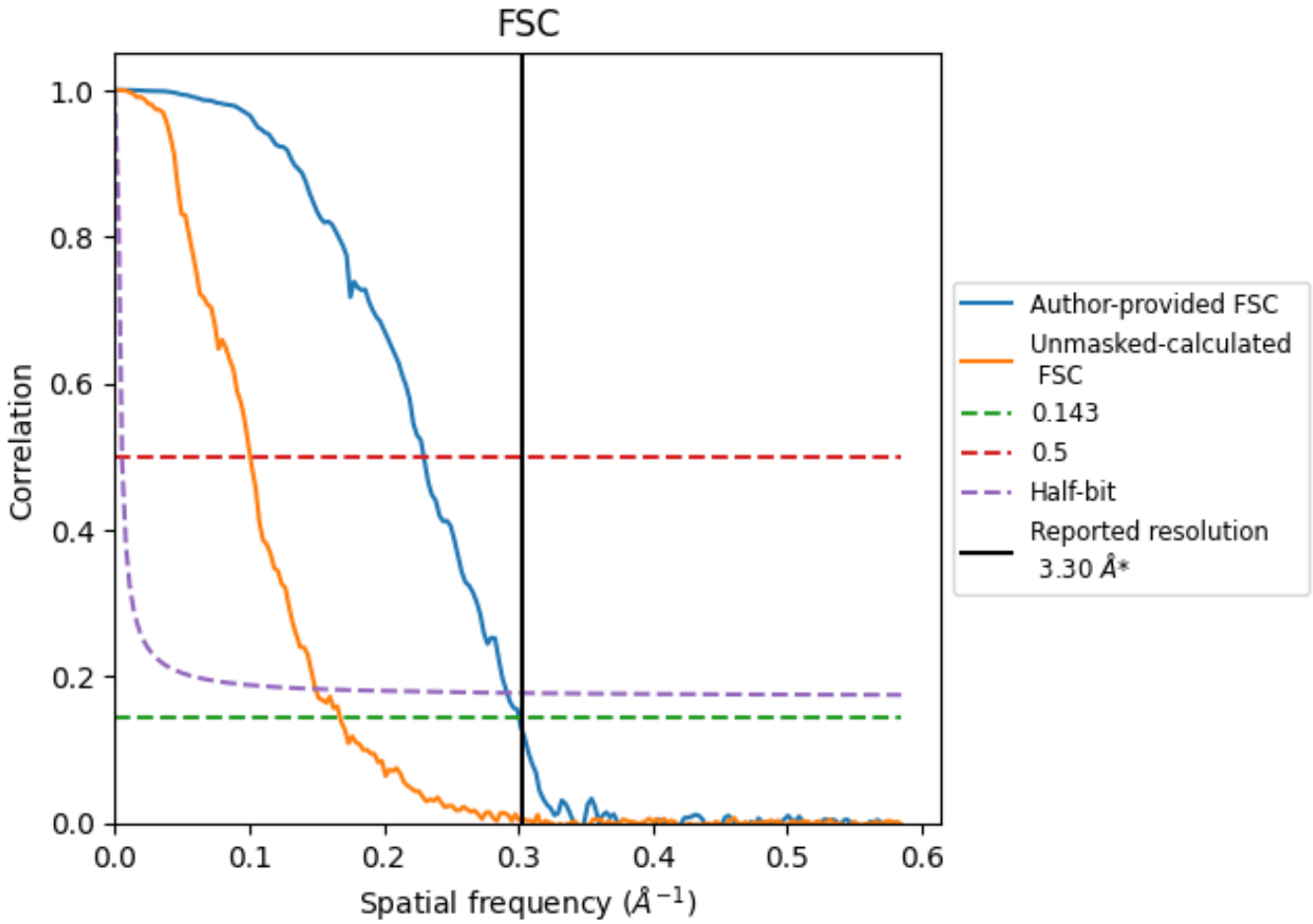


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

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 0.303 Å^{-1}

8.2 Resolution estimates (i)

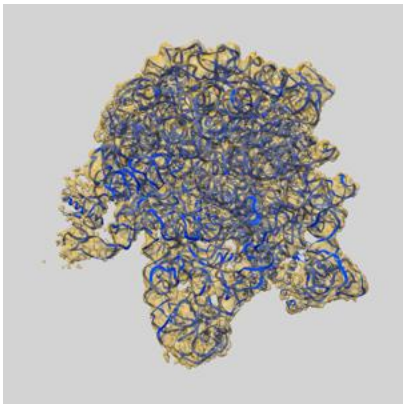
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.33	4.35	3.43
Unmasked-calculated*	5.97	9.93	6.70

*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 5.97 differs from the reported value 3.3 by more than 10 %

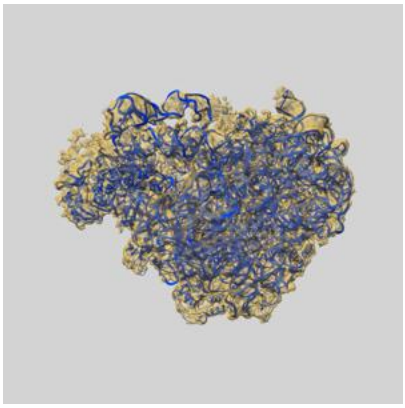
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-44849 and PDB model 9BS0. Per-residue inclusion information can be found in section 3 on page 9.

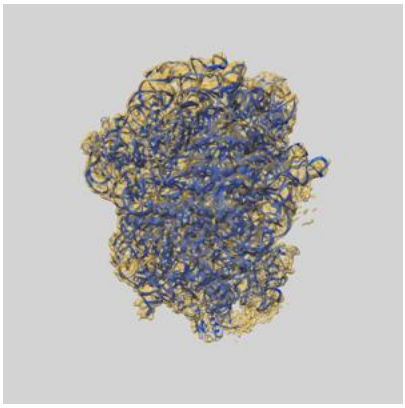
9.1 Map-model overlay



X



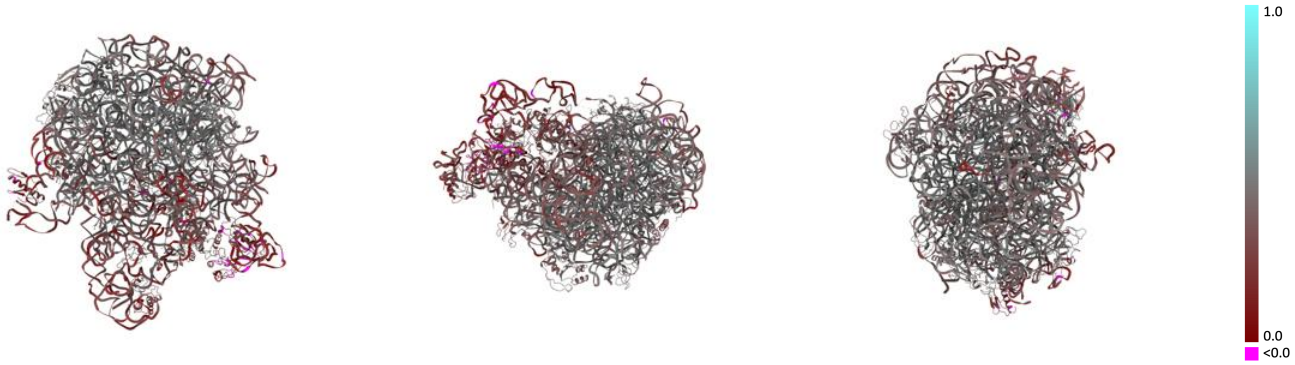
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.255 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.

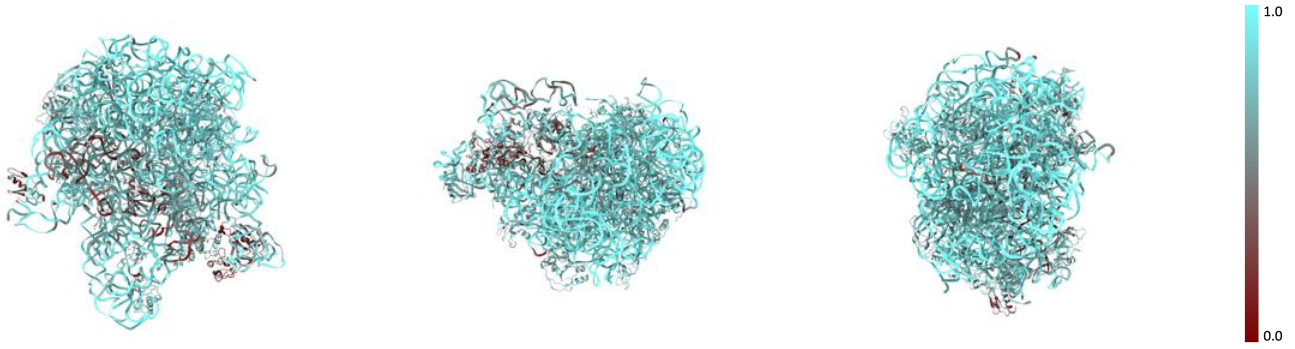
9.2 Q-score mapped to coordinate model (i)



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.

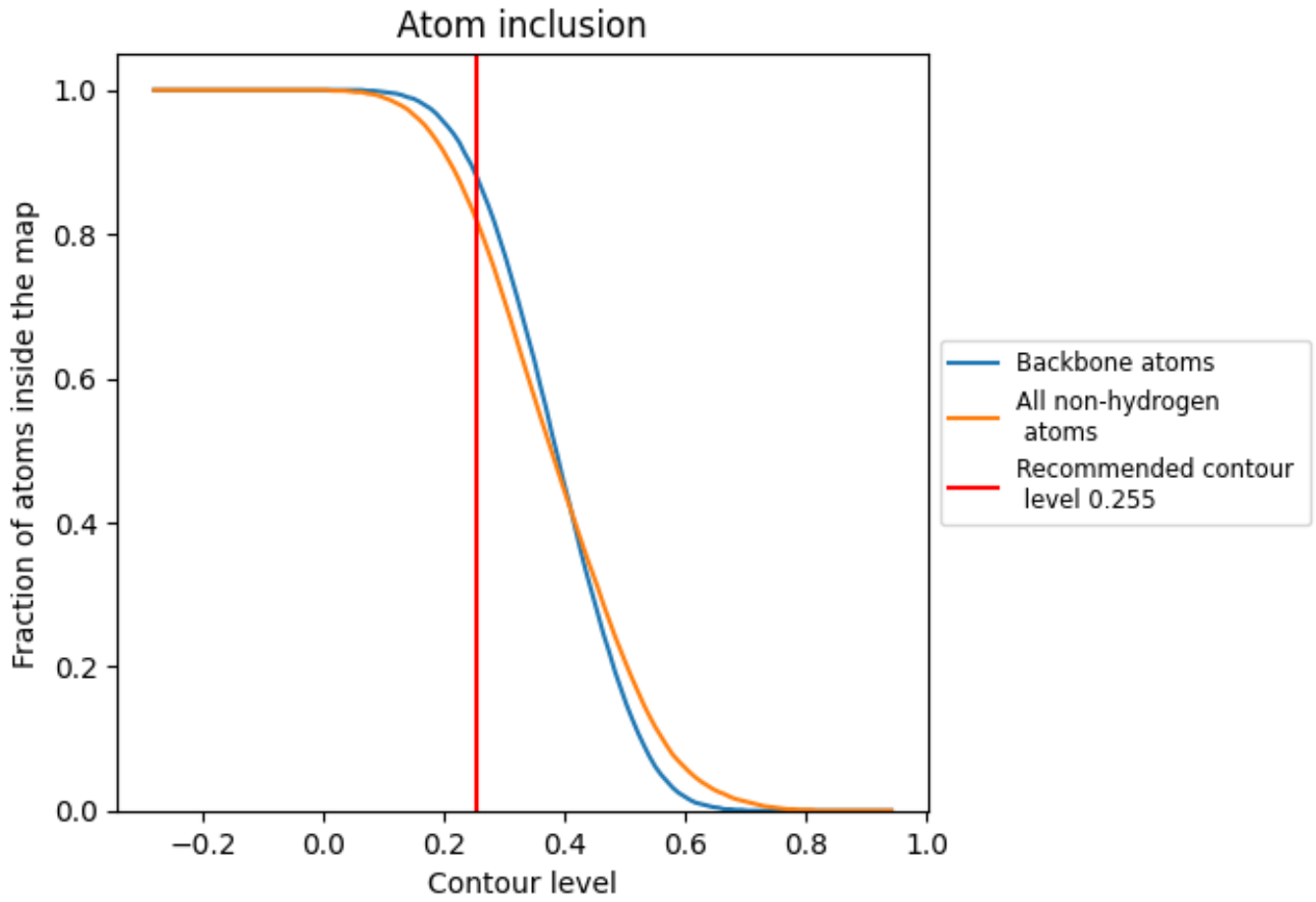
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.255).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 82% 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 (0.255) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8170	0.3900
A	0.8760	0.3950
B	0.8790	0.2760
C	0.7050	0.4410
D	0.6730	0.4380
E	0.7060	0.4210
F	0.3720	0.2340
G	0.7180	0.4260
H	0.6880	0.4240
I	0.6780	0.3970
J	0.7370	0.4270
K	0.7280	0.4280
L	0.7680	0.4470
M	0.7280	0.4420
N	0.7180	0.4530
O	0.7090	0.4390
P	0.7550	0.4150
Q	0.6910	0.4120
R	0.7090	0.3410
S	0.6730	0.3920
T	0.7280	0.4430
U	0.7570	0.4790
V	0.6720	0.2970
W	0.5640	0.3520
Y	0.2440	0.1470
Z	0.5950	0.3740