



wwPDB EM Validation Summary Report ⓘ

Mar 2, 2024 – 07:57 pm GMT

PDB ID : 8CEC
EMDB ID : EMD-16605
Title : Rnase R bound to a 30S degradation intermediate (State I - head-turning)
Authors : Paternoga, H.; Dimitrova-Paternoga, L.; Wilson, D.N.
Deposited on : 2023-02-01
Resolution : 3.57 Å (reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

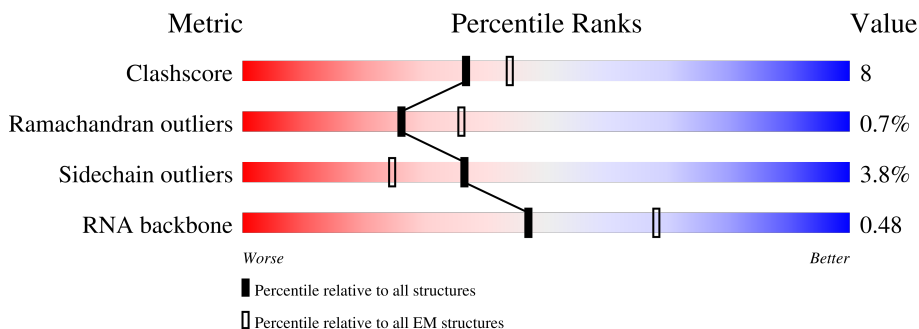
EMDB validation analysis : 0.0.1.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 3.57 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 $\leq 5\%$. 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	1554	
2	B	7	
3	C	779	
4	D	246	
5	F	200	
6	G	166	
7	I	132	

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Mol	Chain	Length	Quality of chain
8	L	138	
9	O	89	
10	P	90	
11	Q	87	
12	S	88	
13	T	95	
14	U	79	
15	V	131	
16	H	218	
17	K	156	
18	N	130	
19	R	102	
20	X	121	
21	Y	61	
22	a	92	

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 51964 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 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	1333	28597	12753	5245	9266	1333	0	0

- Molecule 2 is a RNA chain called RNA Substrate.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	7	154	70	35	42	7	0	0

- Molecule 3 is a protein called Ribonuclease R.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	708	5650	3559	962	1102	27	0	0

- Molecule 4 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	218	1757	1119	309	323	6	0	0

- Molecule 5 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	185	1490	942	276	270	2	0	0

- Molecule 6 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	158	1170	736	216	216	2	0	0

- Molecule 7 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	I	131	1036	655	191	187	3	0	0

- Molecule 8 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	L	136	1052	653	211	186	2	0	0

- Molecule 9 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	O	85	710	436	144	129	1	0	0

- Molecule 10 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	P	88	695	441	128	124	2	0	0

- Molecule 11 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	Q	84	691	435	128	126	2	0	0

- Molecule 12 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	S	83	637	390	130	116	1	0	0

- Molecule 13 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	T	95	784	492	138	152	2	0	0

- Molecule 14 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	U	64	Total	C	N	O	S	0	0
			518	332	96	88	2		

- Molecule 15 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	V	101	Total	C	N	O	S	0	0
			730	450	136	143	1		

- Molecule 16 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	205	Total	C	N	O	S	0	0
			1615	1009	303	300	3		

- Molecule 17 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	149	Total	C	N	O	S	0	0
			1181	740	220	215	6		

- Molecule 18 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	108	Total	C	N	O	S	0	0
			826	510	160	155	1		

- Molecule 19 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	95	Total	C	N	O	S	0	0
			761	479	139	141	2		

- Molecule 20 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	X	108	Total	C	N	O	0	0
			868	534	176	158		

- Molecule 21 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	Y	49	409	263	79	63	4	0	0

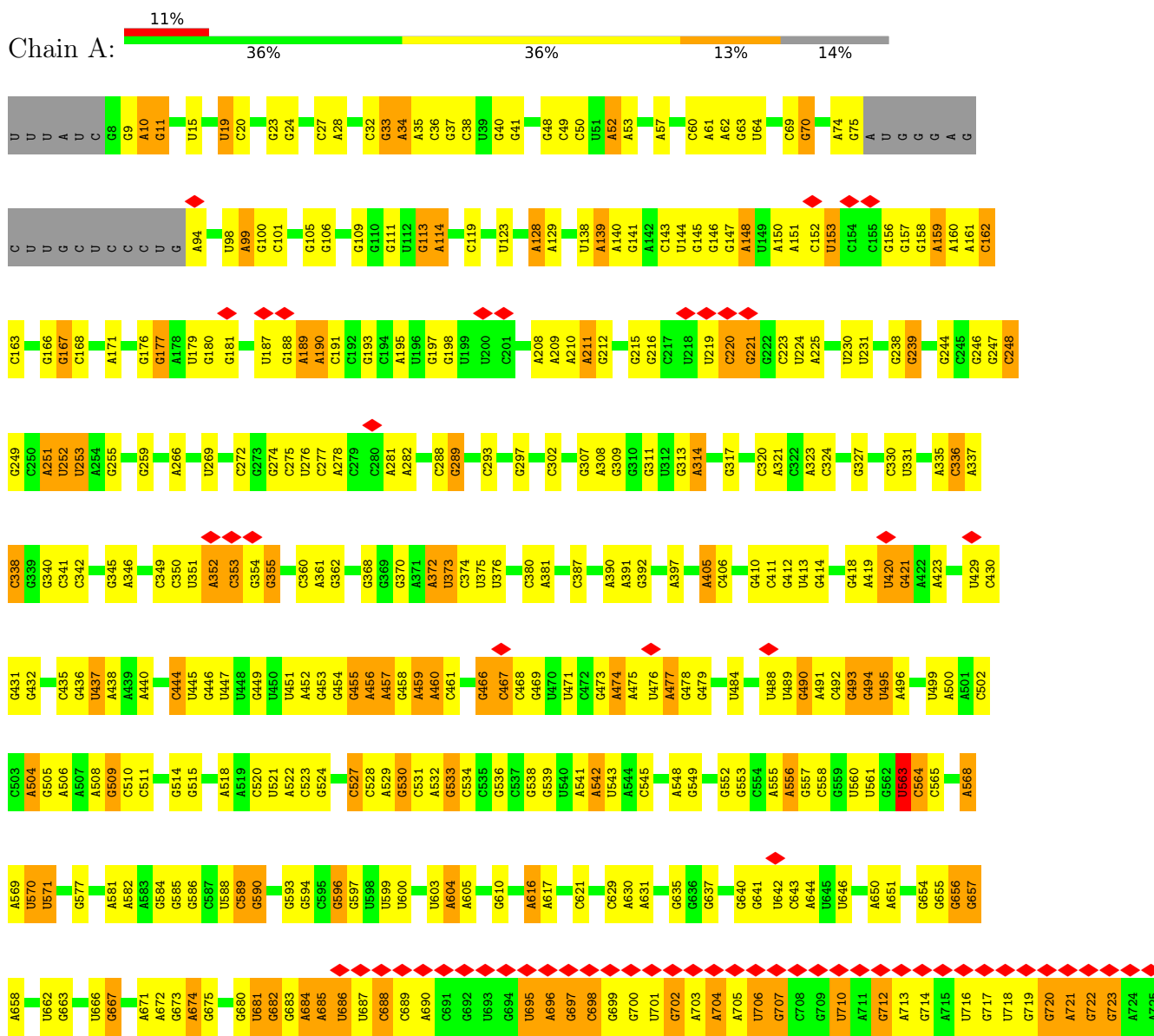
- Molecule 22 is a protein called 30S ribosomal protein S19.

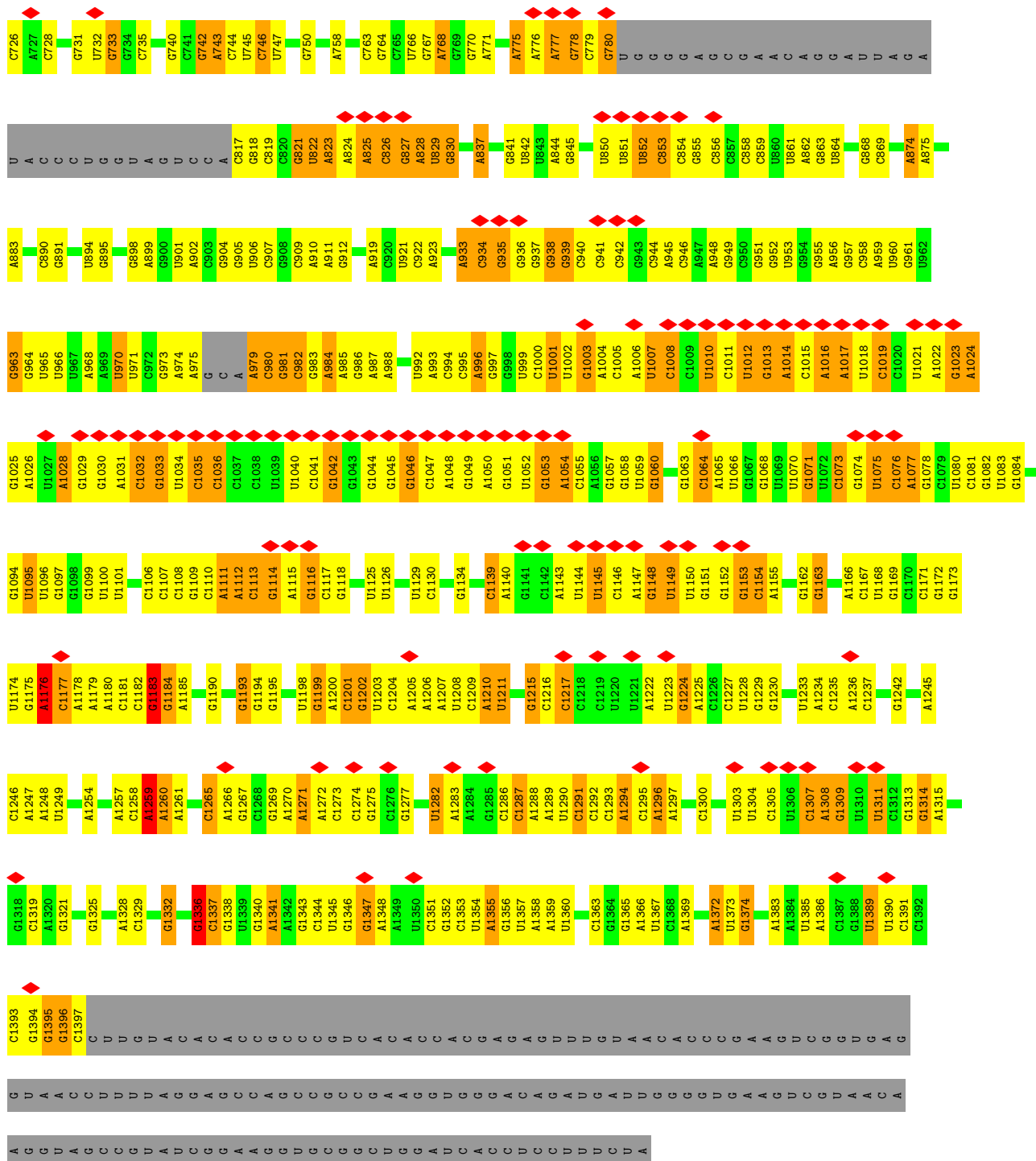
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	a	78	633	409	112	110	2	0	0

3 Residue-property plots [i](#)

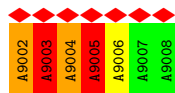
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 16S rRNA

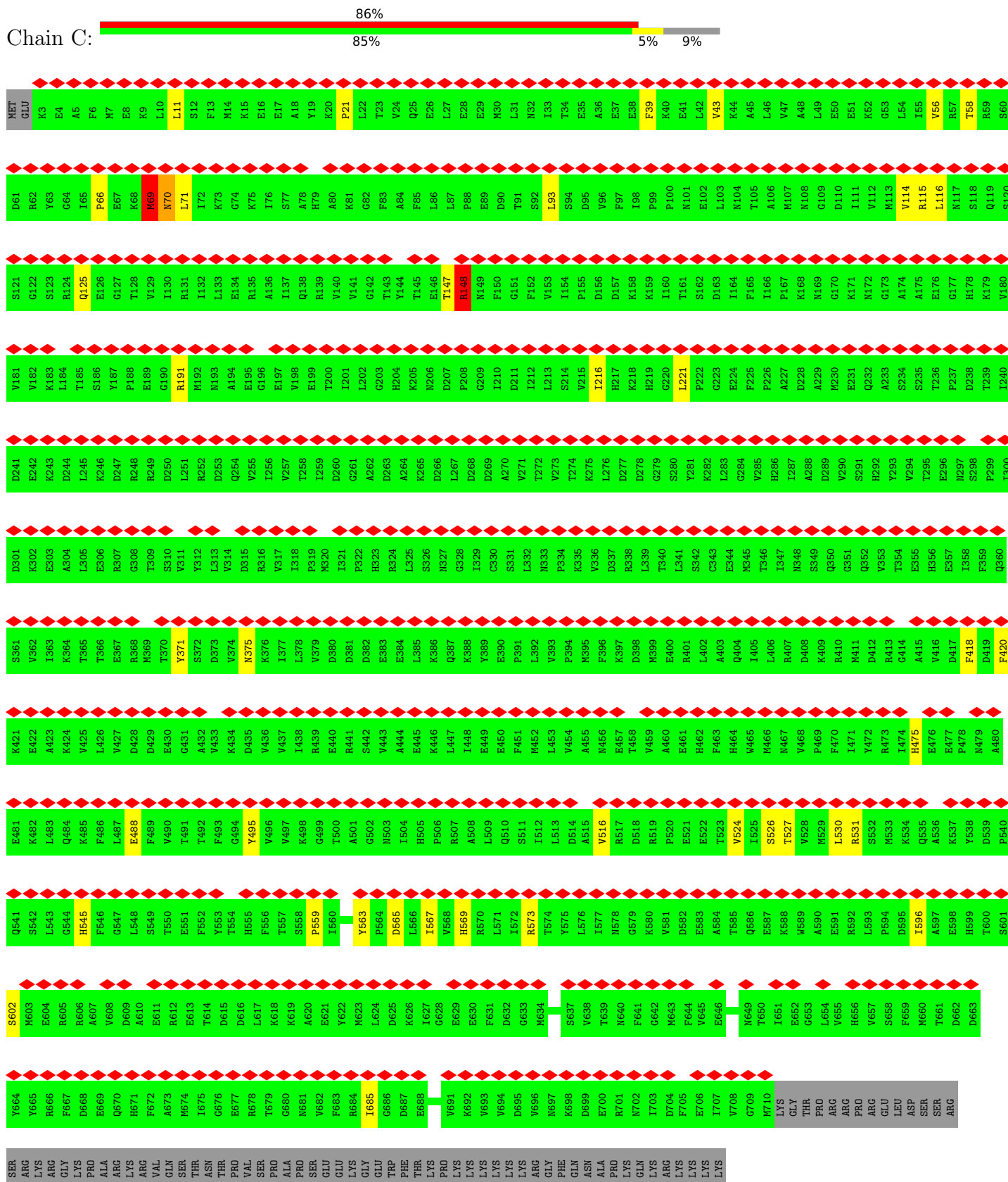




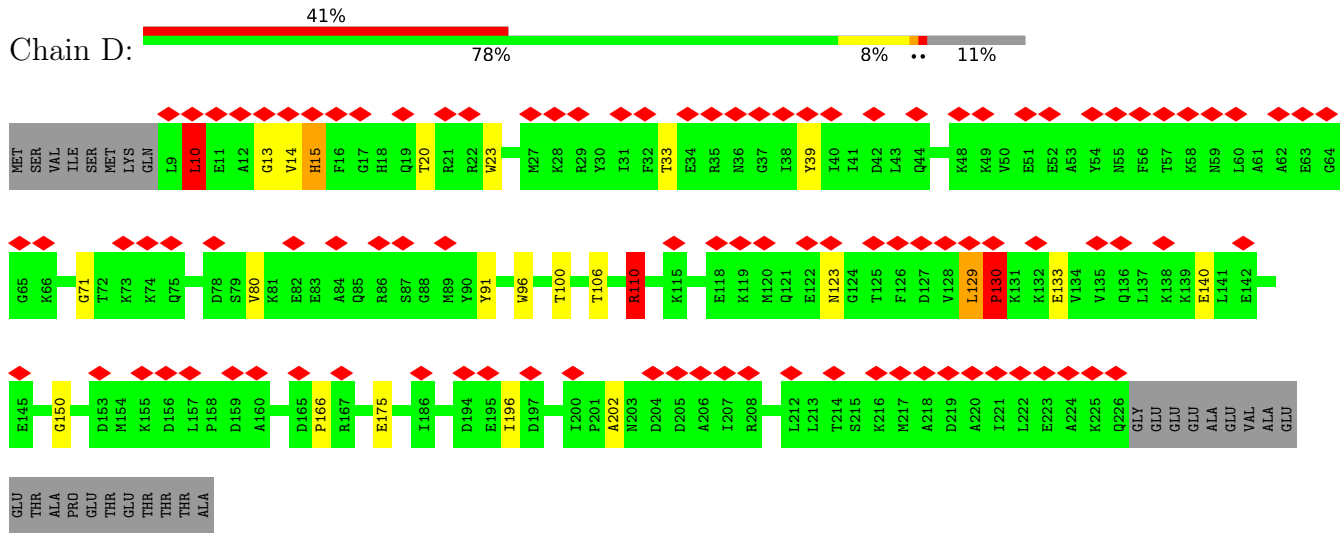
- Molecule 2: RNA Substrate



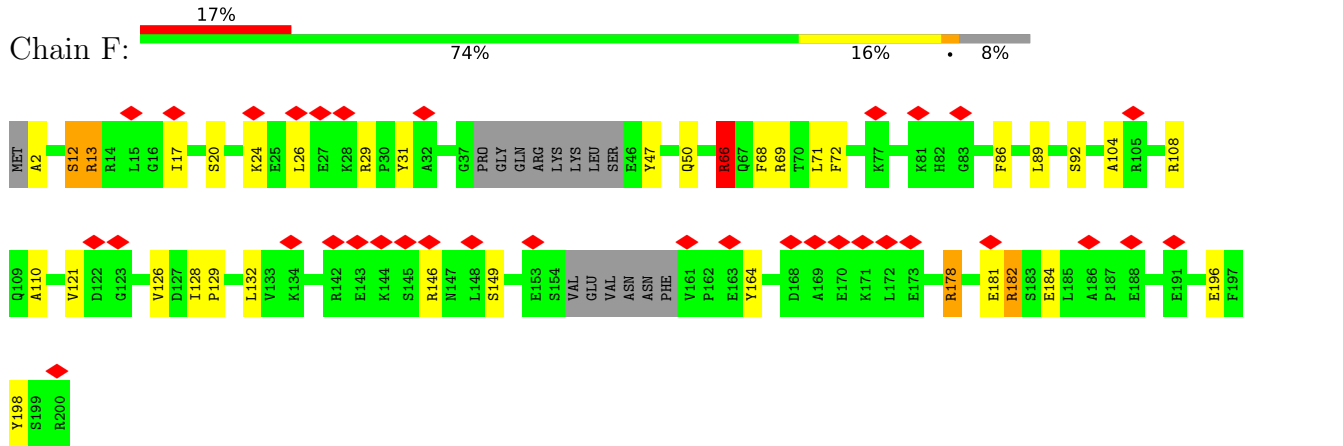
- Molecule 3: Ribonuclease R



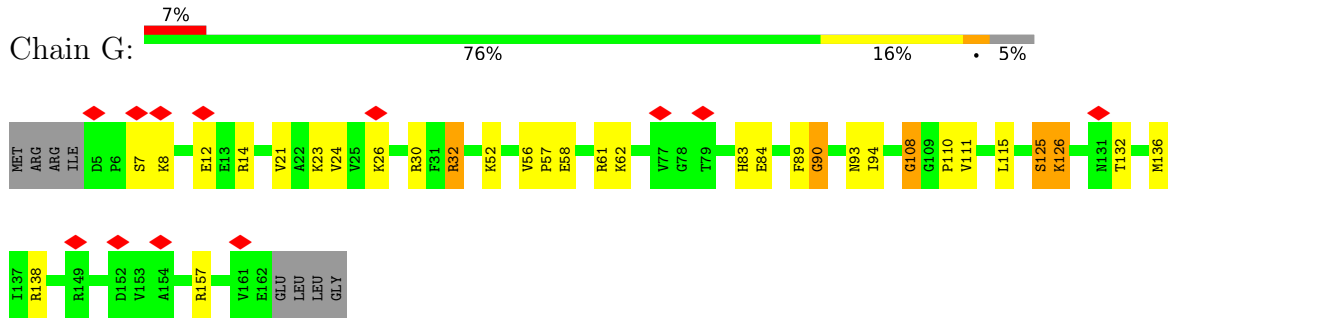
• Molecule 4: 30S ribosomal protein S2



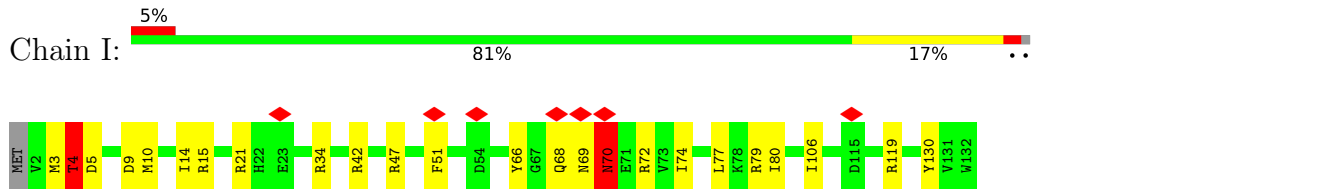
• Molecule 5: 30S ribosomal protein S4



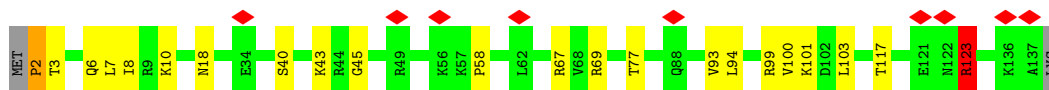
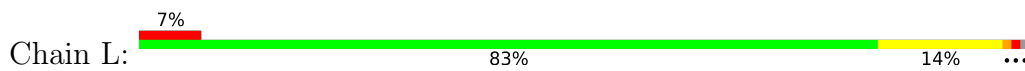
• Molecule 6: 30S ribosomal protein S5



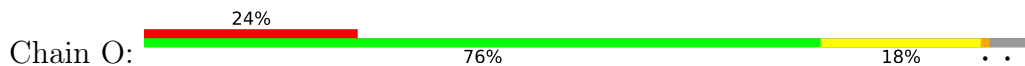
• Molecule 7: 30S ribosomal protein S8



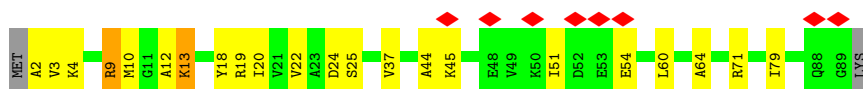
• Molecule 8: 30S ribosomal protein S12



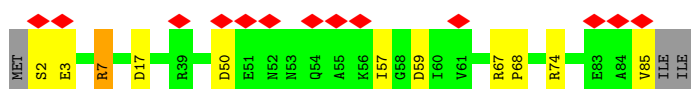
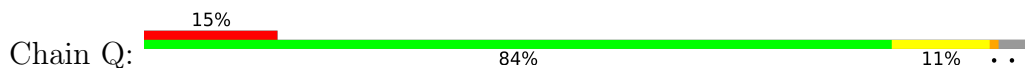
• Molecule 9: 30S ribosomal protein S15



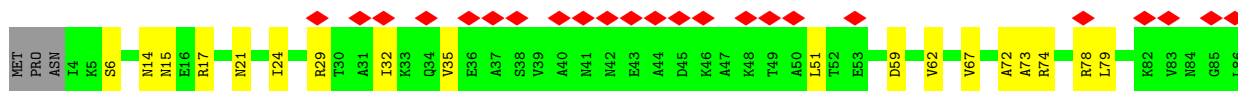
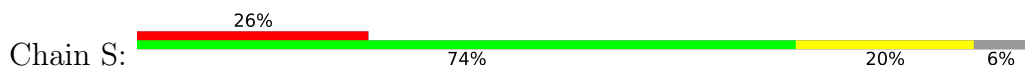
• Molecule 10: 30S ribosomal protein S16



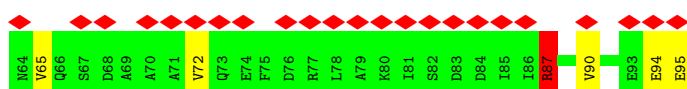
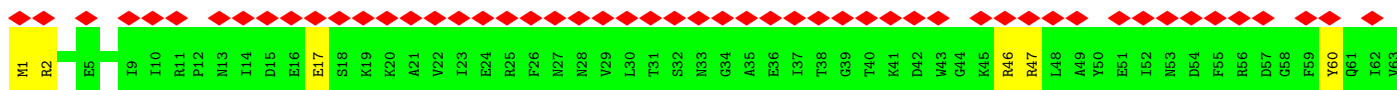
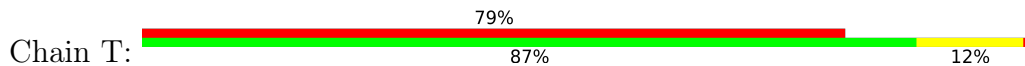
• Molecule 11: 30S ribosomal protein S17



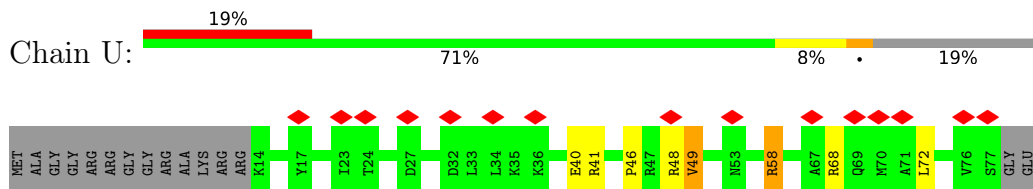
• Molecule 12: 30S ribosomal protein S20



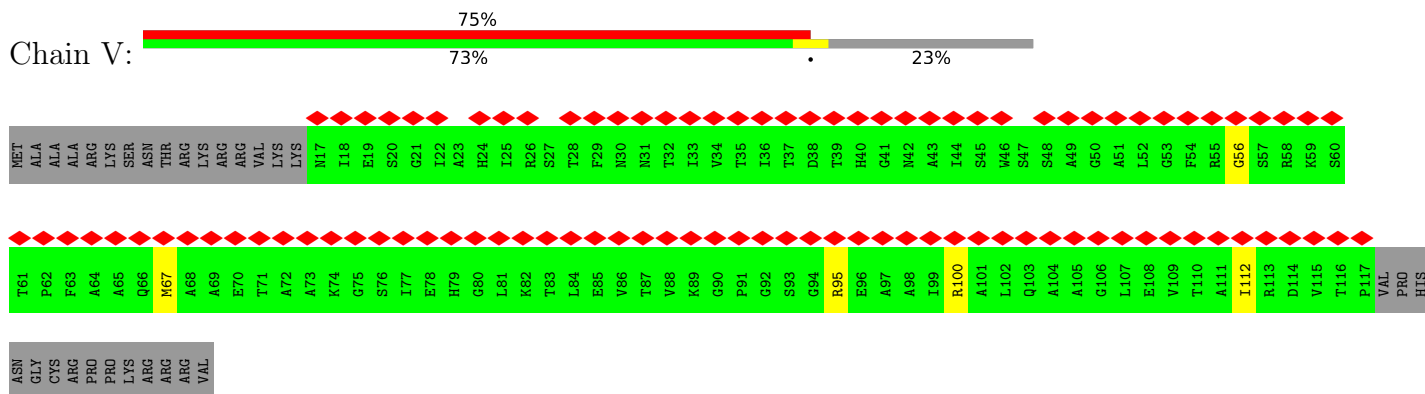
• Molecule 13: 30S ribosomal protein S6



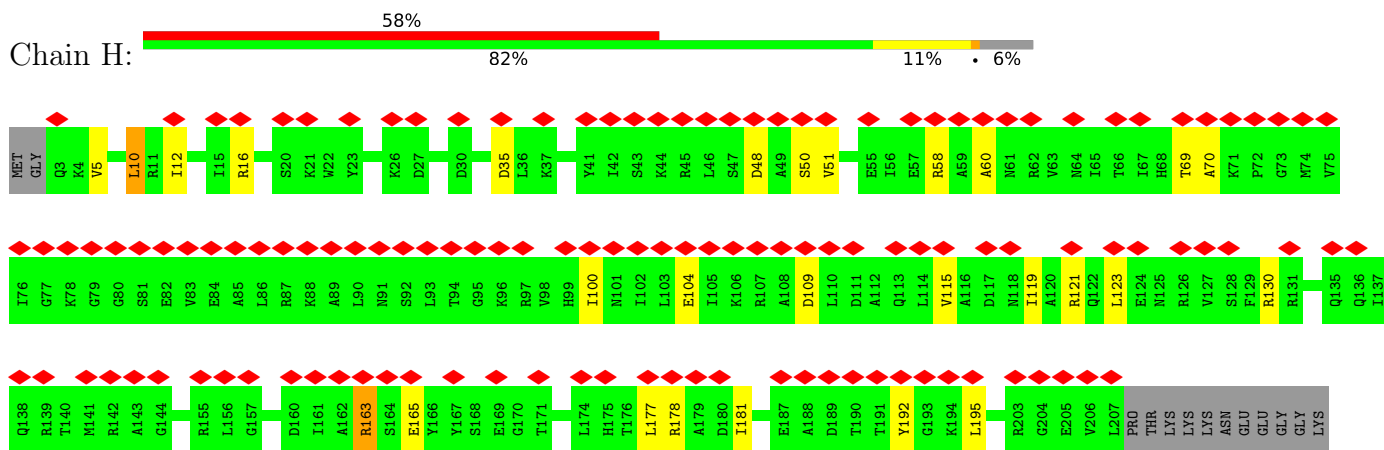
• Molecule 14: 30S ribosomal protein S18



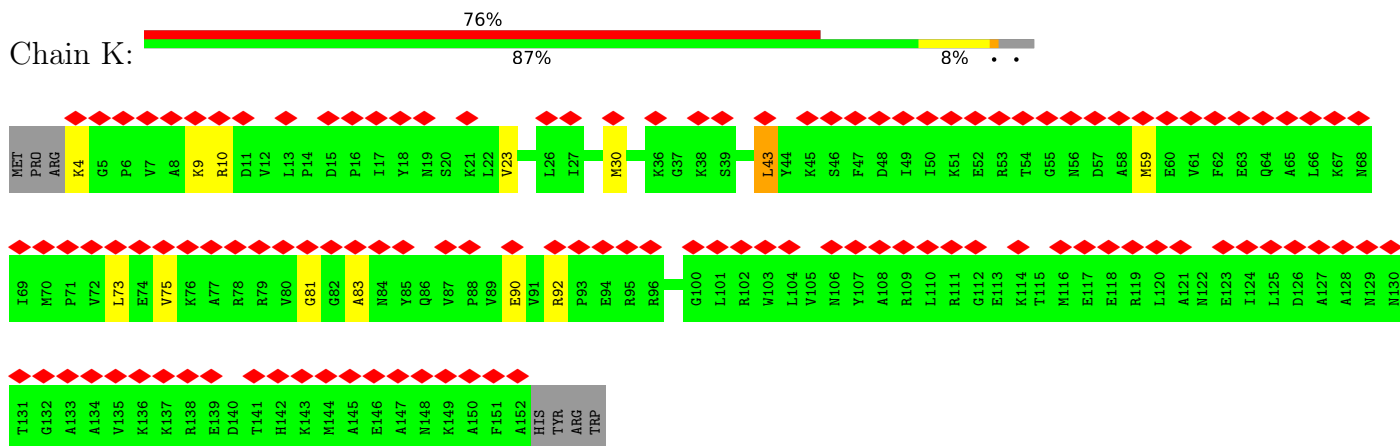
• Molecule 15: 30S ribosomal protein S11



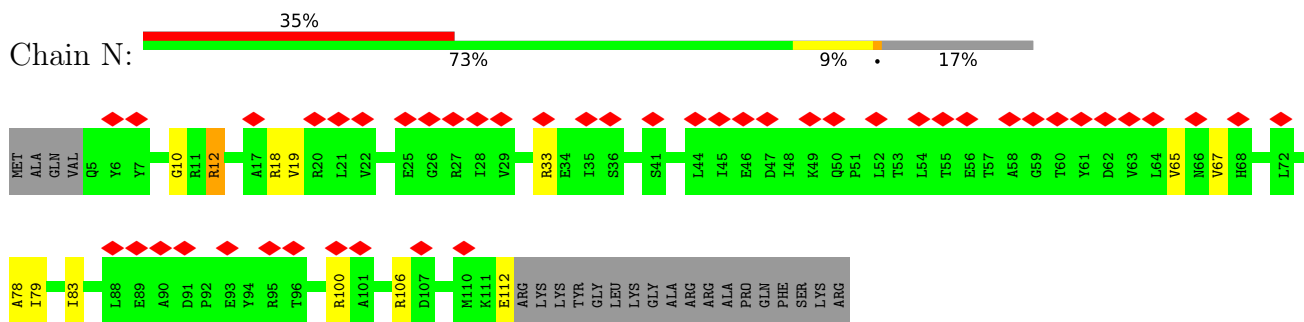
• Molecule 16: 30S ribosomal protein S3



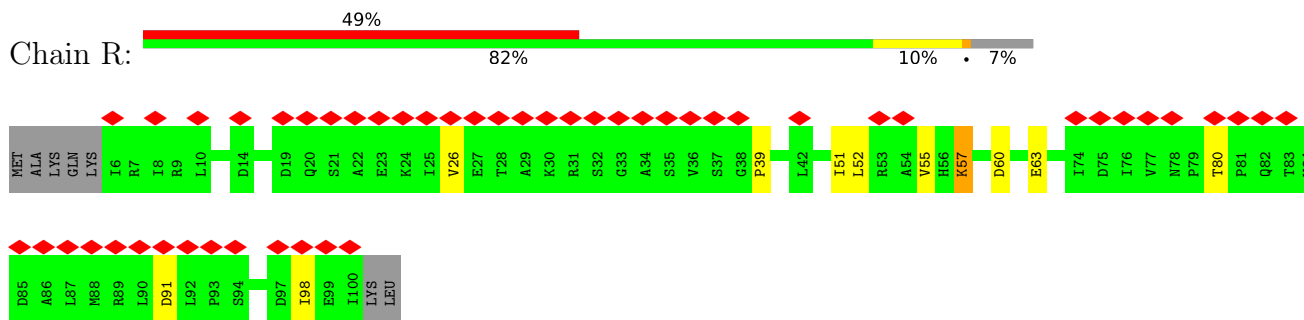
• Molecule 17: 30S ribosomal protein S7



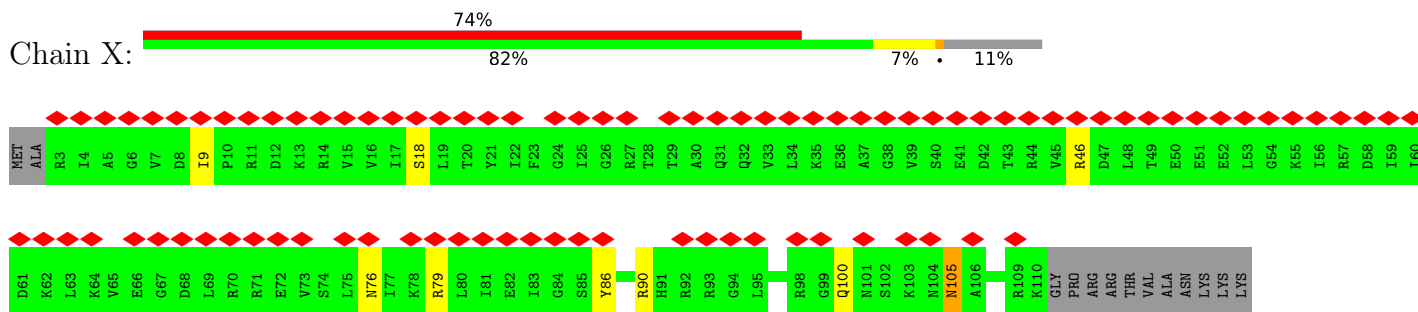
• Molecule 18: 30S ribosomal protein S9



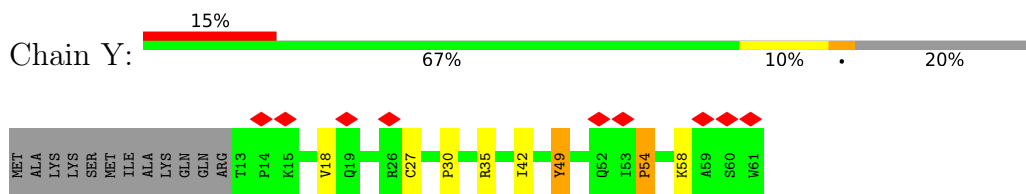
• Molecule 19: 30S ribosomal protein S10



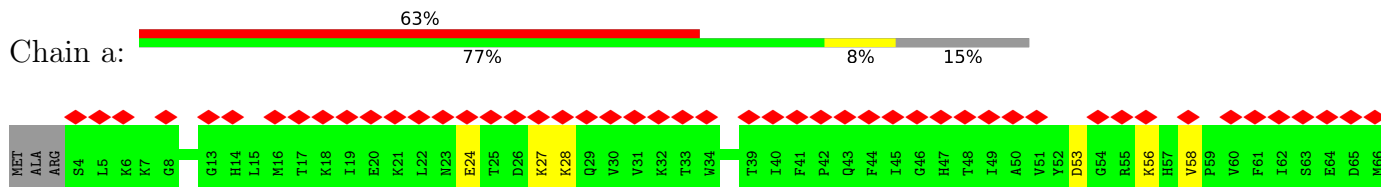
• Molecule 20: 30S ribosomal protein S13

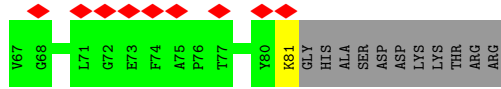


• Molecule 21: 30S ribosomal protein S14



• Molecule 22: 30S ribosomal protein S19





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	15566	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	900	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.094	Depositor
Minimum map value	-0.032	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0204	Depositor
Map size (Å)	307.2, 307.2, 307.2	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8, 0.8, 0.8	Depositor

5 Model quality i

5.1 Standard geometry i

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	0.65	2/32015 (0.0%)	0.93	15/49936 (0.0%)
2	B	0.81	0/174	1.81	9/269 (3.3%)
3	C	0.36	0/5748	0.76	1/7760 (0.0%)
4	D	0.44	0/1782	0.97	2/2392 (0.1%)
5	F	0.53	1/1517 (0.1%)	1.01	1/2036 (0.0%)
6	G	0.51	0/1182	1.07	1/1591 (0.1%)
7	I	0.48	0/1048	1.05	1/1407 (0.1%)
8	L	0.50	0/1069	1.10	2/1435 (0.1%)
9	O	0.50	0/718	1.06	0/960
10	P	0.56	0/708	1.07	2/950 (0.2%)
11	Q	0.50	0/699	1.07	0/933
12	S	0.45	0/639	1.01	0/852
13	T	0.39	0/795	0.91	3/1067 (0.3%)
14	U	0.48	0/526	1.06	1/705 (0.1%)
15	V	0.37	0/740	0.72	0/1002
16	H	0.38	0/1637	0.77	0/2203
17	K	0.34	0/1196	0.74	0/1604
18	N	0.40	0/836	0.77	0/1128
19	R	0.39	0/773	0.81	0/1044
20	X	0.35	0/873	0.75	0/1166
21	Y	0.43	0/419	0.99	1/558 (0.2%)
22	a	0.36	0/649	0.77	0/872
All	All	0.57	3/55743 (0.0%)	0.92	39/81870 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	4
4	D	0	4
5	F	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	G	0	6
7	I	0	4
8	L	0	3
9	O	0	1
10	P	0	3
11	Q	0	3
12	S	0	2
13	T	0	3
14	U	0	2
16	H	0	6
18	N	0	2
20	X	0	1
All	All	0	48

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	946	C	O3'-P	5.66	1.68	1.61
1	A	979	A	P-O5'	5.37	1.65	1.59
5	F	12	SER	CA-CB	-5.19	1.45	1.52

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	590	G	O5'-P-OP1	-9.98	96.72	105.70
4	D	110	ARG	NE-CZ-NH2	-8.20	116.20	120.30
2	B	9002	A	N1-C6-N6	-8.19	113.69	118.60
3	C	475	HIS	CB-CA-C	7.38	125.15	110.40
2	B	9002	A	C5-C6-N6	7.24	129.49	123.70

There are no chirality outliers.

5 of 48 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	148	ARG	Sidechain
3	C	573	ARG	Sidechain
3	C	69	MET	Peptide,Mainchain
4	D	10	LEU	Peptide
4	D	110	ARG	Sidechain

5.2 Too-close contacts

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	28597	0	14401	556	0
2	B	154	0	78	19	0
3	C	5650	0	5619	55	0
4	D	1757	0	1830	29	0
5	F	1490	0	1518	17	0
6	G	1170	0	1245	13	0
7	I	1036	0	1095	11	0
8	L	1052	0	1112	7	0
9	O	710	0	735	11	0
10	P	695	0	721	8	0
11	Q	691	0	728	7	0
12	S	637	0	696	9	0
13	T	784	0	777	2	0
14	U	518	0	555	4	0
15	V	730	0	735	4	0
16	H	1615	0	1655	8	0
17	K	1181	0	1235	6	0
18	N	826	0	849	4	0
19	R	761	0	795	4	0
20	X	868	0	925	5	0
21	Y	409	0	427	5	0
22	a	633	0	649	0	0
All	All	51964	0	38380	723	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 723 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)
1:A:281:A:O2'	1:A:282:A:H5'	1.53	1.09
1:A:775:A:O2'	1:A:776:A:H5'	1.51	1.07
1:A:1094:G:H2'	1:A:1095:U:C5	2.02	0.93
1:A:11:G:H5'	6:G:108:GLY:HA3	1.49	0.92
1:A:1015:C:H4'	1:A:1048:A:H1'	1.52	0.92

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	706/779 (91%)	687 (97%)	18 (2%)	1 (0%)	51 84
4	D	216/246 (88%)	196 (91%)	19 (9%)	1 (0%)	29 67
5	F	179/200 (90%)	165 (92%)	11 (6%)	3 (2%)	9 44
6	G	156/166 (94%)	141 (90%)	11 (7%)	4 (3%)	5 35
7	I	129/132 (98%)	115 (89%)	11 (8%)	3 (2%)	6 38
8	L	134/138 (97%)	125 (93%)	9 (7%)	0	100 100
9	O	83/89 (93%)	77 (93%)	6 (7%)	0	100 100
10	P	86/90 (96%)	80 (93%)	5 (6%)	1 (1%)	13 51
11	Q	82/87 (94%)	74 (90%)	7 (8%)	1 (1%)	13 51
12	S	81/88 (92%)	75 (93%)	6 (7%)	0	100 100
13	T	93/95 (98%)	87 (94%)	5 (5%)	1 (1%)	14 53
14	U	62/79 (78%)	58 (94%)	4 (6%)	0	100 100
15	V	99/131 (76%)	95 (96%)	4 (4%)	0	100 100
16	H	203/218 (93%)	170 (84%)	32 (16%)	1 (0%)	29 67
17	K	147/156 (94%)	138 (94%)	7 (5%)	2 (1%)	11 48
18	N	106/130 (82%)	100 (94%)	6 (6%)	0	100 100
19	R	93/102 (91%)	87 (94%)	6 (6%)	0	100 100
20	X	106/121 (88%)	102 (96%)	4 (4%)	0	100 100
21	Y	47/61 (77%)	43 (92%)	3 (6%)	1 (2%)	7 40
22	a	76/92 (83%)	72 (95%)	2 (3%)	2 (3%)	5 35
All	All	2884/3200 (90%)	2687 (93%)	176 (6%)	21 (1%)	26 62

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	130	PRO
5	F	24	LYS
6	G	8	LYS
6	G	26	LYS
7	I	4	THR

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	628/692 (91%)	622 (99%)	6 (1%)	76 89
4	D	189/212 (89%)	185 (98%)	4 (2%)	53 79
5	F	159/173 (92%)	151 (95%)	8 (5%)	24 59
6	G	123/130 (95%)	118 (96%)	5 (4%)	30 64
7	I	111/112 (99%)	107 (96%)	4 (4%)	35 67
8	L	114/116 (98%)	107 (94%)	7 (6%)	18 53
9	O	80/83 (96%)	75 (94%)	5 (6%)	18 52
10	P	74/76 (97%)	70 (95%)	4 (5%)	22 57
11	Q	77/80 (96%)	75 (97%)	2 (3%)	46 74
12	S	66/70 (94%)	63 (96%)	3 (4%)	27 62
13	T	84/84 (100%)	79 (94%)	5 (6%)	19 54
14	U	56/64 (88%)	54 (96%)	2 (4%)	35 67
15	V	74/100 (74%)	73 (99%)	1 (1%)	67 85
16	H	168/178 (94%)	158 (94%)	10 (6%)	19 54
17	K	125/132 (95%)	118 (94%)	7 (6%)	21 56
18	N	85/102 (83%)	80 (94%)	5 (6%)	19 54
19	R	86/92 (94%)	79 (92%)	7 (8%)	11 43
20	X	94/104 (90%)	92 (98%)	2 (2%)	53 79
21	Y	44/54 (82%)	41 (93%)	3 (7%)	16 49
22	a	70/81 (86%)	65 (93%)	5 (7%)	14 48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2507/2735 (92%)	2412 (96%)	95 (4%)	36 66

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	H	12	ILE
17	K	59	MET
16	H	48	ASP
16	H	195	LEU
18	N	100	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
20	X	76	ASN
20	X	100	GLN
22	a	14	HIS
9	O	46	HIS
14	U	69	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1329/1554 (85%)	334 (25%)	75 (5%)
2	B	6/7 (85%)	3 (50%)	0
All	All	1335/1561 (85%)	337 (25%)	75 (5%)

5 of 337 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	10	A
1	A	11	G
1	A	32	C
1	A	33	G

5 of 75 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1111	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1344	C
1	A	1139	C
1	A	1266	A
1	A	490	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](#)

There are no ligands in this entry.

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.

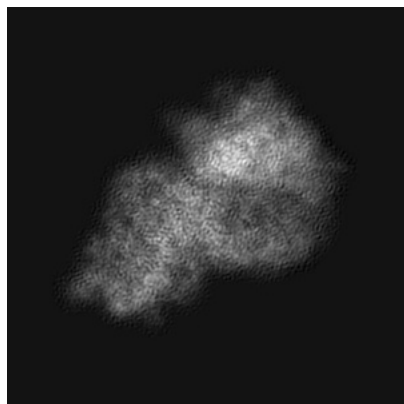
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16605. These allow visual inspection of the internal detail of the map and identification of artifacts.

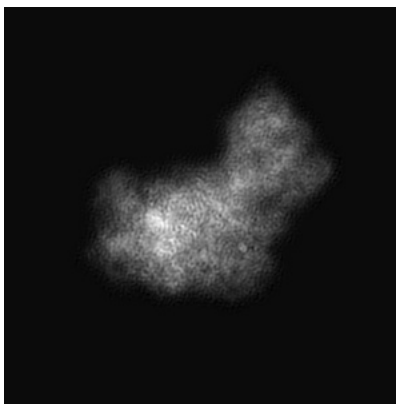
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

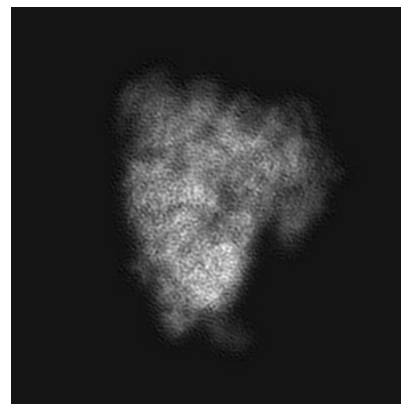
6.1.1 Primary map



X

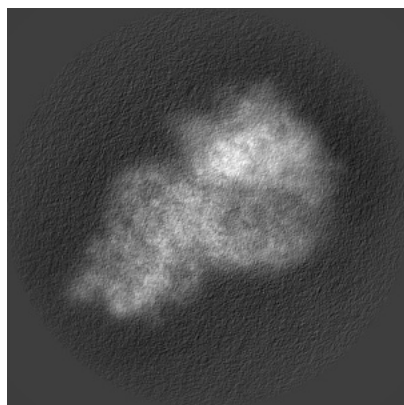


Y

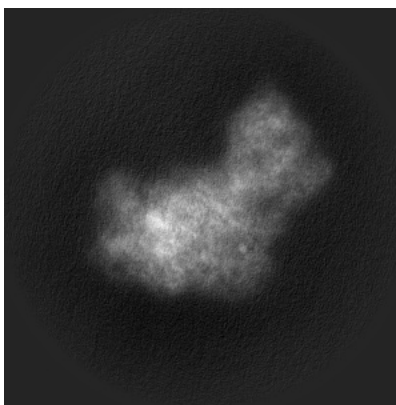


Z

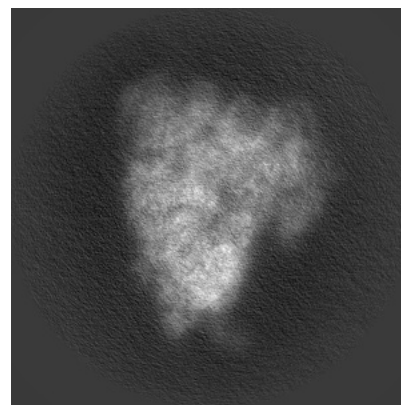
6.1.2 Raw map



X



Y

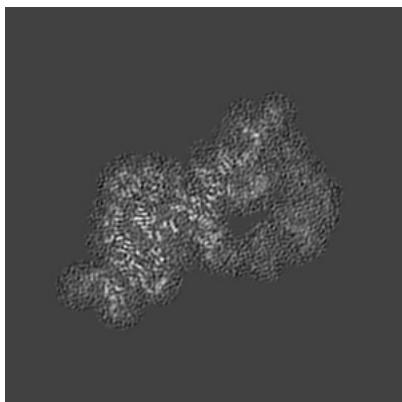


Z

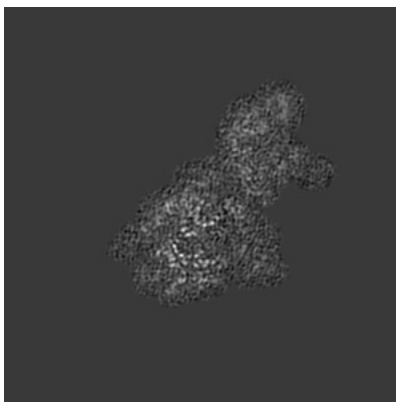
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

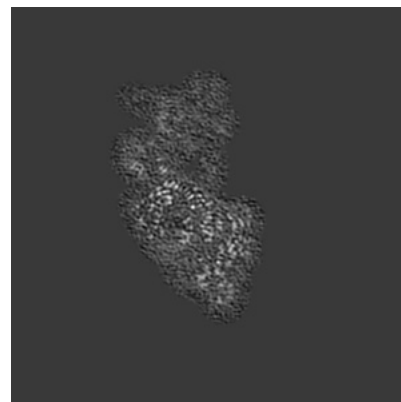
6.2.1 Primary map



X Index: 192

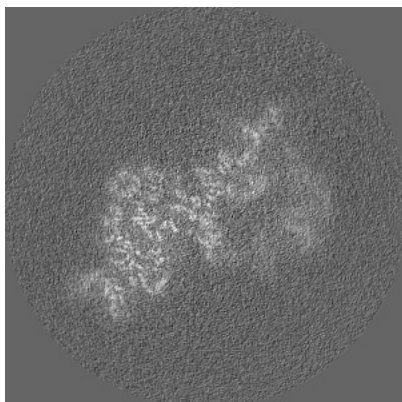


Y Index: 192

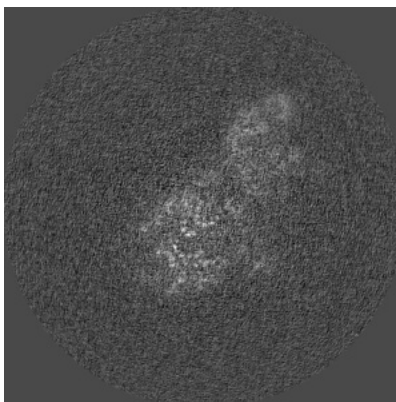


Z Index: 192

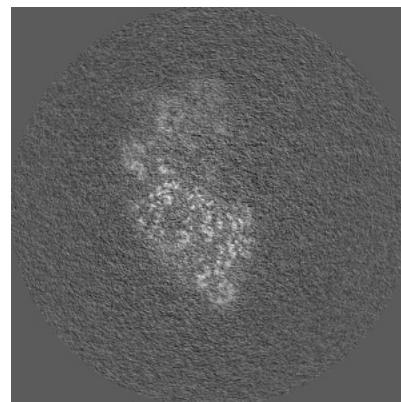
6.2.2 Raw map



X Index: 192



Y Index: 192

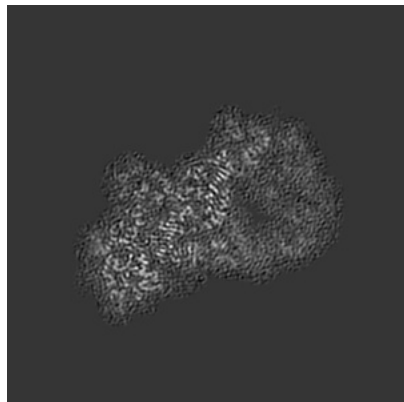


Z Index: 192

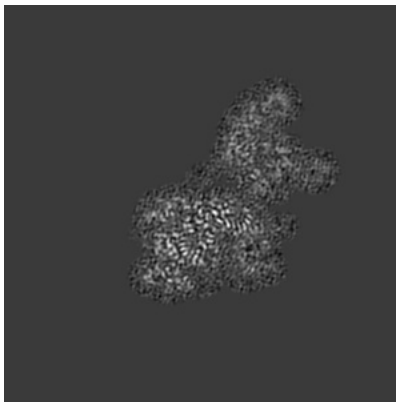
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

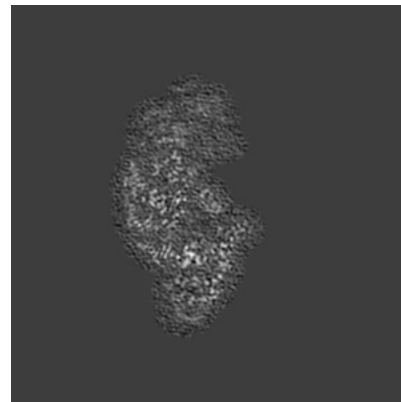
6.3.1 Primary map



X Index: 177

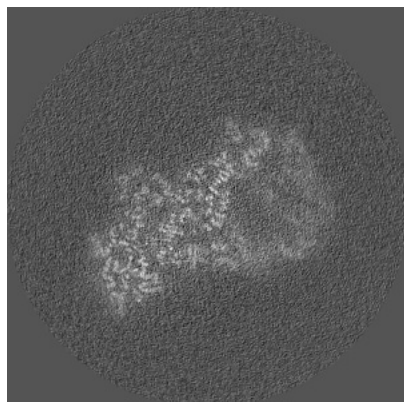


Y Index: 200

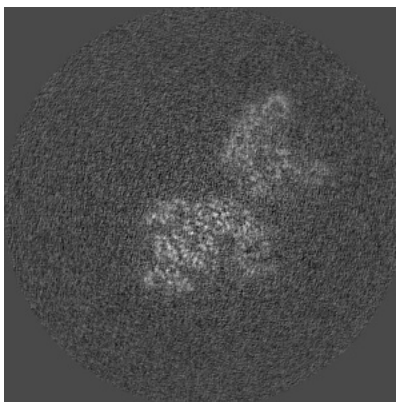


Z Index: 161

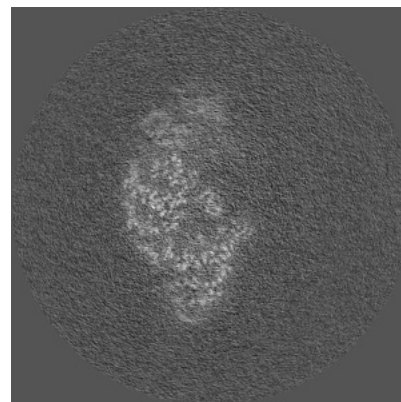
6.3.2 Raw map



X Index: 177



Y Index: 200

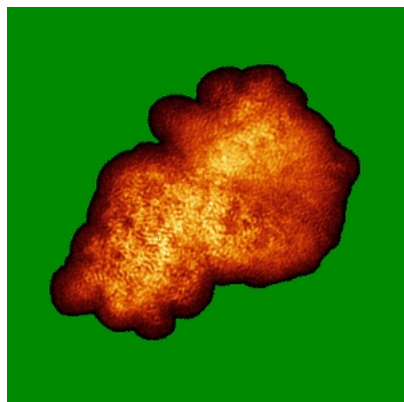


Z Index: 162

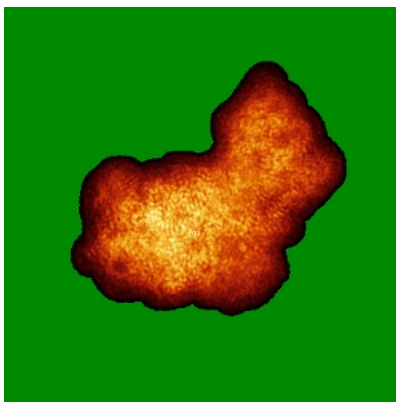
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

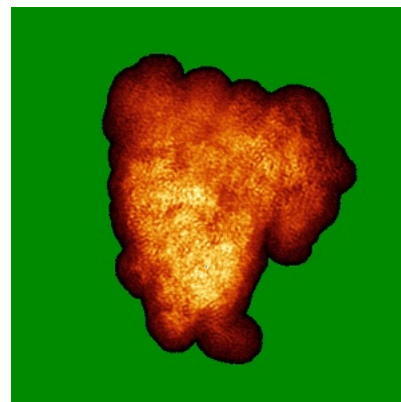
6.4.1 Primary map



X

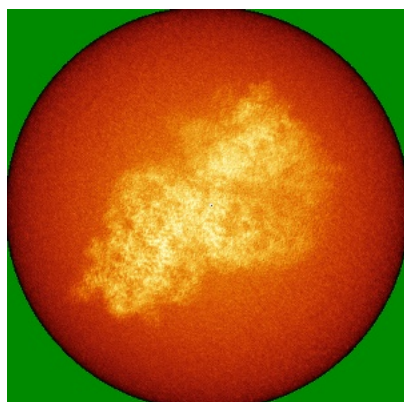


Y

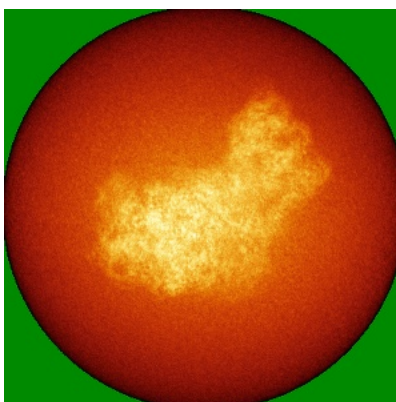


Z

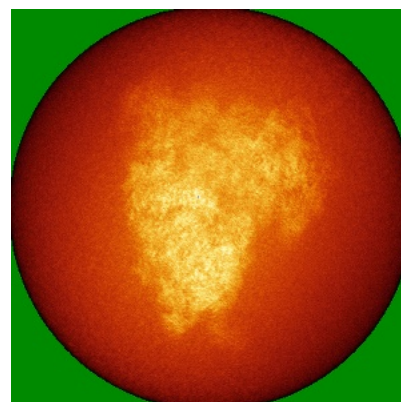
6.4.2 Raw map



X



Y

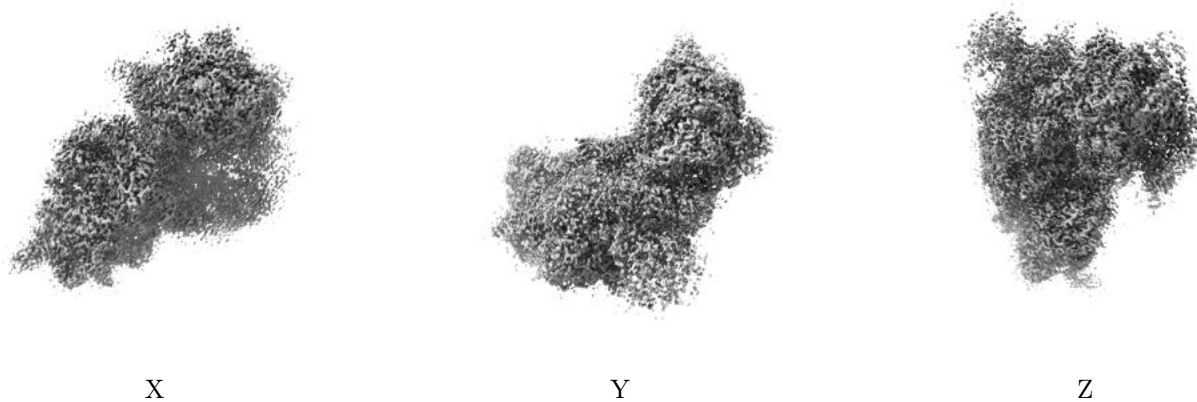


Z

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.

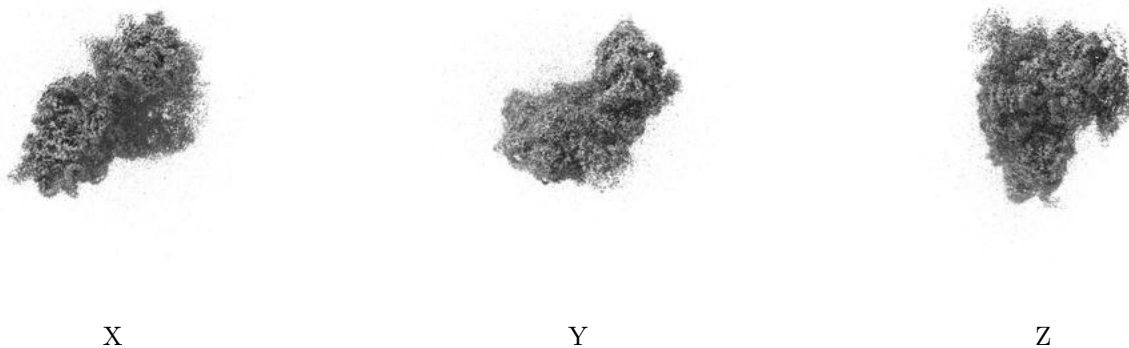
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0204. 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



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.

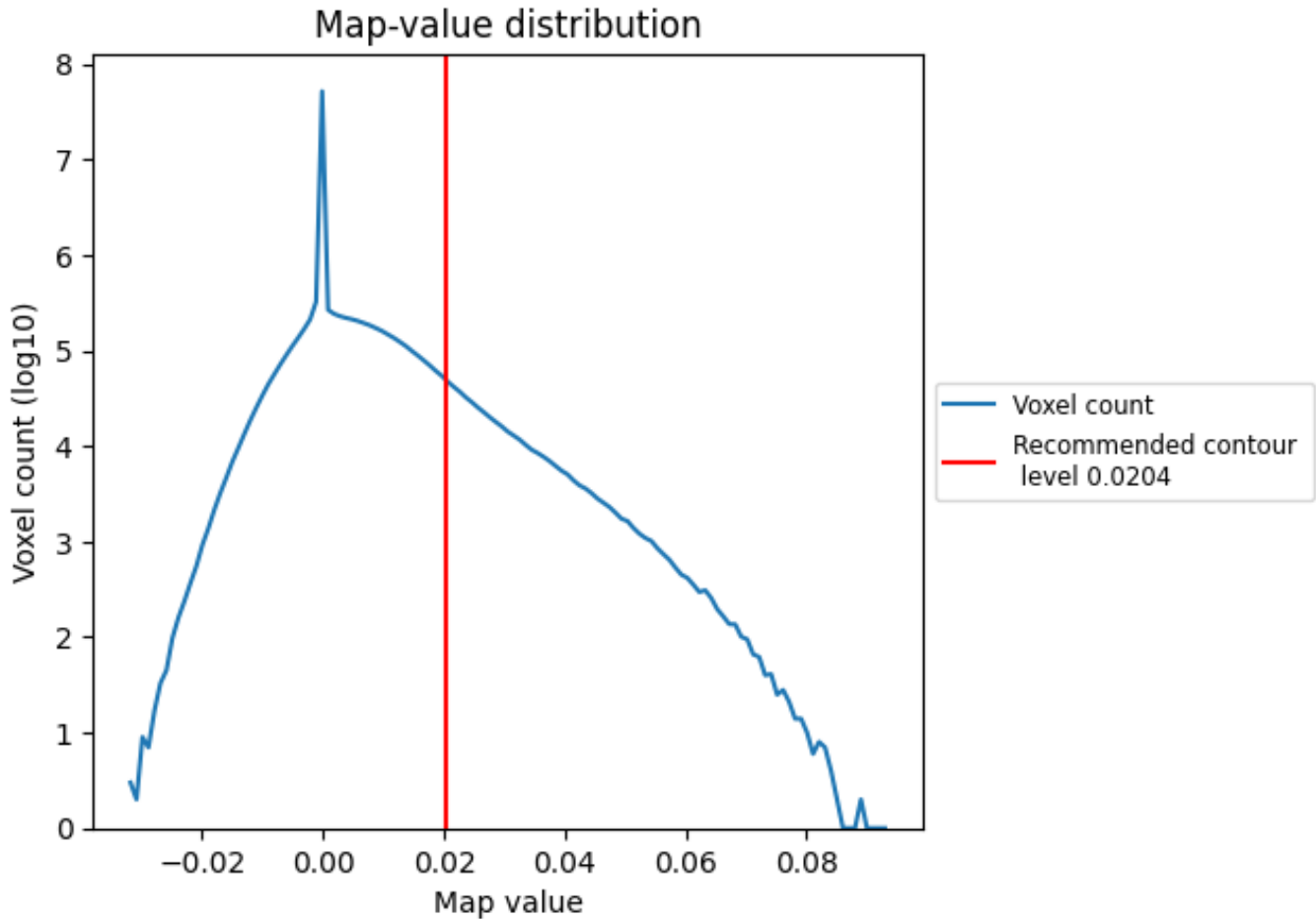
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

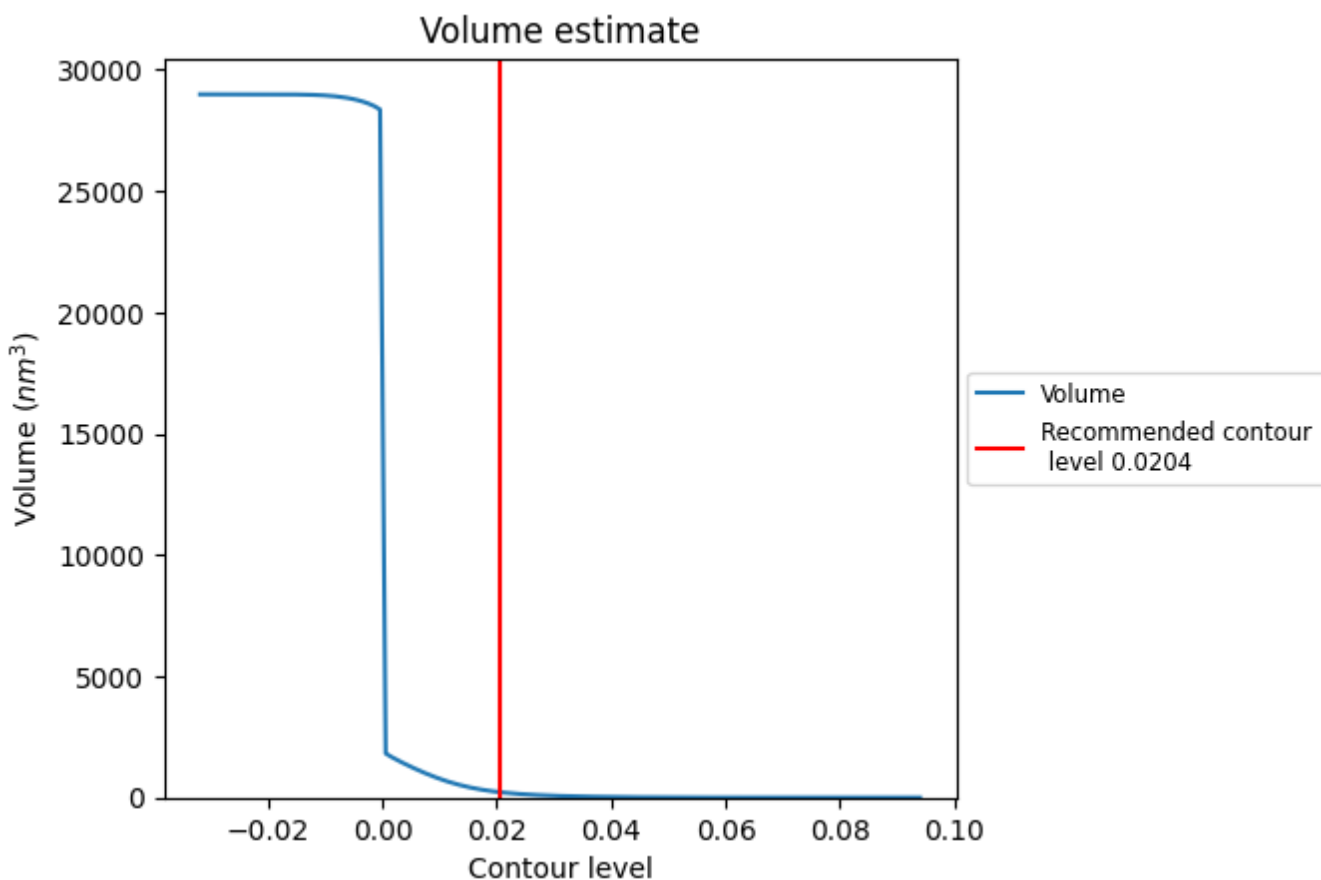
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

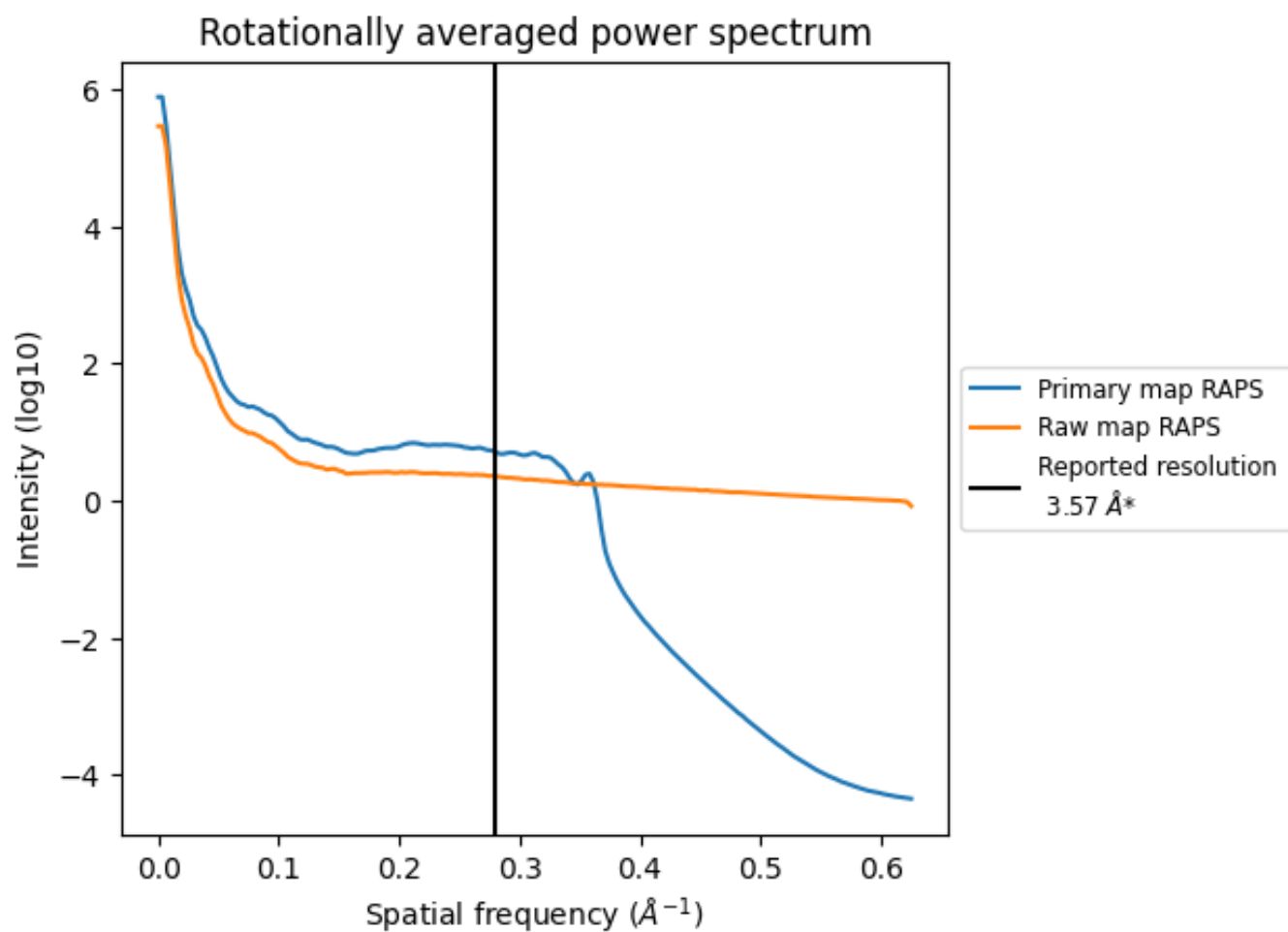
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 226 nm^3 ; this corresponds to an approximate mass of 204 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](#)

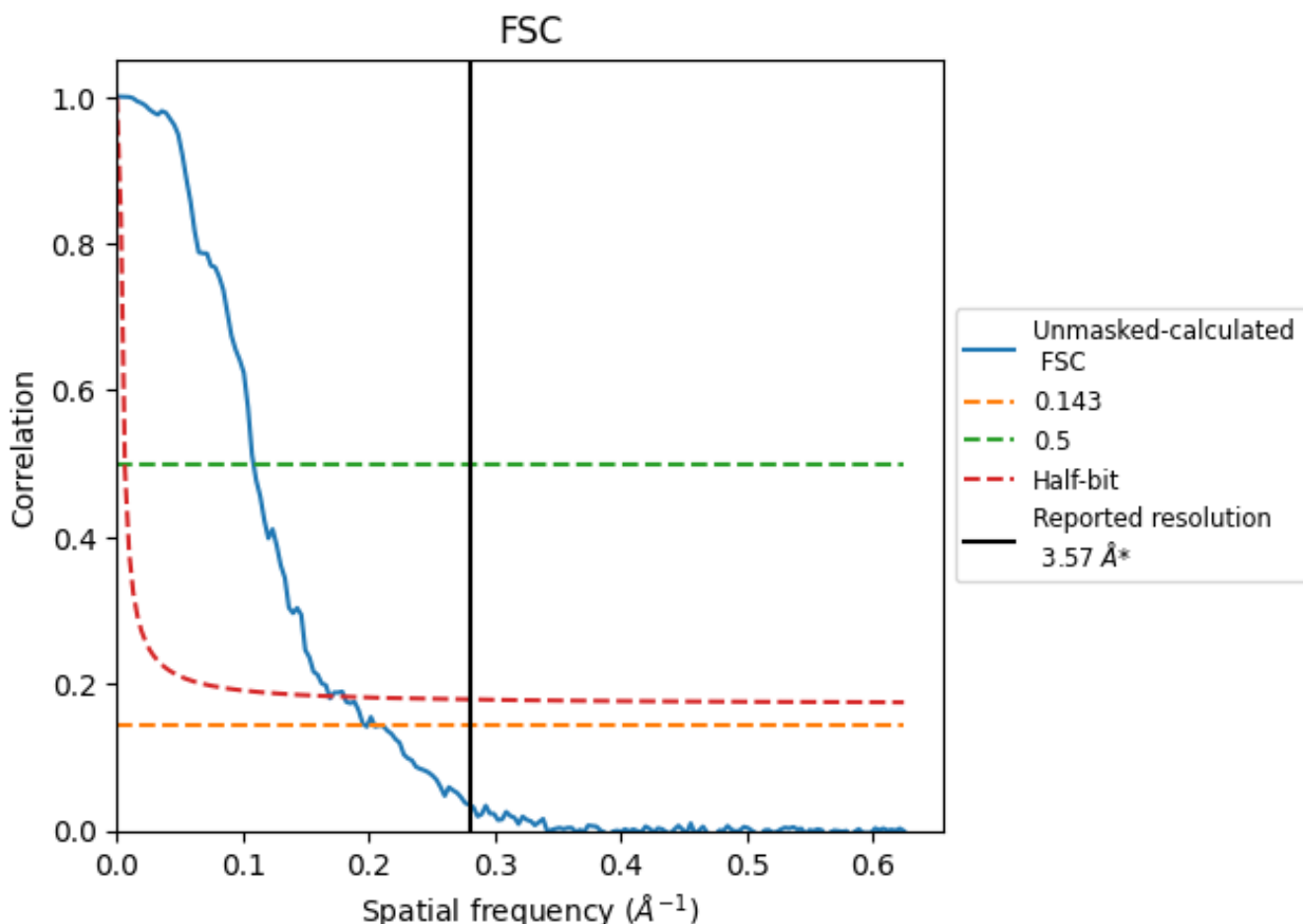


*Reported resolution corresponds to spatial frequency of 0.280 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.280 Å⁻¹

8.2 Resolution estimates [i](#)

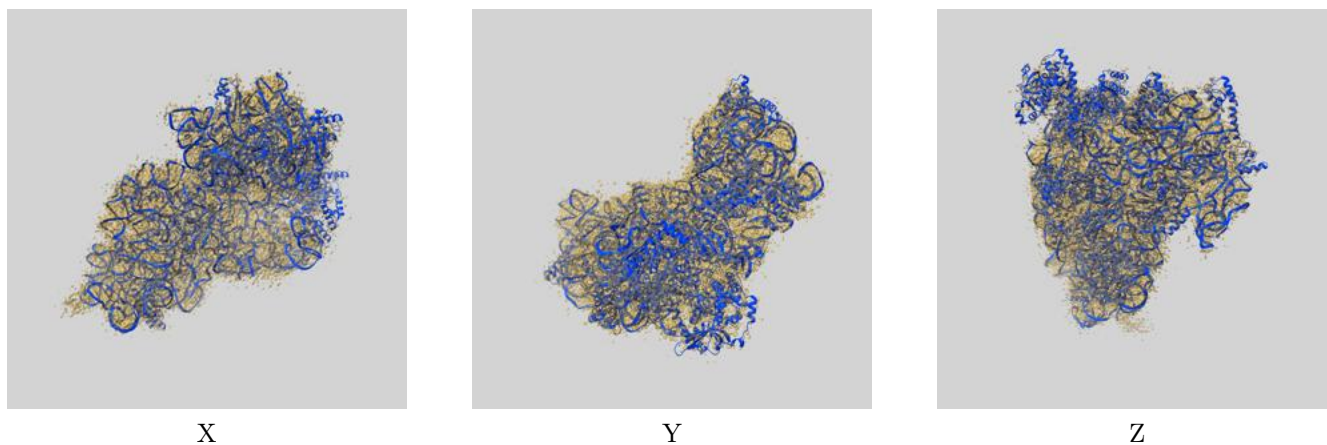
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.57	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.07	9.22	5.93

*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 5.07 differs from the reported value 3.57 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16605 and PDB model 8CEC. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



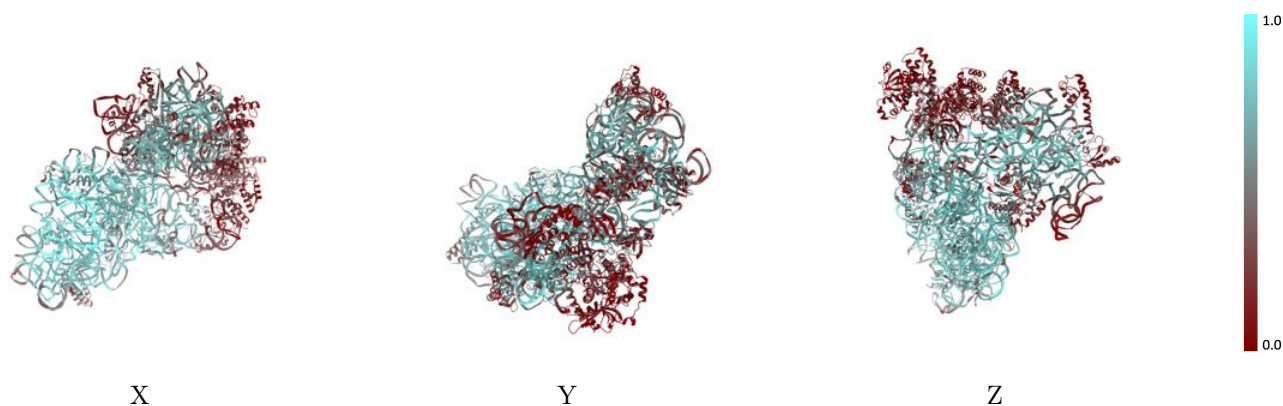
The images above show the 3D surface view of the map at the recommended contour level 0.0204 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



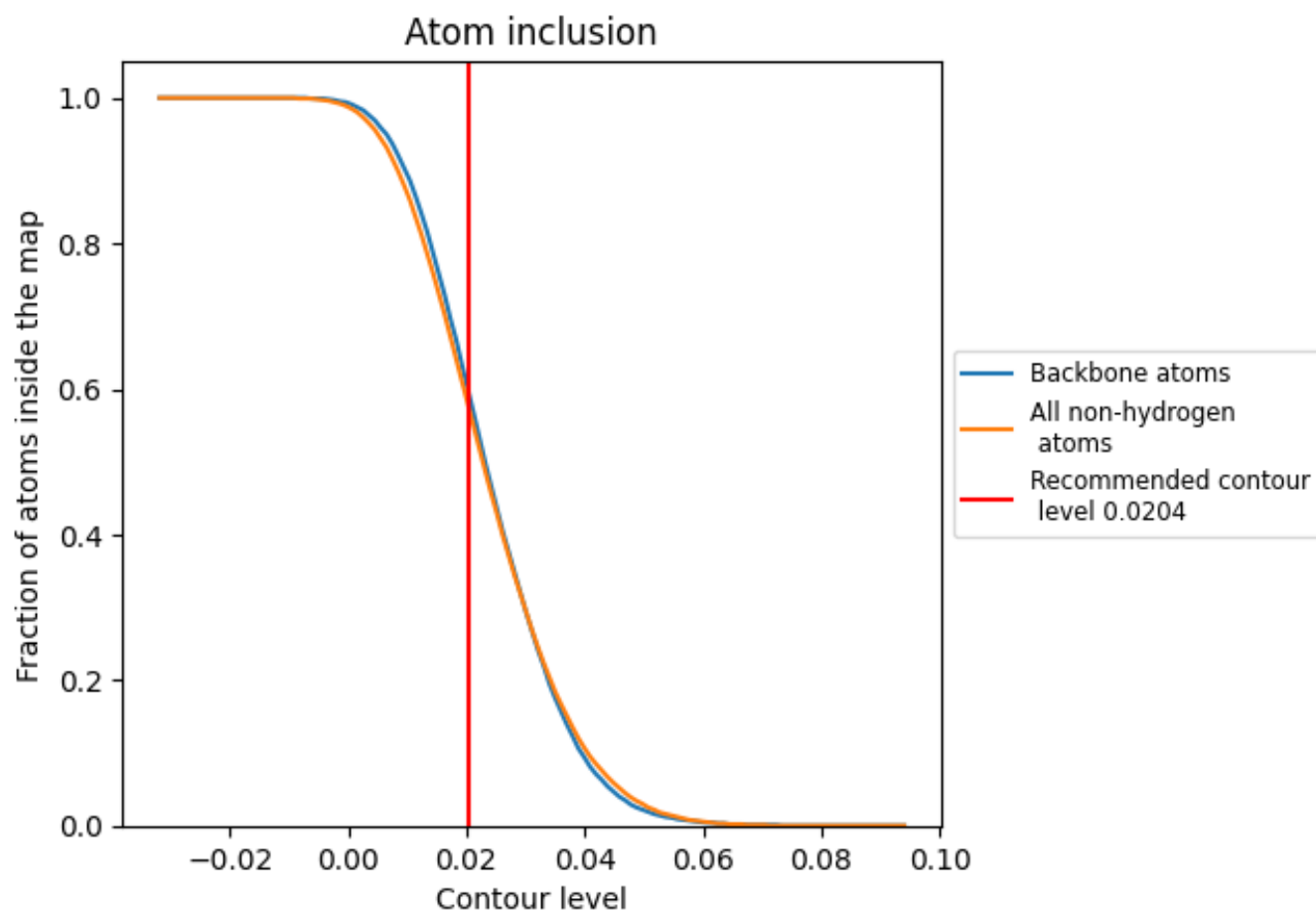
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.0204).















































9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 57% 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 (0.0204) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5750	 0.3880
A	 0.7190	 0.4410
B	 0.2340	 0.2130
C	 0.1160	 0.1560
D	 0.4360	 0.3750
F	 0.6370	 0.4650
G	 0.7240	 0.5030
H	 0.3650	 0.2800
I	 0.7190	 0.5070
K	 0.2370	 0.2060
L	 0.6810	 0.4880
N	 0.4610	 0.3390
O	 0.5990	 0.4510
P	 0.7320	 0.5090
Q	 0.6580	 0.4820
R	 0.4110	 0.3180
S	 0.5740	 0.4350
T	 0.2790	 0.3180
U	 0.5500	 0.4460
V	 0.0990	 0.1610
X	 0.2020	 0.2110
Y	 0.6140	 0.4150
a	 0.2730	 0.2700

