wwPDB EM Validation Summary Report ⓘ

Mar 19, 2024 – 01:12 PM JST

PDB ID	:	5XYI
EMDB ID	:	EMD-6788
Title	:	Small subunit of Trichomonas vaginalis ribosome
Authors	:	Li, Z.; Guo, Q.; Zheng, L.; Ji, Y.; Xie, Y.; Lai, D.; Lun, Z.; Suo, X.; Gao, N.
Deposited on	:	2017-07-08
Resolution	:	3.35 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:

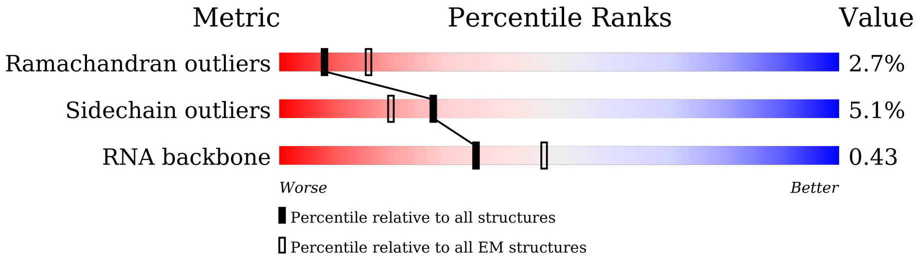
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

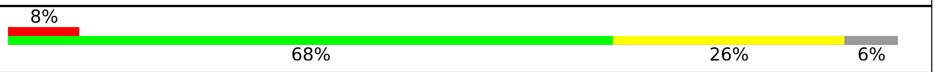
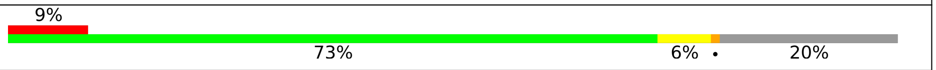
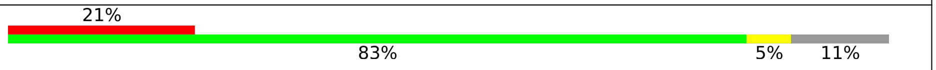
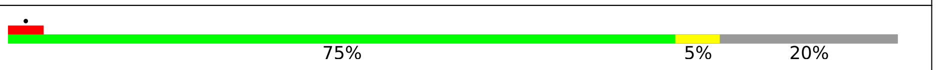
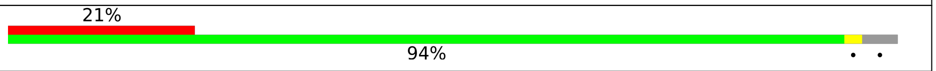
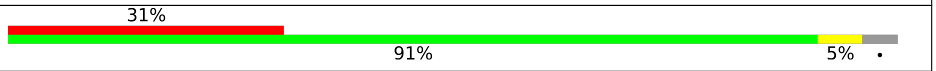
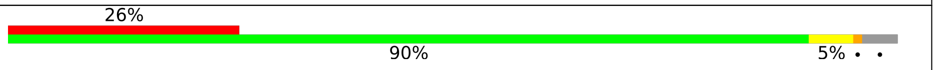
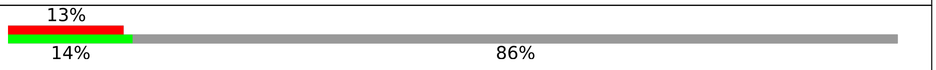
The reported resolution of this entry is 3.35 Å.

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)
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	2	1577	
2	A	256	
3	B	247	
4	C	272	
5	D	216	
6	E	255	
7	F	193	
8	G	216	

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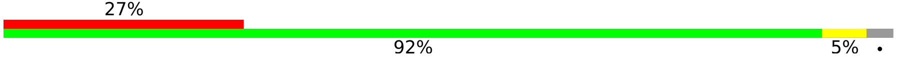
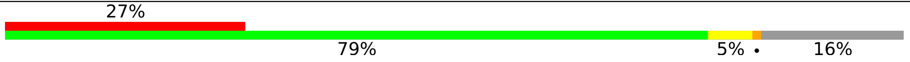
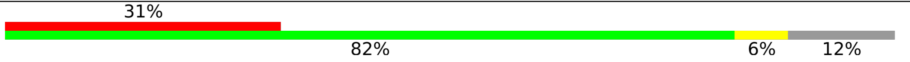
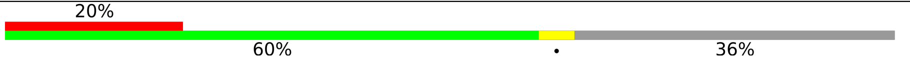
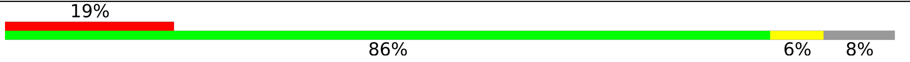
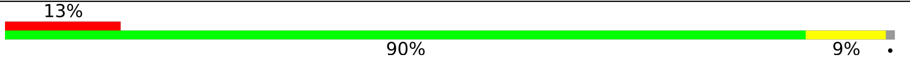
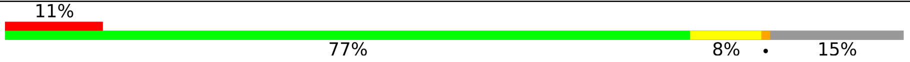
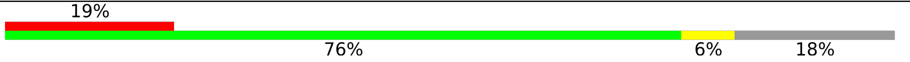
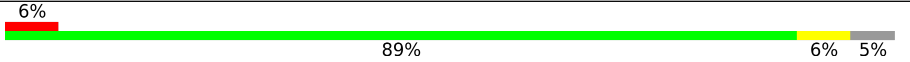
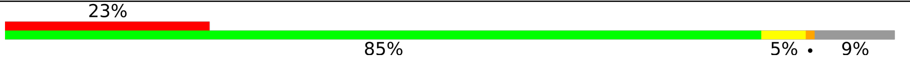
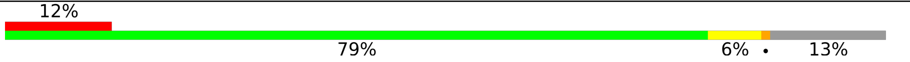
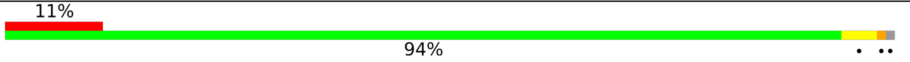
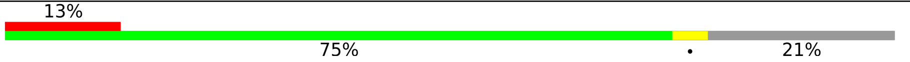
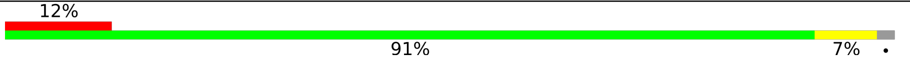
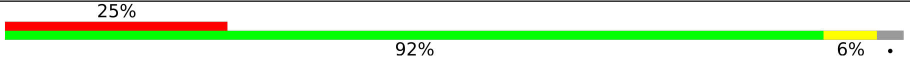
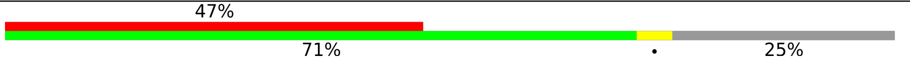
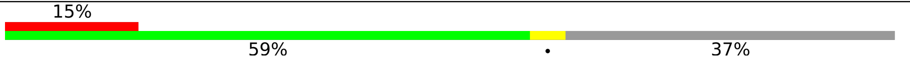
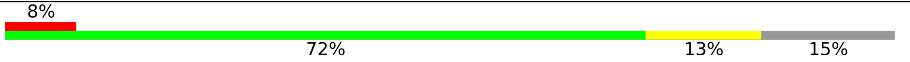
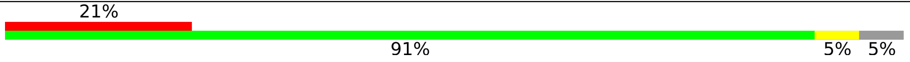
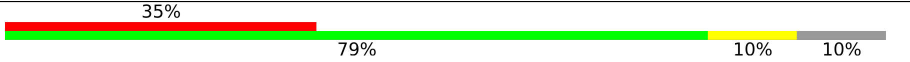
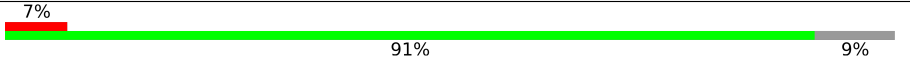
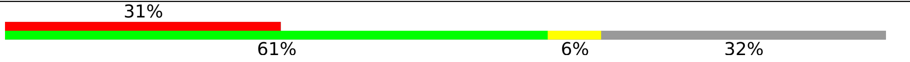
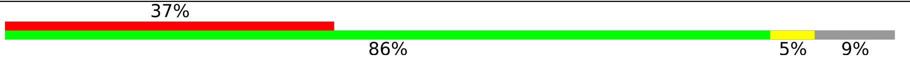
Mol	Chain	Length	Quality of chain
9	H	168	
10	I	197	
11	J	185	
12	K	141	
13	L	155	
14	M	124	
15	N	151	
16	O	159	
17	P	144	
18	Q	140	
19	R	129	
20	S	155	
21	T	148	
22	U	123	
23	V	89	
24	W	130	
25	X	144	
26	Y	140	
27	Z	115	
28	a	118	
29	b	86	
30	c	68	
31	d	57	
32	e	62	
33	g	335	

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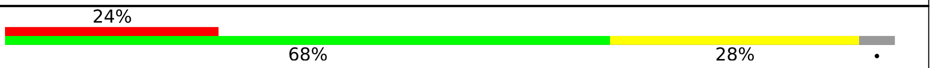
Mol	Chain	Length	Quality of chain
34	n	25	

2 Entry composition ⓘ

There are 34 unique types of molecules in this entry. The entry contains 65924 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 18S.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1490	31820	14210	5694	10426	1490	0	0

- Molecule 2 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	204	1603	1028	266	294	15	0	0

- Molecule 3 is a protein called Ribosomal protein S3Ae, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	219	1747	1103	314	318	12	0	0

- Molecule 4 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	217	1685	1082	299	298	6	0	0

- Molecule 5 is a protein called Ribosomal protein S3, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	D	208	1655	1039	311	296	9	0	0

- Molecule 6 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	E	246	1935	1236	362	329	8	0	0

- Molecule 7 is a protein called 40s ribosomal protein S5-B, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	186	Total	C	N	O	S	0	0
			1476	915	279	273	9		

- Molecule 8 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	G	31	Total	C	N	O	0	0
			155	93	31	31		

- Molecule 9 is a protein called 40S ribosomal protein S7, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	163	Total	C	N	O	S	0	0
			1276	811	230	234	1		

- Molecule 10 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	166	Total	C	N	O	S	0	0
			1300	811	253	232	4		

- Molecule 11 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	162	Total	C	N	O	S	0	0
			1321	833	252	233	3		

- Molecule 12 is a protein called Plectin/S10 domain containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	90	Total	C	N	O	S	0	0
			731	472	125	128	6		

- Molecule 13 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	142	Total	C	N	O	S	0	0
			1160	742	222	193	3		

- Molecule 14 is a protein called Ribosomal protein L7Ae, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	M	103	509	303	103	103	0	0

- Molecule 15 is a protein called 40S ribosomal protein S13, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	N	150	1190	749	234	202	5	0	0

- Molecule 16 is a protein called Ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	O	135	1005	615	205	182	3	0	0

- Molecule 17 is a protein called Ribosomal protein S19, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	P	118	962	624	176	159	3	0	0

- Molecule 18 is a protein called 40S ribosomal protein S16, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	Q	133	1043	660	196	182	5	0	0

- Molecule 19 is a protein called 40S ribosomal protein S17-B, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	R	118	961	603	181	171	6	0	0

- Molecule 20 is a protein called Ribosomal protein S13p/S18e, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	S	135	1077	668	219	183	7	0	0

- Molecule 21 is a protein called Ribosomal protein S19e, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	T	146	1148	725	219	200	4	0	0

- Molecule 22 is a protein called Ribosomal protein S10p/S20e, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	U	97	777	487	150	137	3	0	0

- Molecule 23 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	V	87	671	418	118	131	4	0	0

- Molecule 24 is a protein called Ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	W	128	1001	637	182	175	7	0	0

- Molecule 25 is a protein called 40S ribosomal protein S23, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	X	140	1062	670	206	182	4	0	0

- Molecule 26 is a protein called Ribosomal protein S24e, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	Y	105	792	506	144	141	1	0	0

- Molecule 27 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	Z	73	560	356	99	102	3	0	0

- Molecule 28 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	a	100	815	503	168	136	8	0	0

- Molecule 29 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	b	82	632	395	114	119	4	0	0

- Molecule 30 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
30	c	61	475	290	96	89	0	0

- Molecule 31 is a protein called 40S ribosomal protein S29, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	d	52	438	272	95	67	4	0	0

- Molecule 32 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	e	42	337	211	71	54	1	0	0

- Molecule 33 is a protein called Guanine nucleotide-binding protein beta subunit, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	g	305	2380	1509	417	443	11	0	0

- Molecule 34 is a protein called eL41.

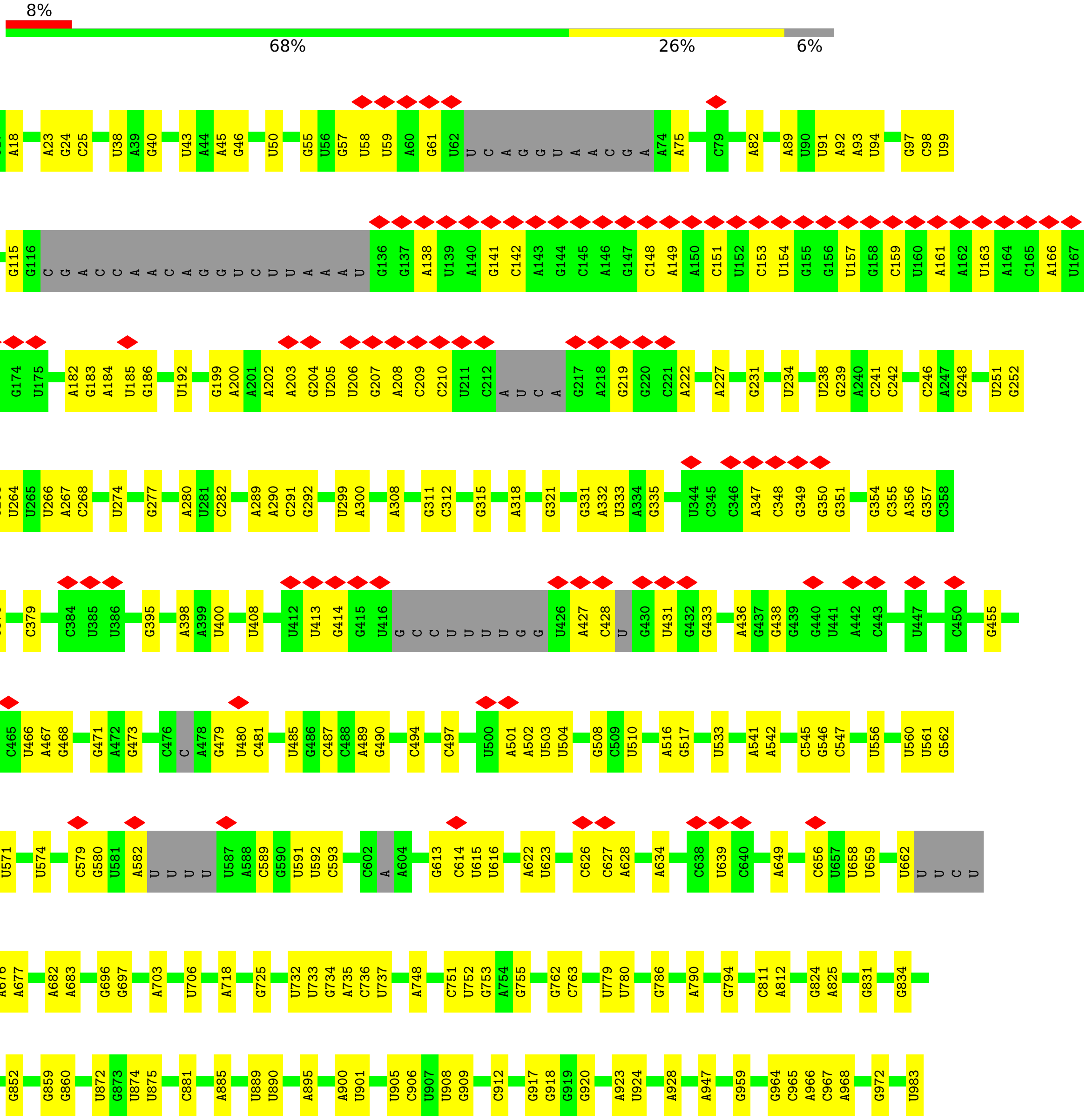
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
34	n	24	225	137	62	26	0	0

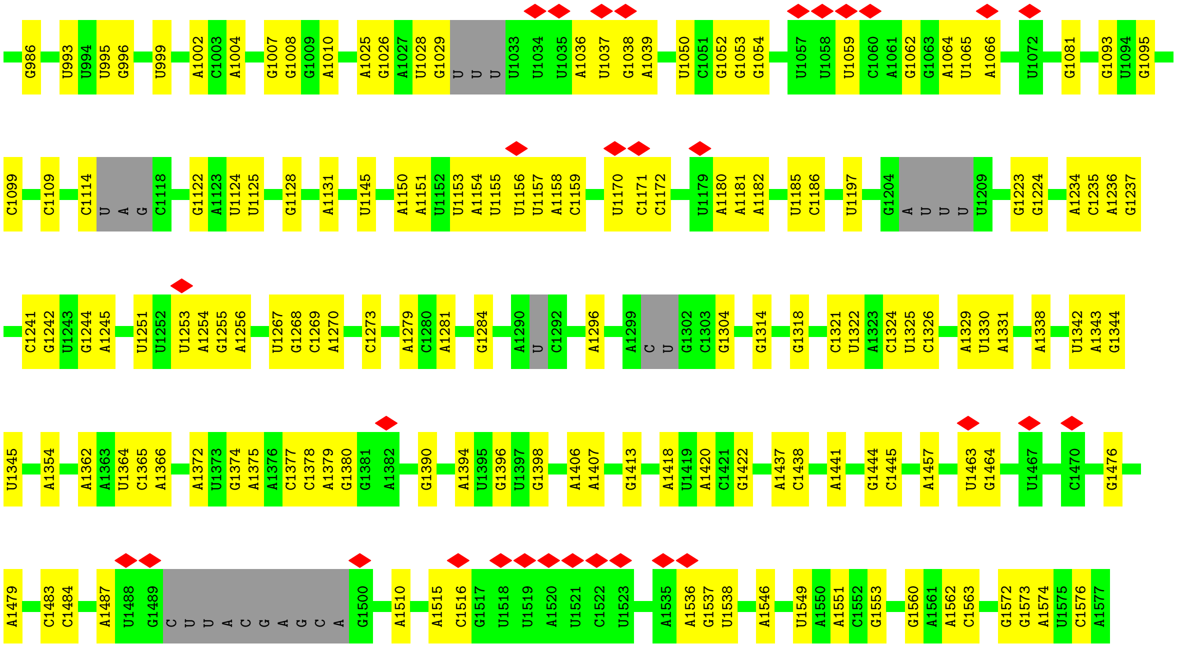
3 Residue-property plots ⓘ

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: 18S

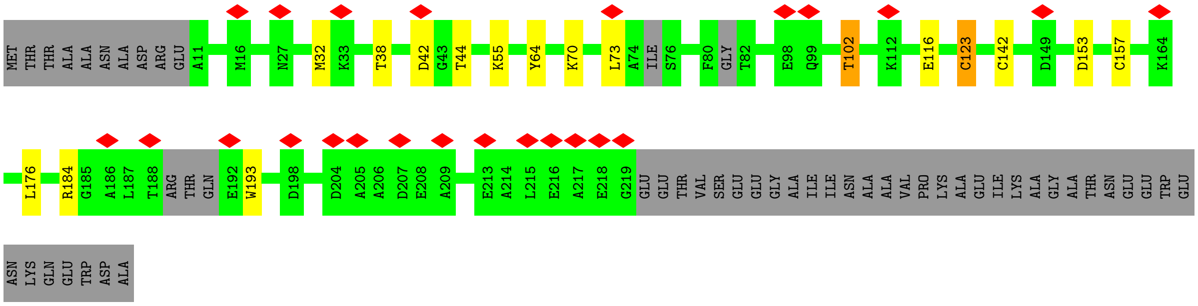
Chain 2:





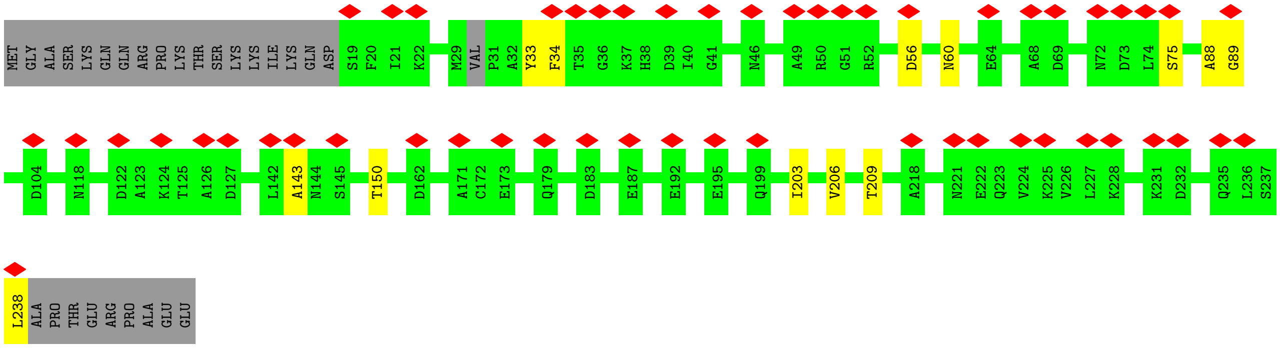
- Molecule 2: 40S ribosomal protein SA

Chain A:



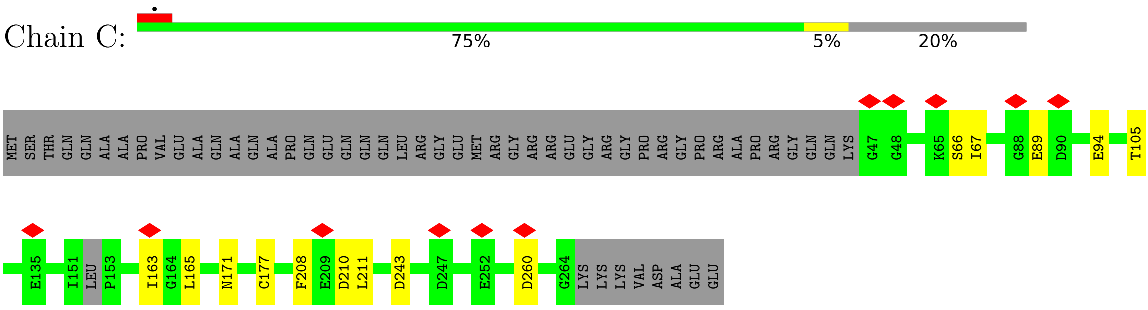
- Molecule 3: Ribosomal protein S3Ae, putative

Chain B:



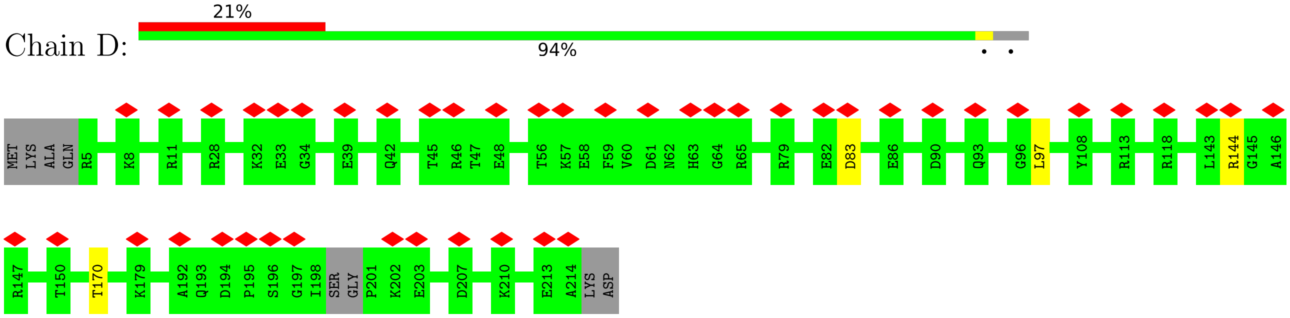
- Molecule 4: Uncharacterized protein

Chain C:



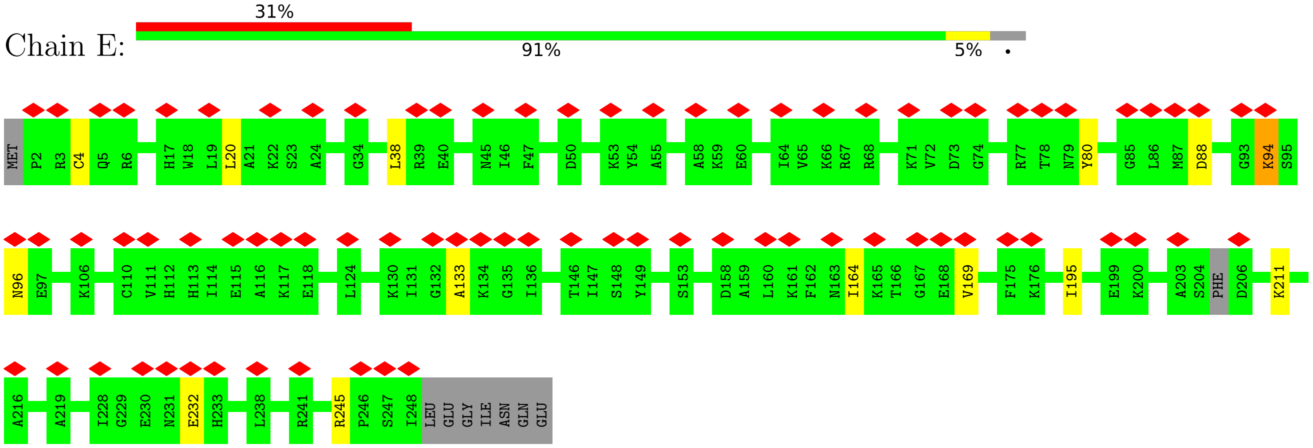
- Molecule 5: Ribosomal protein S3, putative

Chain D:



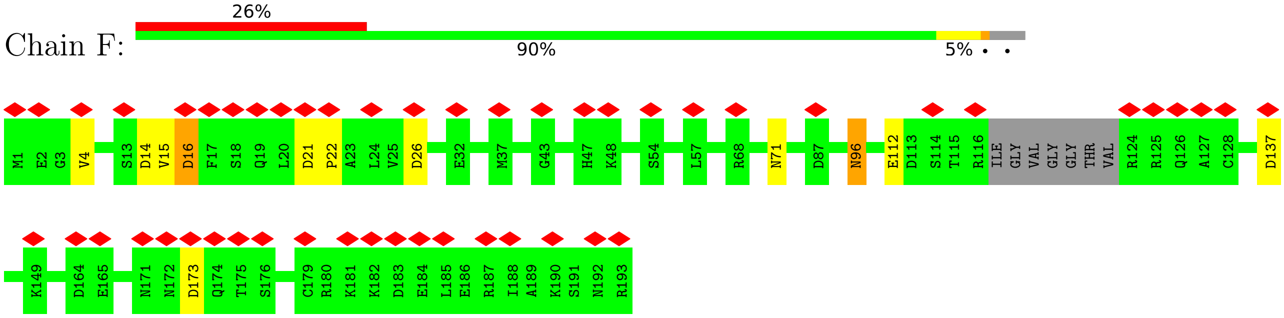
- Molecule 6: 40S ribosomal protein S4

Chain E:



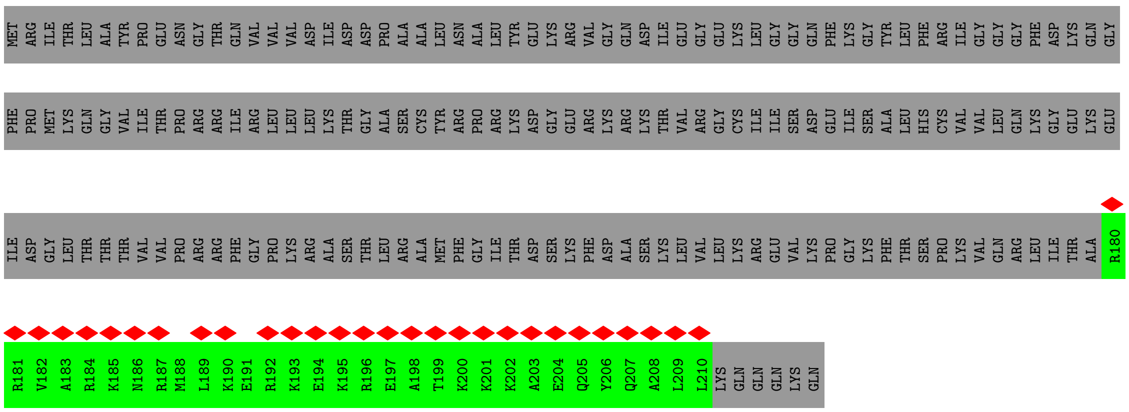
- Molecule 7: 40s ribosomal protein S5-B, putative

Chain F:



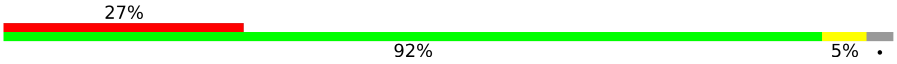
- Molecule 8: 40S ribosomal protein S6

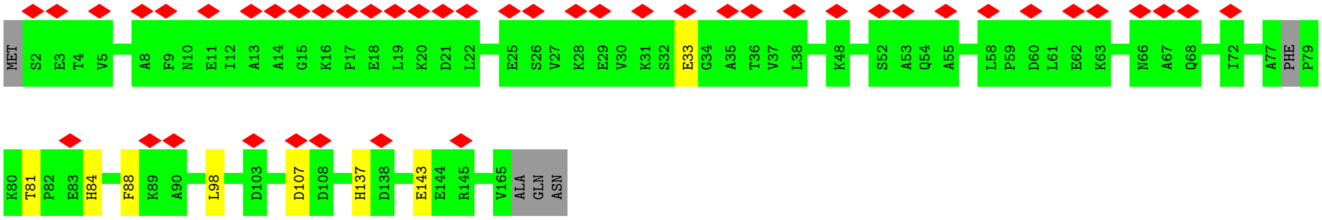
Chain G:



- Molecule 9: 40S ribosomal protein S7, putative

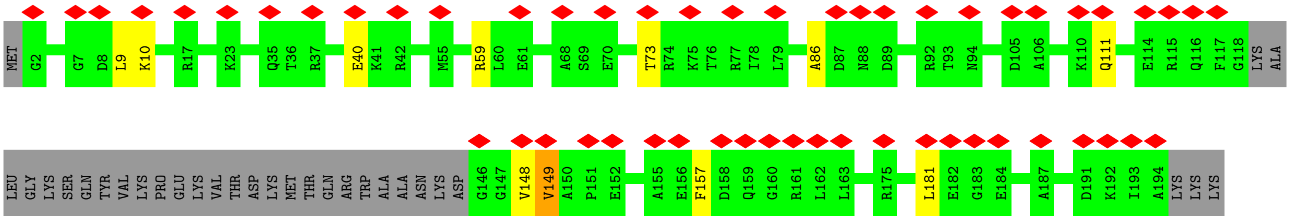
Chain H:





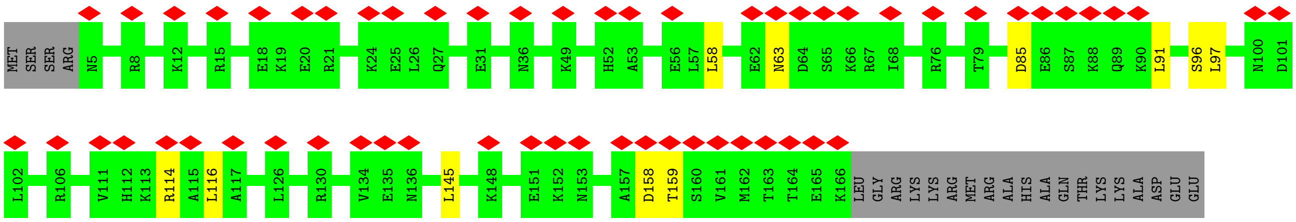
- Molecule 10: 40S ribosomal protein S8

Chain I:



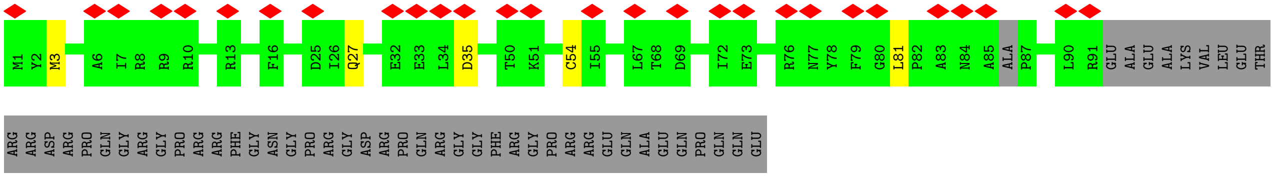
- Molecule 11: Uncharacterized protein

Chain J:



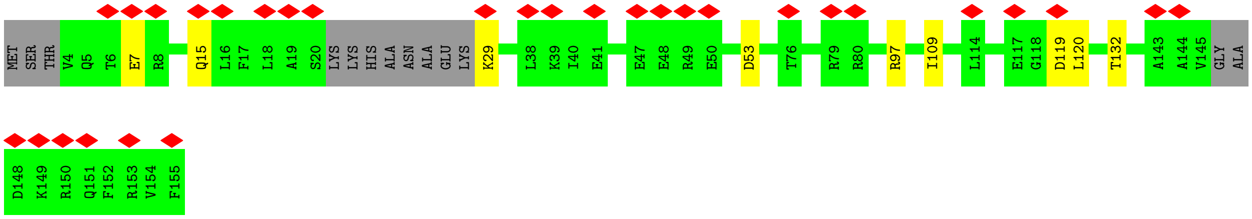
- Molecule 12: Plectin/S10 domain containing protein

Chain K:



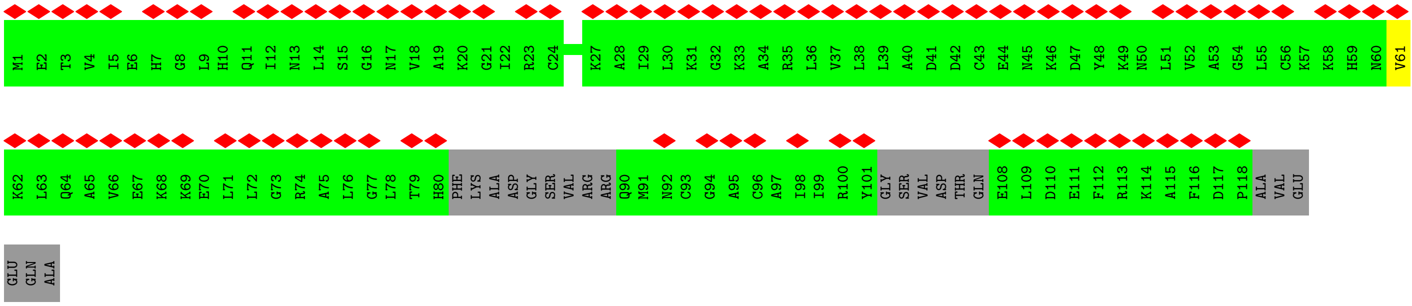
- Molecule 13: Uncharacterized protein

Chain L:



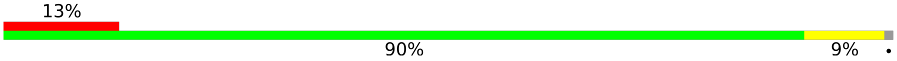
- Molecule 14: Ribosomal protein L7Ae, putative

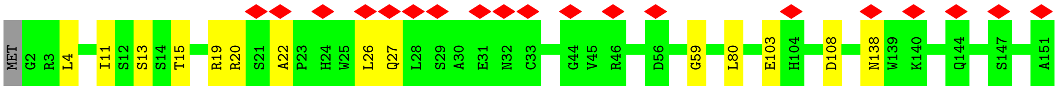
Chain M:



- Molecule 15: 40S ribosomal protein S13, putative

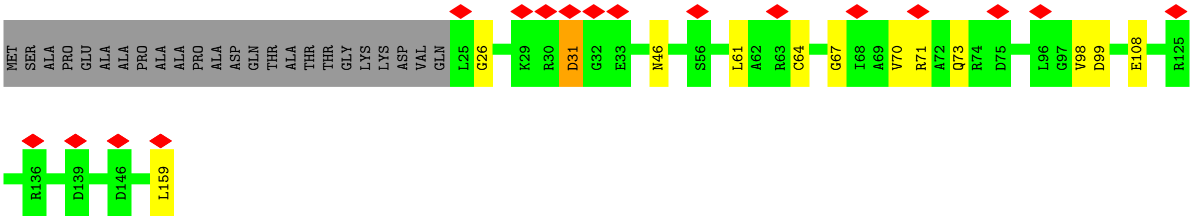
Chain N:





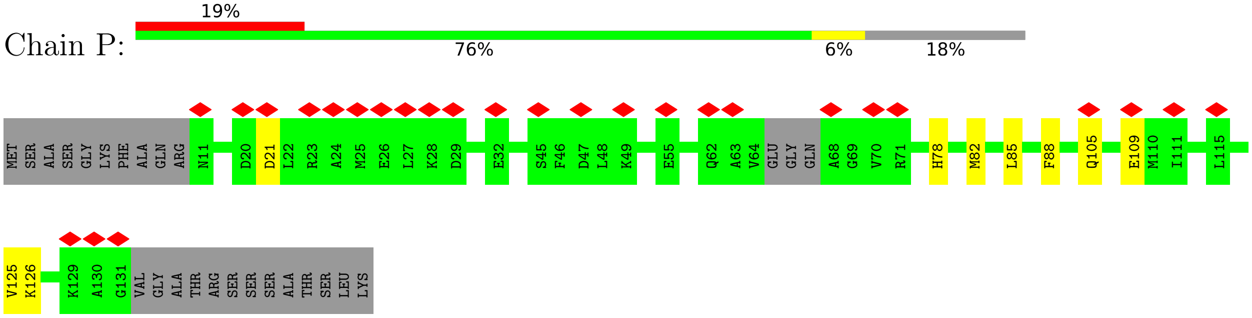
- Molecule 16: Ribosomal protein S14

Chain O:



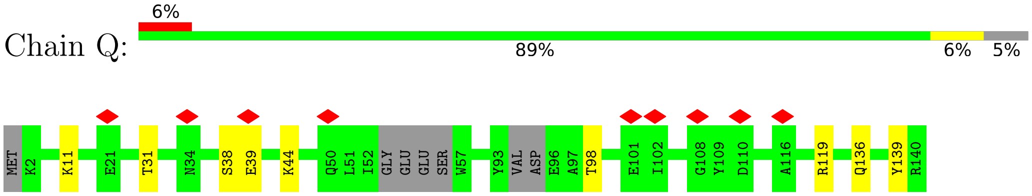
- Molecule 17: Ribosomal protein S19, putative

Chain P:



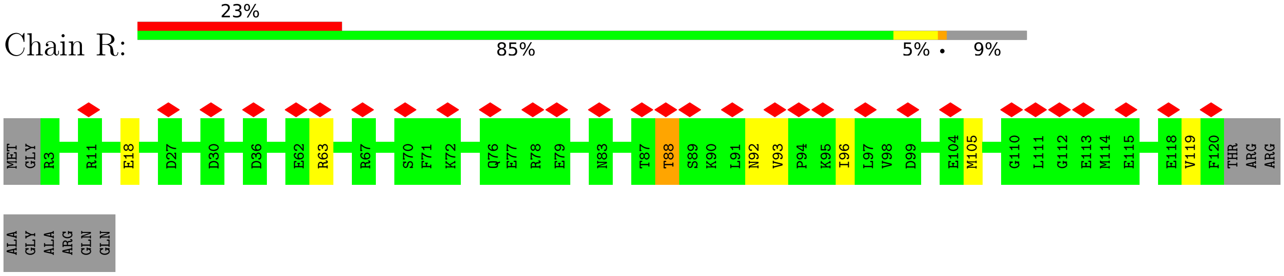
- Molecule 18: 40S ribosomal protein S16, putative

Chain Q:



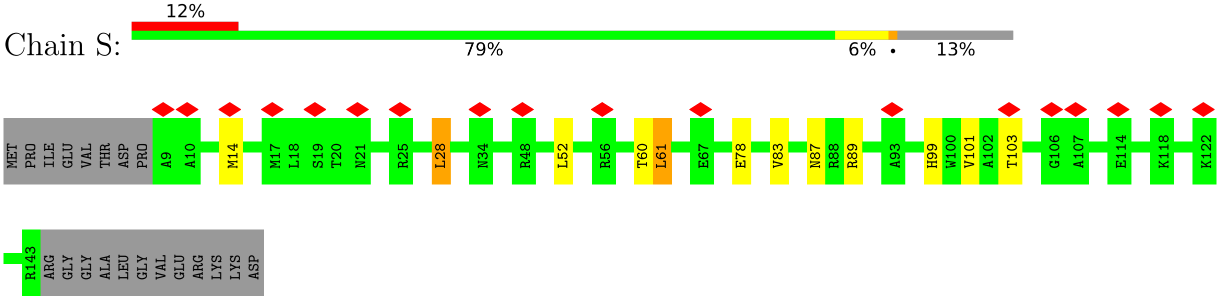
- Molecule 19: 40S ribosomal protein S17-B, putative

Chain R:



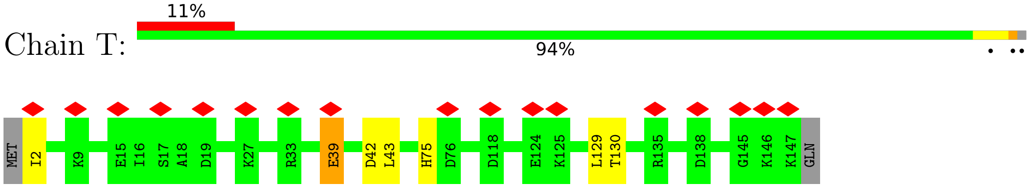
- Molecule 20: Ribosomal protein S13p/S18e, putative

Chain S:



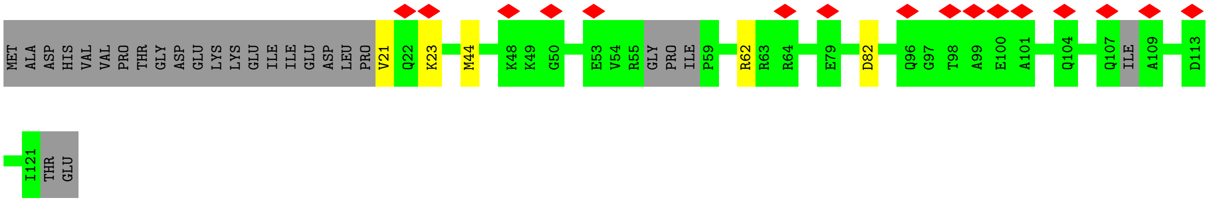
- Molecule 21: Ribosomal protein S19e, putative

Chain T:



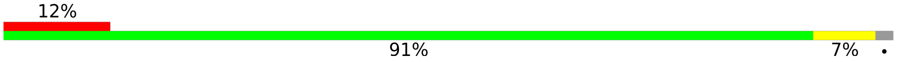
- Molecule 22: Ribosomal protein S10p/S20e, putative

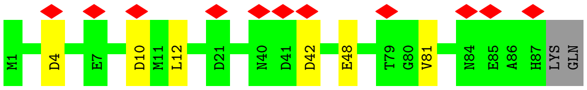
Chain U:



- Molecule 23: 40S ribosomal protein S21

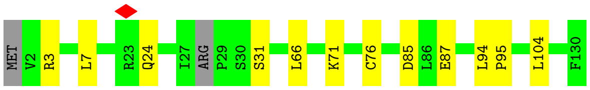
Chain V:





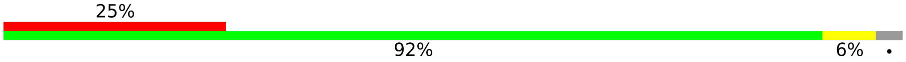
- Molecule 24: Ribosomal protein S15a

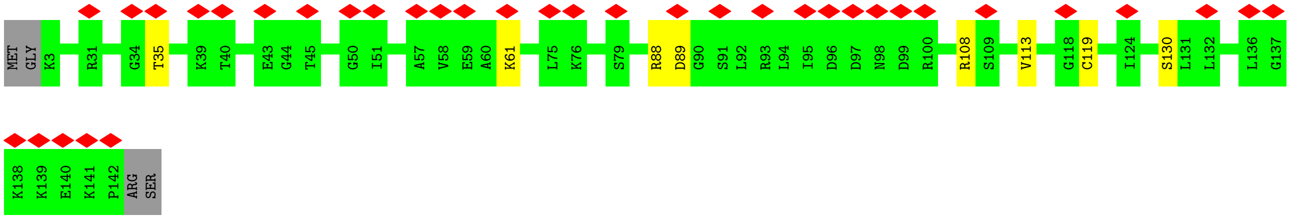
Chain W:



- Molecule 25: 40S ribosomal protein S23, putative

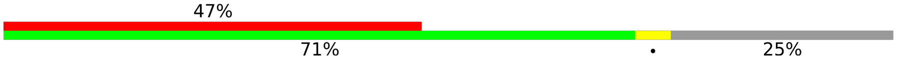
Chain X:

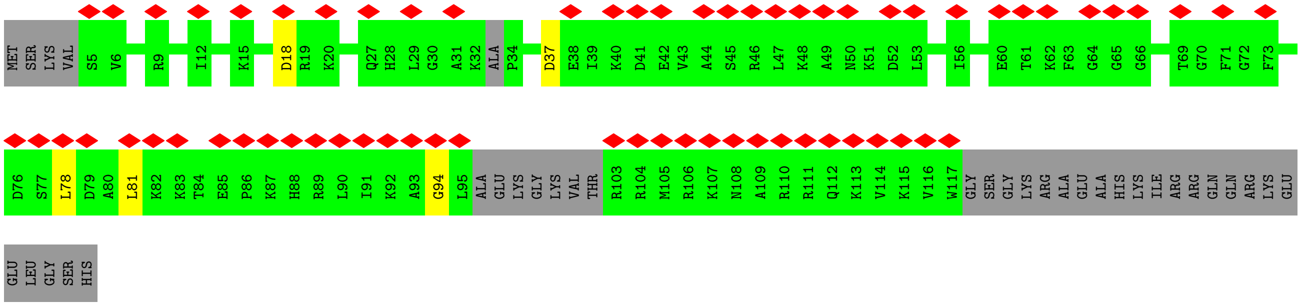




- Molecule 26: Ribosomal protein S24e, putative

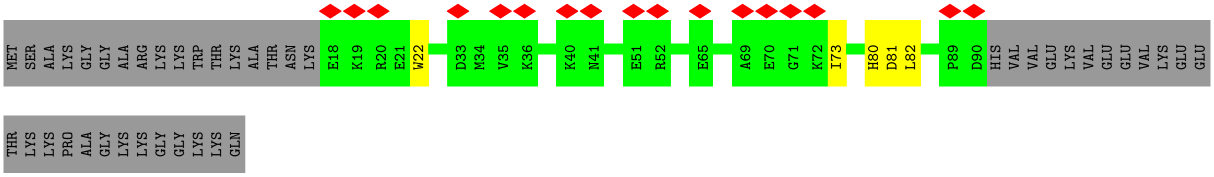
Chain Y:





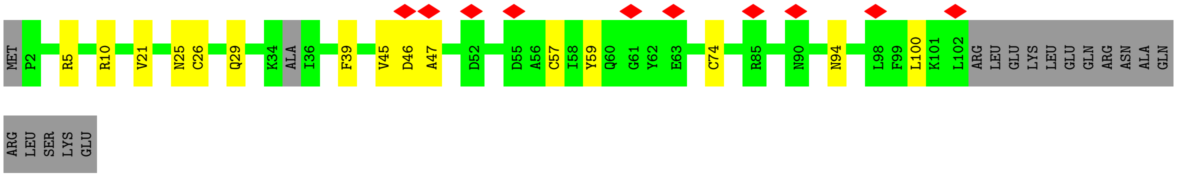
- Molecule 27: Uncharacterized protein

Chain Z:



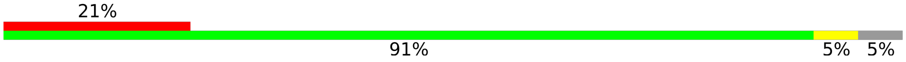
- Molecule 28: 40S ribosomal protein S26

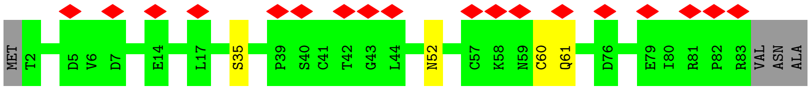
Chain a:



- Molecule 29: 40S ribosomal protein S27

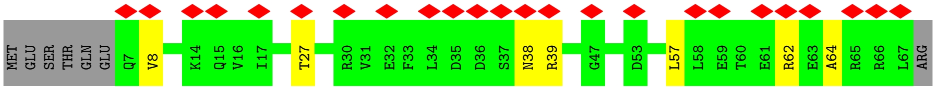
Chain b:





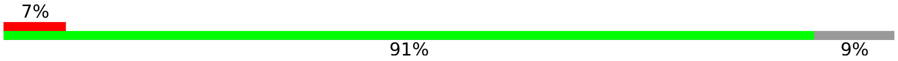
- Molecule 30: Uncharacterized protein

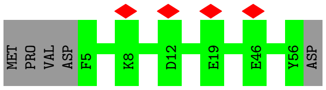
Chain c:



- Molecule 31: 40S ribosomal protein S29, putative

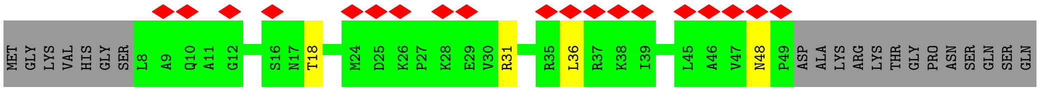
Chain d:





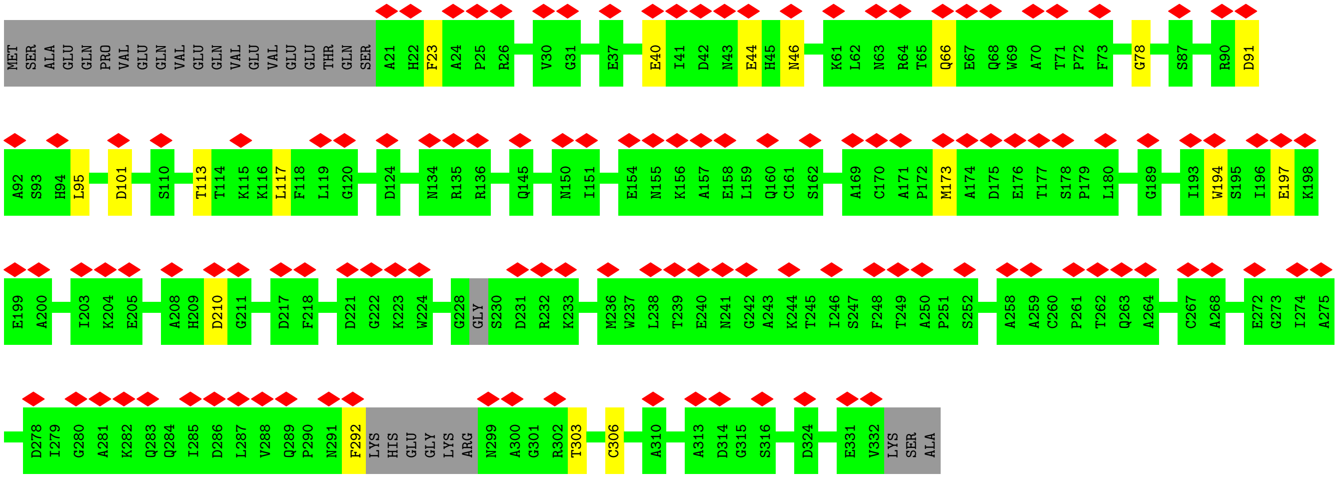
- Molecule 32: 40S ribosomal protein S30

Chain e:



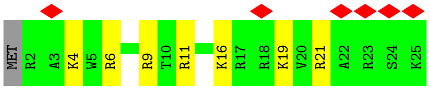
- Molecule 33: Guanine nucleotide-binding protein beta subunit, putative

Chain g:



- Molecule 34: eL41

Chain n:



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	57162	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 $(e^-/\text{Å}^2)$	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.268	Depositor
Minimum map value	-0.139	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.036	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	2	0.22	0/35582	0.68	0/55428
2	A	0.38	0/1634	0.55	0/2210
3	B	0.35	0/1777	0.57	0/2389
4	C	0.39	0/1722	0.57	0/2318
5	D	0.36	0/1675	0.56	0/2242
6	E	0.35	0/1974	0.56	0/2657
7	F	0.38	0/1497	0.64	0/2010
8	G	0.37	0/154	0.40	0/214
9	H	0.38	0/1295	0.56	0/1746
10	I	0.40	0/1322	0.60	0/1778
11	J	0.34	0/1344	0.56	0/1808
12	K	0.43	0/749	0.60	0/1013
13	L	0.34	0/1181	0.57	0/1585
14	M	0.34	0/507	0.60	0/701
15	N	0.40	0/1213	0.62	0/1634
16	O	0.35	0/1017	0.70	0/1366
17	P	0.40	0/983	0.61	0/1320
18	Q	0.39	0/1057	0.62	0/1418
19	R	0.41	0/975	0.60	0/1305
20	S	0.42	0/1093	0.67	0/1467
21	T	0.36	0/1172	0.56	0/1576
22	U	0.37	0/785	0.62	0/1053
23	V	0.43	0/682	0.64	0/924
24	W	0.35	0/1015	0.56	0/1358
25	X	0.36	0/1076	0.61	0/1441
26	Y	0.37	0/802	0.55	0/1073
27	Z	0.36	0/570	0.55	0/770
28	a	0.40	0/829	0.69	0/1110
29	b	0.40	0/645	0.61	0/880
30	c	0.33	0/475	0.61	0/635
31	d	0.39	0/445	0.66	0/588
32	e	0.35	0/341	0.55	0/454
33	g	0.37	0/2440	0.53	0/3324
34	n	0.70	0/226	0.93	0/290

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.31	0/70254	0.64	0/102085

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	
2	A	196/256 (77%)	180 (92%)	11 (6%)	5 (3%)	5	28
3	B	215/247 (87%)	195 (91%)	11 (5%)	9 (4%)	3	19
4	C	213/272 (78%)	193 (91%)	15 (7%)	5 (2%)	6	31
5	D	204/216 (94%)	188 (92%)	15 (7%)	1 (0%)	29	63
6	E	242/255 (95%)	210 (87%)	26 (11%)	6 (2%)	5	29
7	F	182/193 (94%)	158 (87%)	16 (9%)	8 (4%)	2	18
8	G	29/216 (13%)	29 (100%)	0	0	100	100
9	H	159/168 (95%)	146 (92%)	10 (6%)	3 (2%)	8	34
10	I	162/197 (82%)	147 (91%)	10 (6%)	5 (3%)	4	25
11	J	160/185 (86%)	138 (86%)	16 (10%)	6 (4%)	3	21
12	K	86/141 (61%)	80 (93%)	6 (7%)	0	100	100
13	L	136/155 (88%)	121 (89%)	14 (10%)	1 (1%)	22	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	M	97/124 (78%)	84 (87%)	12 (12%)	1 (1%)	15	49
15	N	148/151 (98%)	128 (86%)	14 (10%)	6 (4%)	3	19
16	O	133/159 (84%)	104 (78%)	21 (16%)	8 (6%)	1	11
17	P	114/144 (79%)	102 (90%)	10 (9%)	2 (2%)	8	35
18	Q	127/140 (91%)	108 (85%)	14 (11%)	5 (4%)	3	20
19	R	116/129 (90%)	101 (87%)	11 (10%)	4 (3%)	3	23
20	S	133/155 (86%)	119 (90%)	10 (8%)	4 (3%)	4	26
21	T	144/148 (97%)	133 (92%)	9 (6%)	2 (1%)	11	40
22	U	91/123 (74%)	84 (92%)	6 (7%)	1 (1%)	14	46
23	V	85/89 (96%)	73 (86%)	9 (11%)	3 (4%)	3	23
24	W	124/130 (95%)	113 (91%)	10 (8%)	1 (1%)	19	53
25	X	138/144 (96%)	124 (90%)	10 (7%)	4 (3%)	4	26
26	Y	99/140 (71%)	84 (85%)	13 (13%)	2 (2%)	7	33
27	Z	71/115 (62%)	66 (93%)	2 (3%)	3 (4%)	3	19
28	a	96/118 (81%)	84 (88%)	6 (6%)	6 (6%)	1	10
29	b	80/86 (93%)	71 (89%)	6 (8%)	3 (4%)	3	21
30	c	59/68 (87%)	51 (86%)	3 (5%)	5 (8%)	1	5
31	d	50/57 (88%)	48 (96%)	2 (4%)	0	100	100
32	e	40/62 (64%)	38 (95%)	2 (5%)	0	100	100
33	g	299/335 (89%)	263 (88%)	30 (10%)	6 (2%)	7	33
34	n	22/25 (88%)	20 (91%)	2 (9%)	0	100	100
All	All	4250/5143 (83%)	3783 (89%)	352 (8%)	115 (3%)	8	27

5 of 115 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	42	ASP
3	B	88	ALA
7	F	15	VAL
7	F	26	ASP
10	I	149	VAL

5.3.2 Protein sidechains ⓘ

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	
2	A	172/211 (82%)	158 (92%)	14 (8%)	11	38
3	B	192/216 (89%)	188 (98%)	4 (2%)	53	77
4	C	174/216 (81%)	165 (95%)	9 (5%)	23	55
5	D	176/182 (97%)	173 (98%)	3 (2%)	60	80
6	E	209/217 (96%)	200 (96%)	9 (4%)	29	60
7	F	161/165 (98%)	155 (96%)	6 (4%)	34	63
9	H	137/141 (97%)	132 (96%)	5 (4%)	35	64
10	I	131/158 (83%)	124 (95%)	7 (5%)	22	54
11	J	141/168 (84%)	136 (96%)	5 (4%)	36	66
12	K	77/116 (66%)	72 (94%)	5 (6%)	17	48
13	L	124/137 (90%)	116 (94%)	8 (6%)	17	48
14	M	1/101 (1%)	1 (100%)	0	100	100
15	N	125/126 (99%)	117 (94%)	8 (6%)	17	48
16	O	99/115 (86%)	93 (94%)	6 (6%)	18	50
17	P	105/124 (85%)	98 (93%)	7 (7%)	16	47
18	Q	108/114 (95%)	104 (96%)	4 (4%)	34	63
19	R	104/111 (94%)	99 (95%)	5 (5%)	25	57
20	S	112/128 (88%)	102 (91%)	10 (9%)	9	34
21	T	120/122 (98%)	114 (95%)	6 (5%)	24	56
22	U	87/110 (79%)	83 (95%)	4 (5%)	27	59
23	V	72/74 (97%)	69 (96%)	3 (4%)	30	60
24	W	107/109 (98%)	96 (90%)	11 (10%)	7	27
25	X	112/115 (97%)	108 (96%)	4 (4%)	35	64
26	Y	77/118 (65%)	74 (96%)	3 (4%)	32	62
27	Z	60/93 (64%)	58 (97%)	2 (3%)	38	67
28	a	91/107 (85%)	82 (90%)	9 (10%)	8	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	b	76/79 (96%)	75 (99%)	1 (1%)	69	84
30	c	52/59 (88%)	50 (96%)	2 (4%)	33	63
31	d	46/51 (90%)	46 (100%)	0	100	100
32	e	35/51 (69%)	31 (89%)	4 (11%)	5	22
33	g	256/282 (91%)	244 (95%)	12 (5%)	26	58
34	n	22/23 (96%)	15 (68%)	7 (32%)	0	1
All	All	3561/4139 (86%)	3378 (95%)	183 (5%)	27	55

5 of 183 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	T	2	ILE
26	Y	37	ASP
21	T	129	LEU
24	W	24	GLN
28	a	21	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
18	Q	80	GLN
26	Y	14	ASN
18	Q	91	GLN
21	T	70	GLN
27	Z	30	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1472/1577 (93%)	406 (27%)	47 (3%)

5 of 406 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	3	U
1	2	4	U
1	2	16	C
1	2	18	A

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Mol	**Chain**	**Res**	**Type**
1	2	24	G

5 of 47 RNA pucker outliers are listed below:

Mol	**Chain**	**Res**	**Type**
1	2	917	G
1	2	1154	A
1	2	966	A
1	2	1059	U
1	2	1244	G

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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.

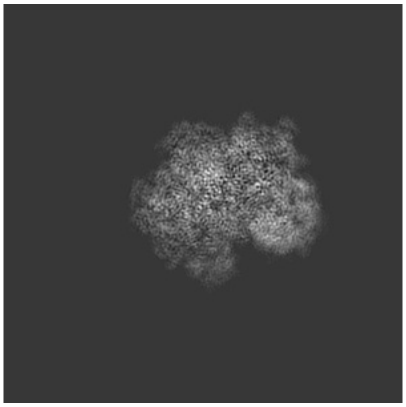
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6788. These allow visual inspection of the internal detail of the map and identification of artifacts.

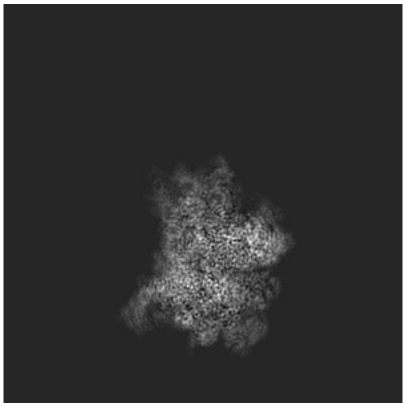
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

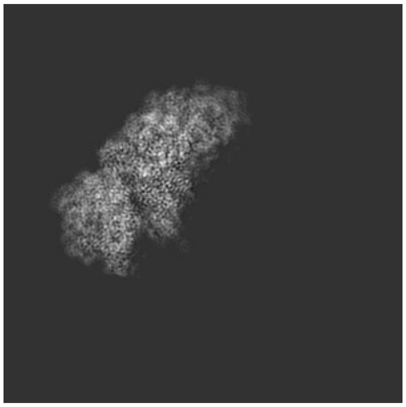
6.1.1 Primary map



X



Y

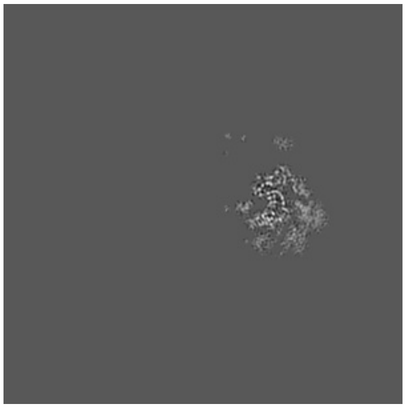


Z

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

6.2 Central slices

6.2.1 Primary map



X Index: 160

Y Index: 160

Z Index: 160

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map

X Index: 128

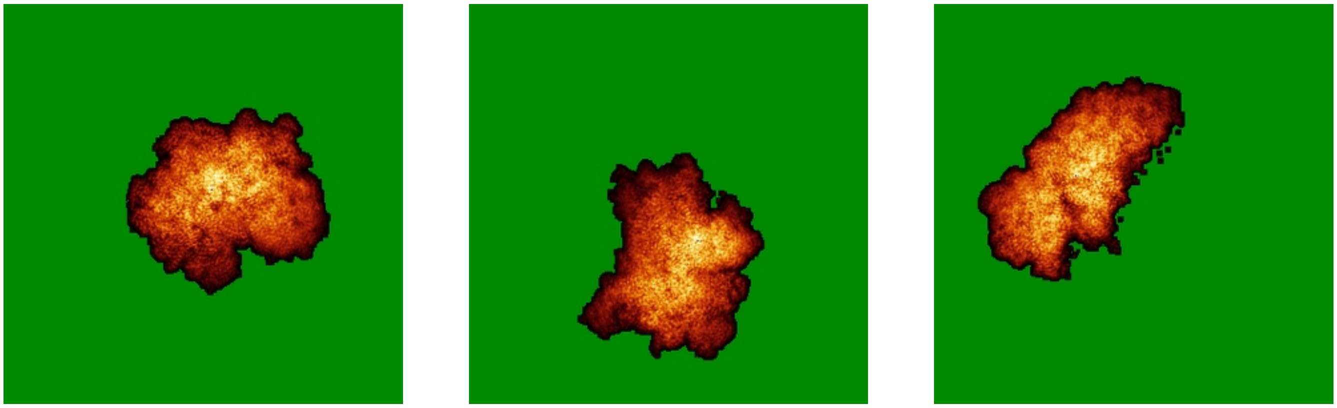
Y Index: 167

Z Index: 173

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

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

6.4.1 Primary map



X

Y

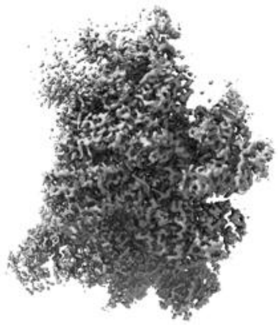
Z

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 0.036. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

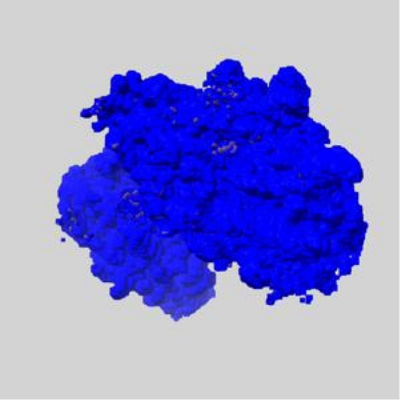
6.6 Mask visualisation

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

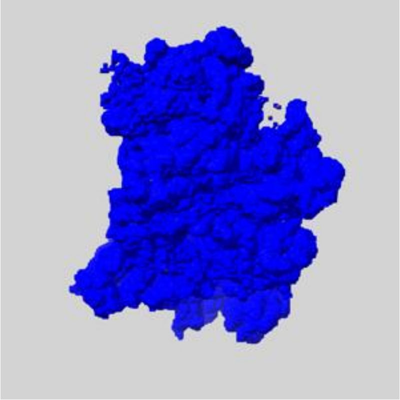
A mask typically either:

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

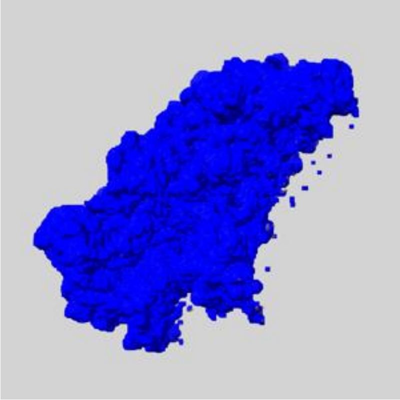
6.6.1 emd_6788_msk_1.map



X



Y

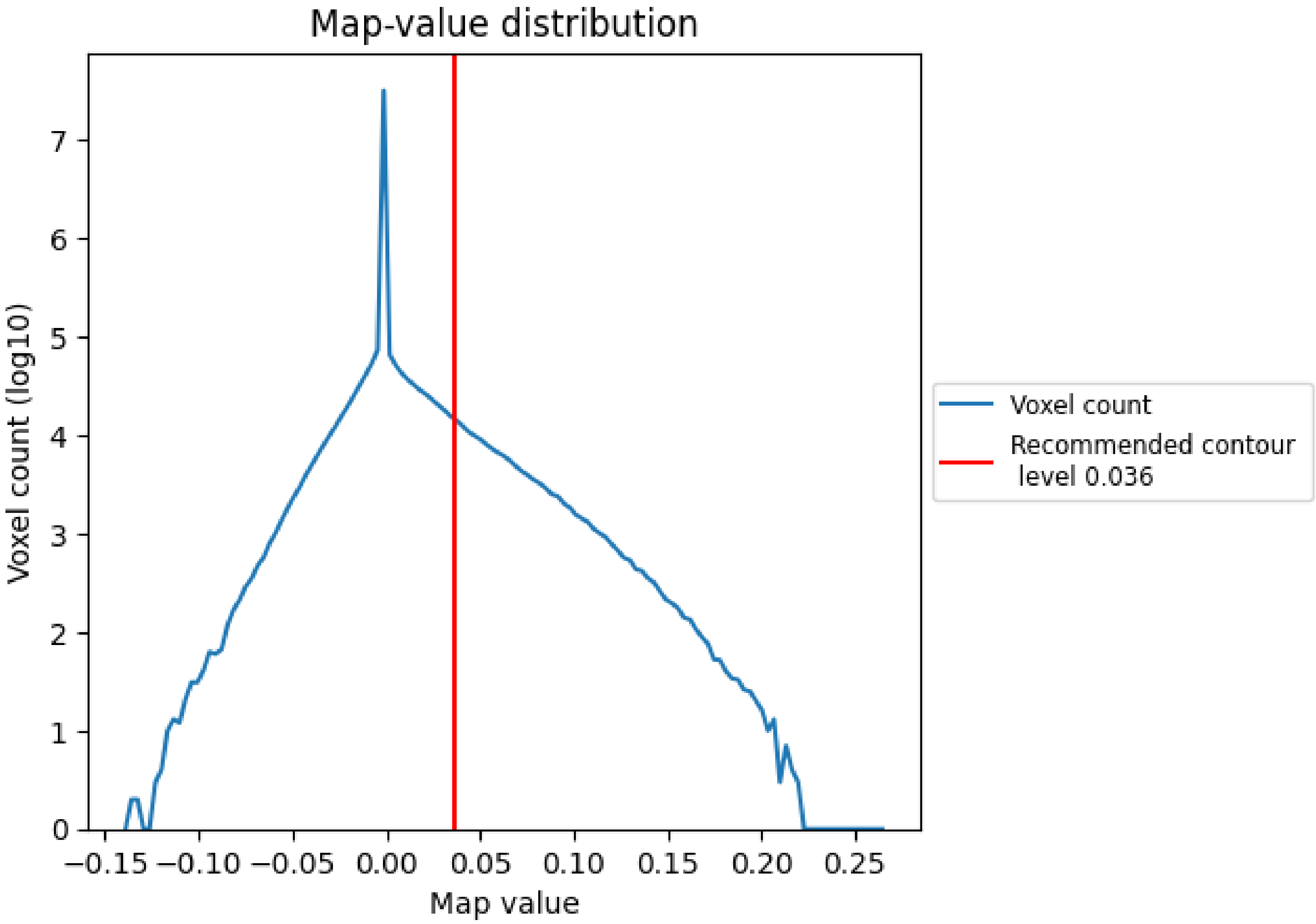


Z

7 Map analysis ⓘ

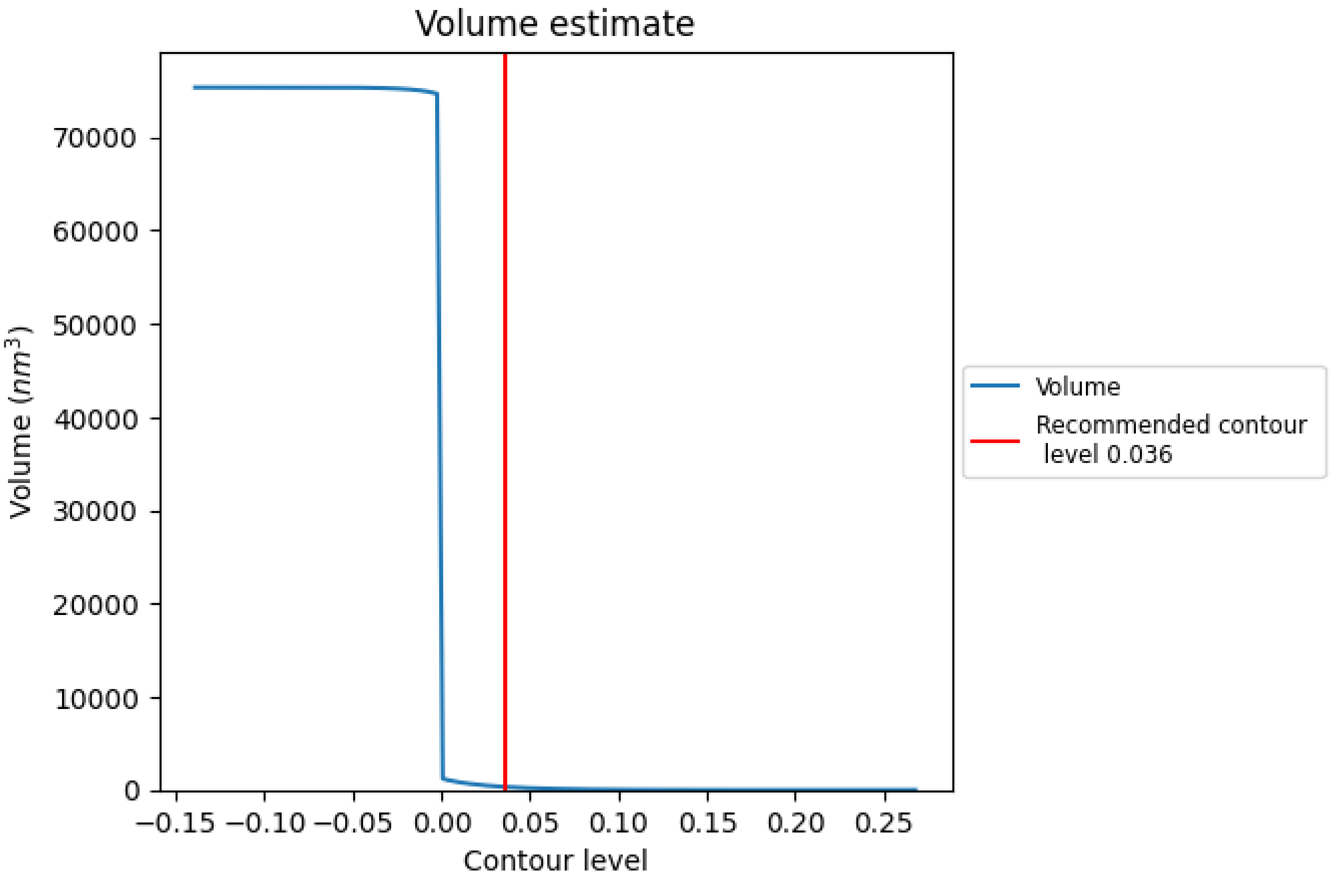
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

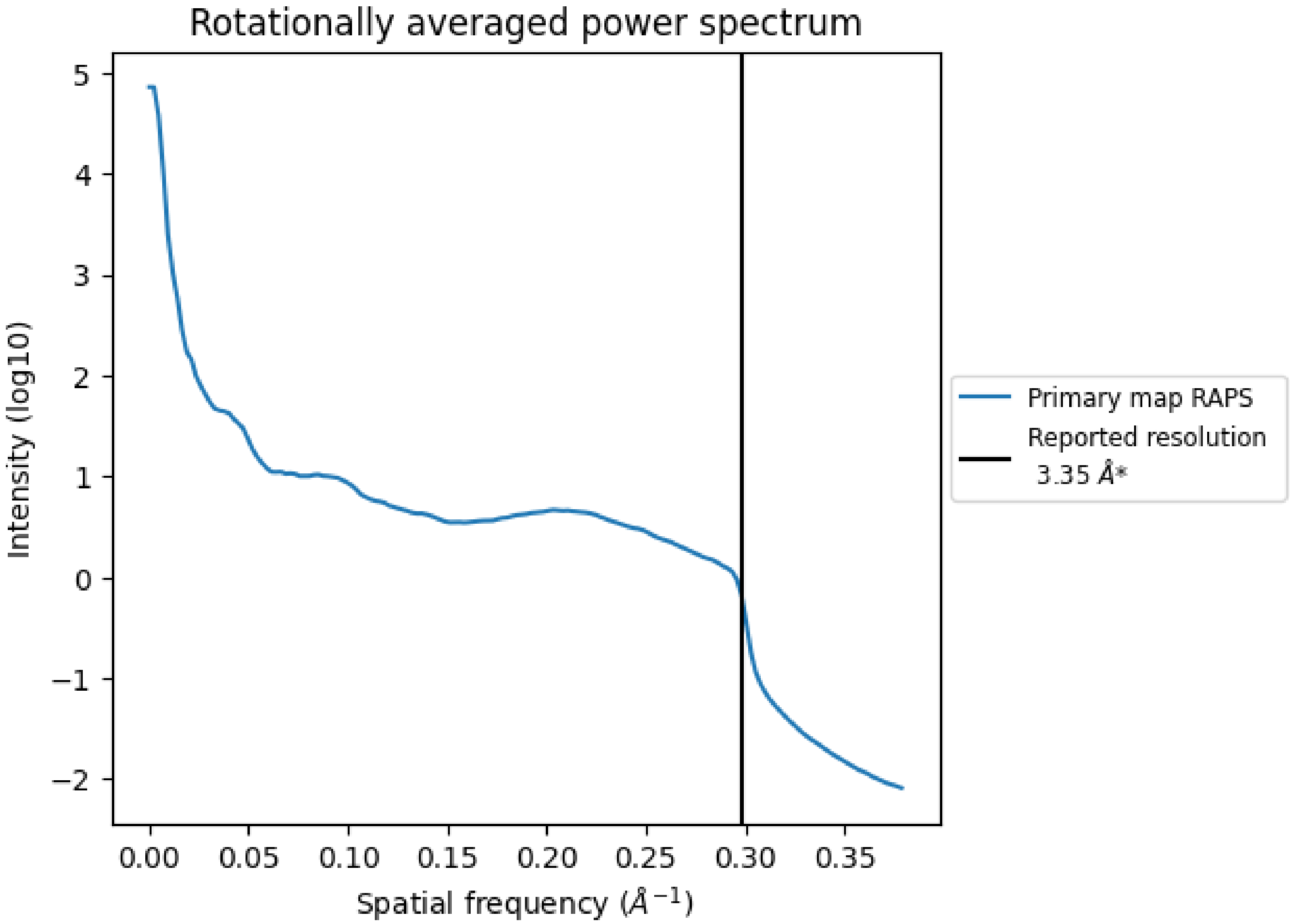
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 325 nm^3; this corresponds to an approximate mass of 294 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 ⓘ

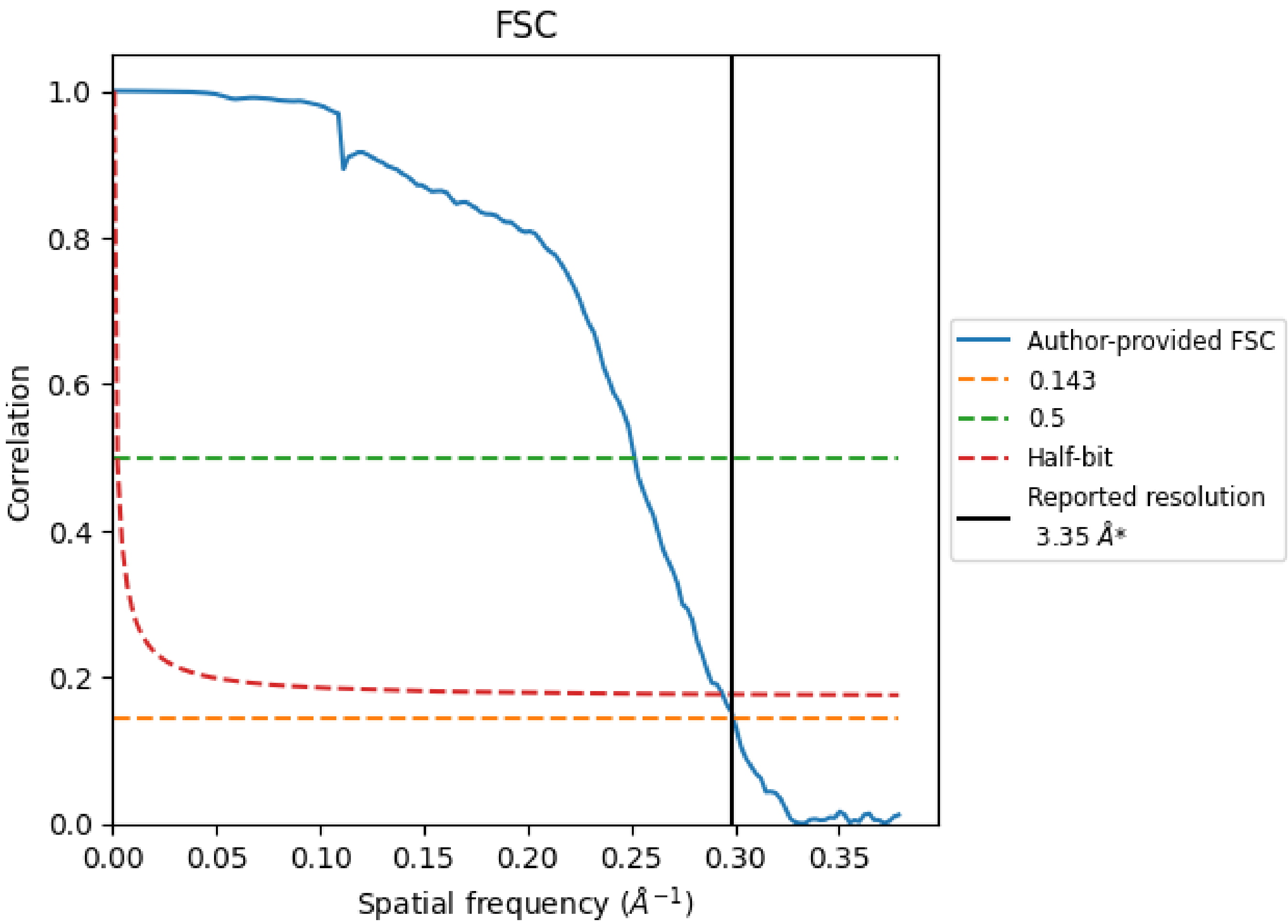


*Reported resolution corresponds to spatial frequency of 0.299 Å^{-1}

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 0.299 Å^{-1}

8.2 Resolution estimates ⓘ

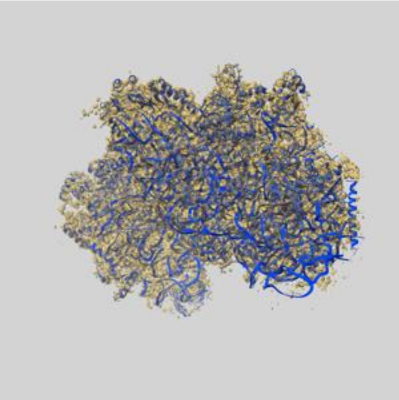
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.35	-	-
Author-provided FSC curve	3.34	3.98	3.40
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

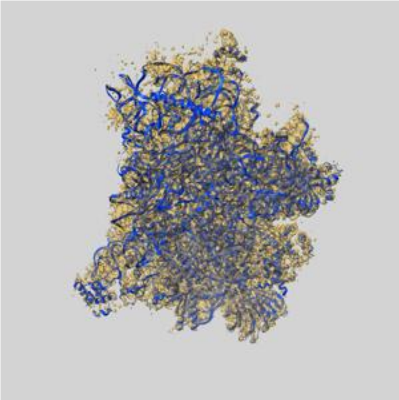
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-6788 and PDB model 5XYI. Per-residue inclusion information can be found in section 3 on page 10.

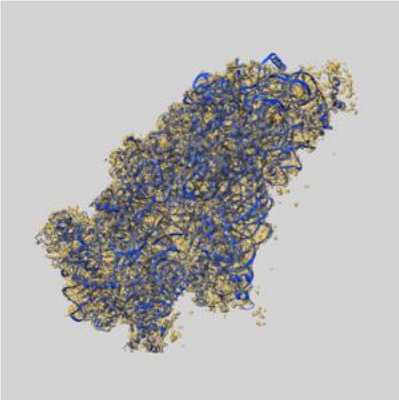
9.1 Map-model overlay ⓘ



X



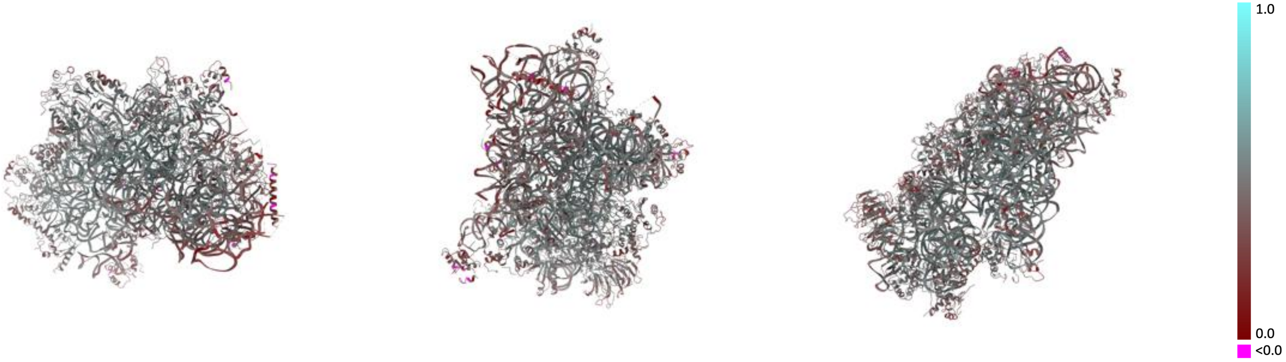
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.036 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

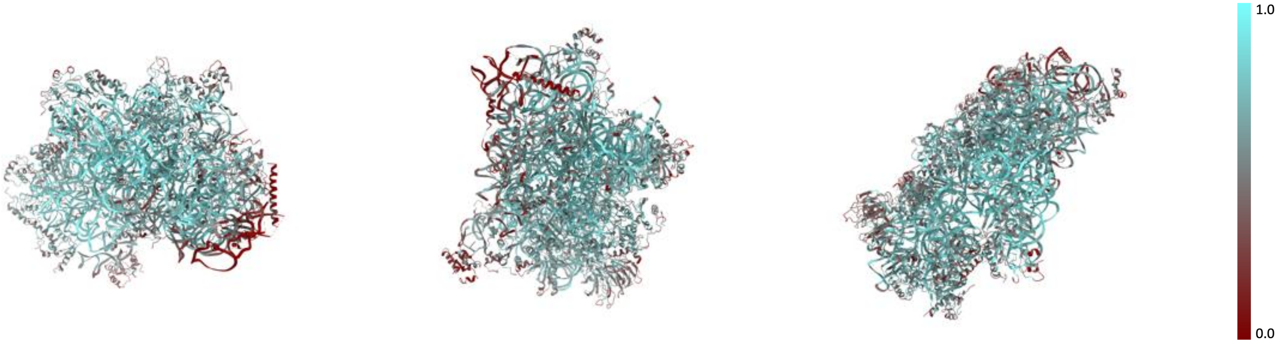
9.2 Q-score mapped to coordinate model ⓘ



X Y Z

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

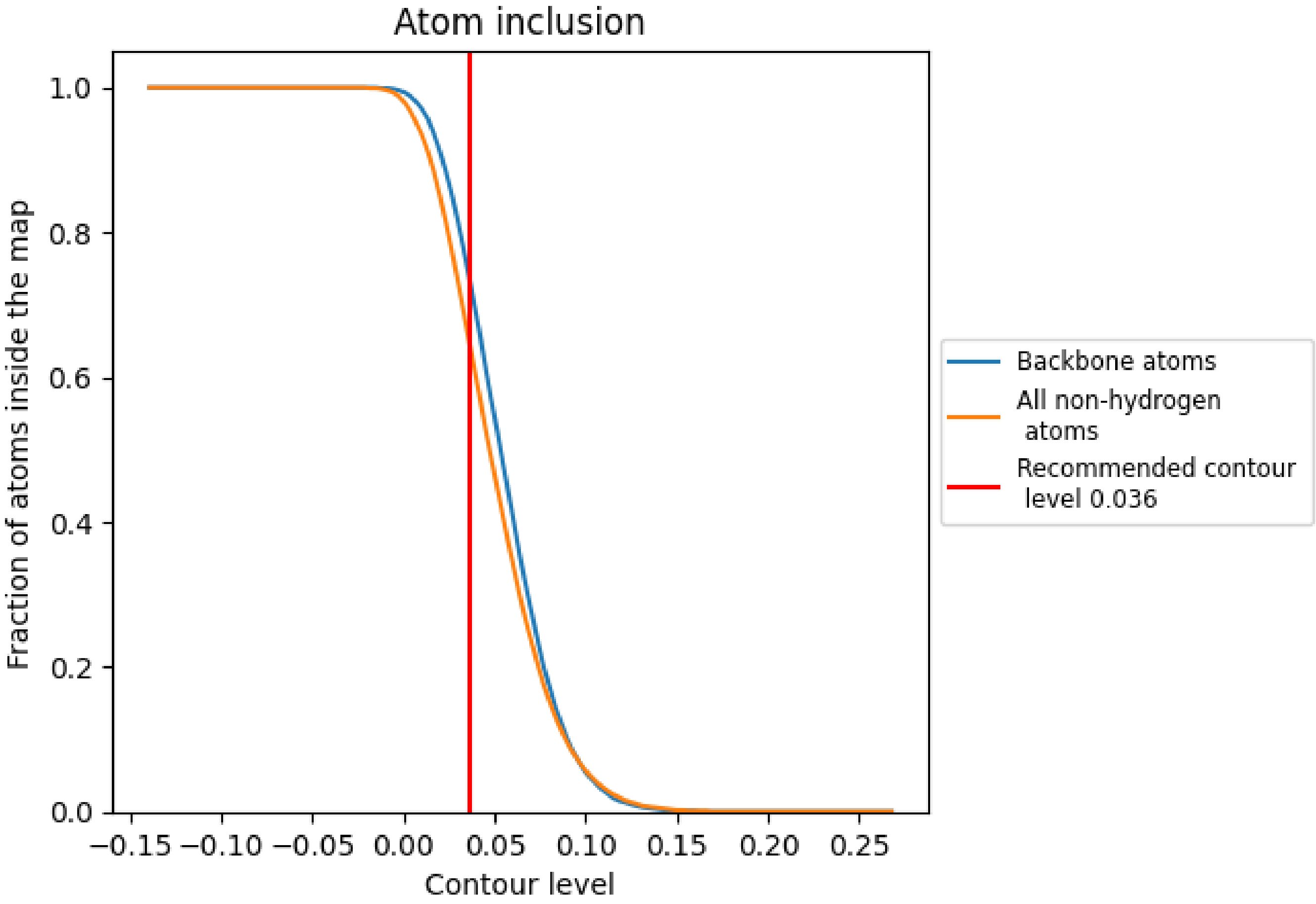
9.3 Atom inclusion mapped to coordinate model ⓘ



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.036).

9.4 Atom inclusion ⓘ



At the recommended contour level, 74% of all backbone atoms, 65% 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 (0.036) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6530	0.4480
2	0.7470	0.4670
A	0.6390	0.4370
B	0.5600	0.4280
C	0.7060	0.4920
D	0.5580	0.4360
E	0.4870	0.4080
F	0.5390	0.4280
G	0.0970	0.2080
H	0.5350	0.4150
I	0.5290	0.4220
J	0.5000	0.4110
K	0.5310	0.4070
L	0.5810	0.4420
M	0.2060	0.2850
N	0.6140	0.4490
O	0.6340	0.4640
P	0.5560	0.4240
Q	0.6600	0.4790
R	0.5680	0.3970
S	0.6140	0.4540
T	0.6450	0.4630
U	0.6080	0.4500
V	0.6440	0.4520
W	0.7240	0.4880
X	0.5390	0.4380
Y	0.3530	0.3540
Z	0.5210	0.3970
a	0.7020	0.4960
b	0.5590	0.4200
c	0.4400	0.4370
d	0.6860	0.4860
e	0.4290	0.3820
g	0.4660	0.3860
n	0.5740	0.4270