



wwPDB EM Validation Summary Report ⓘ

Nov 27, 2022 – 06:04 AM EST

PDB ID : 6OKK
EMDB ID : EMD-2660
Title : Cryo-EM structure of the Plasmodium falciparum 80S ribosome bound to the anti-protozoan drug emetine, small subunit
Authors : Wong, W.; Scheres, S.H.W.
Deposited on : 2019-04-13
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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

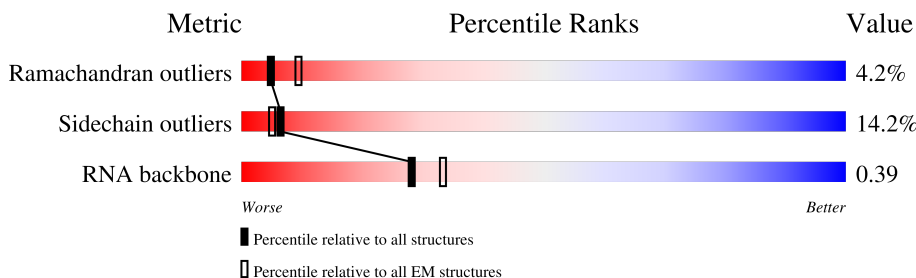
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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)
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	2092	31% (Poor fit) 53% (0 outliers), 24% (1 outlier), 23% (2+ outliers)
2	B	262	47% (Poor fit) 63% (0 outliers), 15% (1 outlier), 20% (2+ outliers)
3	C	263	57% (Poor fit) 63% (0 outliers), 11% (1 outlier), 26% (2+ outliers)
4	D	221	71% (Poor fit) 63% (0 outliers), 8% (1 outlier), 29% (2+ outliers)
5	E	189	52% (Poor fit) 84% (0 outliers), 14% (1 outlier), 2% (2+ outliers)
6	F	261	50% (Poor fit) 82% (0 outliers), 16% (1 outlier), 2% (2+ outliers)
7	G	272	35% (Poor fit) 69% (0 outliers), 13% (1 outlier), 18% (2+ outliers)
8	H	306	52% (Poor fit) 55% (0 outliers), 11% (1 outlier), 33% (2+ outliers)

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Mol	Chain	Length	Quality of chain
9	I	195	92% 75% 16% 8%
10	J	194	76% 84% 11%
11	K	130	31% 78% 18%
12	L	218	26% 67% 11% 21%
13	M	144	96% 87% 9%
14	N	118	82% 64% 15% 17%
15	O	137	58% 49% 9% 42%
16	P	151	42% 72% 10% 16%
17	Q	145	39% 89% 10%
18	R	141	70% 64% 6% 30%
19	S	156	82% 67% 15% 18%
20	T	54	89% 78% 11% 11%
21	U	151	47% 81% 18%
22	V	161	29% 71% 16% 9%
23	W	137	69% 57% 12% 31%
24	X	145	66% 57% 9% 34%
25	Y	170	91% 76% 14% 9%
26	Z	82	65% 71% 16% 12%
27	a	133	55% 76% 14% 10%
28	b	105	39% 34% 5% 61%
29	c	107	40% 76% 13% 11%
30	d	82	63% 76% 16% 7%
31	e	67	84% 81% 6% 13%
32	f	58	50% 64% 10% 26%
33	g	74	89% 59% 41%

2 Entry composition [i](#)

There are 36 unique types of molecules in this entry. The entry contains 68866 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	1608	34277	15347	6109	11213	1608	0	0

- Molecule 2 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	210	1713	1097	301	303	12	0	0

- Molecule 3 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	195	1538	990	266	273	9	0	0

- Molecule 4 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	157	1228	782	225	214	7	0	0

- Molecule 5 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	185	1508	959	287	260	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	257	2061	1320	377	356	8	0	0

- Molecule 7 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	224	1757	1132	307	309	9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	204	1644	1042	313	283	6	0	0

- Molecule 9 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	180	1424	893	263	258	10	0	0

- Molecule 10 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	188	1528	982	264	278	4	0	0

- Molecule 11 is a protein called 40S ribosomal protein S15A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	129	1037	665	189	178	5	0	0

- Molecule 12 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	172	1392	878	266	244	4	0	0

- Molecule 13 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	138	1098	704	200	193	1	0	0

- Molecule 14 is a protein called 40S ribosomal protein S20e.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	98	Total	C	N	O	S	0	0
			772	484	135	148	5		

- Molecule 15 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	79	Total	C	N	O	S	0	0
			686	450	116	118	2		

- Molecule 16 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	127	Total	C	N	O	S	0	0
			953	591	184	175	3		

- Molecule 17 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	144	Total	C	N	O	S	0	0
			1129	712	222	193	2		

- Molecule 18 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	98	Total	C	N	O	S	0	0
			746	474	123	145	4		

- Molecule 19 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	128	Total	C	N	O	S	0	0
			1042	655	204	179	4		

- Molecule 20 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	48	Total	C	N	O	S	0	0
			404	252	85	63	4		

- Molecule 21 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	149	Total	C	N	O	S	0	0
			1202	769	220	210	3		

- Molecule 22 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	146	Total	C	N	O	S	0	0
			1206	772	227	200	7		

- Molecule 23 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	95	Total	C	N	O	S	0	0
			785	498	149	135	3		

- Molecule 24 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	96	Total	C	N	O	S	0	0
			776	497	137	138	4		

- Molecule 25 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	154	Total	C	N	O	S	0	0
			1266	811	239	214	2		

- Molecule 26 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	72	Total	C	N	O	S	0	0
			556	346	102	104	4		

- Molecule 27 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	120	Total	C	N	O	S	0	0
			981	629	188	162	2		

- Molecule 28 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
28	b	41	320	208	56	56	0	0

- Molecule 29 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	c	95	781	478	169	128	6	0	0

- Molecule 30 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	d	76	586	368	102	107	9	0	0

- Molecule 31 is a protein called 40S ribosomal protein S28e.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
31	e	58	451	282	90	79	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
32	f	43	345	213	75	57	0	0

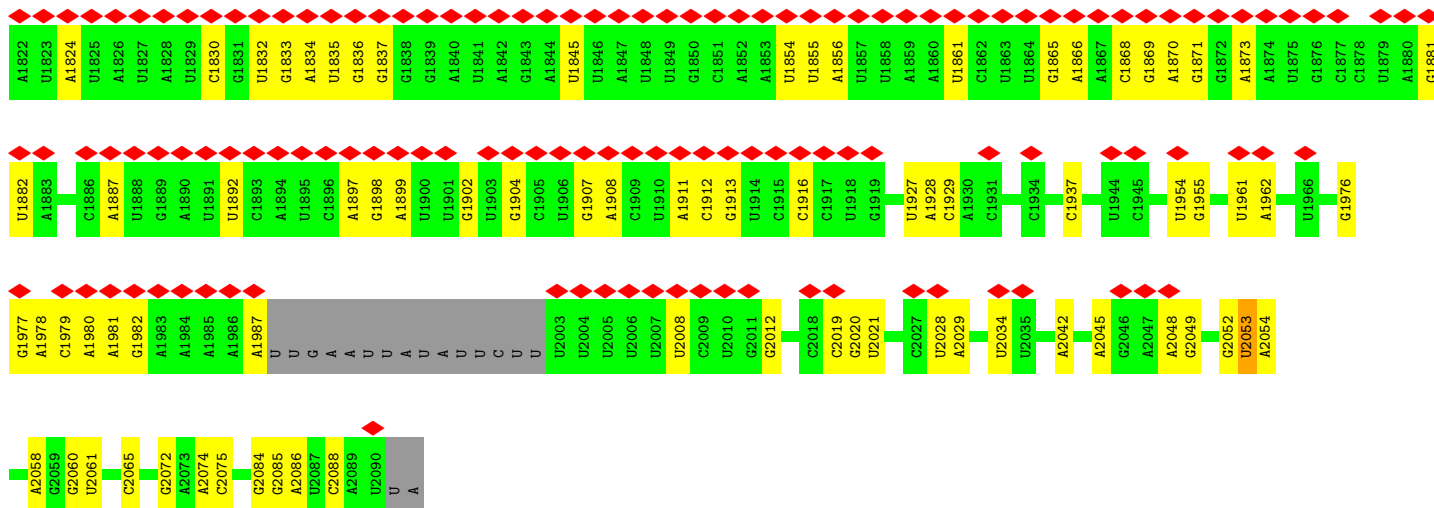
- Molecule 33 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
33	g	74	1571	702	275	521	73	0	0

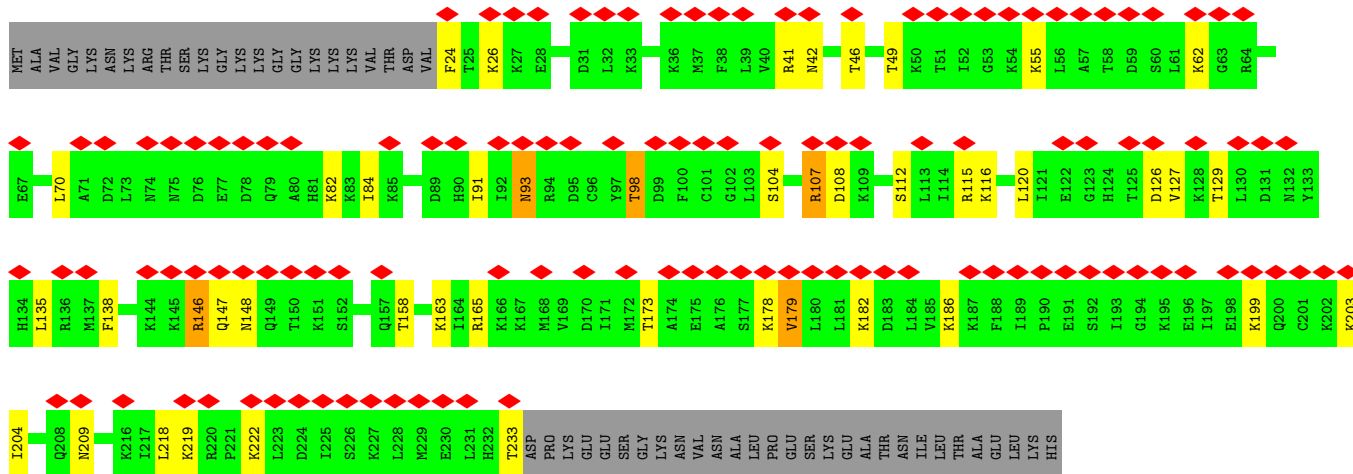
- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
34	A	67	67	67	0

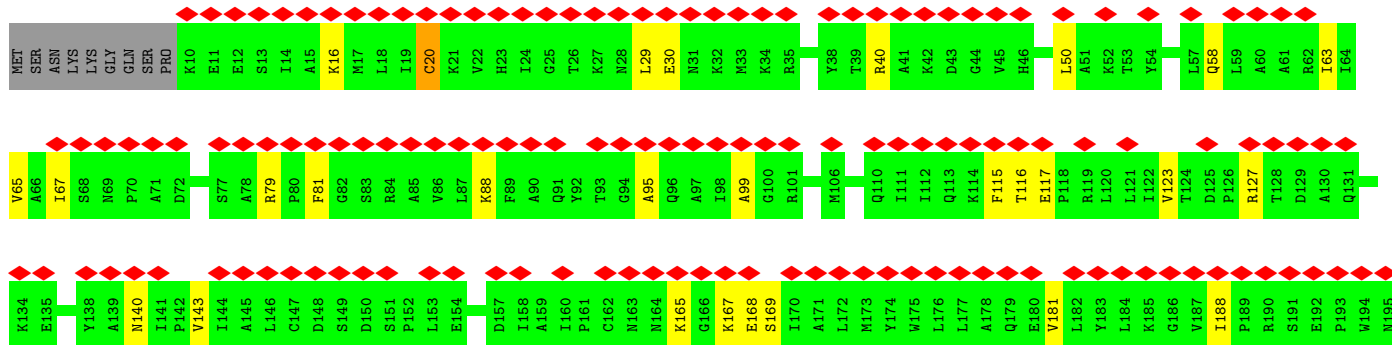
- Molecule 35 is emetine (three-letter code: 34G) (formula: C₂₉H₄₀N₂O₄).

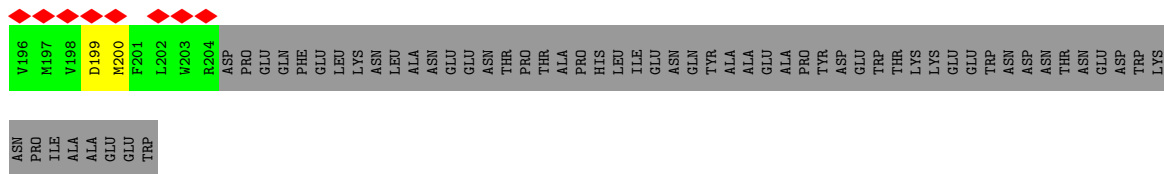


• Molecule 2: 40S ribosomal protein S3a

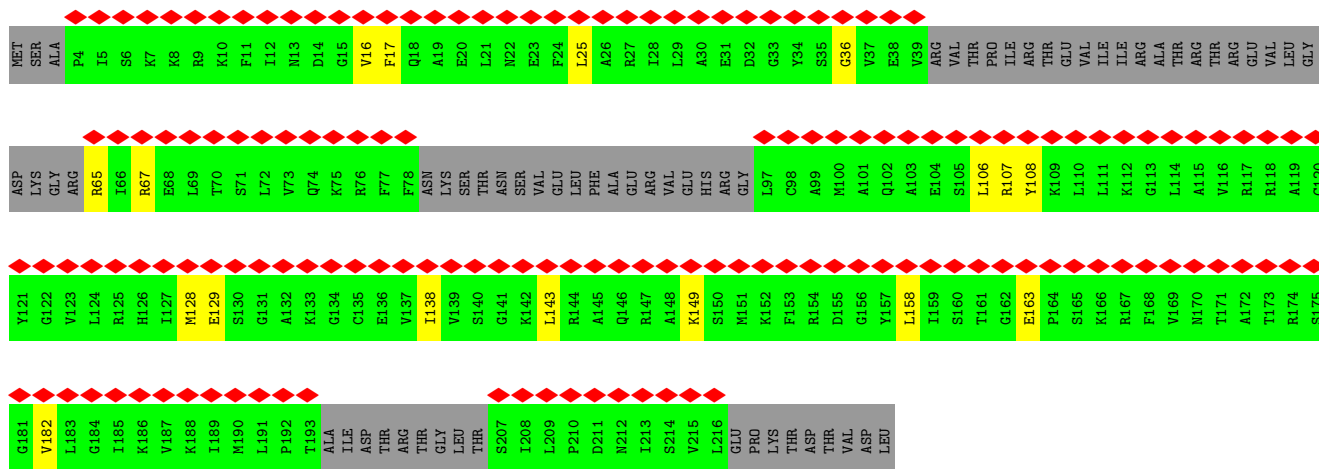


• Molecule 3: 40S ribosomal protein SA

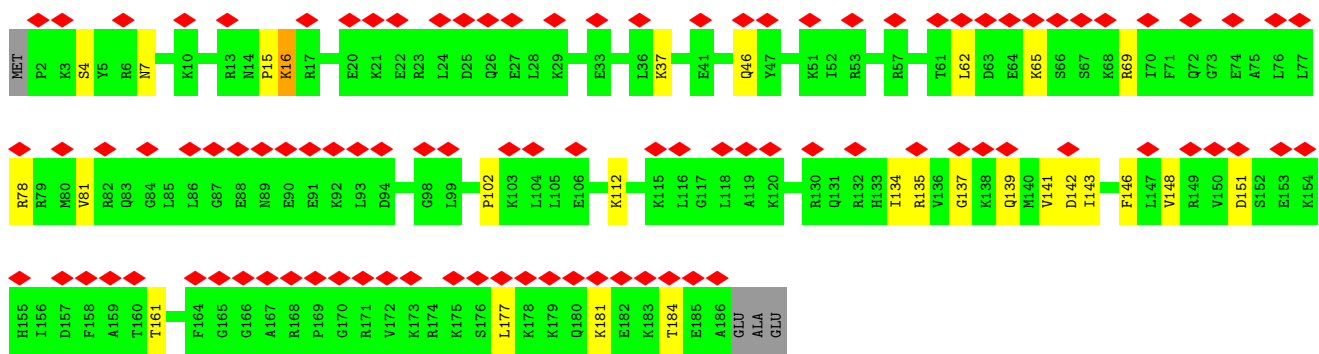
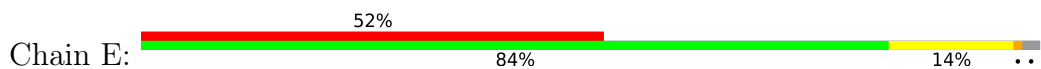




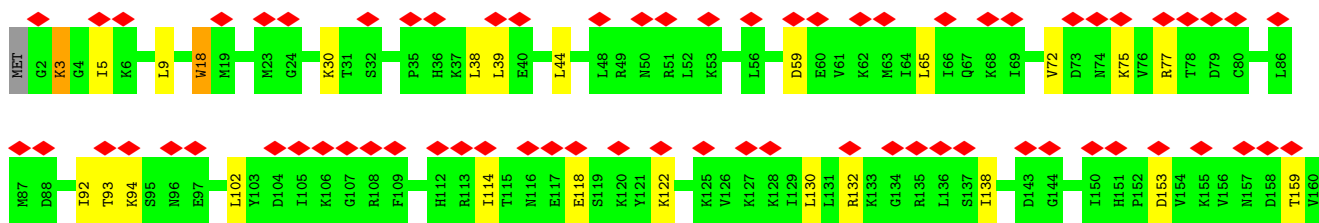
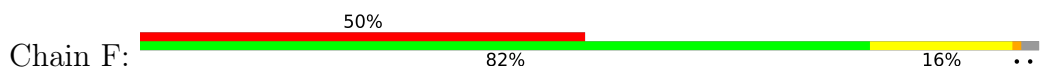
• Molecule 4: 40S ribosomal protein S3

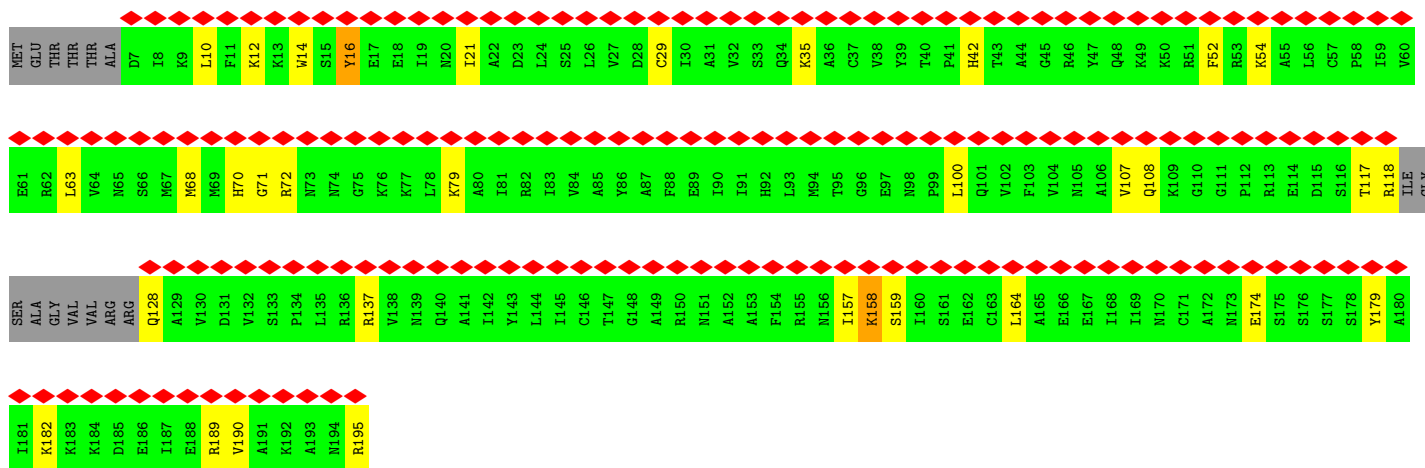


• Molecule 5: 40S ribosomal protein S9

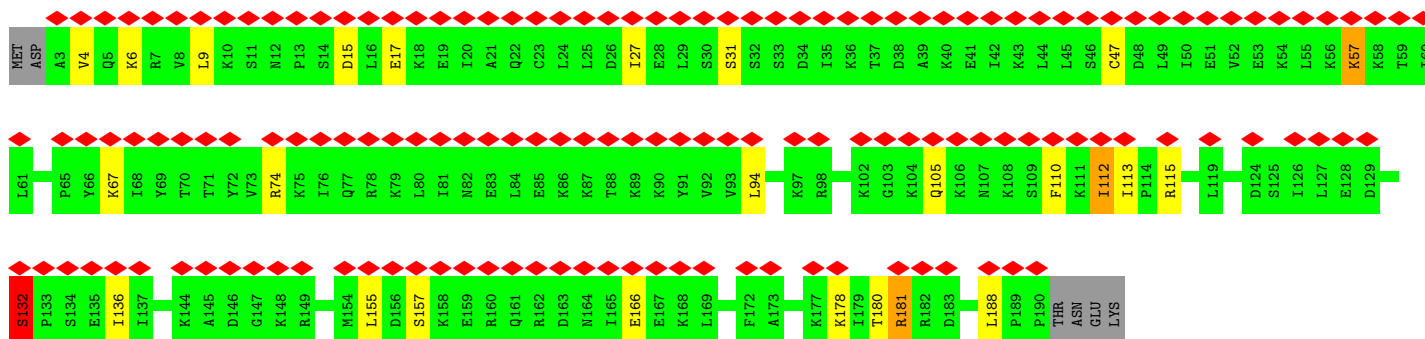
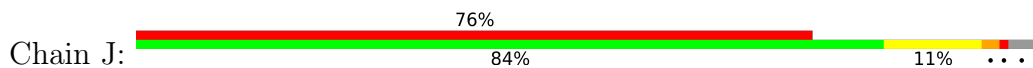


• Molecule 6: 40S ribosomal protein S4

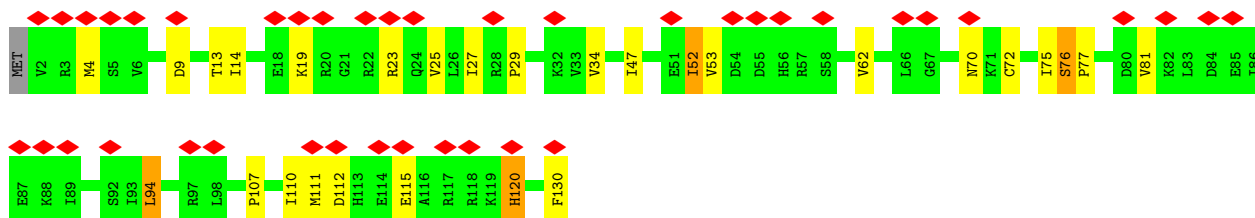
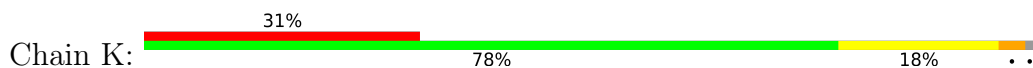




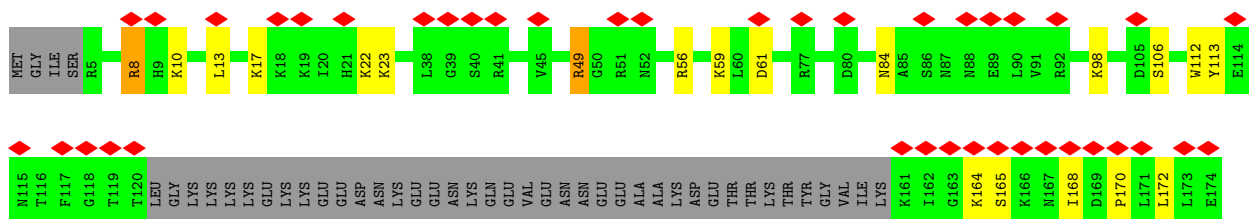
• Molecule 10: 40S ribosomal protein S7

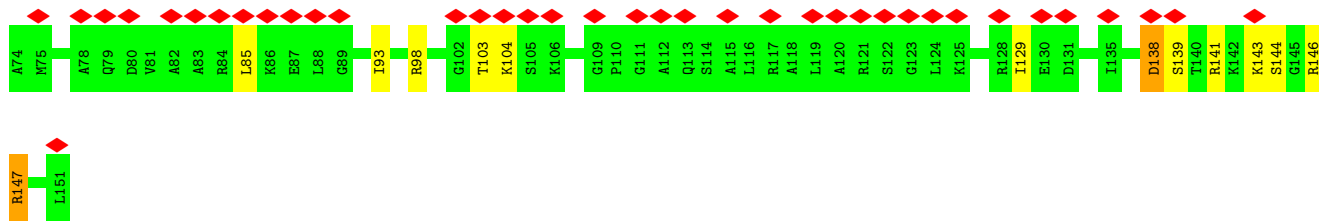


• Molecule 11: 40S ribosomal protein S15A

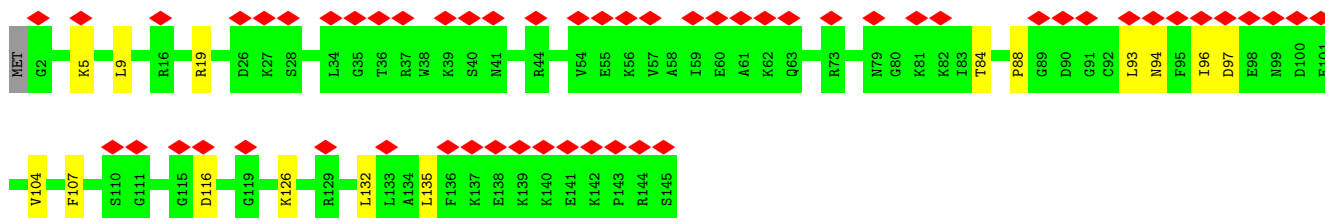
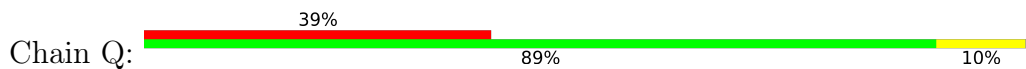


• Molecule 12: 40S ribosomal protein S8

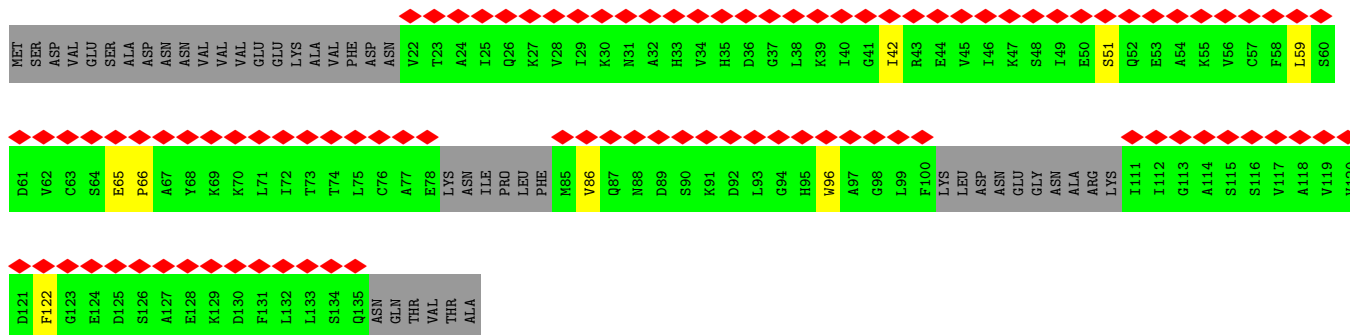




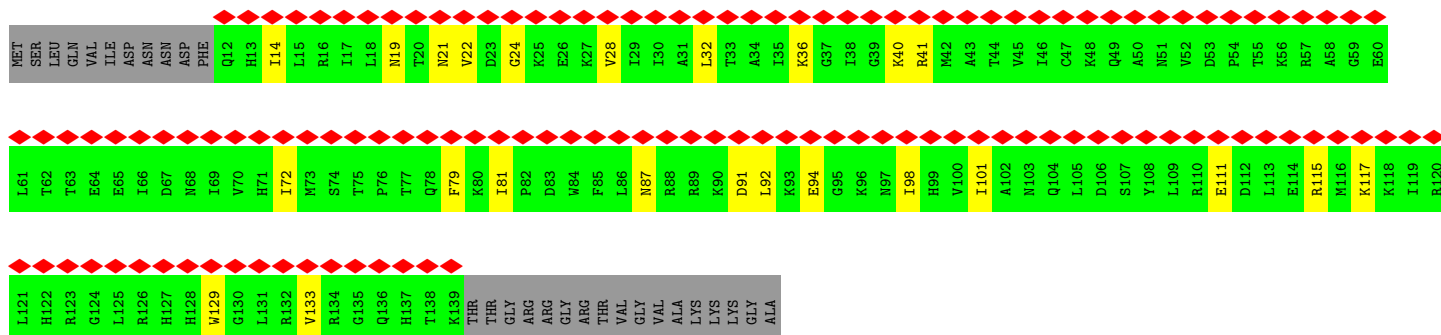
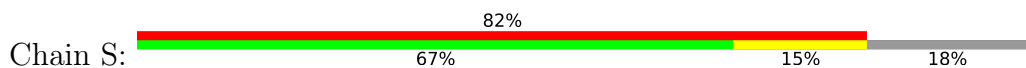
- Molecule 17: 40S ribosomal protein S23



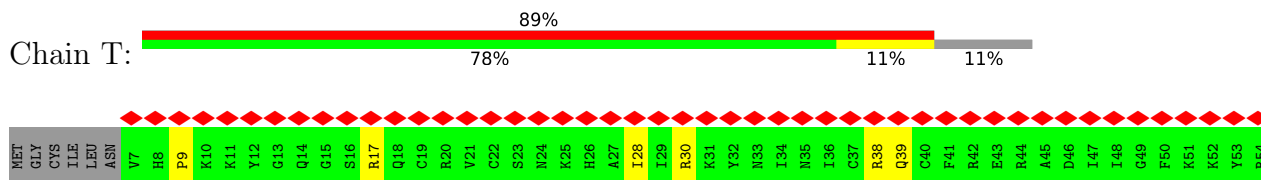
- Molecule 18: 40S ribosomal protein S12



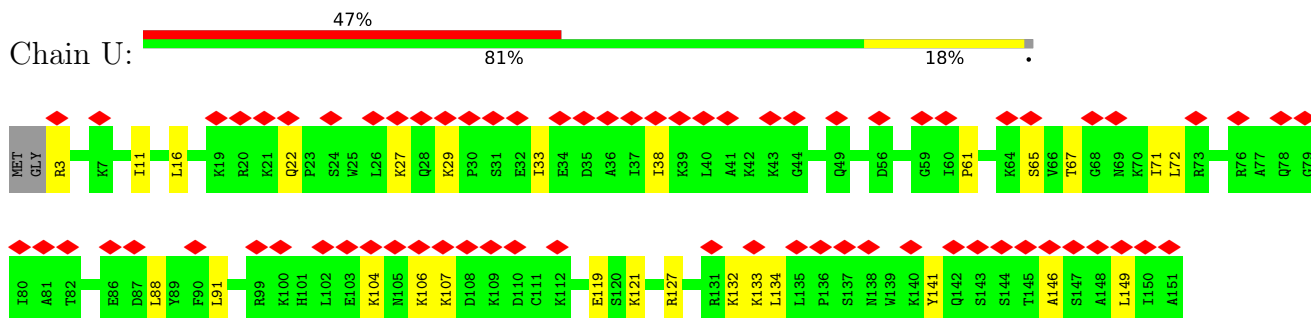
- Molecule 19: 40S ribosomal protein S18



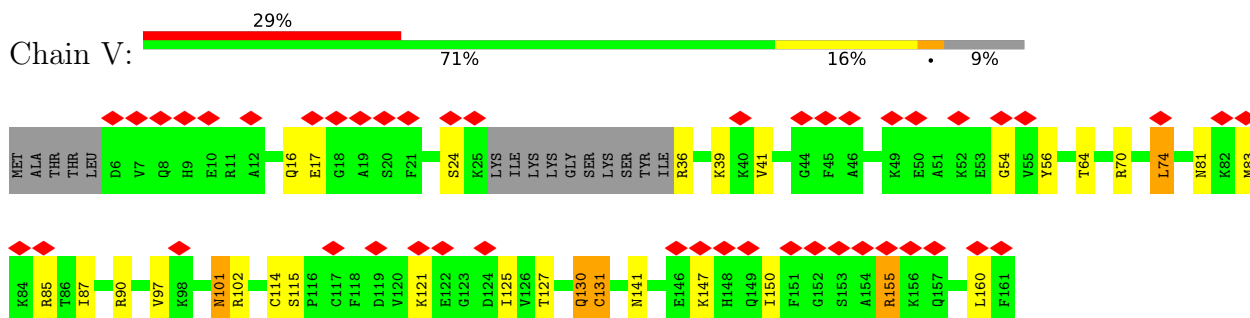
- Molecule 20: 40S ribosomal protein S29



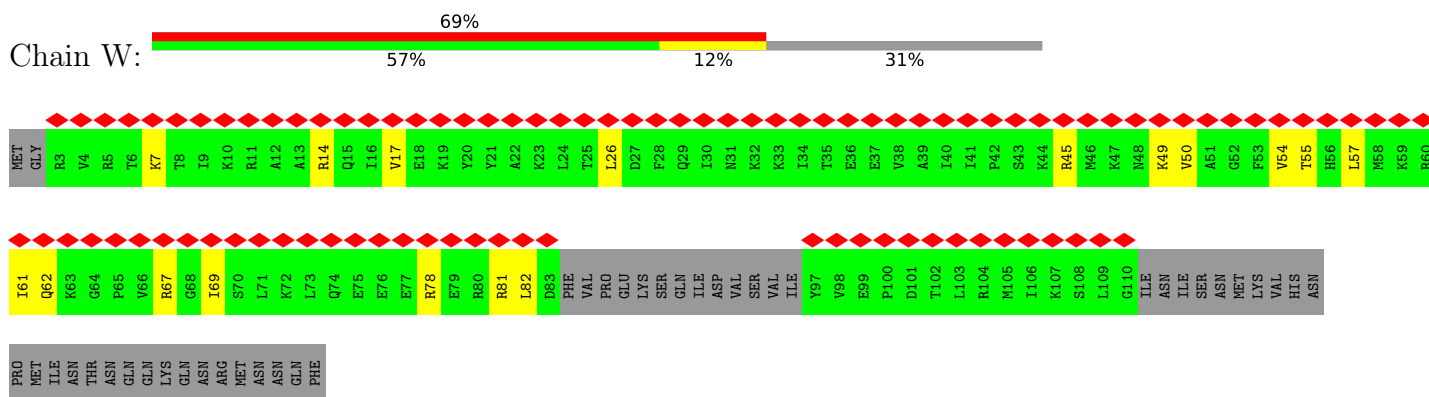
• Molecule 21: 40S ribosomal protein S15



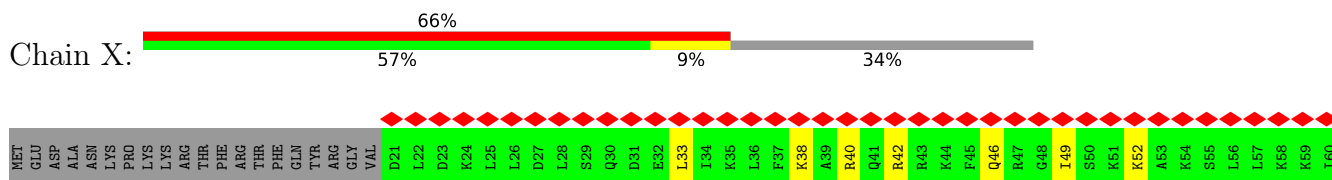
• Molecule 22: 40S ribosomal protein S11

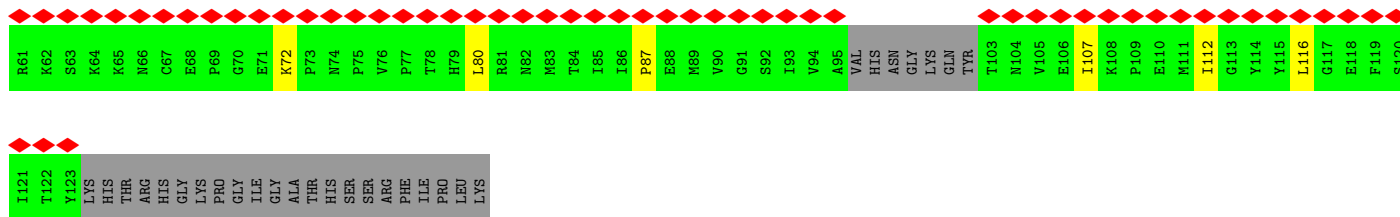


• Molecule 23: 40S ribosomal protein S17

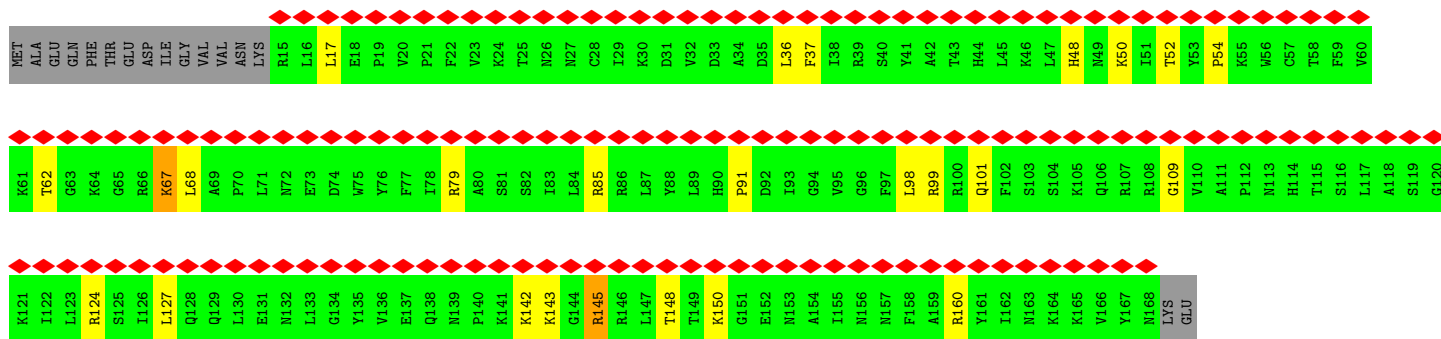
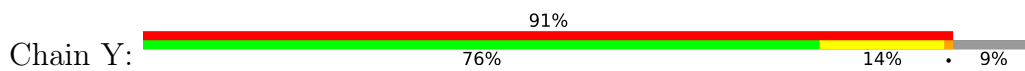


• Molecule 24: 40S ribosomal protein S19

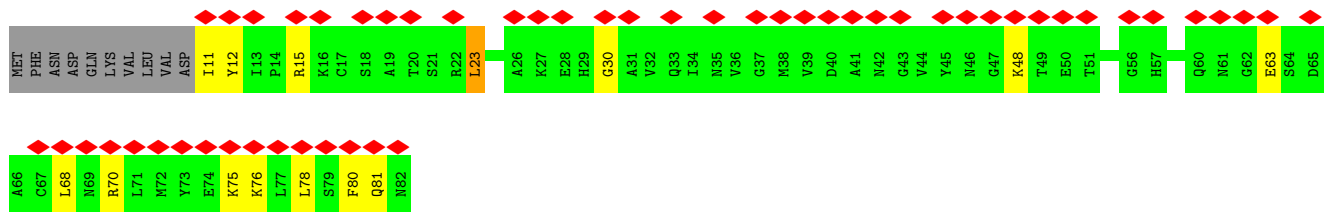




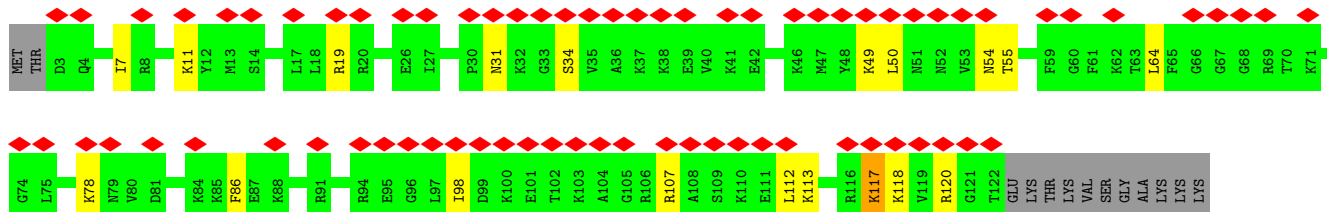
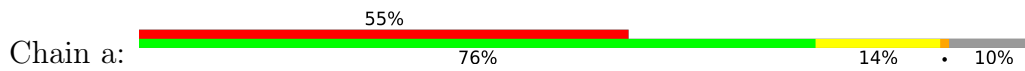
• Molecule 25: 40S ribosomal protein S19



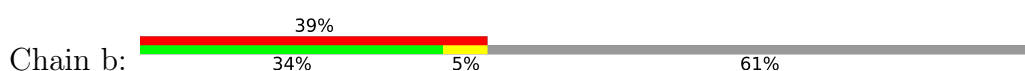
• Molecule 26: 40S ribosomal protein S21

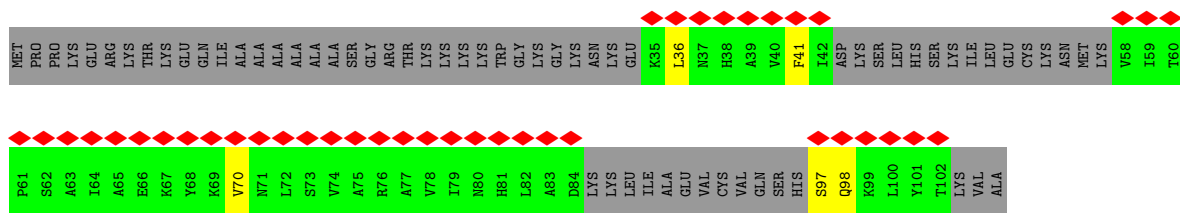


• Molecule 27: 40S ribosomal protein S24

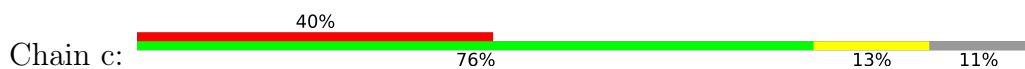


• Molecule 28: 40S ribosomal protein S25

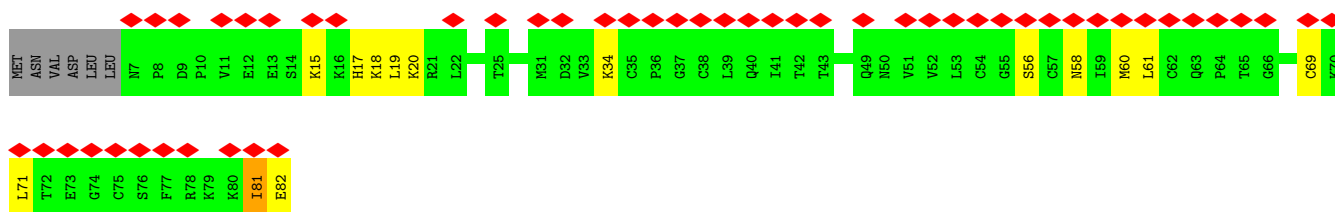
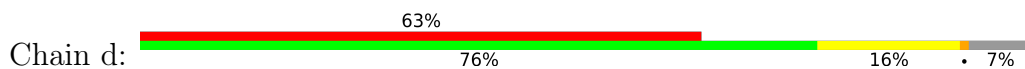




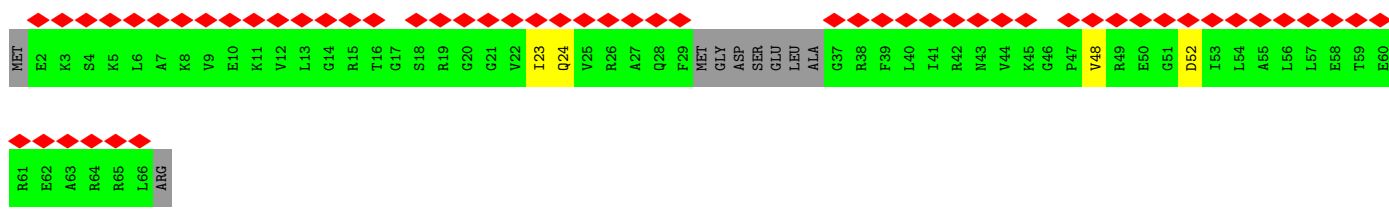
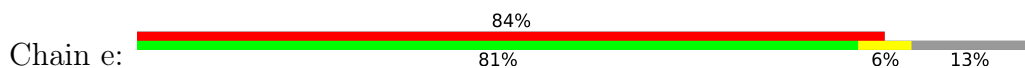
• Molecule 29: 40S ribosomal protein S26



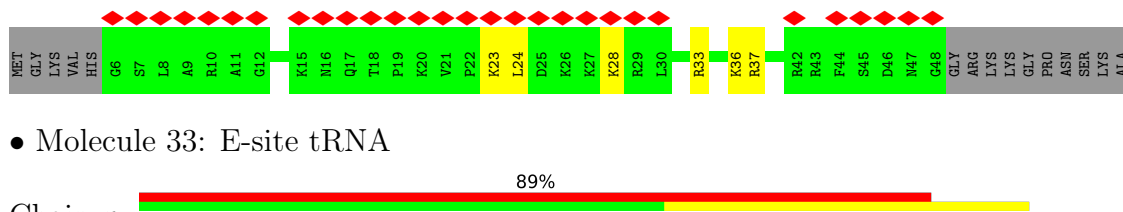
• Molecule 30: 40S ribosomal protein S27



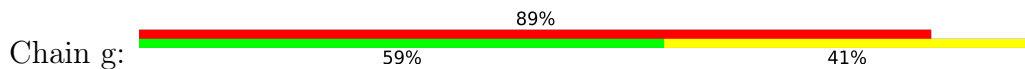
• Molecule 31: 40S ribosomal protein S28e

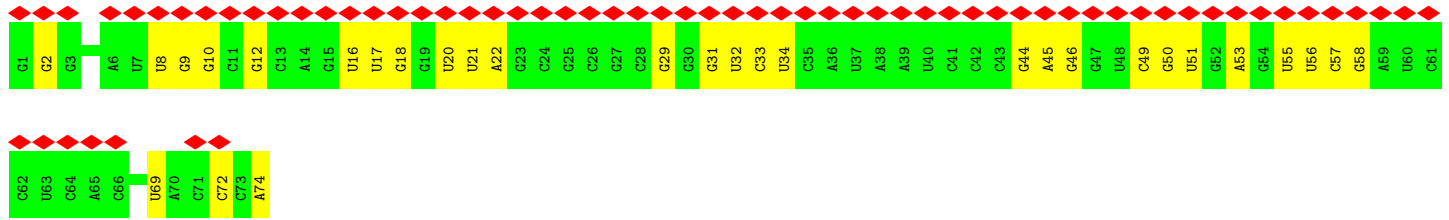


• Molecule 32: 40S ribosomal protein S30



• Molecule 33: E-site tRNA





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	105247	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.962	Depositor
Minimum map value	-0.545	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.044	Depositor
Recommended contour level	0.18	Depositor
Map size (Å)	482.40002, 482.40002, 482.40002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	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: ZN, 34G, MG

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	0.35	3/38345 (0.0%)	0.75	16/59689 (0.0%)
2	B	0.46	0/1737	0.81	0/2321
3	C	0.43	0/1569	0.79	0/2129
4	D	0.46	0/1240	0.79	1/1652 (0.1%)
5	E	0.47	0/1532	0.87	0/2048
6	F	0.47	0/2097	0.80	1/2819 (0.0%)
7	G	0.48	0/1799	0.78	0/2429
8	H	0.43	0/1661	0.77	0/2205
9	I	0.47	0/1443	0.86	0/1936
10	J	0.45	0/1544	0.78	0/2064
11	K	0.51	0/1054	0.92	1/1411 (0.1%)
12	L	0.51	0/1416	0.82	1/1890 (0.1%)
13	M	0.45	0/1113	0.71	0/1487
14	N	0.46	0/780	0.81	0/1053
15	O	0.48	0/705	0.73	0/950
16	P	0.47	0/965	0.88	1/1295 (0.1%)
17	Q	0.47	0/1149	0.80	0/1532
18	R	0.47	0/754	0.66	0/1013
19	S	0.48	0/1058	0.82	0/1420
20	T	0.42	0/411	0.72	0/544
21	U	0.45	0/1223	0.87	0/1634
22	V	0.50	0/1233	0.79	1/1645 (0.1%)
23	W	0.47	0/792	0.86	0/1053
24	X	0.49	0/787	0.81	0/1050
25	Y	0.46	0/1294	0.86	1/1742 (0.1%)
26	Z	0.44	0/564	0.78	0/758
27	a	0.49	0/994	0.86	0/1317
28	b	0.48	0/323	0.67	0/435
29	c	0.48	0/793	0.90	0/1055
30	d	0.45	0/597	0.73	0/801
31	e	0.40	0/452	0.64	0/599
32	f	0.42	0/348	0.80	0/458

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	g	0.24	0/1754	0.72	0/2732
All	All	0.41	3/73526 (0.0%)	0.77	23/107166 (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
2	B	0	1
10	J	0	1
11	K	0	3
12	L	0	1
19	S	0	1
21	U	0	1
24	X	0	1
27	a	0	1
All	All	0	10

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	788	A	O3'-P	7.96	1.70	1.61
1	A	789	U	C1'-N1	6.92	1.59	1.48
1	A	788	A	C1'-N9	-5.25	1.39	1.46

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	788	A	P-O3'-C3'	-10.80	106.73	119.70
1	A	788	A	OP2-P-O3'	7.77	122.30	105.20
1	A	2053	U	C2'-C3'-O3'	7.75	126.56	109.50
1	A	850	G	C2'-C3'-O3'	7.70	126.44	109.50
1	A	1381	C	C2'-C3'-O3'	7.21	125.35	109.50

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	148	ASN	Peptide
10	J	132	SER	Peptide

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Mol	Chain	Res	Type	Group
11	K	27	ILE	Peptide
11	K	76	SER	Peptide
11	K	94	LEU	Peptide

5.2 Too-close contacts [i](#)

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

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	
2	B	208/262 (79%)	169 (81%)	27 (13%)	12 (6%)	1	11
3	C	193/263 (73%)	163 (84%)	22 (11%)	8 (4%)	3	17
4	D	149/221 (67%)	129 (87%)	17 (11%)	3 (2%)	7	32
5	E	183/189 (97%)	159 (87%)	19 (10%)	5 (3%)	5	26
6	F	255/261 (98%)	217 (85%)	31 (12%)	7 (3%)	5	26
7	G	222/272 (82%)	195 (88%)	20 (9%)	7 (3%)	4	22
8	H	200/306 (65%)	173 (86%)	19 (10%)	8 (4%)	3	18
9	I	176/195 (90%)	153 (87%)	14 (8%)	9 (5%)	2	13
10	J	186/194 (96%)	160 (86%)	17 (9%)	9 (5%)	2	14
11	K	127/130 (98%)	104 (82%)	16 (13%)	7 (6%)	2	11
12	L	166/218 (76%)	134 (81%)	23 (14%)	9 (5%)	2	12
13	M	136/144 (94%)	116 (85%)	13 (10%)	7 (5%)	2	13
14	N	96/118 (81%)	83 (86%)	8 (8%)	5 (5%)	2	13
15	O	77/137 (56%)	66 (86%)	10 (13%)	1 (1%)	12	40
16	P	125/151 (83%)	103 (82%)	18 (14%)	4 (3%)	4	22
17	Q	142/145 (98%)	128 (90%)	13 (9%)	1 (1%)	22	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	R	92/141 (65%)	73 (79%)	13 (14%)	6 (6%)	1	9
19	S	126/156 (81%)	100 (79%)	17 (14%)	9 (7%)	1	7
20	T	46/54 (85%)	43 (94%)	2 (4%)	1 (2%)	6	30
21	U	147/151 (97%)	133 (90%)	10 (7%)	4 (3%)	5	26
22	V	142/161 (88%)	123 (87%)	9 (6%)	10 (7%)	1	7
23	W	91/137 (66%)	80 (88%)	7 (8%)	4 (4%)	2	16
24	X	92/145 (63%)	82 (89%)	6 (6%)	4 (4%)	2	16
25	Y	152/170 (89%)	134 (88%)	12 (8%)	6 (4%)	3	18
26	Z	70/82 (85%)	62 (89%)	3 (4%)	5 (7%)	1	7
27	a	118/133 (89%)	104 (88%)	9 (8%)	5 (4%)	3	17
28	b	35/105 (33%)	30 (86%)	5 (14%)	0	100	100
29	c	93/107 (87%)	80 (86%)	10 (11%)	3 (3%)	4	22
30	d	74/82 (90%)	48 (65%)	21 (28%)	5 (7%)	1	8
31	e	54/67 (81%)	50 (93%)	4 (7%)	0	100	100
32	f	41/58 (71%)	34 (83%)	4 (10%)	3 (7%)	1	7
All	All	4014/4955 (81%)	3428 (85%)	419 (10%)	167 (4%)	5	17

5 of 167 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	84	ILE
2	B	93	ASN
2	B	147	GLN
2	B	179	VAL
3	C	20	CYS

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	
2	B	195/238 (82%)	158 (81%)	37 (19%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	167/227 (74%)	144 (86%)	23 (14%)	3	16
4	D	132/188 (70%)	119 (90%)	13 (10%)	8	29
5	E	160/167 (96%)	137 (86%)	23 (14%)	3	15
6	F	233/237 (98%)	194 (83%)	39 (17%)	2	10
7	G	191/222 (86%)	161 (84%)	30 (16%)	2	12
8	H	181/279 (65%)	151 (83%)	30 (17%)	2	10
9	I	154/165 (93%)	128 (83%)	26 (17%)	2	9
10	J	177/183 (97%)	156 (88%)	21 (12%)	5	21
11	K	115/116 (99%)	94 (82%)	21 (18%)	1	7
12	L	152/193 (79%)	136 (90%)	16 (10%)	7	25
13	M	116/122 (95%)	110 (95%)	6 (5%)	23	54
14	N	91/109 (84%)	70 (77%)	21 (23%)	1	3
15	O	76/129 (59%)	65 (86%)	11 (14%)	3	14
16	P	99/119 (83%)	83 (84%)	16 (16%)	2	10
17	Q	120/121 (99%)	106 (88%)	14 (12%)	5	21
18	R	83/121 (69%)	81 (98%)	2 (2%)	49	73
19	S	113/136 (83%)	99 (88%)	14 (12%)	4	19
20	T	43/48 (90%)	38 (88%)	5 (12%)	5	22
21	U	132/133 (99%)	110 (83%)	22 (17%)	2	10
22	V	131/144 (91%)	106 (81%)	25 (19%)	1	6
23	W	86/127 (68%)	73 (85%)	13 (15%)	3	13
24	X	88/130 (68%)	80 (91%)	8 (9%)	9	31
25	Y	137/151 (91%)	117 (85%)	20 (15%)	3	14
26	Z	60/70 (86%)	50 (83%)	10 (17%)	2	10
27	a	103/115 (90%)	89 (86%)	14 (14%)	3	16
28	b	35/88 (40%)	30 (86%)	5 (14%)	3	15
29	c	87/98 (89%)	76 (87%)	11 (13%)	4	19
30	d	70/76 (92%)	60 (86%)	10 (14%)	3	15
31	e	46/54 (85%)	42 (91%)	4 (9%)	10	34
32	f	36/47 (77%)	33 (92%)	3 (8%)	11	36
All	All	3609/4353 (83%)	3096 (86%)	513 (14%)	6	15

5 of 513 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	Z	70	ARG
27	a	112	LEU
26	Z	68	LEU
8	H	184	LEU
8	H	158	ILE

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

Mol	Chain	Res	Type
27	a	54	ASN
27	a	52	ASN
11	K	64	ASN
23	W	31	ASN
11	K	24	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1586/2092 (75%)	474 (29%)	71 (4%)
33	g	73/74 (98%)	30 (41%)	0
All	All	1659/2166 (76%)	504 (30%)	71 (4%)

5 of 504 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	A
1	A	4	C
1	A	5	U
1	A	17	C
1	A	25	C

5 of 71 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1813	U
1	A	1819	U
1	A	1897	A
1	A	752	U
1	A	614	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 69 ligands modelled in this entry, 68 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	34G	P	201	-	39,39,39	2.72	8 (20%)	51,56,56	2.03	15 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	34G	P	201	-	-	11/14/49/49	0/5/5/5

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	P	201	34G	CBC-CBG	-11.48	1.41	1.52
35	P	201	34G	CBD-CBH	-7.09	1.40	1.52
35	P	201	34G	CAM-CAX	-5.83	1.41	1.51
35	P	201	34G	CAL-CAW	-5.82	1.41	1.51
35	P	201	34G	CAK-CAL	2.59	1.57	1.50

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	P	201	34G	CAE-OAV-CBB	-5.64	109.01	117.53
35	P	201	34G	CAD-OAU-CBA	-4.53	110.69	117.53
35	P	201	34G	CAL-CAK-NAR	4.46	115.22	109.04
35	P	201	34G	CAW-CBC-CBG	-4.40	117.11	121.63
35	P	201	34G	CAB-OAS-CAY	-3.63	112.05	117.53

There are no chirality outliers.

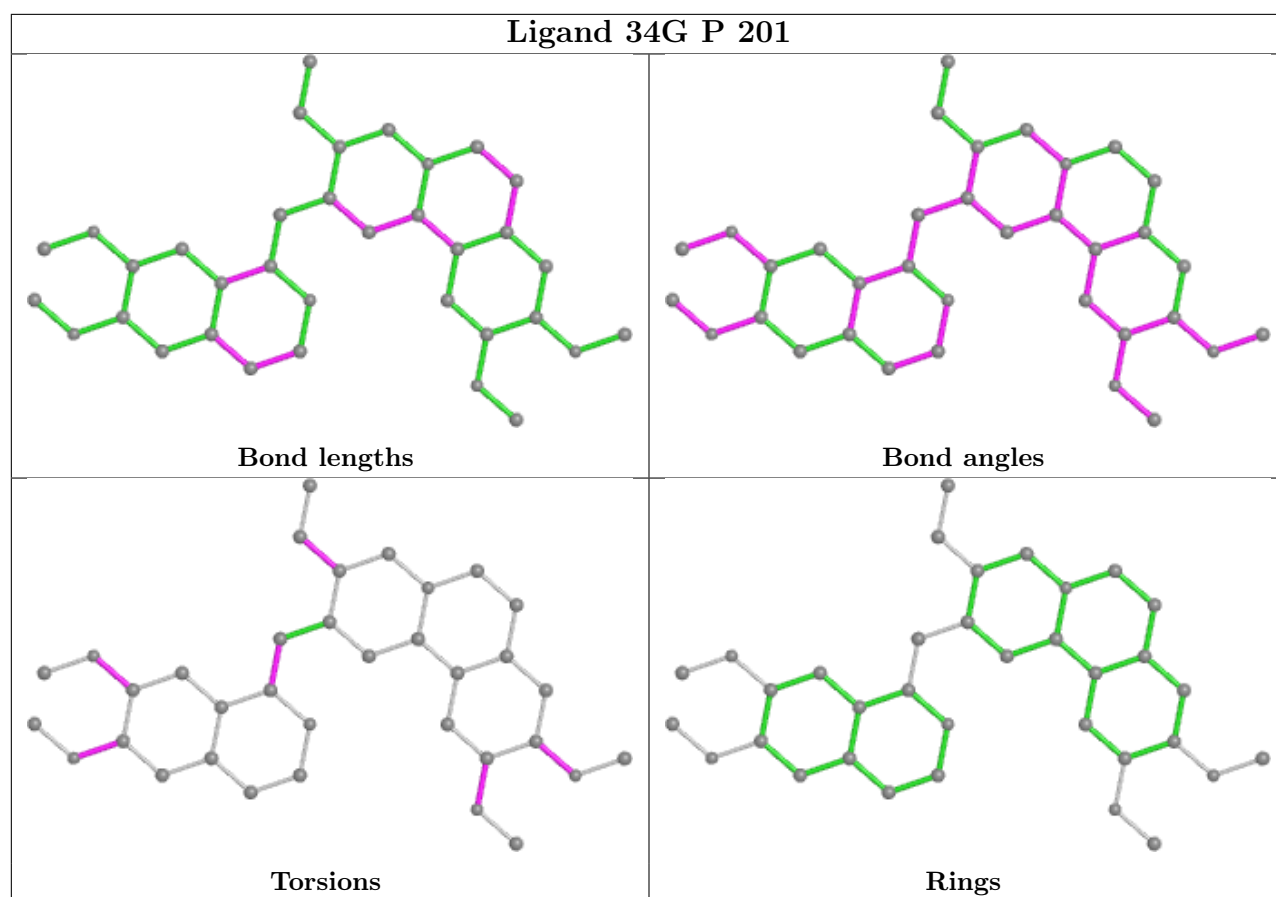
5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	P	201	34G	CBF-CAO-CBG-NAR
35	P	201	34G	CAY-CBA-OAU-CAD
35	P	201	34G	CBA-CAY-OAS-CAB
35	P	201	34G	CBB-CAZ-OAT-CAC
35	P	201	34G	CAH-CBA-OAU-CAD

There are no ring outliers.

No monomer is involved in short contacts.

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 than 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.



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.

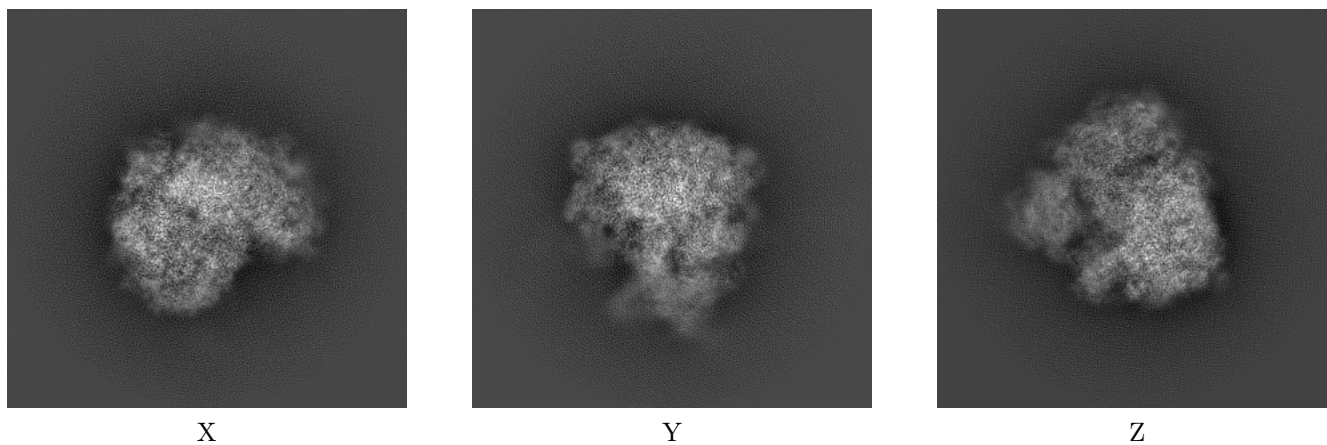
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2660. 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 [i](#)

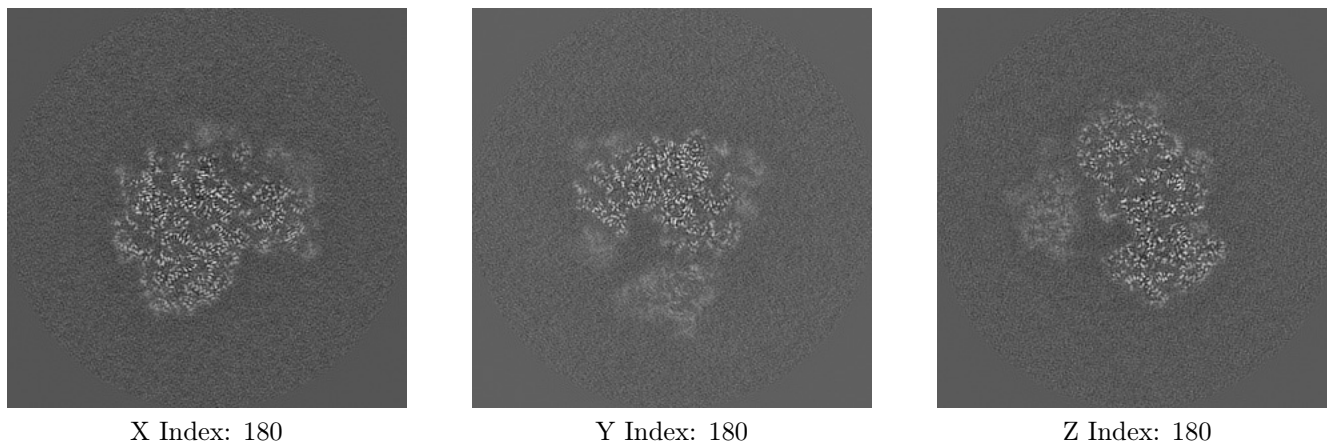
6.1.1 Primary map



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

6.2 Central slices [i](#)

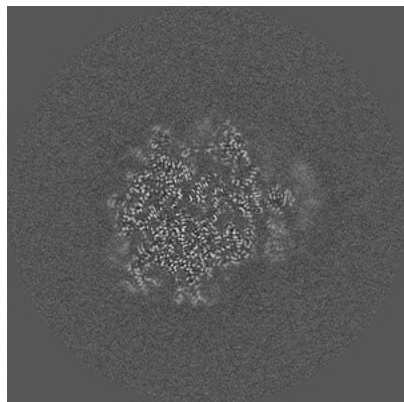
6.2.1 Primary map



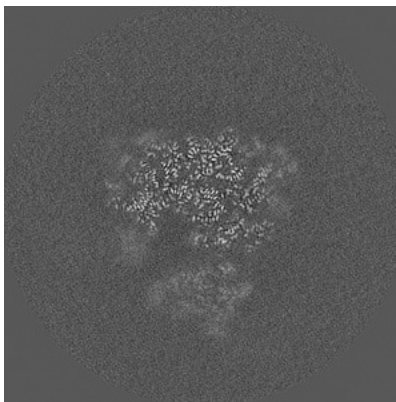
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

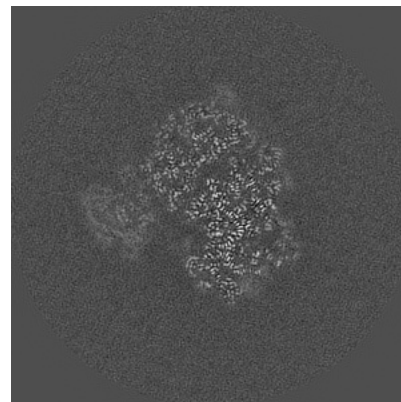
6.3.1 Primary map



X Index: 201



Y Index: 183



Z Index: 187

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.18. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

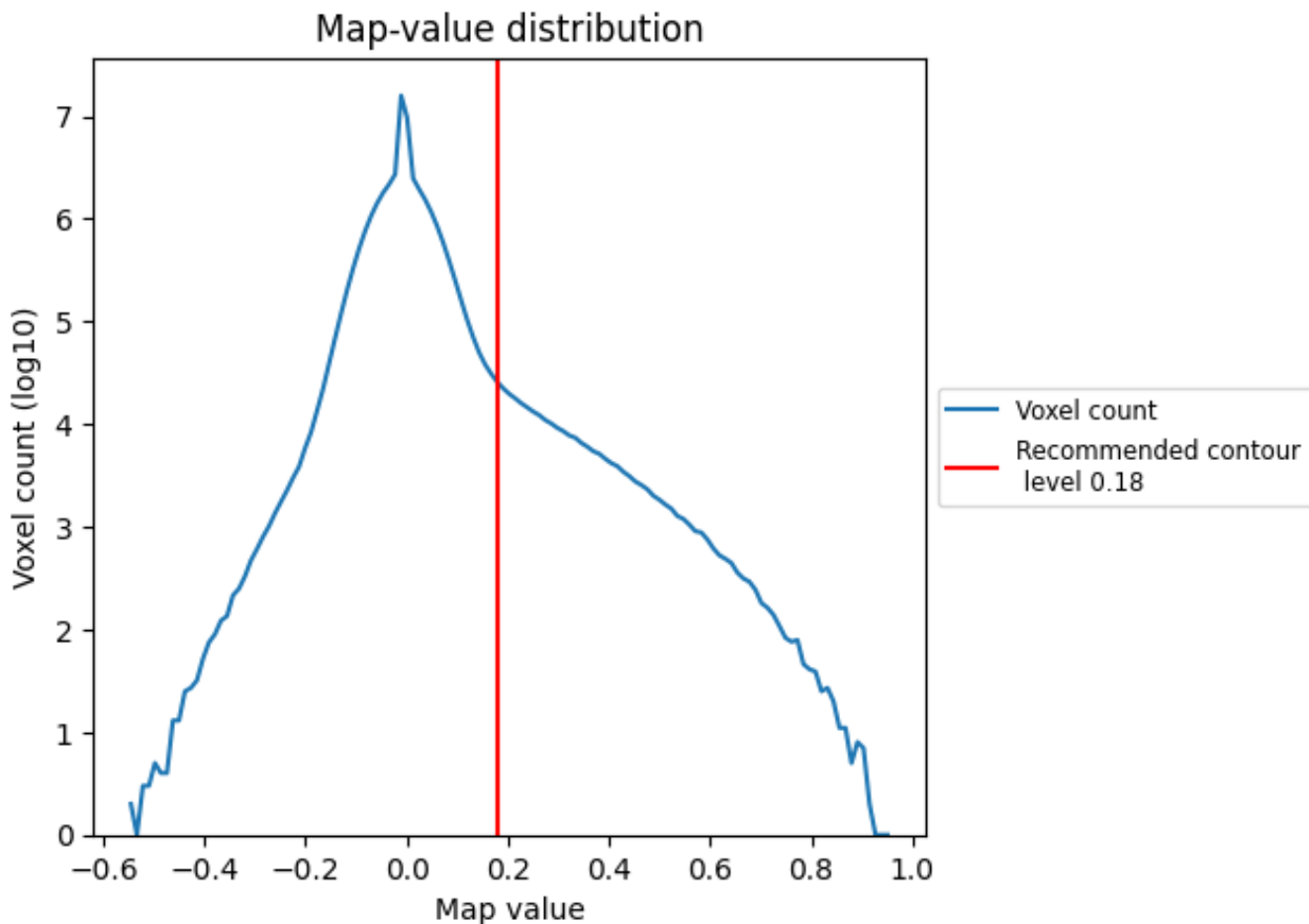
6.5 Mask visualisation

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

7 Map analysis [i](#)

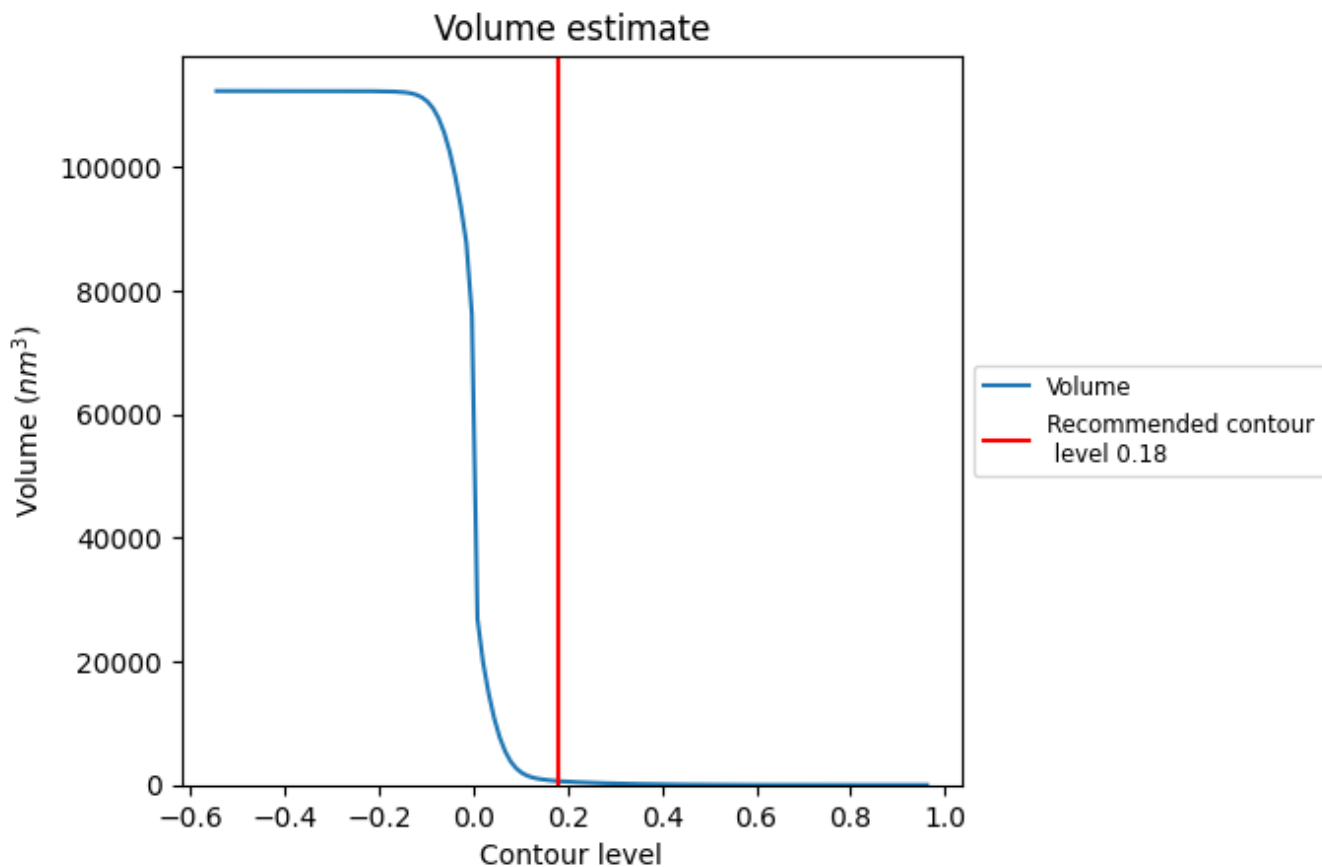
This section contains the results of statistical analysis of the map.

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.

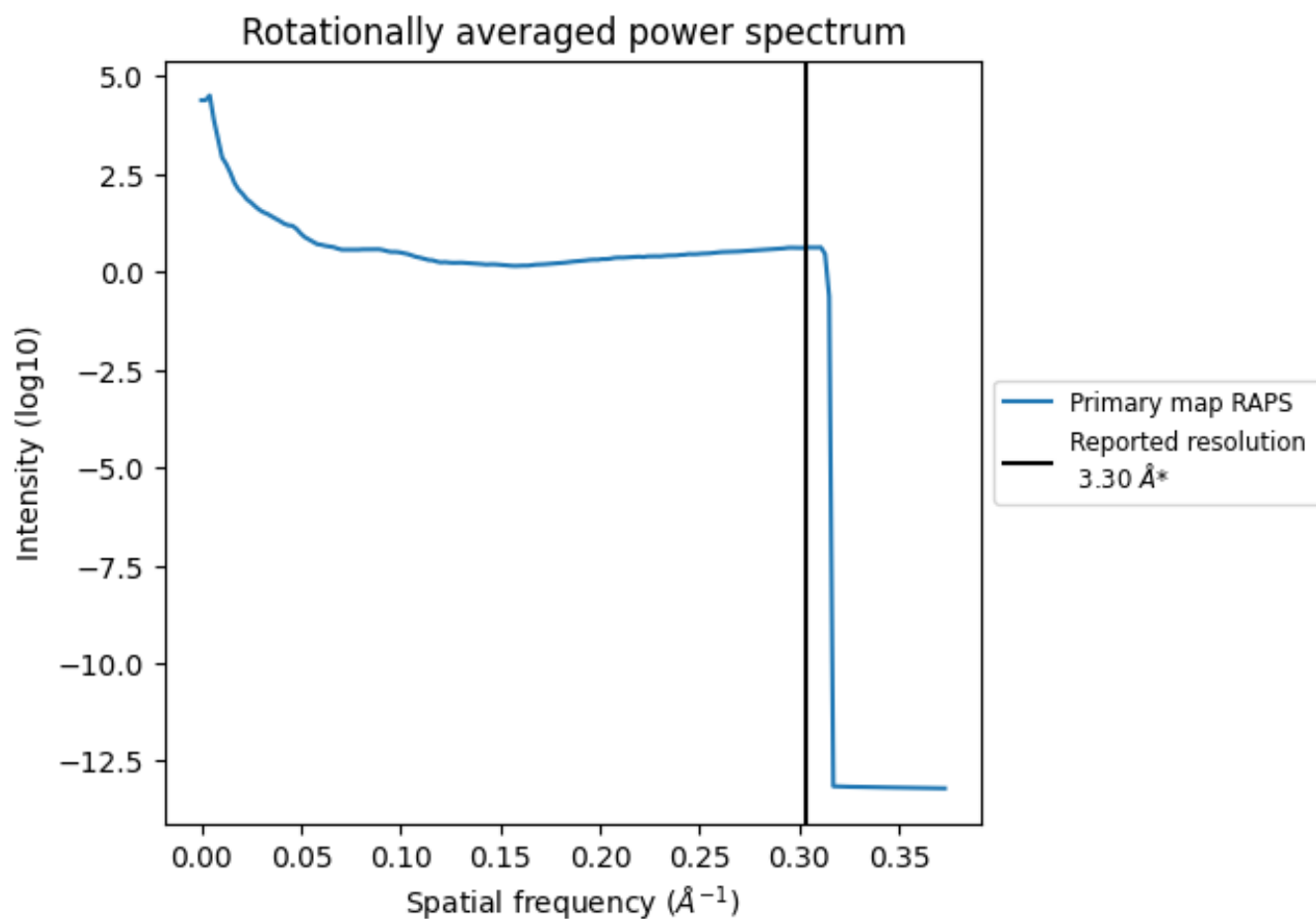
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 628 nm^3 ; this corresponds to an approximate mass of 567 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

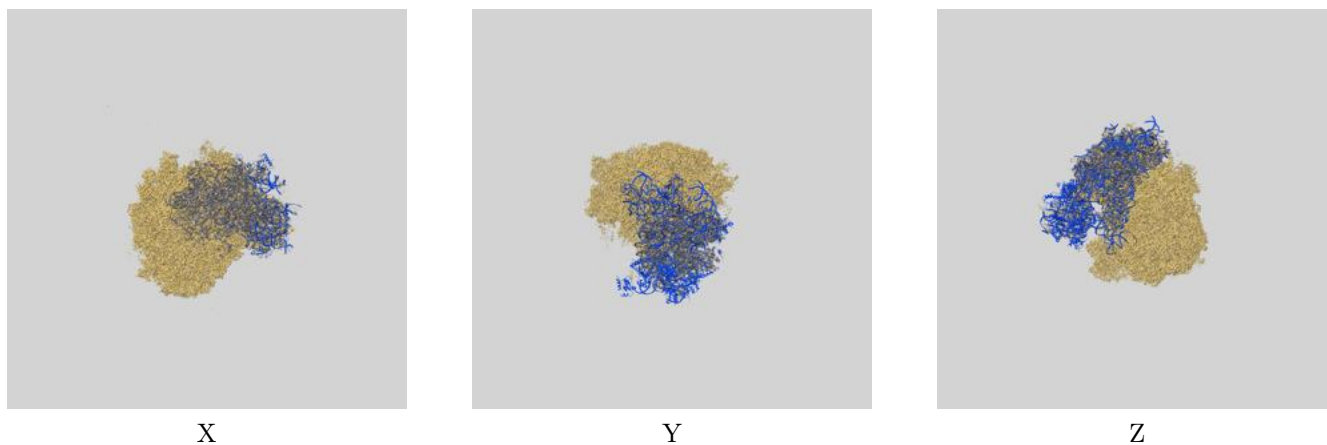
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

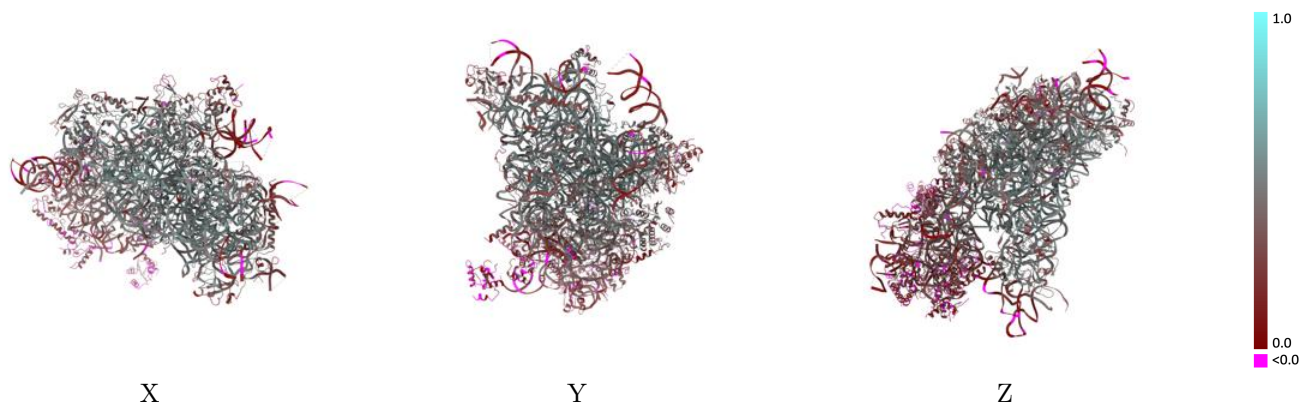
This section contains information regarding the fit between EMDB map EMD-2660 and PDB model 6OKK. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



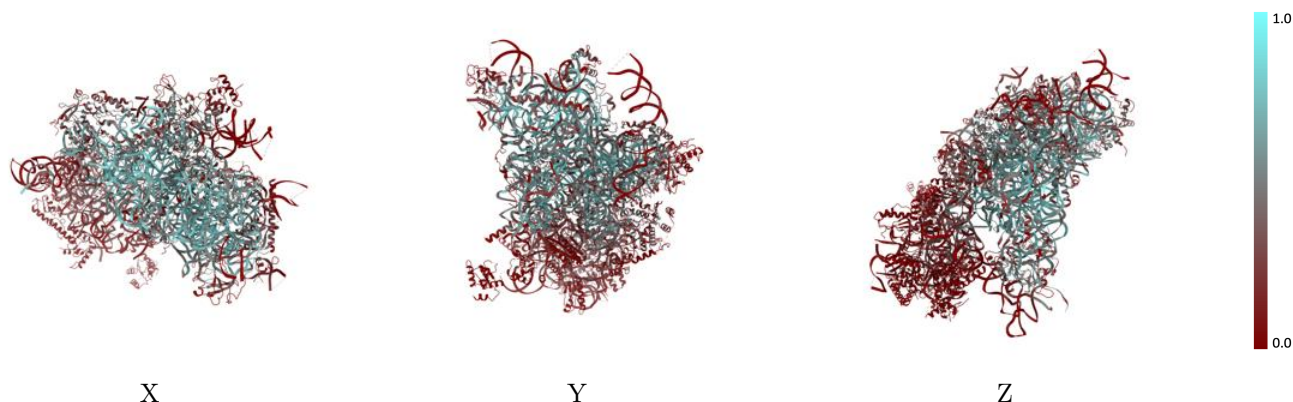
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



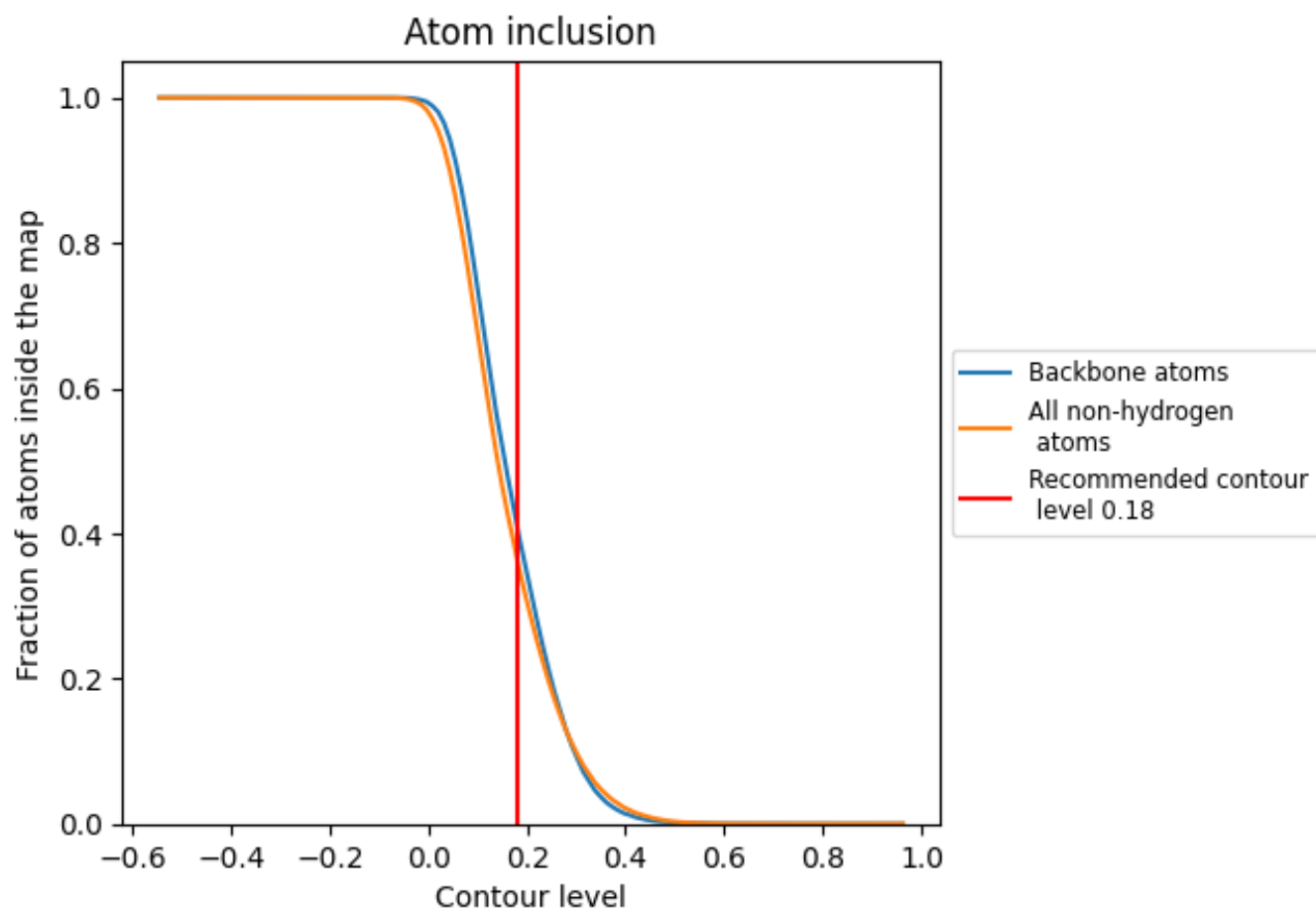
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.18).





































































9.4 Atom inclusion [i](#)



At the recommended contour level, 41% of all backbone atoms, 36% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3644	 0.3790
A	 0.4755	 0.4230
B	 0.3418	 0.4140
C	 0.2555	 0.3820
D	 0.0293	 0.2310
E	 0.4114	 0.4190
F	 0.4003	 0.4470
G	 0.4196	 0.4510
H	 0.2631	 0.3570
I	 0.0216	 0.1940
J	 0.1951	 0.3310
K	 0.4906	 0.4900
L	 0.4789	 0.4540
M	 0.0234	 0.2020
N	 0.0225	 0.1880
O	 0.0075	 0.1390
P	 0.4046	 0.4550
Q	 0.4394	 0.4680
R	 0.0000	 0.0500
S	 0.0118	 0.1580
T	 0.0515	 0.2420
U	 0.4271	 0.4530
V	 0.4945	 0.4920
W	 0.0395	 0.2040
X	 0.0039	 0.1120
Y	 0.0391	 0.2040
Z	 0.3028	 0.4060
a	 0.3463	 0.3870
b	 0.0158	 0.1430
c	 0.4477	 0.4660
d	 0.2892	 0.3760
e	 0.0368	 0.2170
f	 0.3012	 0.3950
g	 0.1426	 0.1840

