



## wwPDB EM Validation Summary Report ⓘ

Nov 13, 2024 – 10:11 AM EST

PDB ID : 3J7A  
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.; Bai, X.C.; Brown, A.; Fernandez, I.S.; Hanssen, E.; Condrón, M.; Tan, Y.H.; Baum, J.; Scheres, S.H.W.  
Deposited on : 2014-06-03  
Resolution : 3.20 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](mailto: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>.

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

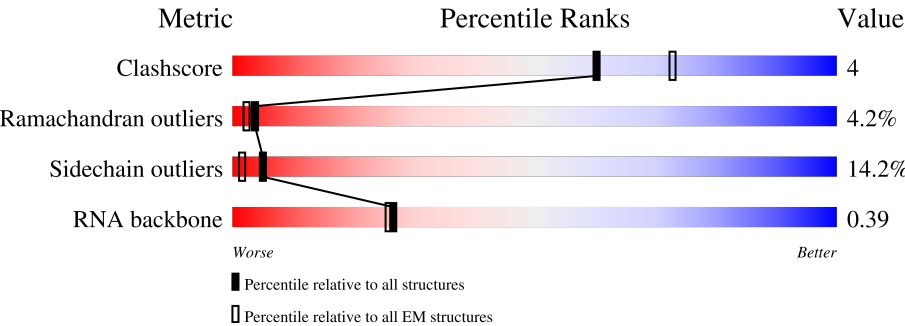
EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 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 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>44%</div> <div>45% 26% 5% 23%</div> </div>
2	B	262	<div> <div>76%</div> <div>53% 22% 5% 20%</div> </div>
3	C	263	<div> <div>70%</div> <div>55% 17% • 26%</div> </div>
4	D	221	<div> <div>71%</div> <div>56% 14% • 29%</div> </div>
5	E	189	<div> <div>67%</div> <div>71% 26% ••</div> </div>
6	F	261	<div> <div>59%</div> <div>71% 23% ••</div> </div>
7	G	272	<div> <div>65%</div> <div>65% 15% • 18%</div> </div>

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Mol	Chain	Length	Quality of chain
8	H	306	
9	I	195	
10	J	194	
11	K	130	
12	L	218	
13	M	144	
14	N	118	
15	O	137	
16	P	151	
17	Q	145	
18	R	141	
19	S	156	
20	T	54	
21	U	151	
22	V	161	
23	W	137	
24	X	145	
25	Y	170	
26	Z	82	
27	1	133	
28	2	105	
29	3	107	
30	4	82	
31	5	67	
32	6	58	

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Mol	Chain	Length	Quality of chain
33	7	74	<div><div></div><div>100%</div><div>53%</div><div>46%</div><div>.</div></div>

## 2 Entry composition

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
1	A	1608	Total	C	N	O	P	0	0
			34277	15347	6109	11213	1608		

- Molecule 2 is a protein called 40S ribosomal protein eS1.

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

- Molecule 3 is a protein called 40S ribosomal protein uS2.

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

- Molecule 4 is a protein called 40S ribosomal protein uS3.

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

- Molecule 5 is a protein called 40S ribosomal protein uS4.

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

- Molecule 6 is a protein called 40S ribosomal protein eS4.

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

- Molecule 7 is a protein called 40S ribosomal protein uS5.

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

- Molecule 8 is a protein called 40S ribosomal protein eS6.

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

- Molecule 9 is a protein called 40S ribosomal protein uS7.

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

- Molecule 10 is a protein called 40S ribosomal protein eS7.

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

- Molecule 11 is a protein called 40S ribosomal protein uS8.

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

- Molecule 12 is a protein called 40S ribosomal protein eS8.

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

- Molecule 13 is a protein called 40S ribosomal protein uS9.

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

- Molecule 14 is a protein called 40S ribosomal protein uS10.

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 eS10.

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 uS11.

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 uS12.

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 eS12.

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 uS13.

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 uS14.

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 uS15.

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 uS17.

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 eS17.

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 uS19.

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 eS19.

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 eS21.

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 eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	1	120	Total	C	N	O	S	0	0
			981	629	188	162	2		

- Molecule 28 is a protein called 40S ribosomal protein eS25.



Mol	Chain	Residues	Atoms				AltConf	Trace
28	2	41	Total	C	N	O	0	0
			320	208	56	56		

- Molecule 29 is a protein called 40S ribosomal protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	3	95	Total	C	N	O	S	0	0
			781	478	169	128	6		

- Molecule 30 is a protein called 40S ribosomal protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	4	76	Total	C	N	O	S	0	0
			586	368	102	107	9		

- Molecule 31 is a protein called 40S ribosomal protein eS28.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	5	58	Total	C	N	O	0	0
			451	282	90	79		

- Molecule 32 is a protein called 40S ribosomal protein eS30.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	6	43	Total	C	N	O	0	0
			345	213	75	57		

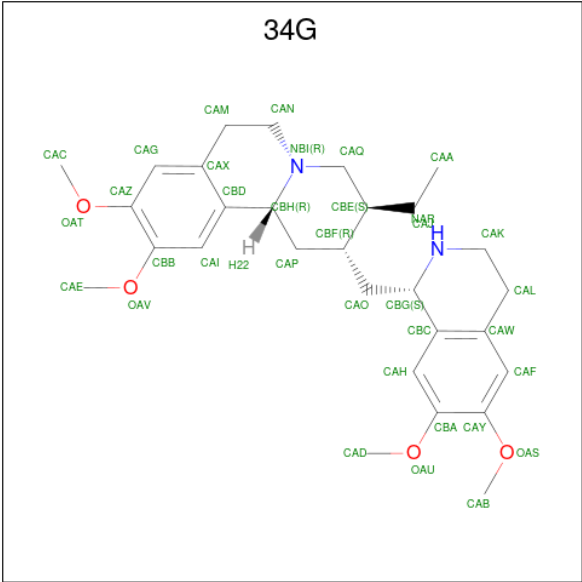
- Molecule 33 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	7	74	Total	C	N	O	P	0	0
			1571	702	275	521	73		

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

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

- Molecule 35 is emetine (three-letter code: 34G) (formula: C<sub>29</sub>H<sub>40</sub>N<sub>2</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				AltConf
35	A	1	Total	C	N	O	0
			35	29	2	4	

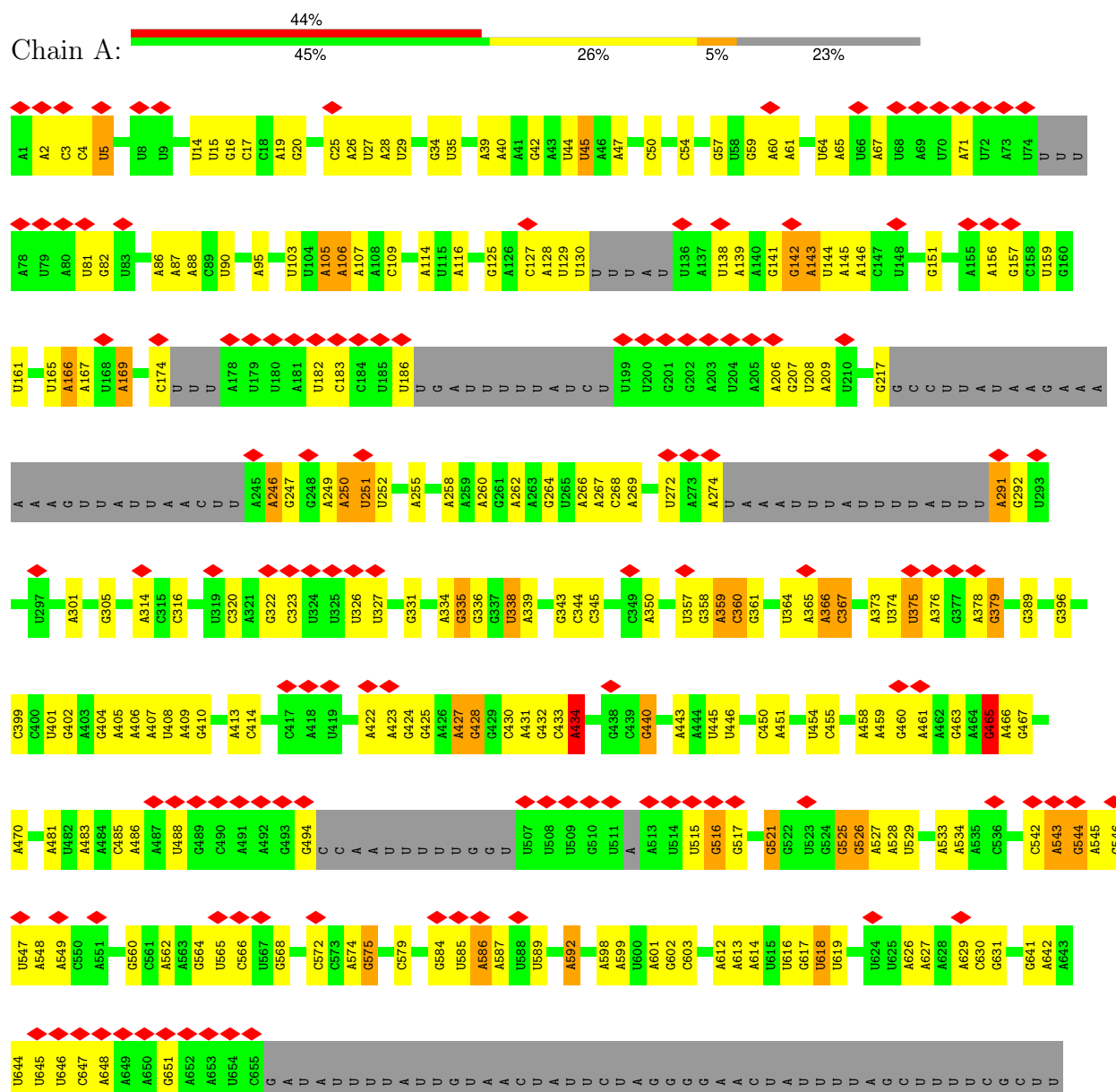
- Molecule 36 is ZINC ION (three-letter code: ZN) (formula: Zn).

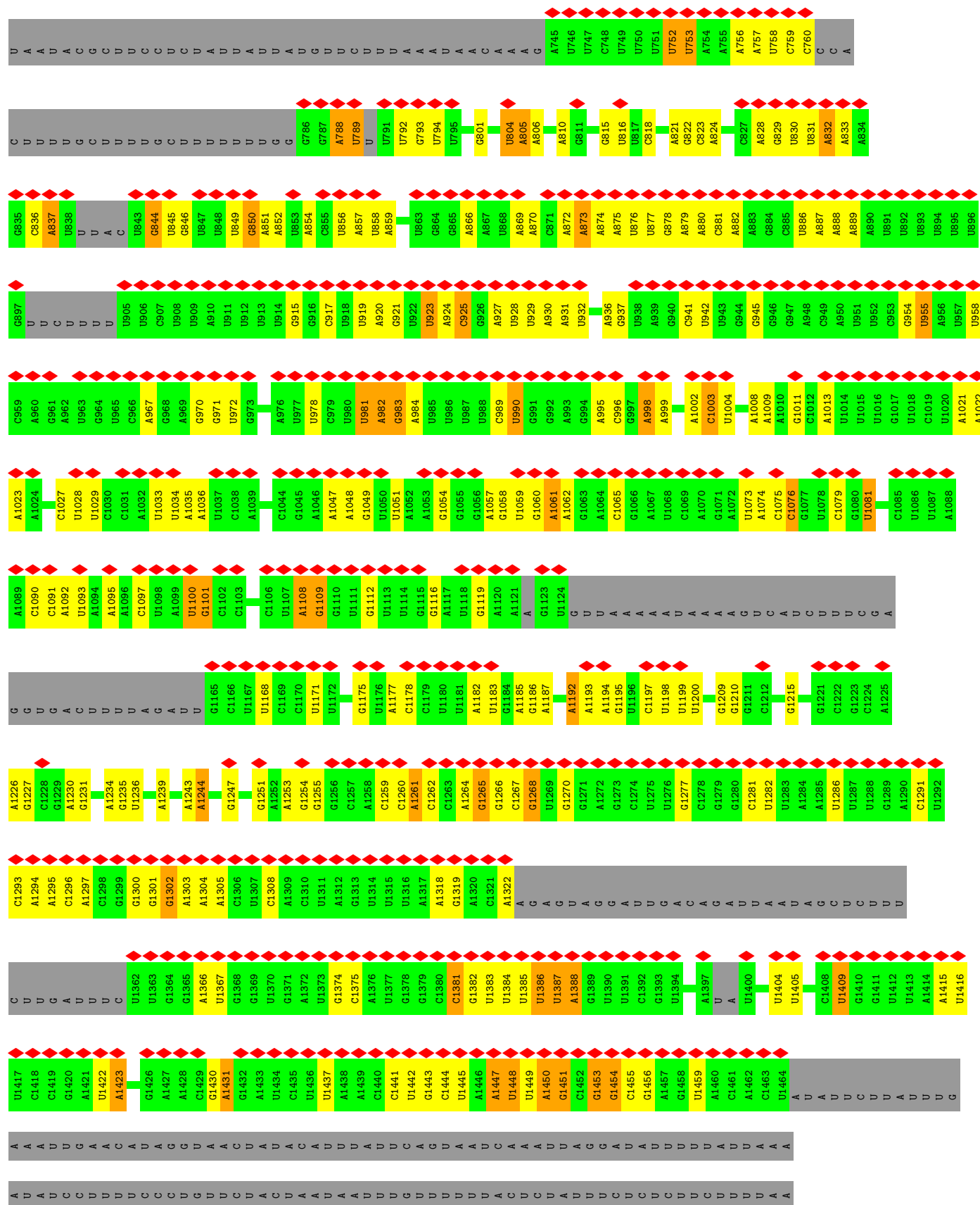
Mol	Chain	Residues	Atoms		AltConf
36	T	1	Total	Zn	0
			1	1	

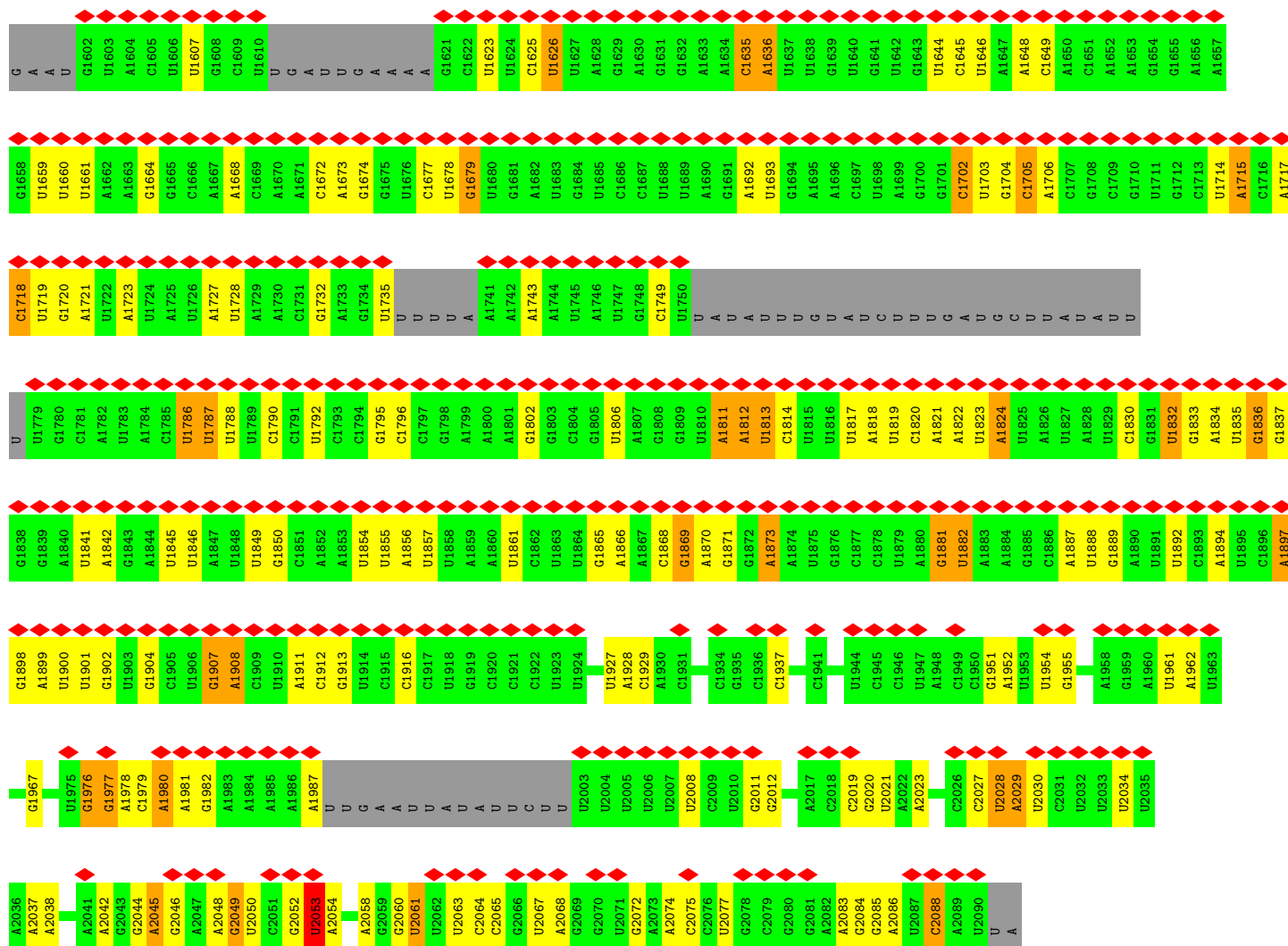
### 3 Residue-property plots

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.

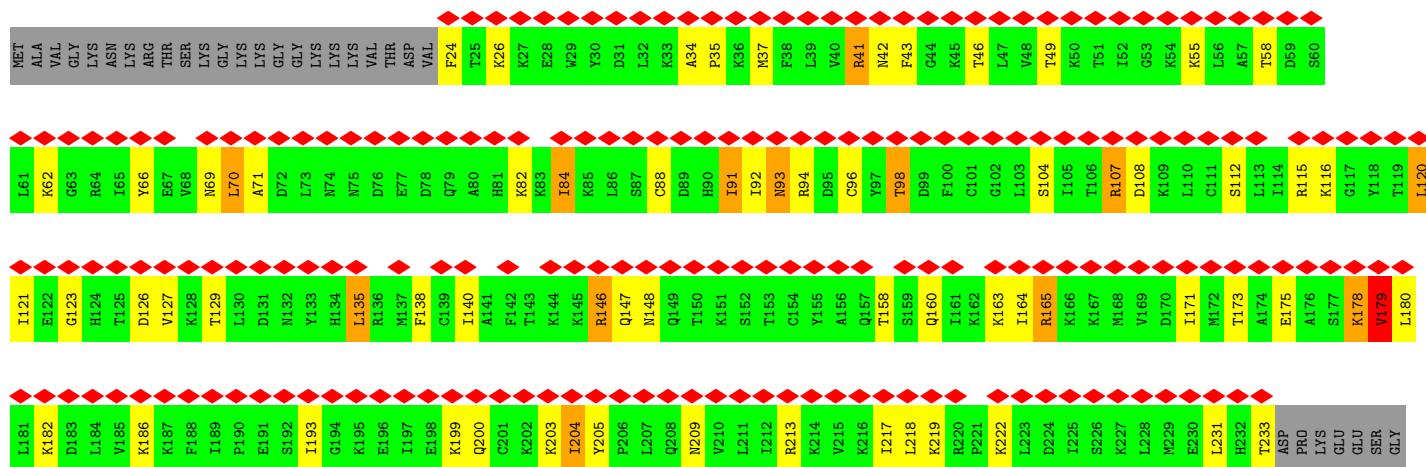
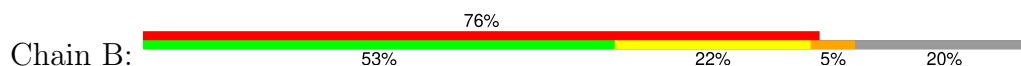
#### • Molecule 1: 18S ribosomal RNA





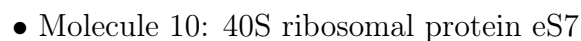


• Molecule 2: 40S ribosomal protein eS1



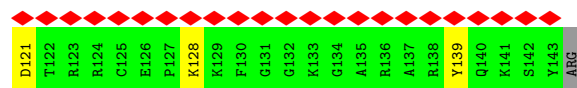




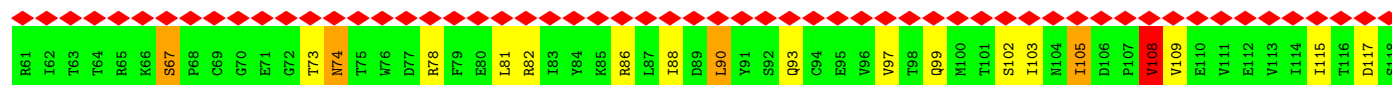
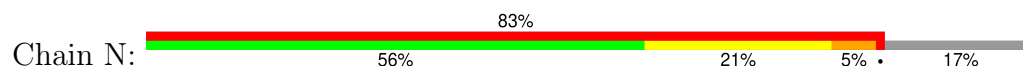




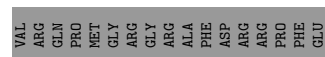




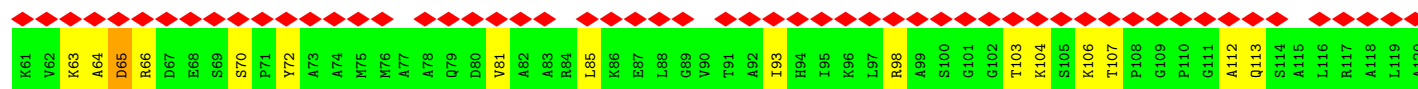
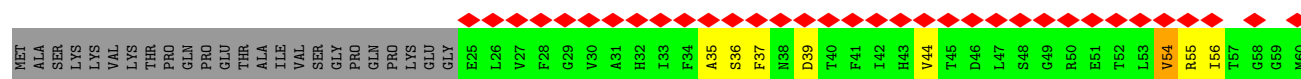
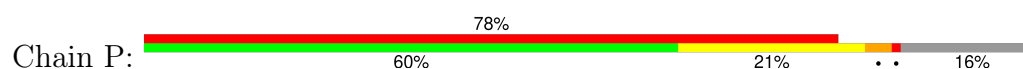
• Molecule 14: 40S ribosomal protein uS10



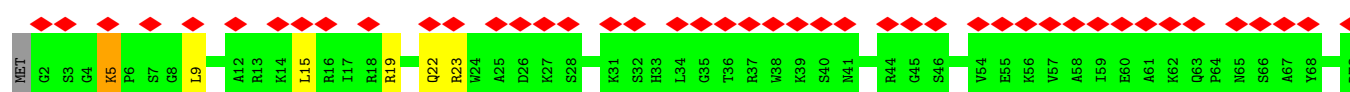
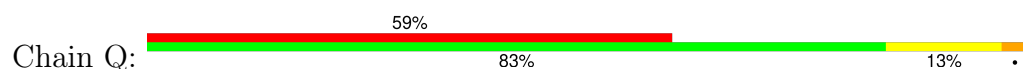
• Molecule 15: 40S ribosomal protein eS10



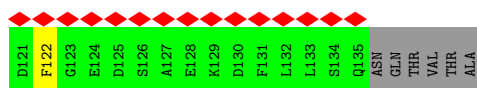
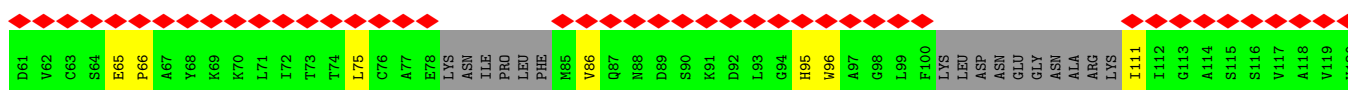
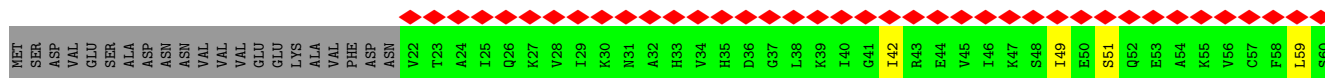
• Molecule 16: 40S ribosomal protein uS11



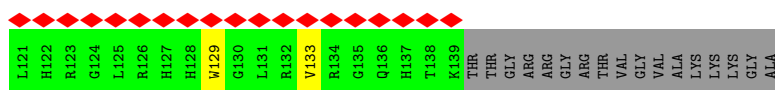
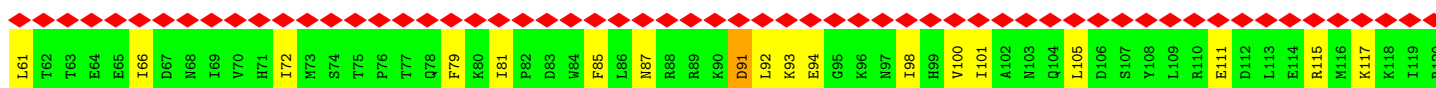
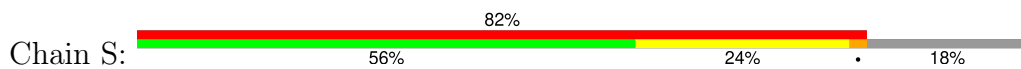
• Molecule 17: 40S ribosomal protein uS12



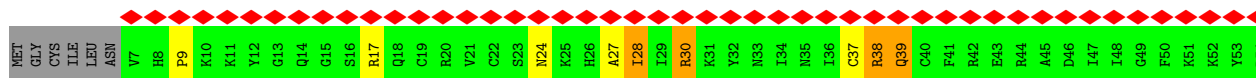
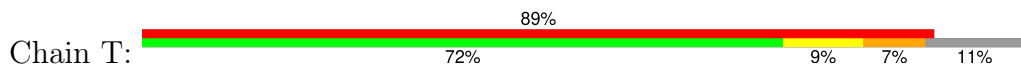
- Molecule 18: 40S ribosomal protein eS12



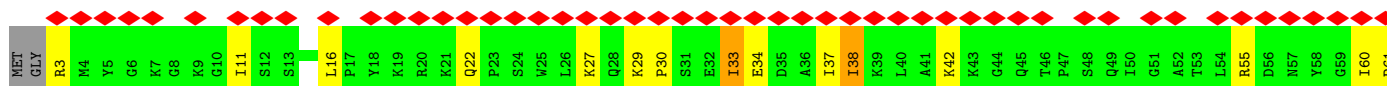
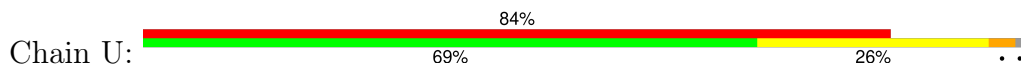
- Molecule 19: 40S ribosomal protein uS13

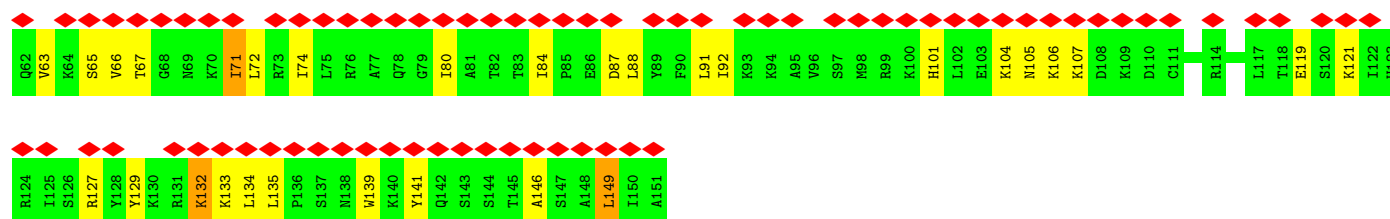


- Molecule 20: 40S ribosomal protein uS14

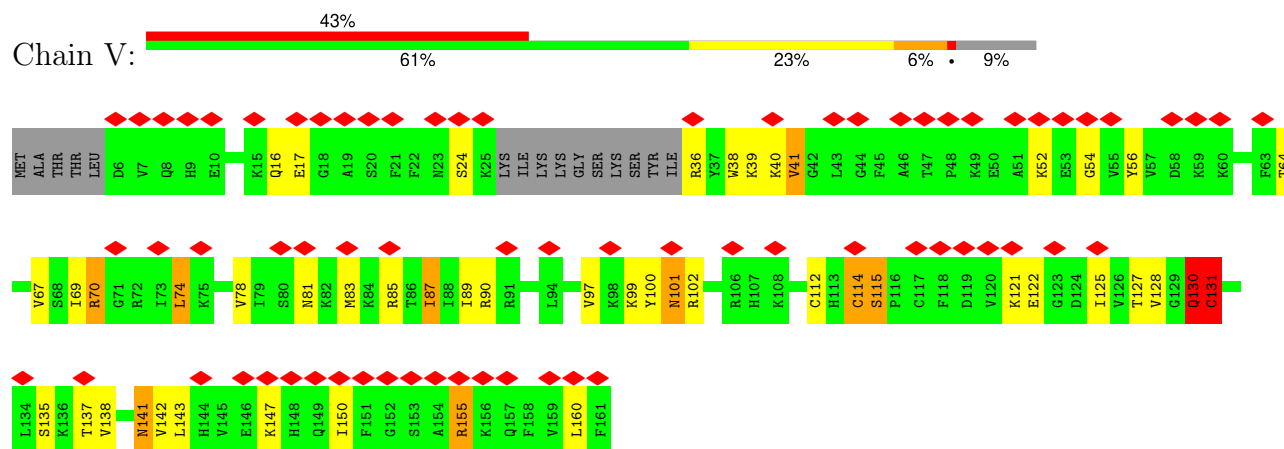


- Molecule 21: 40S ribosomal protein uS15

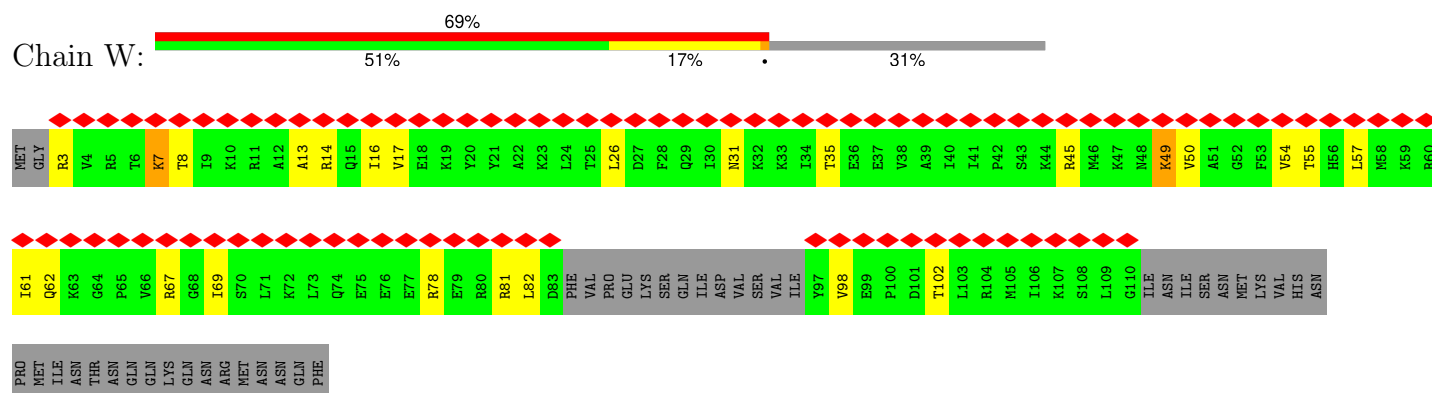




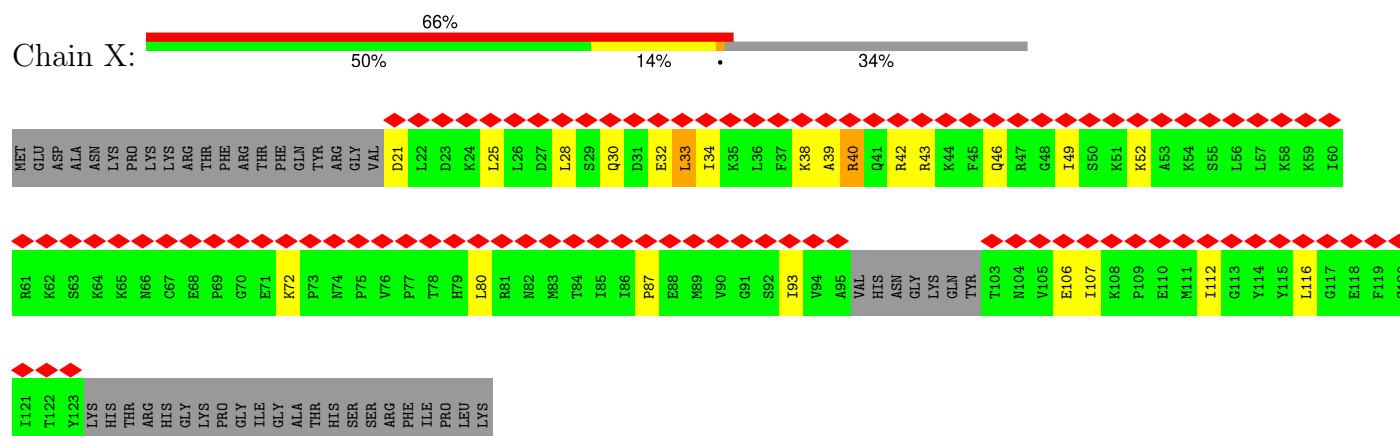
• Molecule 22: 40S ribosomal protein uS17



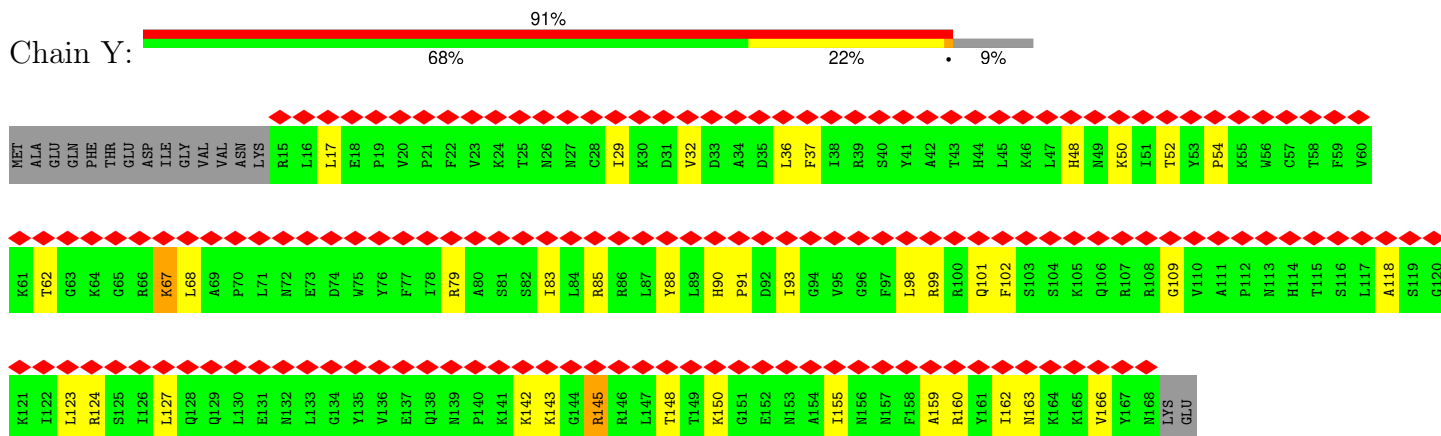
• Molecule 23: 40S ribosomal protein eS17



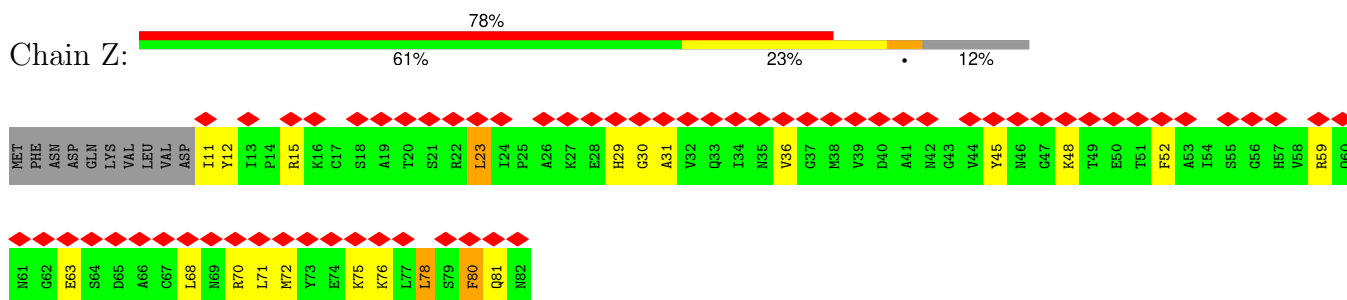
• Molecule 24: 40S ribosomal protein uS19



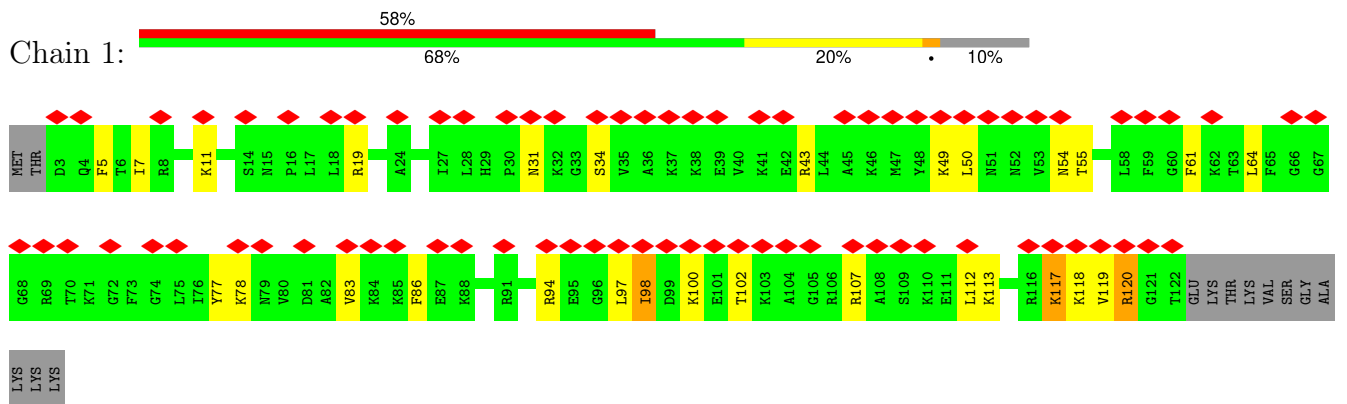
- Molecule 25: 40S ribosomal protein eS19



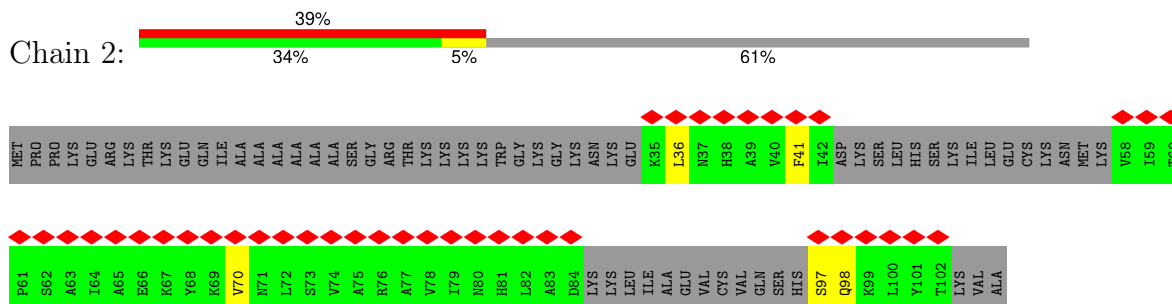
- Molecule 26: 40S ribosomal protein eS21



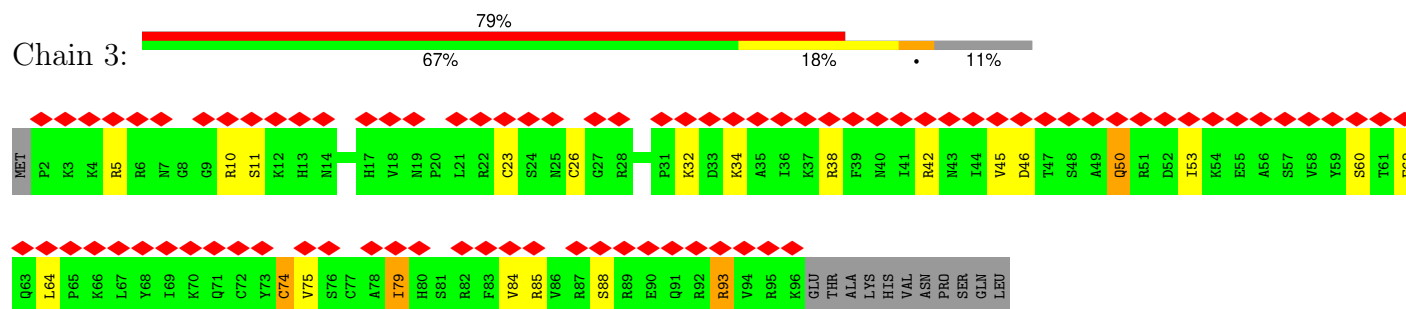
- Molecule 27: 40S ribosomal protein eS24



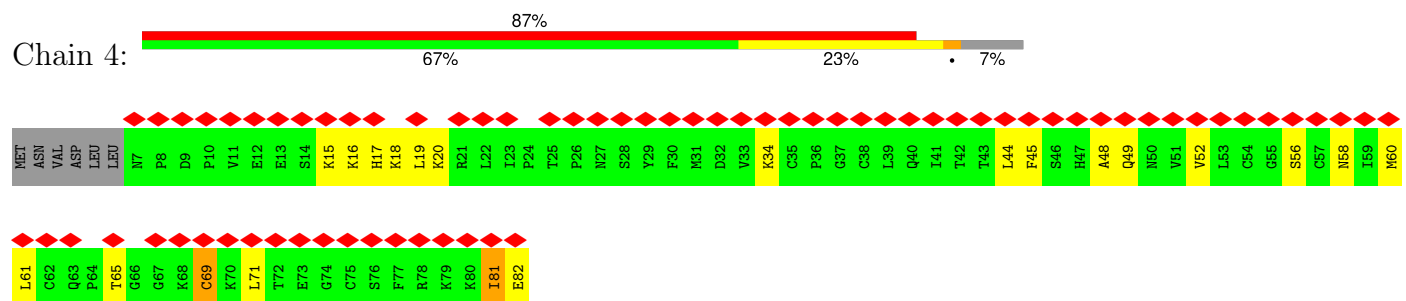
- Molecule 28: 40S ribosomal protein eS25



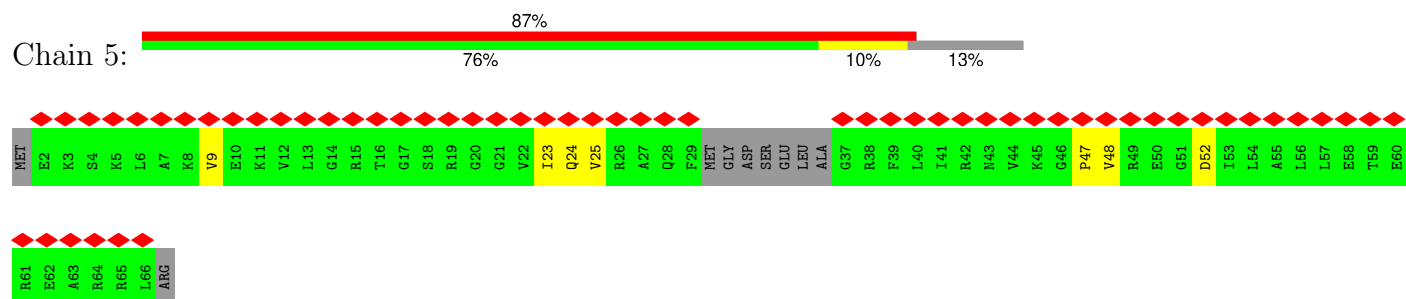
- Molecule 29: 40S ribosomal protein eS26



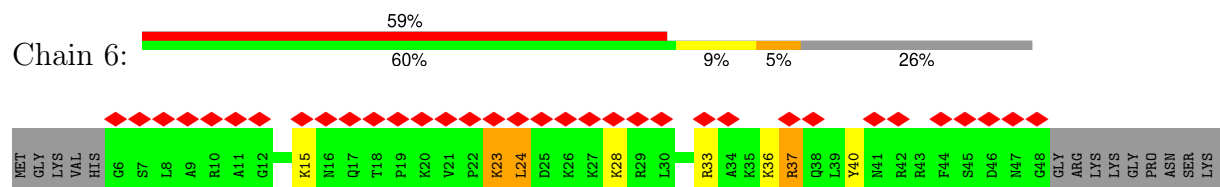
- Molecule 30: 40S ribosomal protein eS27



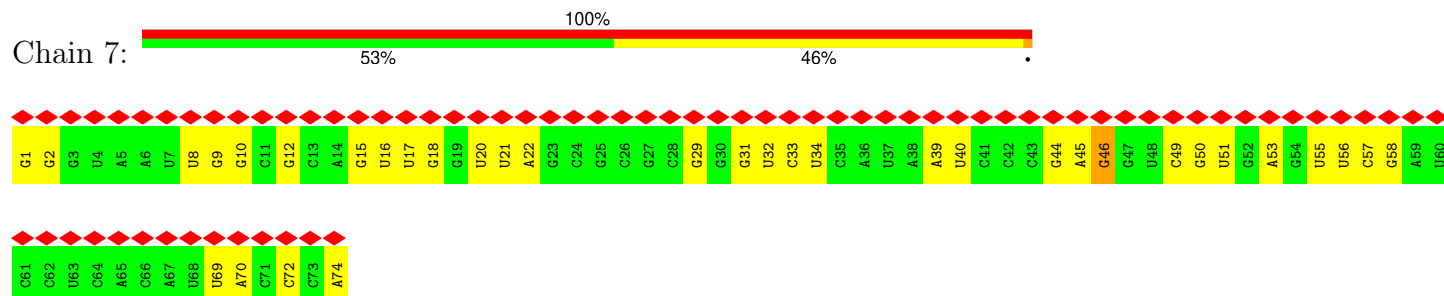
- Molecule 31: 40S ribosomal protein eS28



- Molecule 32: 40S ribosomal protein eS30



- Molecule 33: 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	Each particle	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3800	Depositor
Magnification	104748	Depositor
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 ( $\text{\AA}$ )	482.40002, 482.40002, 482.40002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	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: 34G, ZN, 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	0.45	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	0.73	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	1	0.49	0/994	0.86	0/1317
28	2	0.48	0/323	0.67	0/435
29	3	0.48	0/793	0.90	0/1055
30	4	0.45	0/597	0.73	0/801
31	5	0.40	0/452	0.64	0/599
32	6	0.42	0/348	0.80	0/458



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	7	0.24	0/1754	0.72	0/2732
All	All	0.40	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	1	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	8.01	1.70	1.61
1	A	789	U	C1'-N1	6.93	1.59	1.48
1	A	788	A	C1'-N9	-5.21	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'	-10.85	106.69	119.70
1	A	788	A	OP2-P-O3'	7.78	122.32	105.20
1	A	2053	U	C2'-C3'-O3'	7.76	126.57	109.50
1	A	850	G	C2'-C3'-O3'	7.72	126.49	109.50
1	A	1381	C	C2'-C3'-O3'	7.23	125.40	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

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	34277	0	17246	210	0
2	B	1713	0	1838	25	0
3	C	1538	0	1600	17	0
4	D	1228	0	1311	14	0
5	E	1508	0	1594	16	0
6	F	2061	0	2200	23	0
7	G	1757	0	1811	12	0
8	H	1644	0	1795	15	0
9	I	1424	0	1471	9	0
10	J	1528	0	1680	20	0
11	K	1037	0	1099	16	0
12	L	1392	0	1447	20	0
13	M	1098	0	1183	7	0
14	N	772	0	813	8	0
15	O	686	0	695	7	0
16	P	953	0	997	20	0
17	Q	1129	0	1196	12	0
18	R	746	0	754	2	0
19	S	1042	0	1095	23	0
20	T	404	0	416	5	0
21	U	1202	0	1299	19	0
22	V	1206	0	1239	16	0
23	W	785	0	858	6	0
24	X	776	0	832	9	0
25	Y	1266	0	1316	12	0
26	Z	556	0	558	7	0
27	1	981	0	1065	9	0
28	2	320	0	338	0	0
29	3	781	0	818	12	0
30	4	586	0	604	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	5	451	0	485	2	0
32	6	345	0	381	4	0
33	7	1571	0	797	3	0
34	A	67	0	0	0	0
35	A	35	0	40	2	0
36	T	1	0	0	0	0
All	All	68866	0	52871	522	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 4.

The worst 5 of 522 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)
19:S:33:THR:O	19:S:38:ILE:HG12	1.15	1.32
1:A:759:C:O2	1:A:788:A:C2	1.84	1.30
19:S:35:ILE:O	19:S:38:ILE:CG1	1.76	1.30
1:A:759:C:C2	1:A:788:A:C2	2.30	1.19
19:S:35:ILE:O	19:S:38:ILE:HG13	0.91	1.09

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	
2	B	208/262 (79%)	168 (81%)	28 (14%)	12 (6%)	1	10
3	C	193/263 (73%)	163 (84%)	22 (11%)	8 (4%)	2	17
4	D	149/221 (67%)	129 (87%)	17 (11%)	3 (2%)	6	32
5	E	183/189 (97%)	159 (87%)	19 (10%)	5 (3%)	4	26
6	F	255/261 (98%)	217 (85%)	31 (12%)	7 (3%)	4	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	222/272 (82%)	195 (88%)	20 (9%)	7 (3%)	3	22
8	H	200/306 (65%)	173 (86%)	19 (10%)	8 (4%)	2	18
9	I	176/195 (90%)	153 (87%)	14 (8%)	9 (5%)	1	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%)	1	11
12	L	166/218 (76%)	134 (81%)	23 (14%)	9 (5%)	1	12
13	M	136/144 (94%)	116 (85%)	13 (10%)	7 (5%)	1	13
14	N	96/118 (81%)	83 (86%)	8 (8%)	5 (5%)	1	12
15	O	77/137 (56%)	66 (86%)	10 (13%)	1 (1%)	10	41
16	P	125/151 (83%)	103 (82%)	18 (14%)	4 (3%)	3	22
17	Q	142/145 (98%)	128 (90%)	13 (9%)	1 (1%)	19	54
18	R	92/141 (65%)	73 (79%)	13 (14%)	6 (6%)	1	8
19	S	126/156 (81%)	100 (79%)	17 (14%)	9 (7%)	1	6
20	T	46/54 (85%)	43 (94%)	2 (4%)	1 (2%)	5	30
21	U	147/151 (97%)	133 (90%)	10 (7%)	4 (3%)	4	26
22	V	142/161 (88%)	123 (87%)	9 (6%)	10 (7%)	1	6
23	W	91/137 (66%)	80 (88%)	7 (8%)	4 (4%)	2	15
24	X	92/145 (63%)	82 (89%)	6 (6%)	4 (4%)	2	16
25	Y	152/170 (89%)	134 (88%)	12 (8%)	6 (4%)	2	18
26	Z	70/82 (85%)	62 (89%)	3 (4%)	5 (7%)	1	6
27	1	118/133 (89%)	104 (88%)	9 (8%)	5 (4%)	2	17
28	2	35/105 (33%)	30 (86%)	5 (14%)	0	100	100
29	3	93/107 (87%)	80 (86%)	10 (11%)	3 (3%)	3	22
30	4	74/82 (90%)	48 (65%)	21 (28%)	5 (7%)	1	7
31	5	54/67 (81%)	50 (93%)	4 (7%)	0	100	100
32	6	41/58 (71%)	34 (83%)	4 (10%)	3 (7%)	1	6
All	All	4014/4955 (81%)	3427 (85%)	420 (10%)	167 (4%)	4	17

5 of 167 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	84	ILE
2	B	93	ASN

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Mol	Chain	Res	Type
2	B	147	GLN
2	B	179	VAL
3	C	20	CYS

### 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	B	195/238 (82%)	158 (81%)	37 (19%)	1	6
3	C	167/227 (74%)	144 (86%)	23 (14%)	3	14
4	D	132/188 (70%)	119 (90%)	13 (10%)	6	27
5	E	160/167 (96%)	137 (86%)	23 (14%)	2	13
6	F	233/237 (98%)	194 (83%)	39 (17%)	2	9
7	G	191/222 (86%)	160 (84%)	31 (16%)	2	9
8	H	181/279 (65%)	151 (83%)	30 (17%)	2	9
9	I	154/165 (93%)	128 (83%)	26 (17%)	1	8
10	J	177/183 (97%)	156 (88%)	21 (12%)	4	19
11	K	115/116 (99%)	94 (82%)	21 (18%)	1	7
12	L	152/193 (79%)	136 (90%)	16 (10%)	5	24
13	M	116/122 (95%)	110 (95%)	6 (5%)	19	52
14	N	91/109 (84%)	70 (77%)	21 (23%)	0	3
15	O	76/129 (59%)	65 (86%)	11 (14%)	2	13
16	P	99/119 (83%)	83 (84%)	16 (16%)	2	9
17	Q	120/121 (99%)	106 (88%)	14 (12%)	4	21
18	R	83/121 (69%)	81 (98%)	2 (2%)	44	71
19	S	113/136 (83%)	99 (88%)	14 (12%)	4	18
20	T	43/48 (90%)	38 (88%)	5 (12%)	4	21
21	U	132/133 (99%)	110 (83%)	22 (17%)	2	9
22	V	131/144 (91%)	106 (81%)	25 (19%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	W	86/127 (68%)	73 (85%)	13 (15%)	2	12
24	X	88/130 (68%)	80 (91%)	8 (9%)	7	29
25	Y	137/151 (91%)	117 (85%)	20 (15%)	2	13
26	Z	60/70 (86%)	50 (83%)	10 (17%)	2	9
27	1	103/115 (90%)	89 (86%)	14 (14%)	3	15
28	2	35/88 (40%)	30 (86%)	5 (14%)	2	13
29	3	87/98 (89%)	76 (87%)	11 (13%)	3	18
30	4	70/76 (92%)	60 (86%)	10 (14%)	2	13
31	5	46/54 (85%)	42 (91%)	4 (9%)	8	32
32	6	36/47 (77%)	33 (92%)	3 (8%)	9	35
All	All	3609/4353 (83%)	3095 (86%)	514 (14%)	5	13

5 of 514 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	Z	68	LEU
27	1	107	ARG
26	Z	63	GLU
8	H	183	ARG
8	H	137	ARG

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	1	54	ASN
27	1	52	ASN
11	K	64	ASN
23	W	31	ASN
11	K	24	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1586/2092 (75%)	474 (29%)	71 (4%)
33	7	73/74 (98%)	30 (41%)	3 (4%)
All	All	1659/2166 (76%)	504 (30%)	74 (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 74 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1813	U
33	7	9	G
1	A	1819	U
1	A	1897	A
1	A	752	U

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	A	2168	-	39,39,39	2.75	8 (20%)	51,56,56	1.89	10 (19%)

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	A	2168	-	-	10/14/49/49	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	A	2168	34G	CBC-CBG	-9.18	1.43	1.52
35	A	2168	34G	CAM-CAX	-7.80	1.38	1.51
35	A	2168	34G	CAL-CAW	-5.72	1.41	1.51
35	A	2168	34G	CBD-CBH	-5.64	1.43	1.52
35	A	2168	34G	CAP-CBH	-5.07	1.48	1.53

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	A	2168	34G	CAW-CBC-CBG	-6.34	113.78	121.38
35	A	2168	34G	CAQ-NBI-CBH	5.03	117.45	110.12
35	A	2168	34G	CBF-CAP-CBH	-4.76	102.90	111.76
35	A	2168	34G	CAP-CBF-CBE	-3.90	104.18	110.57
35	A	2168	34G	CAH-CBC-CBG	2.84	126.62	120.67

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	A	2168	34G	CBF-CAO-CBG-NAR
35	A	2168	34G	CBF-CAO-CBG-CBC
35	A	2168	34G	CAZ-CBB-OAV-CAE
35	A	2168	34G	CBA-CAY-OAS-CAB
35	A	2168	34G	CAI-CBB-OAV-CAE

There are no ring outliers.

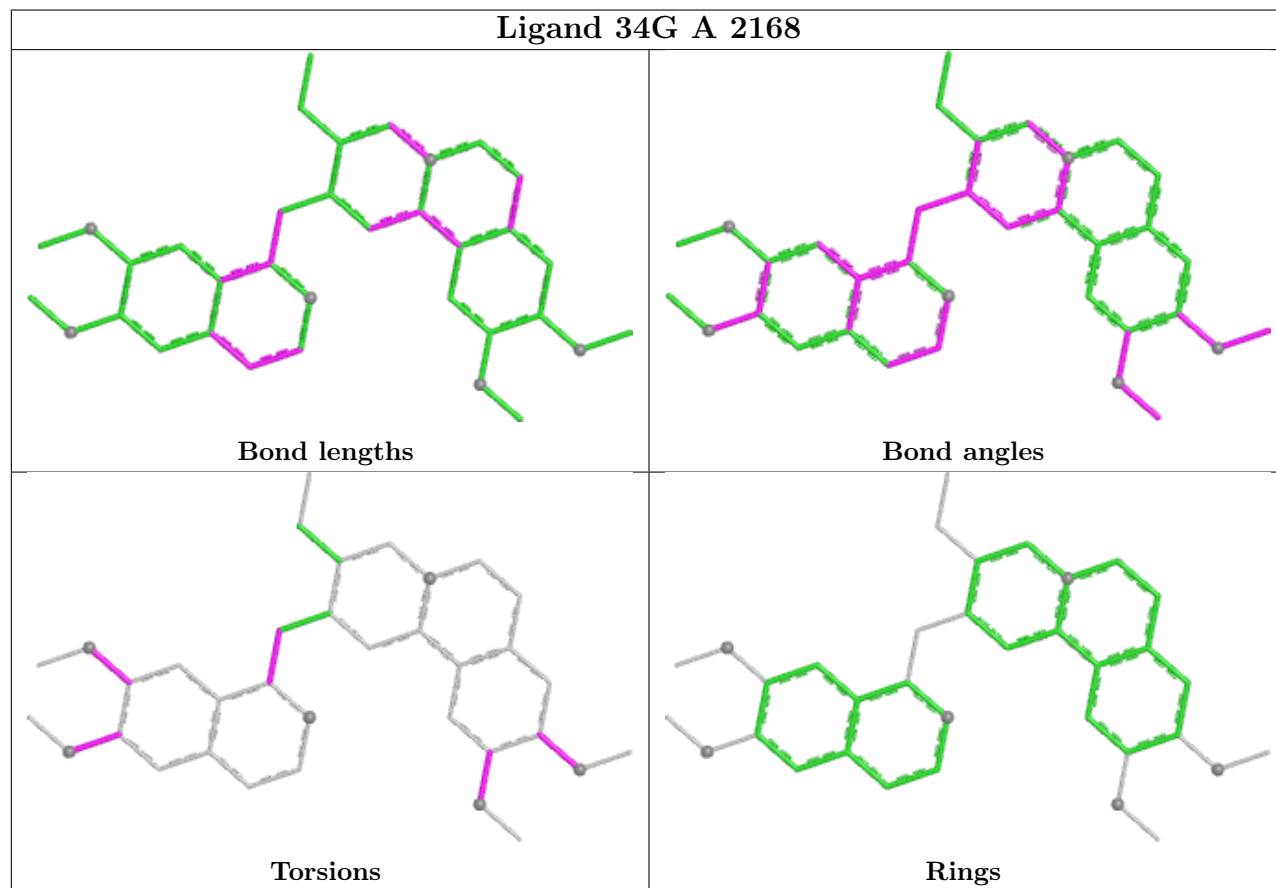
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	A	2168	34G	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In



addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

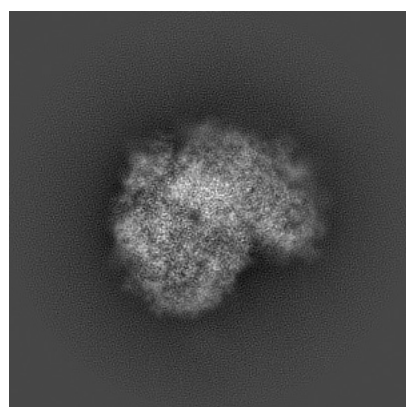
## 6 Map visualisation [i](#)

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.

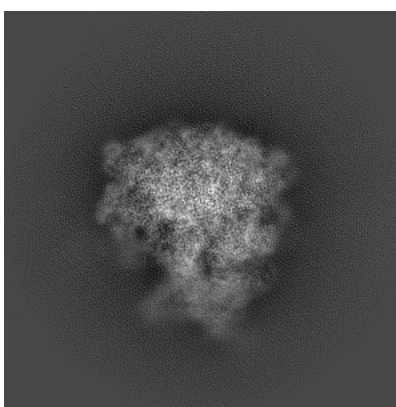
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

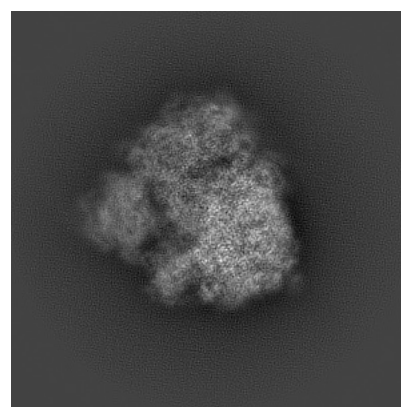
#### 6.1.1 Primary map



X



Y

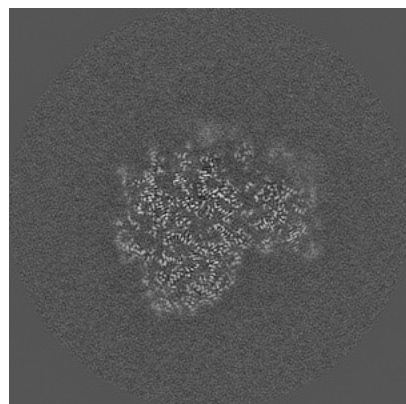


Z

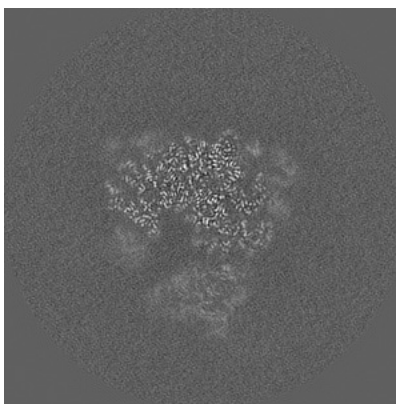
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

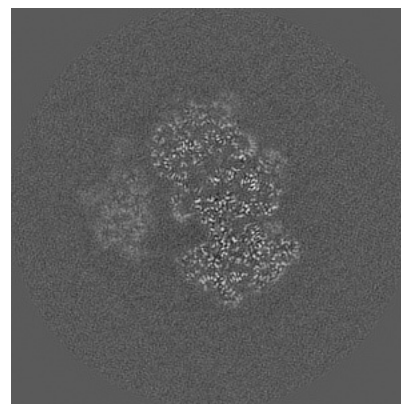
#### 6.2.1 Primary map



X Index: 180



Y Index: 180

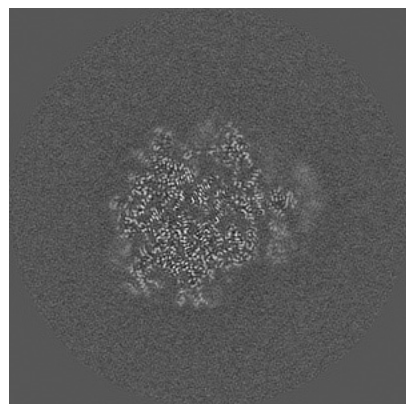


Z Index: 180

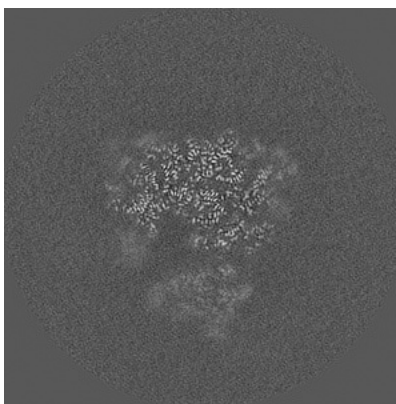
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

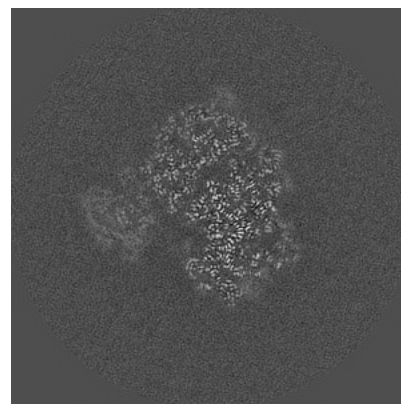
### 6.3.1 Primary map



X Index: 201



Y Index: 183

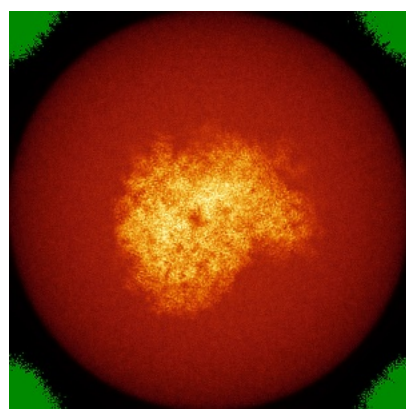


Z Index: 187

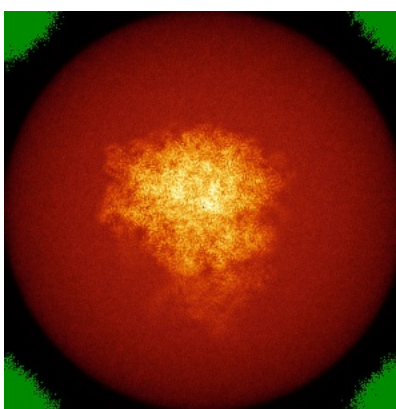
The images above show the largest variance slices of the map in three orthogonal directions.

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

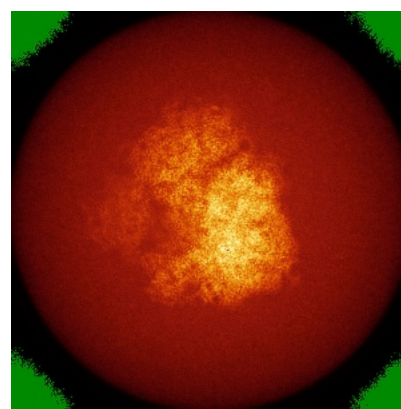
### 6.4.1 Primary map



X



Y

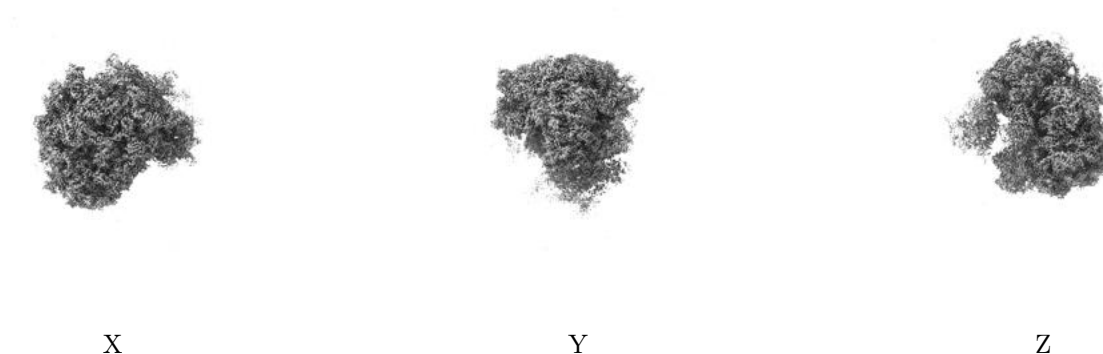


Z

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



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.

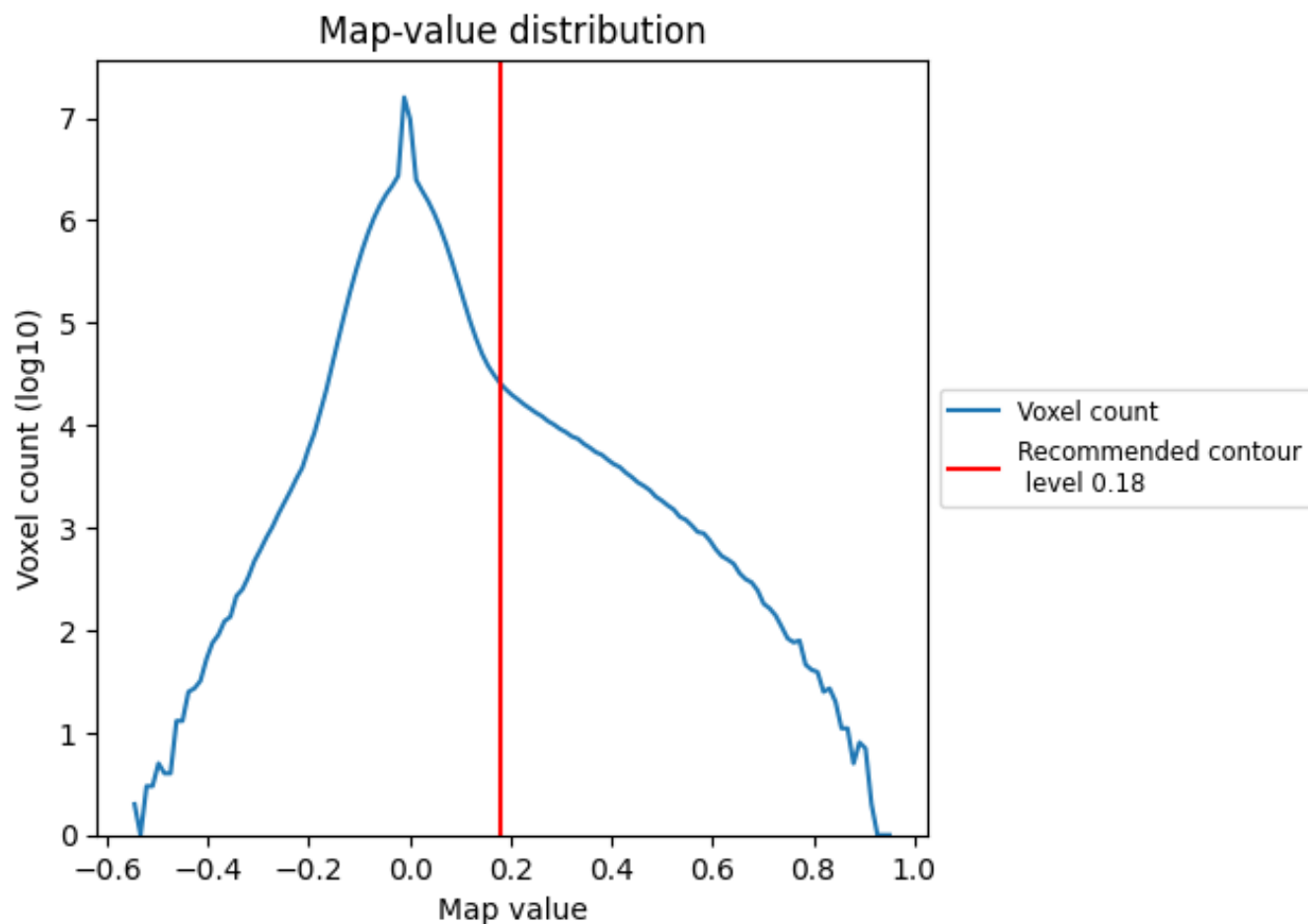
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

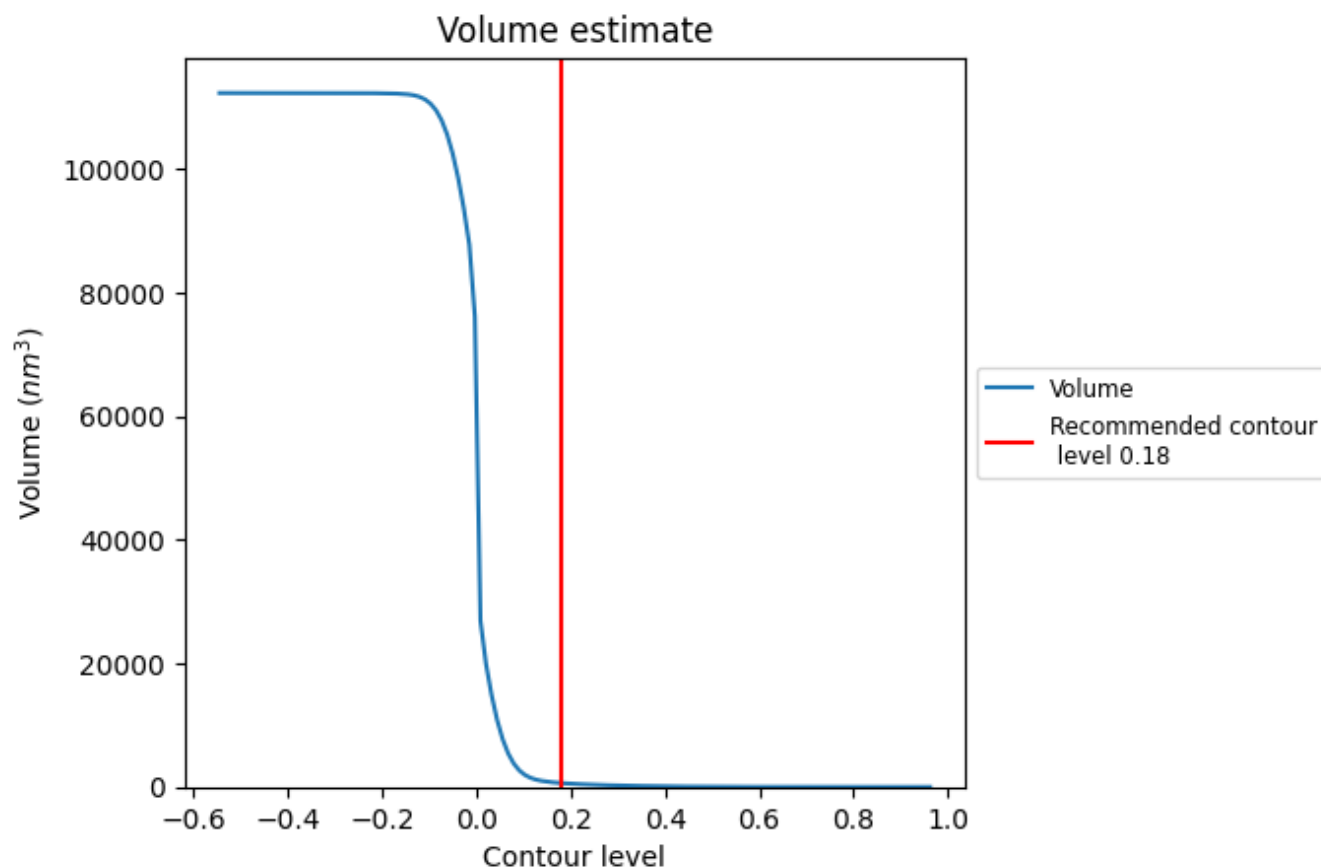
This section contains the results of statistical analysis of the map.

### 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.

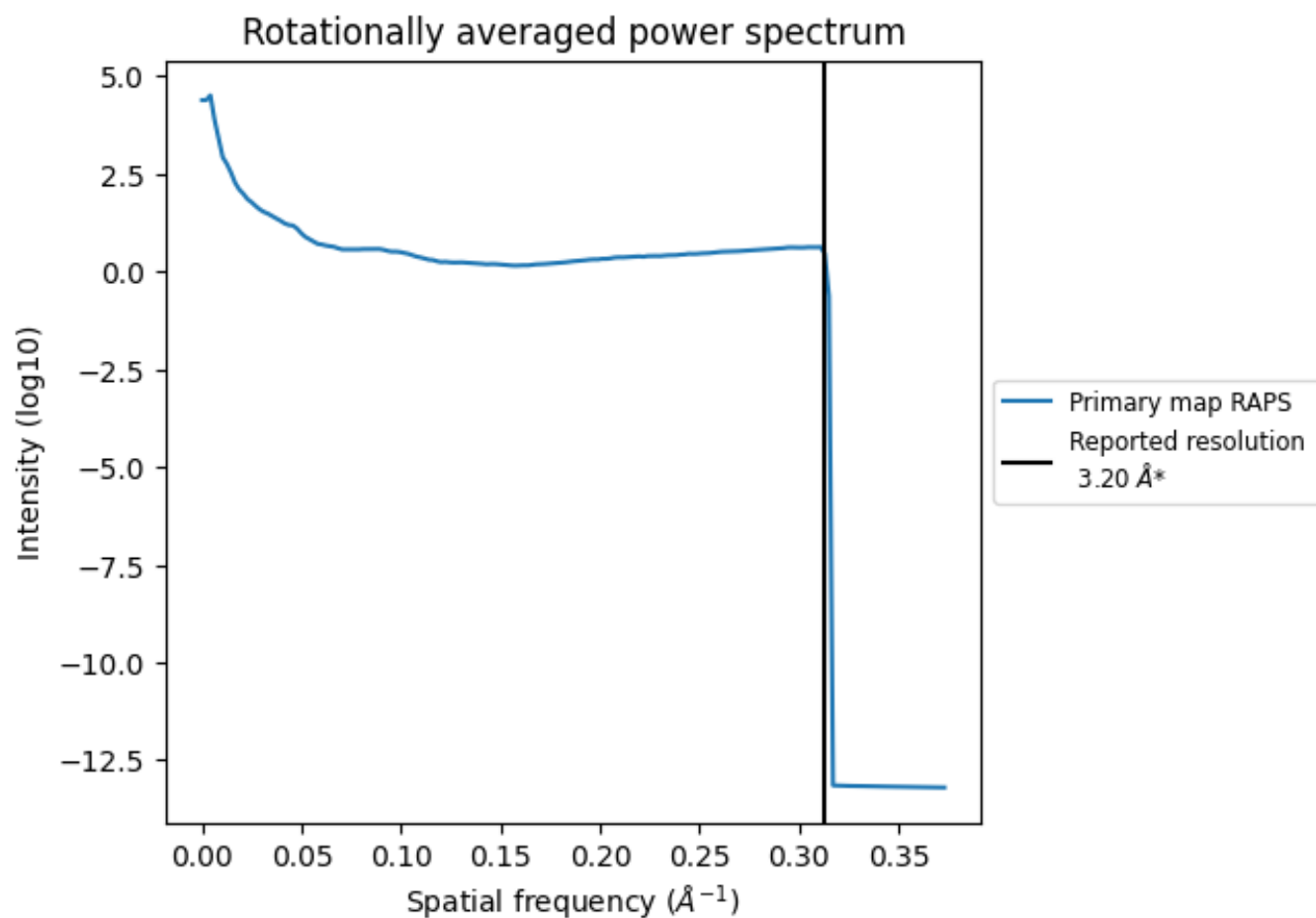
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 628 nm<sup>3</sup>; 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 ⓘ



\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

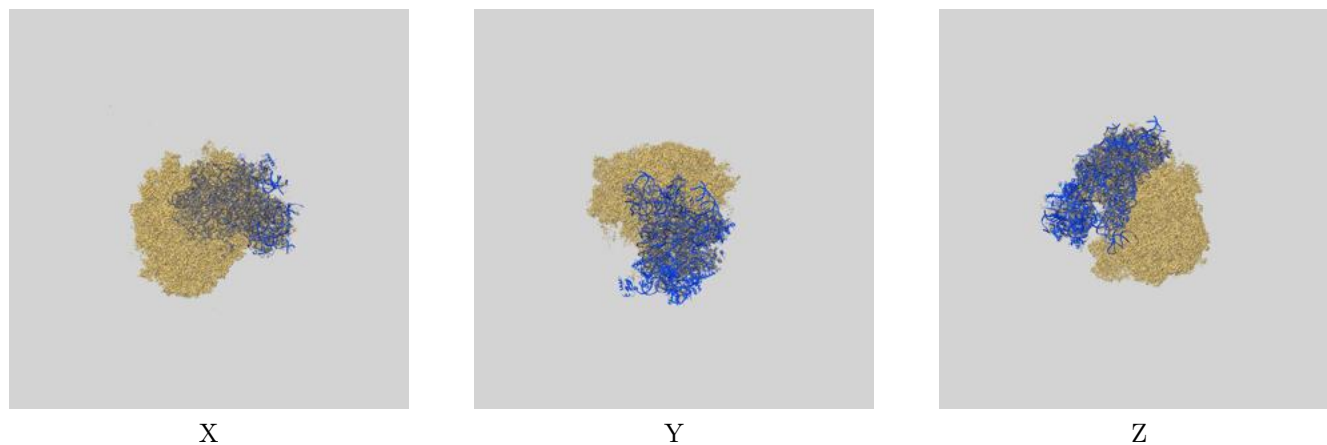
This section was not generated. No FSC curve or half-maps provided.



## 9 Map-model fit [i](#)

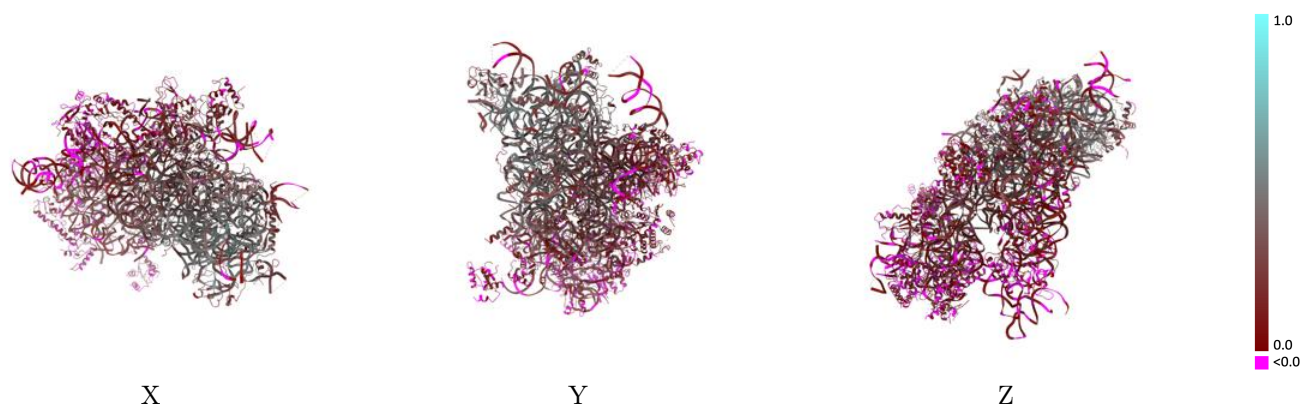
This section contains information regarding the fit between EMDB map EMD-2660 and PDB model 3J7A. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

### 9.1 Map-model overlay [i](#)



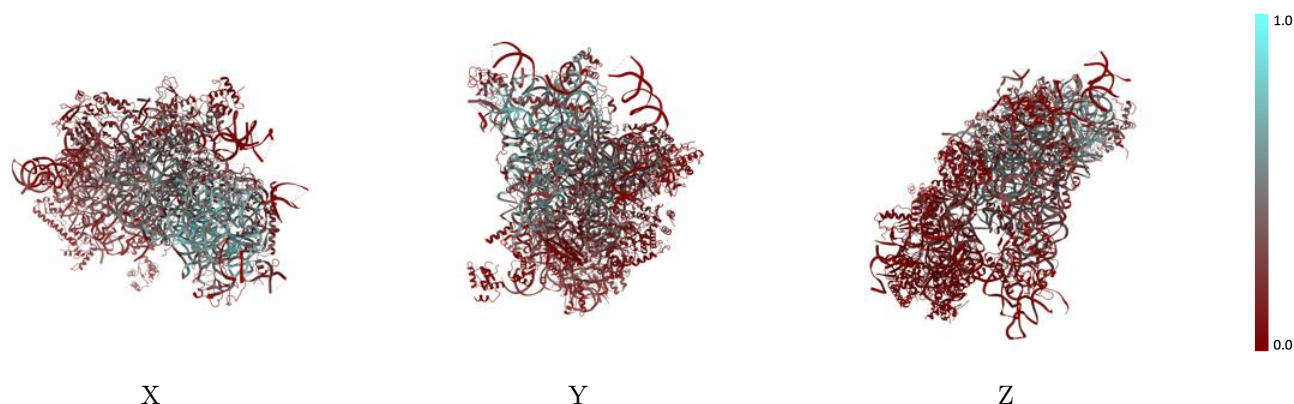
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



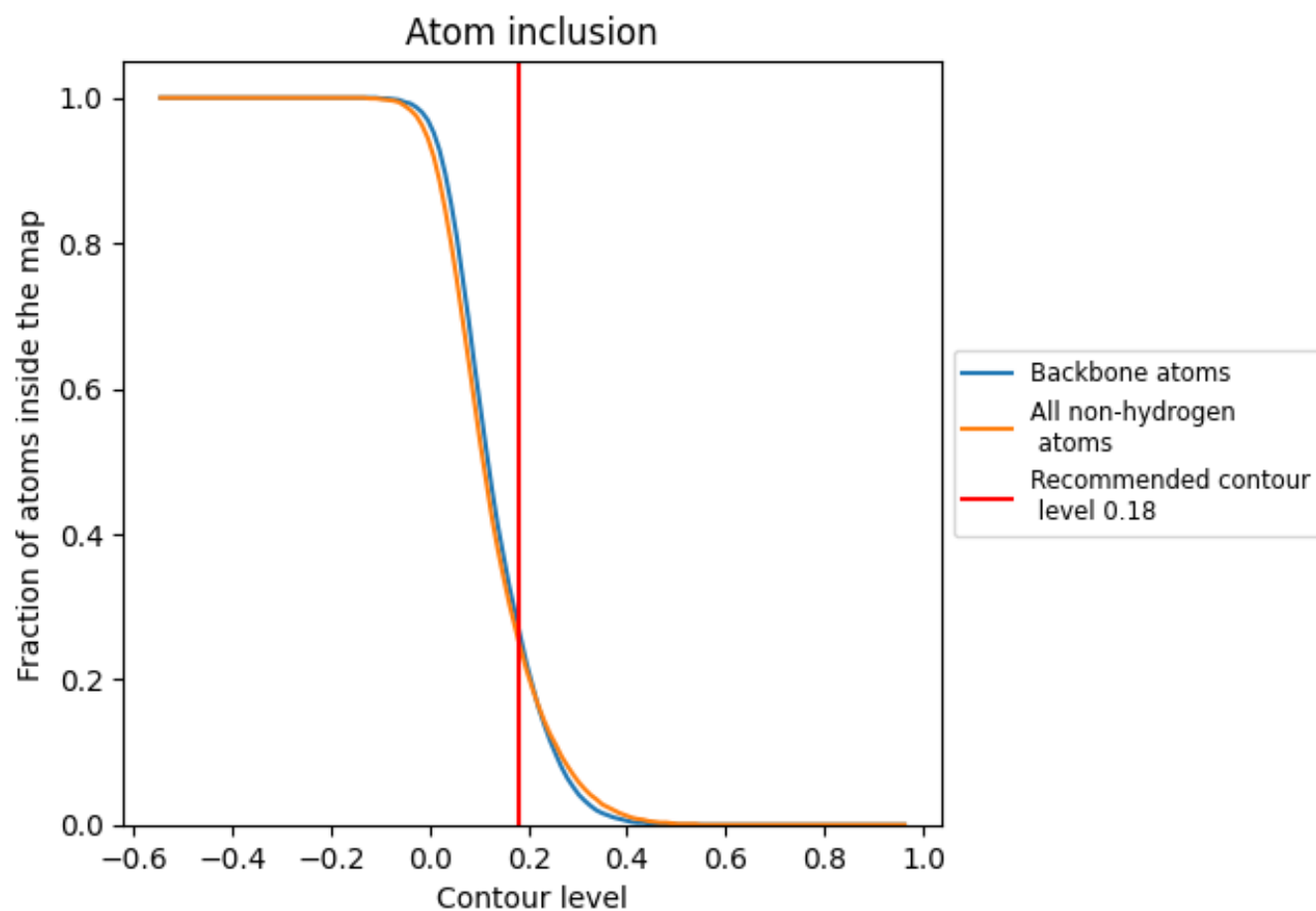
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 27% of all backbone atoms, 25% 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	 0.2530	 0.2310
1	 0.3220	 0.3510
2	 0.0090	 0.0410
3	 0.1660	 0.1200
4	 0.1120	 0.1360
5	 0.0050	 0.0840
6	 0.2530	 0.3130
7	 0.0640	 0.0450
A	 0.3410	 0.2730
B	 0.1220	 0.0800
C	 0.1160	 0.1470
D	 0.0210	 0.1460
E	 0.3260	 0.3110
F	 0.3490	 0.3730
G	 0.2440	 0.2420
H	 0.2490	 0.3400
I	 0.0110	 0.0680
J	 0.0960	 0.1600
K	 0.2870	 0.2510
L	 0.4140	 0.3770
M	 0.0090	 0.0430
N	 0.0150	 0.1240
O	 0.0060	 0.1150
P	 0.1210	 0.0660
Q	 0.3490	 0.3620
R	 0.0000	 0.0290
S	 0.0120	 0.0870
T	 0.0280	 0.1650
U	 0.2120	 0.1940
V	 0.3940	 0.3640
W	 0.0170	 0.1050
X	 0.0050	 0.0480
Y	 0.0220	 0.0770
Z	 0.1490	 0.1730

