



wwPDB EM Validation Summary Report ⓘ

Dec 17, 2022 – 09:01 pm GMT

PDB ID : 6ZMT
EMDB ID : EMD-11301
Title : SARS-CoV-2 Nsp1 bound to a pre-40S-like ribosome complex
Authors : Thoms, M.; Buschauer, R.; Ameismeier, M.; Denk, T.; Kratzat, H.; Mackens-Kiani, T.; Cheng, J.; Berninghausen, O.; Becker, T.; Beckmann, R.
Deposited on : 2020-07-03
Resolution : 3.00 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:

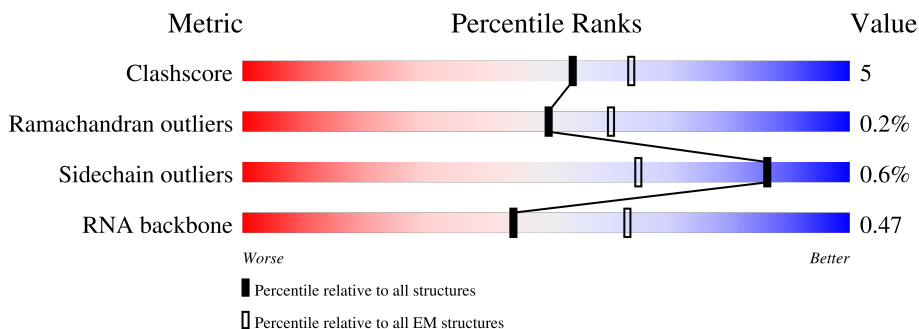
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 3.00 Å.

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







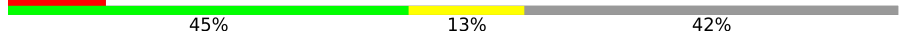












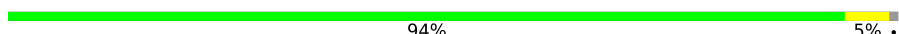

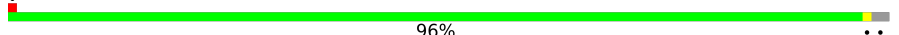


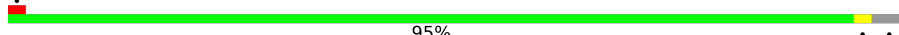

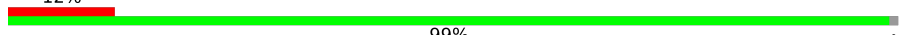
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	B	295	
2	C	264	
3	D	293	
4	E	263	
5	F	243	
6	G	249	
7	H	194	




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Mol	Chain	Length	Quality of chain
8	I	208	 86% 12%
9	J	194	 85% 8% 7%
10	K	204	 11% 72% 20% 7%
11	L	158	 5% 84% 12%
12	M	165	 11% 45% 13% 42%
13	N	151	 86% 13%
14	O	132	 70% 72% 21% 7%
15	P	151	 37% 59% 22% 19%
16	Q	145	 26% 70% 13% 17%
17	R	146	 77% 18% 5%
18	S	135	 79% 16%
19	T	152	 45% 74% 20% 6%
20	U	145	 14% 79% 21%
21	V	119	 22% 68% 17% 15%
22	W	130	 85% 14%
23	X	143	 89% 10%
24	Y	133	 76% 17% 7%
25	Z	83	 94% 5%
26	a	125	 34% 56% 42%
27	b	84	 96%
28	d	69	 22% 88% 12%
29	e	59	 7% 93% 5%
30	f	56	 95%
31	g	156	 18% 40% 59%
32	j	317	 12% 99%

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Mol	Chain	Length	Quality of chain
33	2	1868	
34	i	180	
35	u	804	

2 Entry composition [i](#)

There are 36 unique types of molecules in this entry. The entry contains 76190 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 protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	206	Total	C	N	O	S	0	0
			1624	1035	287	294	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 3 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	218	Total	C	N	O	S	0	0
			1682	1090	289	293	10		

- Molecule 4 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 5 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	225	Total	C	N	O	S	0	0
			1748	1115	315	311	7		

- Molecule 6 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	230	Total	C	N	O	S	0	0
			1862	1164	371	320	7		

- Molecule 7 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	H	186	1501	957	276	267	1	0	0

- Molecule 8 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	I	205	1682	1056	331	290	5	0	0

- Molecule 9 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	180	1499	955	300	242	2	0	0

- Molecule 10 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	K	189	1495	934	284	270	7	0	0

- Molecule 11 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	L	151	1229	782	230	211	6	0	0

- Molecule 12 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	M	95	800	522	142	131	5	0	0

- Molecule 13 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	N	149	1202	770	228	203	1	0	0

- Molecule 14 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	123	Total	C	N	O	S	0	0
			953	598	169	177	9		

- Molecule 15 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	122	Total	C	N	O	S	0	0
			897	555	166	170	6		

- Molecule 16 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	120	Total	C	N	O	S	0	0
			984	625	184	168	7		

- Molecule 17 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	139	Total	C	N	O	S	0	0
			1109	704	210	192	3		

- Molecule 18 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	130	Total	C	N	O	S	0	0
			1050	661	196	189	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	143	Total	C	N	O	S	0	0
			1184	743	240	200	1		

- Molecule 20 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	144	Total	C	N	O	S	0	0
			1122	703	217	199	3		

- Molecule 21 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	V	101	803	504	153	142	4	0	0

- Molecule 22 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	W	129	1034	659	193	176	6	0	0

- Molecule 23 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	X	141	1098	693	219	183	3	0	0

- Molecule 24 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Y	124	1014	641	198	170	5	0	0

- Molecule 25 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Z	82	625	384	116	120	5	0	0

- Molecule 26 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	a	72	574	368	104	101	1	0	0

- Molecule 27 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	b	82	640	402	118	113	7	0	0

- Molecule 28 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	d	61	Total	C	N	O	S	0	0
			479	292	95	90	2		

- Molecule 29 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	e	56	Total	C	N	O	S	0	0
			430	263	95	71	1		

- Molecule 30 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	f	54	Total	C	N	O	S	0	0
			455	284	93	73	5		

- Molecule 31 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	g	64	Total	C	N	O	S	0	0
			477	298	87	85	7		

- Molecule 32 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	j	314	Total	C	N	O	S	0	0
			2440	1537	425	466	12		

- Molecule 33 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	2	1569	Total	C	N	O	P	0	0
			33498	14952	6011	10966	1569		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	1772	C	G	conflict	GB 337376

- Molecule 34 is a protein called Non-structural protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	i	29	239	145	43	50	1	0	0

- Molecule 35 is a protein called Pre-rRNA-processing protein TSR1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	u	615	4954	3179	885	866	24	0	0

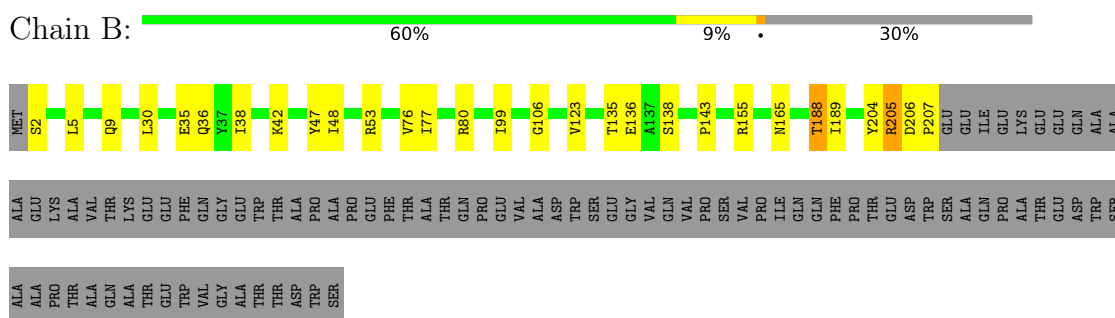
- Molecule 36 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
36	f	1	1	1	0
36	g	1	1	1	0

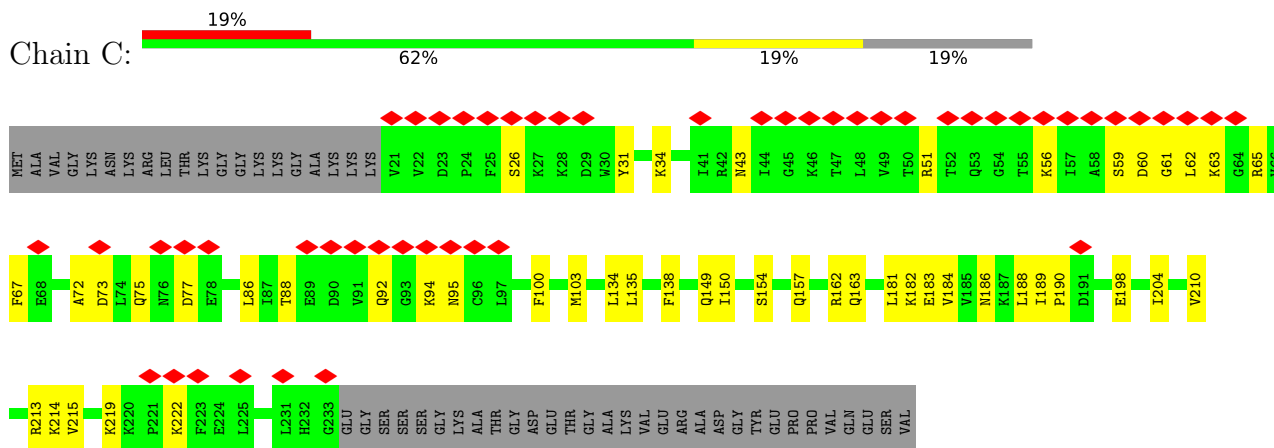
3 Residue-property plots [i](#)

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

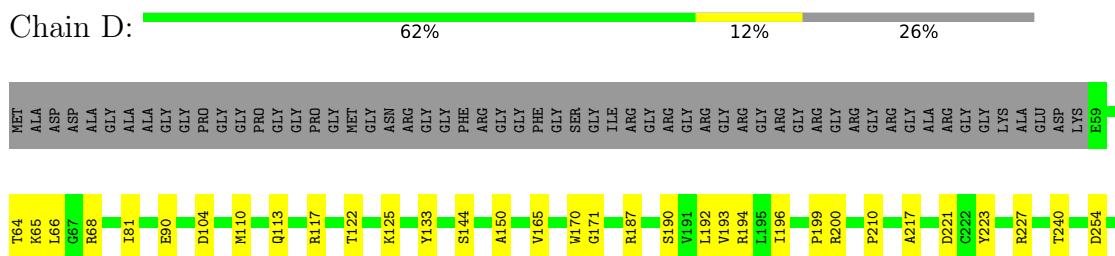
- Molecule 1: 40S ribosomal protein SA

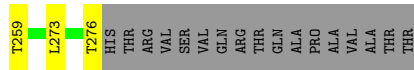


- Molecule 2: 40S ribosomal protein S3a

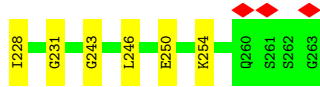
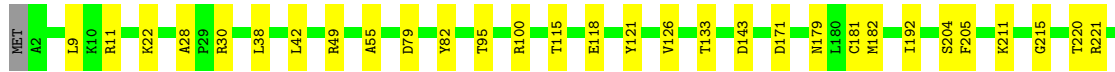
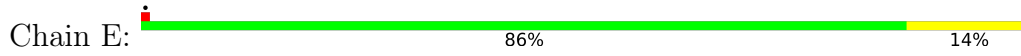


- Molecule 3: 40S ribosomal protein S2

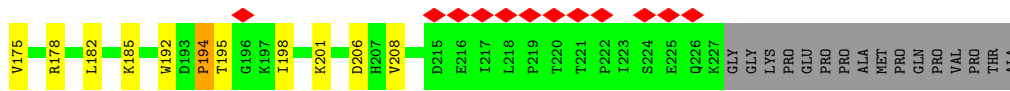
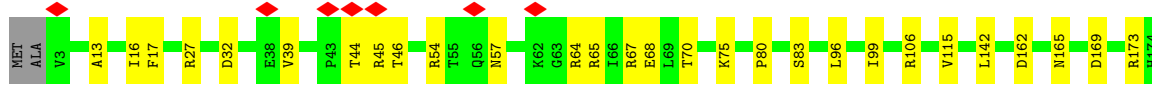
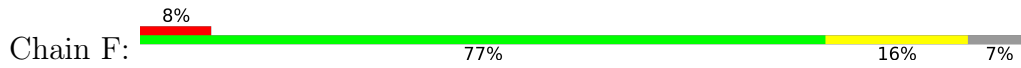




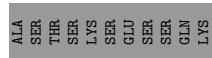
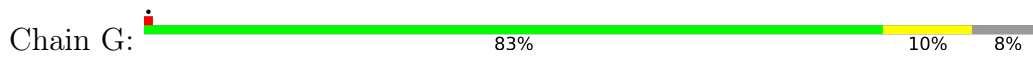
• Molecule 4: 40S ribosomal protein S4, X isoform



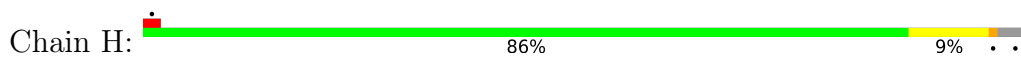
• Molecule 5: 40S ribosomal protein S3



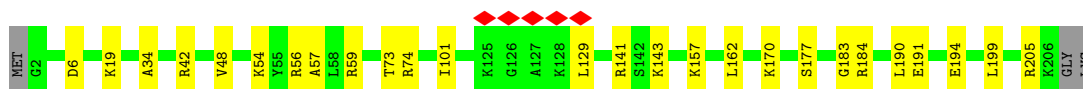
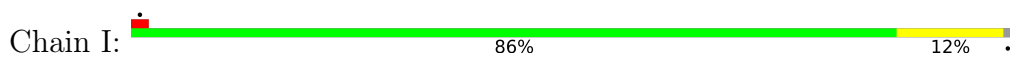
• Molecule 6: 40S ribosomal protein S6

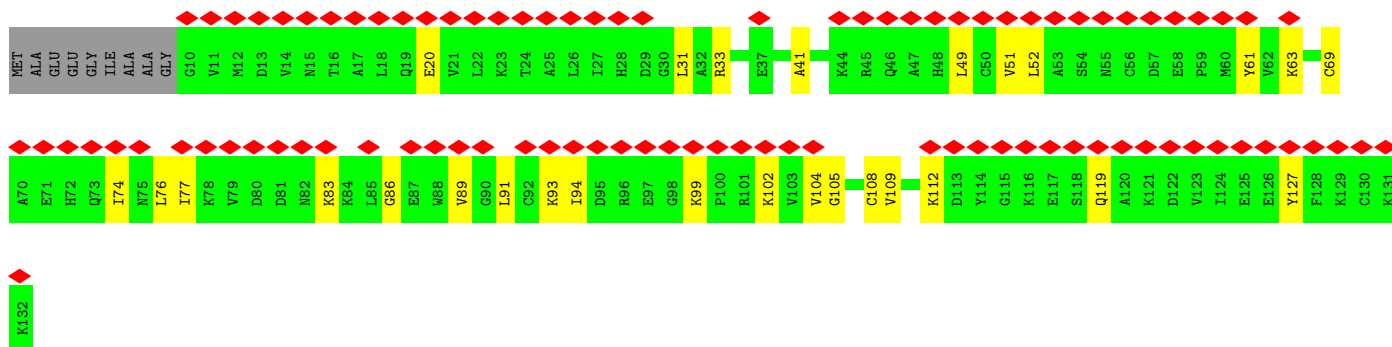


• Molecule 7: 40S ribosomal protein S7

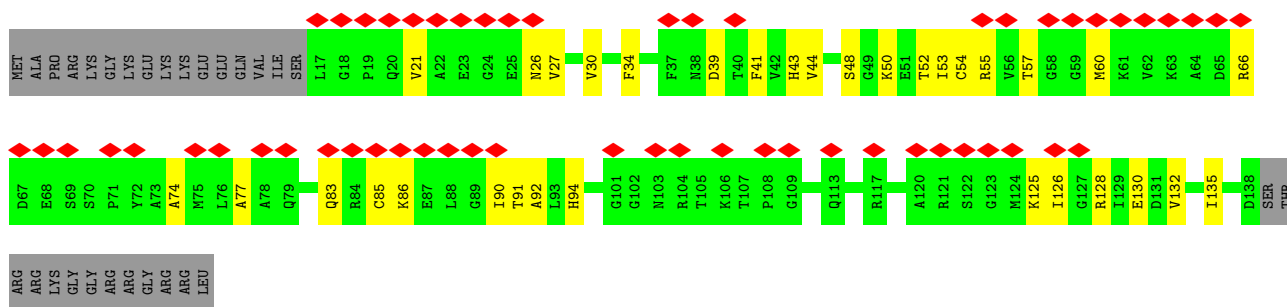


• Molecule 8: 40S ribosomal protein S8

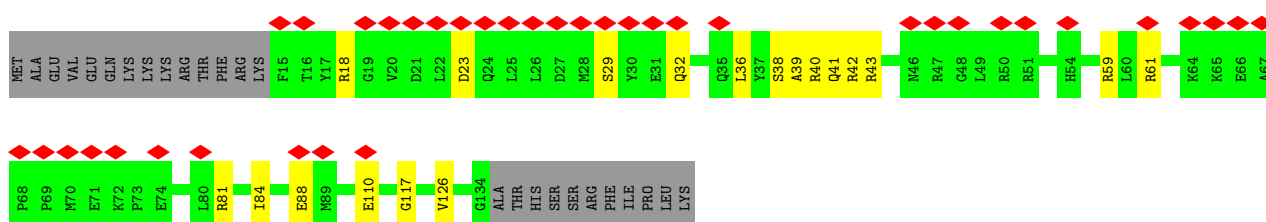




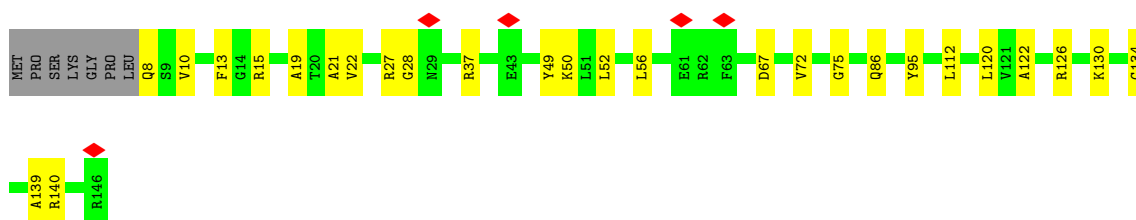
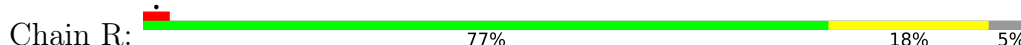
• Molecule 15: 40S ribosomal protein S14



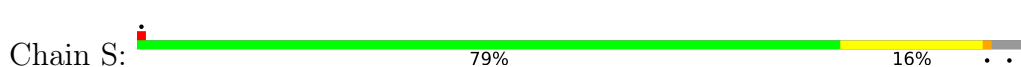
• Molecule 16: 40S ribosomal protein S15

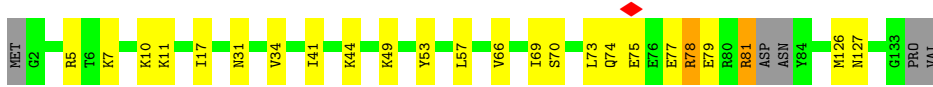


• Molecule 17: 40S ribosomal protein S16

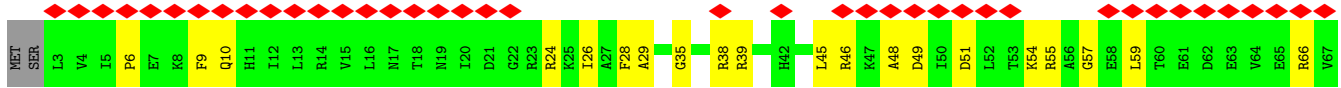
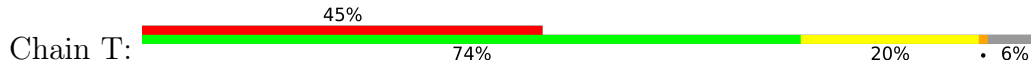


• Molecule 18: 40S ribosomal protein S17

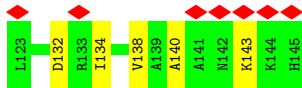
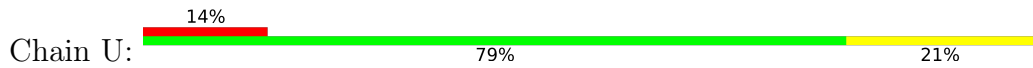




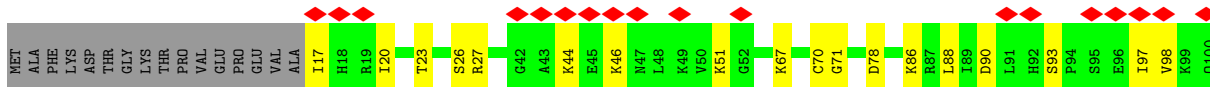
- Molecule 19: 40S ribosomal protein S18



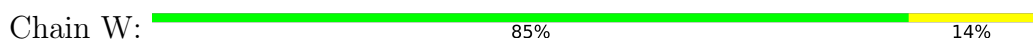
- Molecule 20: 40S ribosomal protein S19



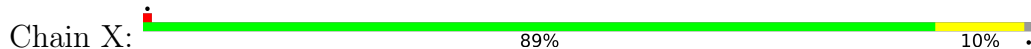
- Molecule 21: 40S ribosomal protein S20

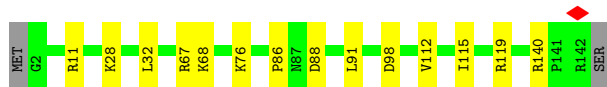


- Molecule 22: 40S ribosomal protein S15a

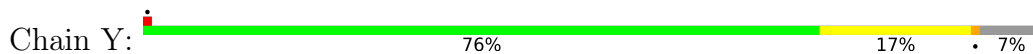


- Molecule 23: 40S ribosomal protein S23





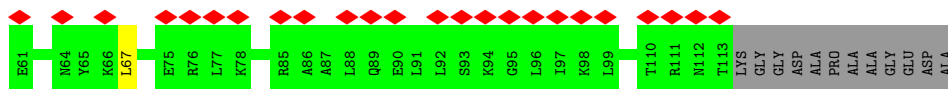
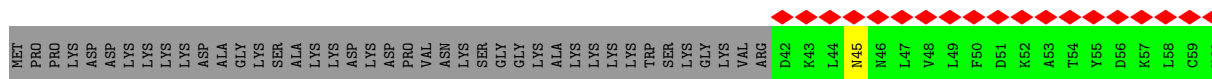
• Molecule 24: 40S ribosomal protein S24



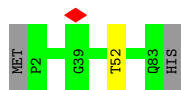
• Molecule 25: 40S ribosomal protein S21



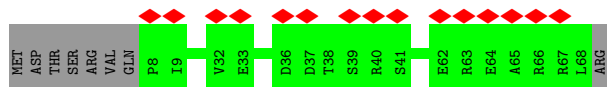
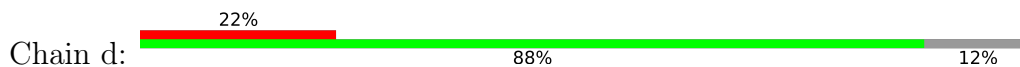
• Molecule 26: 40S ribosomal protein S25



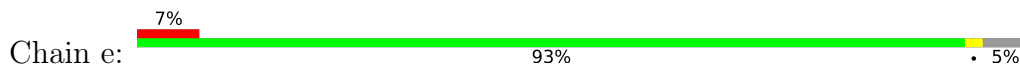
• Molecule 27: 40S ribosomal protein S27

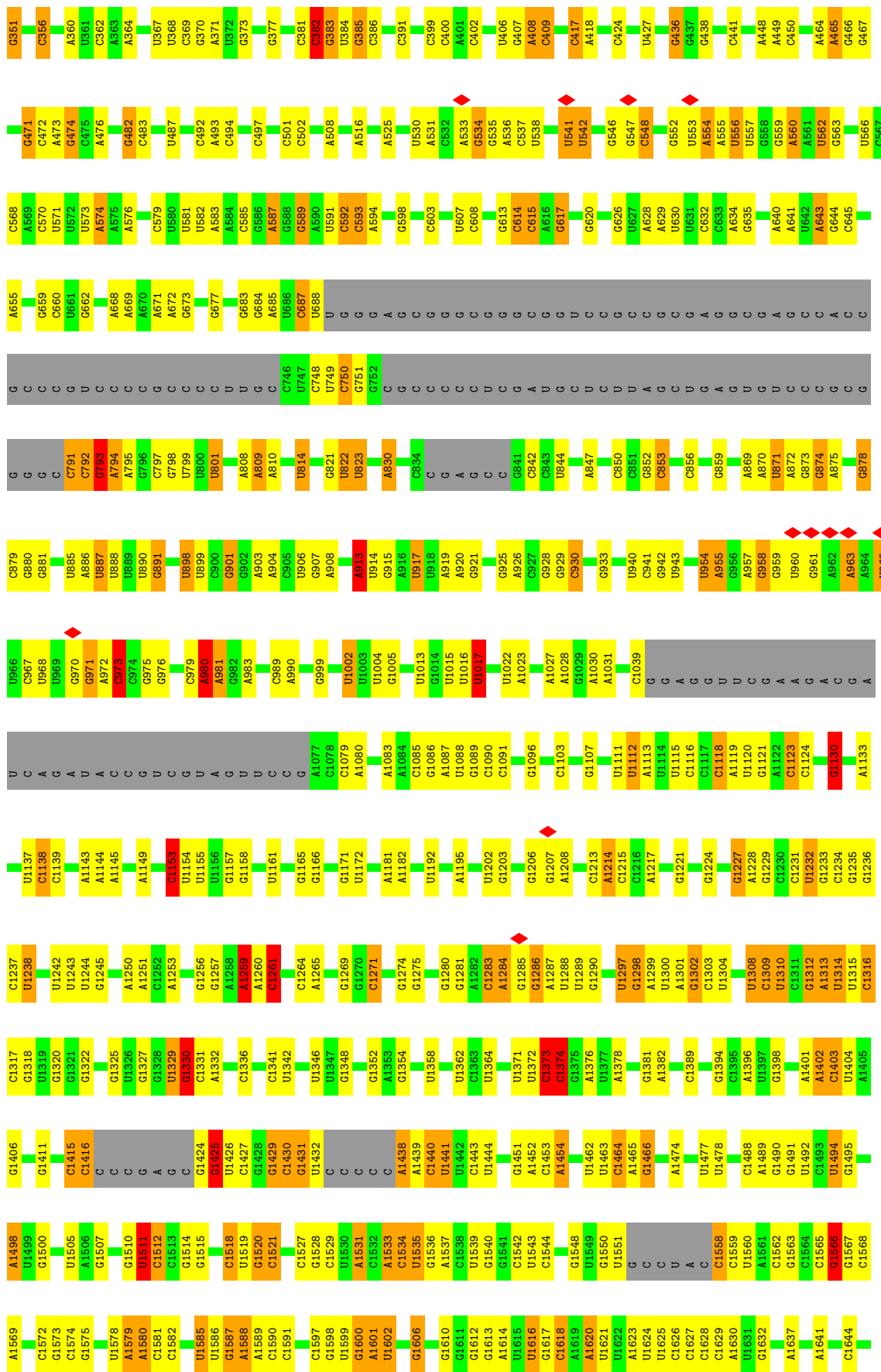


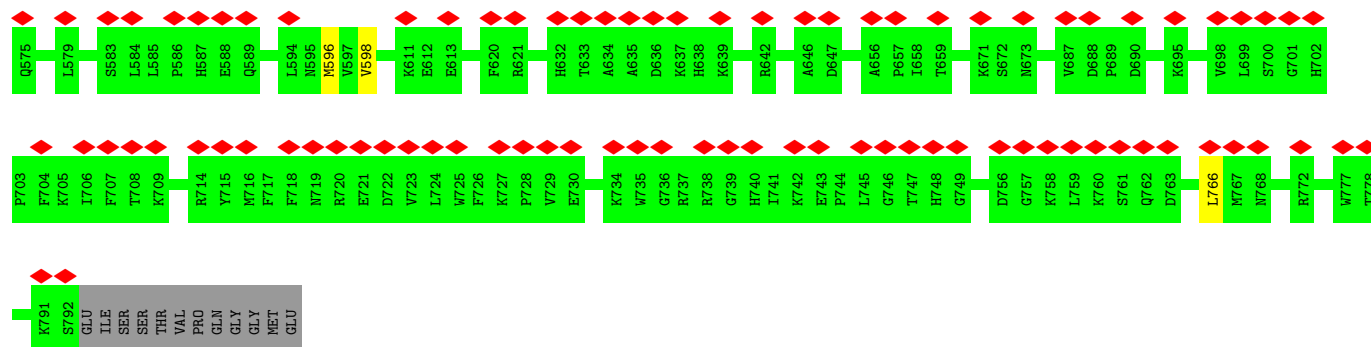
• Molecule 28: 40S ribosomal protein S28



• Molecule 29: 40S ribosomal protein S30







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	35506	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44.8	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	0.380	Depositor
Minimum map value	-0.094	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.038	Depositor
Map size (\AA)	381.24, 381.24, 381.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.059, 1.059, 1.059	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

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	B	0.54	0/1661	0.56	0/2259
2	C	0.31	0/1756	0.54	0/2350
3	D	0.53	0/1718	0.60	1/2322 (0.0%)
4	E	0.54	1/2118 (0.0%)	0.61	1/2849 (0.0%)
5	F	0.36	0/1776	0.58	0/2392
6	G	0.41	0/1885	0.52	0/2510
7	H	0.40	0/1524	0.56	0/2042
8	I	0.49	0/1711	0.55	0/2282
9	J	0.53	0/1524	0.61	1/2035 (0.0%)
10	K	0.31	0/1516	0.54	0/2037
11	L	0.55	0/1250	0.58	0/1673
12	M	0.33	0/824	0.55	0/1112
13	N	0.42	0/1226	0.51	0/1649
14	O	0.29	0/963	0.61	1/1291 (0.1%)
15	P	0.29	0/910	0.52	0/1228
16	Q	0.30	0/1003	0.52	0/1341
17	R	0.32	0/1126	0.55	0/1506
18	S	0.42	0/1063	0.59	0/1424
19	T	0.27	0/1202	0.58	1/1610 (0.1%)
20	U	0.28	0/1142	0.51	0/1530
21	V	0.33	0/813	0.54	0/1092
22	W	0.59	1/1051 (0.1%)	0.60	0/1406
23	X	0.52	0/1116	0.60	0/1490
24	Y	0.48	0/1031	0.60	1/1370 (0.1%)
25	Z	0.48	0/631	0.55	0/844
26	a	0.31	0/580	0.68	1/780 (0.1%)
27	b	0.43	0/653	0.59	0/876
28	d	0.27	0/481	0.53	0/643
29	e	0.41	0/434	0.62	0/571
30	f	0.36	0/466	0.57	0/618
31	g	0.30	0/485	0.55	0/650
32	j	0.29	0/2497	0.54	0/3399

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	2	0.92	3/37453 (0.0%)	1.22	341/58357 (0.6%)
34	i	0.43	0/244	0.45	0/328
35	u	0.30	0/5076	0.57	2/6860 (0.0%)
All	All	0.69	5/80909 (0.0%)	0.95	350/116726 (0.3%)

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
1	B	0	1
5	F	0	1
10	K	0	2
17	R	0	1
22	W	0	1
23	X	0	1
24	Y	0	1
29	e	0	1
All	All	0	9

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	W	93	LEU	C-N	-5.80	1.20	1.34
33	2	64	A	N9-C4	-5.22	1.34	1.37
33	2	501	C	N3-C4	-5.06	1.30	1.33
33	2	1139	C	N3-C4	-5.04	1.30	1.33
4	E	181	CYS	CB-SG	-5.03	1.73	1.81

The worst 5 of 350 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	2	501	C	N1-C2-O2	15.41	128.15	118.90
33	2	501	C	C2-N1-C1'	13.55	133.70	118.80
33	2	501	C	N3-C2-O2	-12.90	112.87	121.90
33	2	293	C	N1-C2-O2	12.39	126.33	118.90
33	2	356	C	N1-C2-O2	11.60	125.86	118.90

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	188	THR	Peptide
5	F	194	PRO	Peptide
10	K	165	ASN	Peptide
10	K	40	ALA	Peptide
17	R	15	ARG	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1624	0	1634	20	0
2	C	1729	0	1803	32	0
3	D	1682	0	1769	23	0
4	E	2076	0	2177	21	0
5	F	1748	0	1844	26	0
6	G	1862	0	2018	20	0
7	H	1501	0	1593	14	0
8	I	1682	0	1769	19	0
9	J	1499	0	1618	11	0
10	K	1495	0	1549	26	0
11	L	1229	0	1302	12	0
12	M	800	0	818	14	0
13	N	1202	0	1289	14	0
14	O	953	0	990	15	0
15	P	897	0	907	26	0
16	Q	984	0	1028	14	0
17	R	1109	0	1174	19	0
18	S	1050	0	1105	19	0
19	T	1184	0	1244	19	0
20	U	1122	0	1153	23	0
21	V	803	0	873	14	0
22	W	1034	0	1080	11	0
23	X	1098	0	1167	9	0
24	Y	1014	0	1082	14	0
25	Z	625	0	628	4	0
26	a	574	0	627	0	0
27	b	640	0	665	0	0
28	d	479	0	507	0	0
29	e	430	0	464	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	f	455	0	446	0	0
31	g	477	0	439	0	0
32	j	2440	0	2396	0	0
33	2	33498	0	16915	218	0
34	i	239	0	211	0	0
35	u	4954	0	5014	0	0
36	f	1	0	0	0	0
36	g	1	0	0	0	0
All	All	76190	0	61298	547	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 5.

The worst 5 of 547 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)
18:S:66:VAL:N	18:S:74:GLN:OE1	1.82	1.11
33:2:1206:G:H1	33:2:1692:U:H3	1.04	0.93
33:2:531:A:H2	33:2:552:G:H1	1.21	0.86
33:2:1656:G:H1	33:2:1668:U:H3	1.26	0.83
33:2:197:U:H3	33:2:202:G:H1	1.25	0.80

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
1	B	204/295 (69%)	193 (95%)	11 (5%)	0	100 100
2	C	211/264 (80%)	200 (95%)	11 (5%)	0	100 100
3	D	216/293 (74%)	205 (95%)	11 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	260/263 (99%)	250 (96%)	10 (4%)	0	100	100
5	F	223/243 (92%)	212 (95%)	10 (4%)	1 (0%)	34	72
6	G	228/249 (92%)	218 (96%)	10 (4%)	0	100	100
7	H	184/194 (95%)	175 (95%)	9 (5%)	0	100	100
8	I	203/208 (98%)	198 (98%)	5 (2%)	0	100	100
9	J	178/194 (92%)	167 (94%)	10 (6%)	1 (1%)	25	64
10	K	187/204 (92%)	170 (91%)	14 (8%)	3 (2%)	9	40
11	L	149/158 (94%)	141 (95%)	8 (5%)	0	100	100
12	M	93/165 (56%)	86 (92%)	7 (8%)	0	100	100
13	N	147/151 (97%)	138 (94%)	9 (6%)	0	100	100
14	O	121/132 (92%)	114 (94%)	7 (6%)	0	100	100
15	P	120/151 (80%)	116 (97%)	4 (3%)	0	100	100
16	Q	118/145 (81%)	114 (97%)	4 (3%)	0	100	100
17	R	137/146 (94%)	132 (96%)	5 (4%)	0	100	100
18	S	126/135 (93%)	117 (93%)	9 (7%)	0	100	100
19	T	141/152 (93%)	132 (94%)	9 (6%)	0	100	100
20	U	142/145 (98%)	139 (98%)	3 (2%)	0	100	100
21	V	99/119 (83%)	96 (97%)	3 (3%)	0	100	100
22	W	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
23	X	139/143 (97%)	135 (97%)	3 (2%)	1 (1%)	22	60
24	Y	122/133 (92%)	114 (93%)	7 (6%)	1 (1%)	19	57
25	Z	80/83 (96%)	78 (98%)	2 (2%)	0	100	100
26	a	70/125 (56%)	67 (96%)	3 (4%)	0	100	100
27	b	80/84 (95%)	74 (92%)	5 (6%)	1 (1%)	12	45
28	d	59/69 (86%)	56 (95%)	3 (5%)	0	100	100
29	e	54/59 (92%)	48 (89%)	6 (11%)	0	100	100
30	f	52/56 (93%)	47 (90%)	4 (8%)	1 (2%)	8	36
31	g	62/156 (40%)	55 (89%)	7 (11%)	0	100	100
32	j	312/317 (98%)	292 (94%)	20 (6%)	0	100	100
34	i	27/180 (15%)	24 (89%)	3 (11%)	0	100	100
35	u	607/804 (76%)	569 (94%)	37 (6%)	1 (0%)	47	82

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5278/6345 (83%)	4996 (95%)	272 (5%)	10 (0%)	50	82

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	K	166	ILE
9	J	161	LEU
5	F	192	TRP
27	b	52	THR
30	f	14	PHE

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	
1	B	172/243 (71%)	169 (98%)	3 (2%)	60	85
2	C	194/231 (84%)	193 (100%)	1 (0%)	88	96
3	D	182/225 (81%)	182 (100%)	0	100	100
4	E	224/225 (100%)	223 (100%)	1 (0%)	91	97
5	F	188/202 (93%)	187 (100%)	1 (0%)	88	96
6	G	200/218 (92%)	199 (100%)	1 (0%)	88	96
7	H	167/174 (96%)	165 (99%)	2 (1%)	71	90
8	I	178/180 (99%)	177 (99%)	1 (1%)	86	95
9	J	160/168 (95%)	160 (100%)	0	100	100
10	K	159/170 (94%)	159 (100%)	0	100	100
11	L	135/142 (95%)	134 (99%)	1 (1%)	84	94
12	M	86/136 (63%)	86 (100%)	0	100	100
13	N	130/131 (99%)	130 (100%)	0	100	100
14	O	104/108 (96%)	102 (98%)	2 (2%)	57	84
15	P	94/119 (79%)	94 (100%)	0	100	100
16	Q	107/130 (82%)	107 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	R	115/121 (95%)	115 (100%)	0	100	100
18	S	116/122 (95%)	111 (96%)	5 (4%)	29	66
19	T	124/132 (94%)	123 (99%)	1 (1%)	81	93
20	U	114/115 (99%)	114 (100%)	0	100	100
21	V	93/107 (87%)	93 (100%)	0	100	100
22	W	112/113 (99%)	112 (100%)	0	100	100
23	X	113/115 (98%)	113 (100%)	0	100	100
24	Y	108/115 (94%)	107 (99%)	1 (1%)	78	92
25	Z	66/67 (98%)	66 (100%)	0	100	100
26	a	64/103 (62%)	63 (98%)	1 (2%)	62	86
27	b	74/76 (97%)	74 (100%)	0	100	100
28	d	54/62 (87%)	54 (100%)	0	100	100
29	e	42/48 (88%)	42 (100%)	0	100	100
30	f	48/49 (98%)	48 (100%)	0	100	100
31	g	46/140 (33%)	45 (98%)	1 (2%)	52	81
32	j	272/275 (99%)	272 (100%)	0	100	100
34	i	26/151 (17%)	26 (100%)	0	100	100
35	u	539/705 (76%)	535 (99%)	4 (1%)	84	94
All	All	4606/5418 (85%)	4580 (99%)	26 (1%)	86	95

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	S	75	GLU
18	S	81	ARG
35	u	596	MET
18	S	79	GLU
19	T	92	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
30	f	45	GLN
35	u	63	GLN
31	g	135	HIS

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Mol	Chain	Res	Type
34	i	158	GLN
35	u	180	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
33	2	1558/1868 (83%)	423 (27%)	41 (2%)

5 of 423 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
33	2	3	C
33	2	17	C
33	2	26	U
33	2	33	G
33	2	41	G

5 of 41 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
33	2	1430	C
33	2	1534	C
33	2	1431	G
33	2	1464	C
33	2	1585	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
33	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1200:A	O3'	1201:U	P	3.10

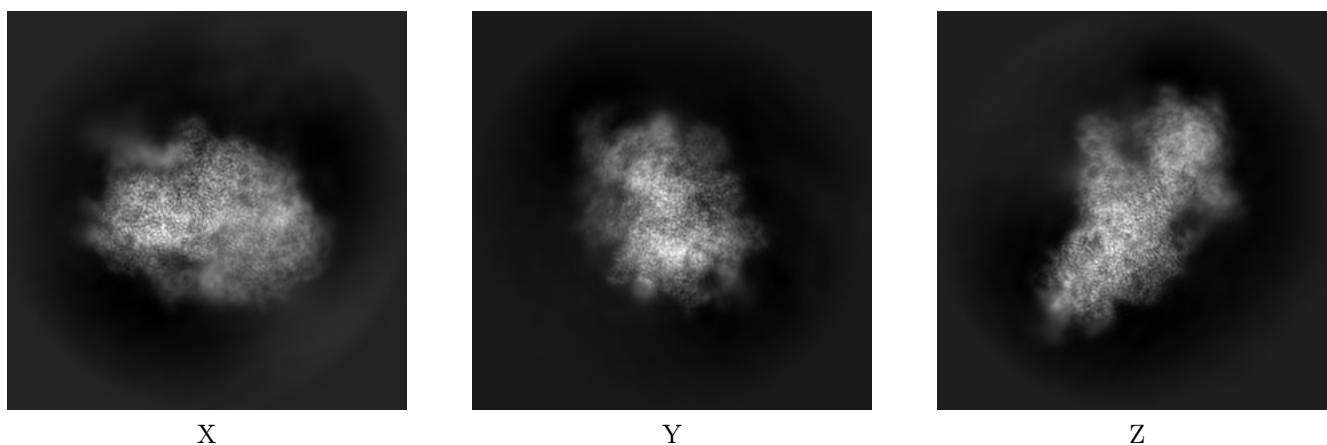
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11301. 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](#)

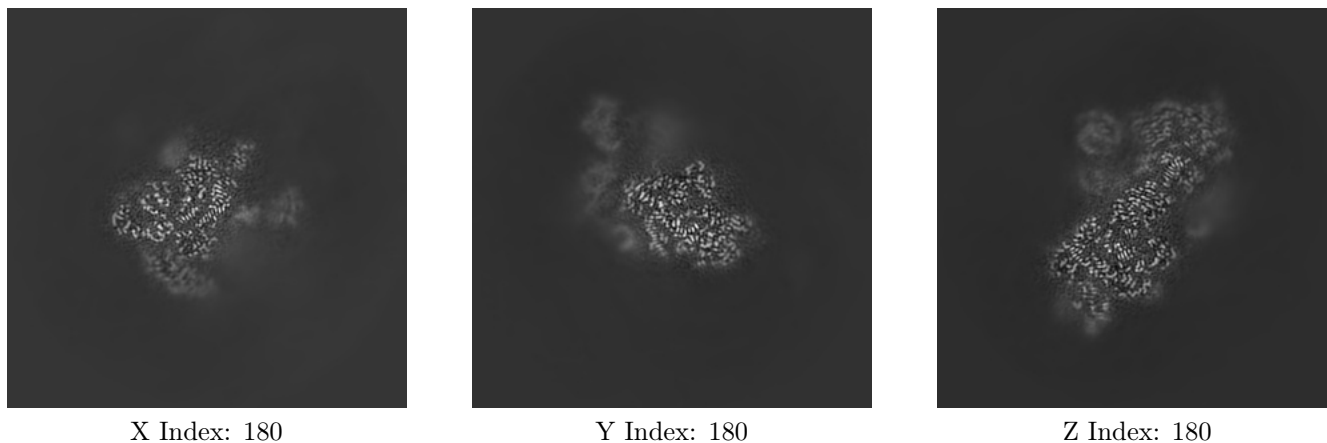
6.1.1 Primary map



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

6.2 Central slices [i](#)

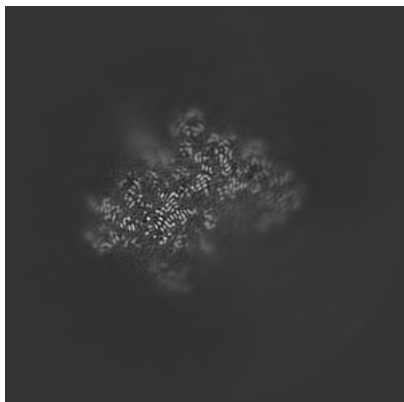
6.2.1 Primary map



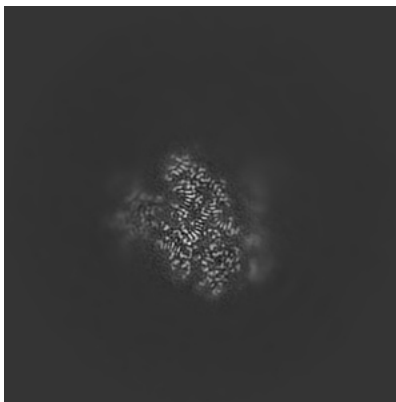
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

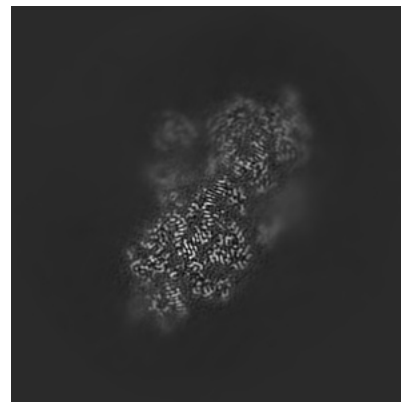
6.3.1 Primary map



X Index: 151



Y Index: 140

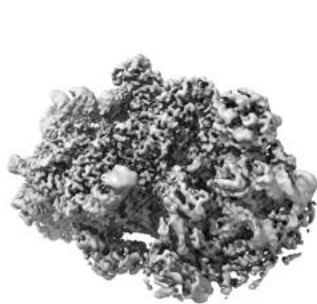


Z Index: 175

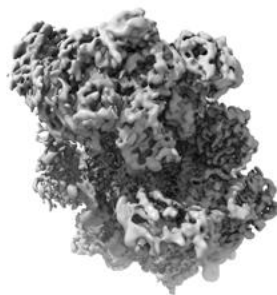
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

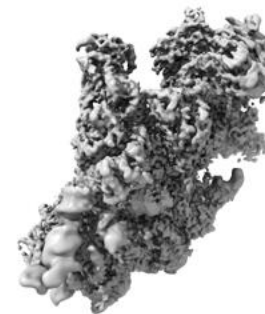
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.038. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

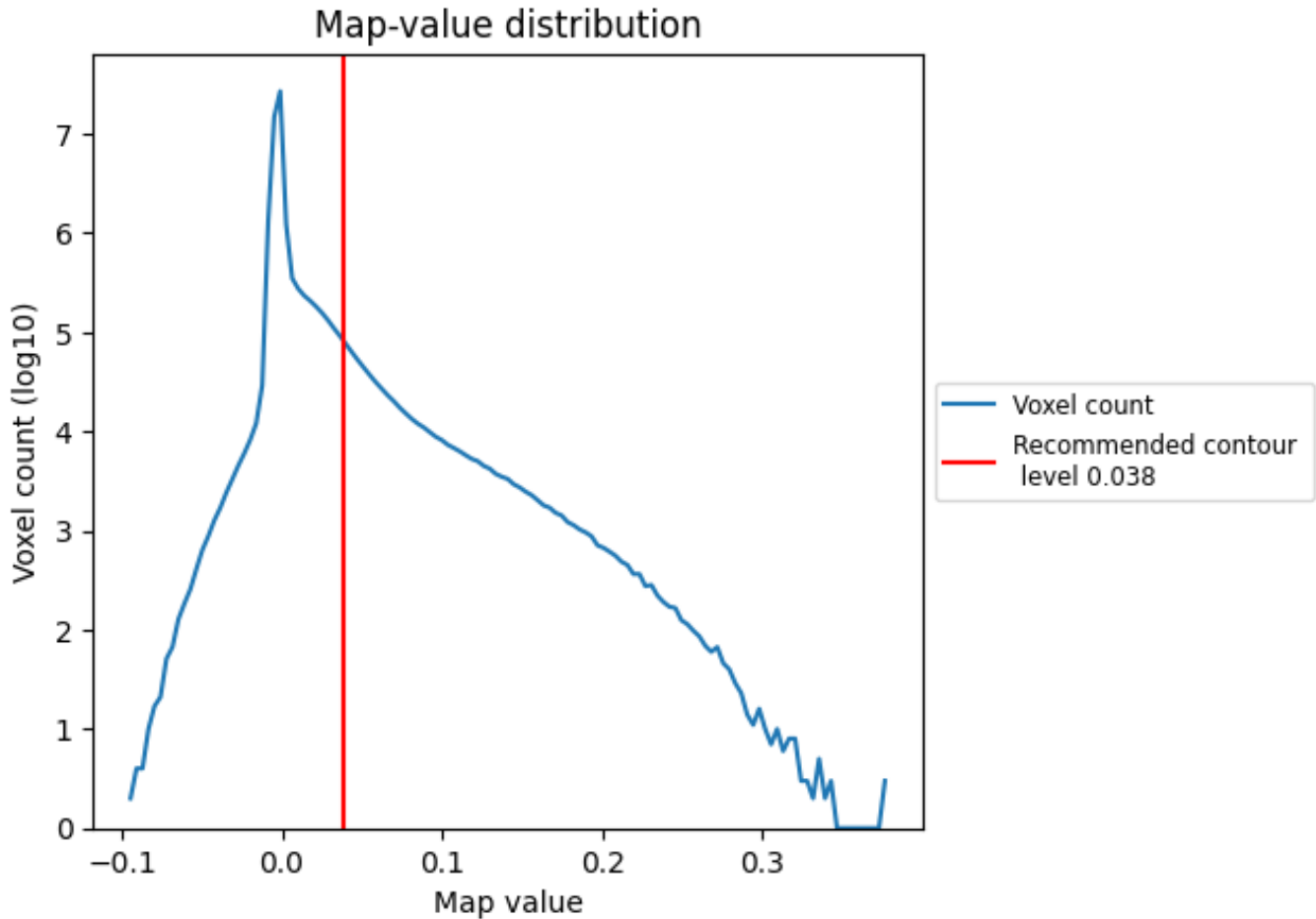
6.5 Mask visualisation

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

7 Map analysis [i](#)

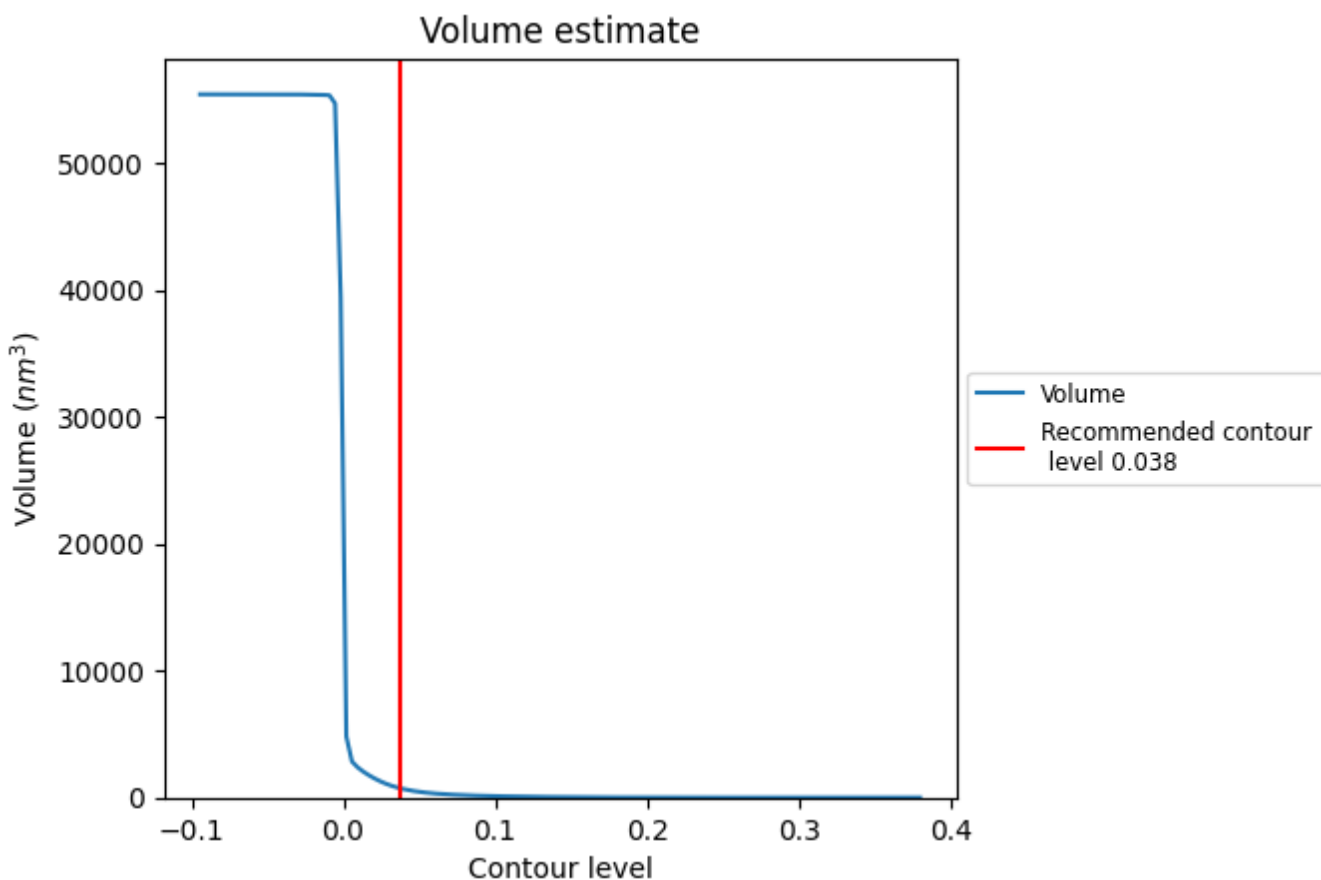
This section contains the results of statistical analysis of the map.

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.

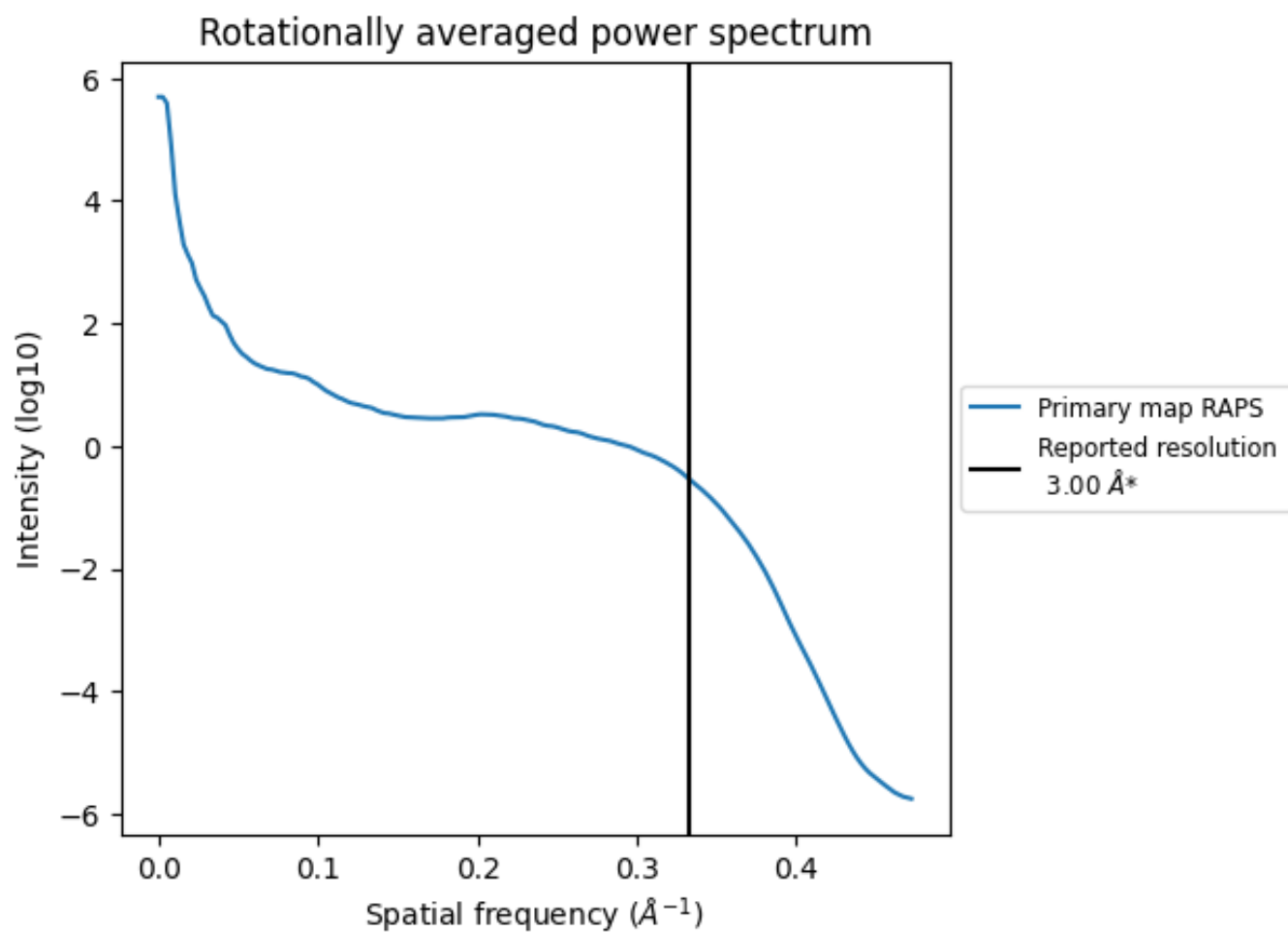
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 718 nm³; this corresponds to an approximate mass of 649 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](#)

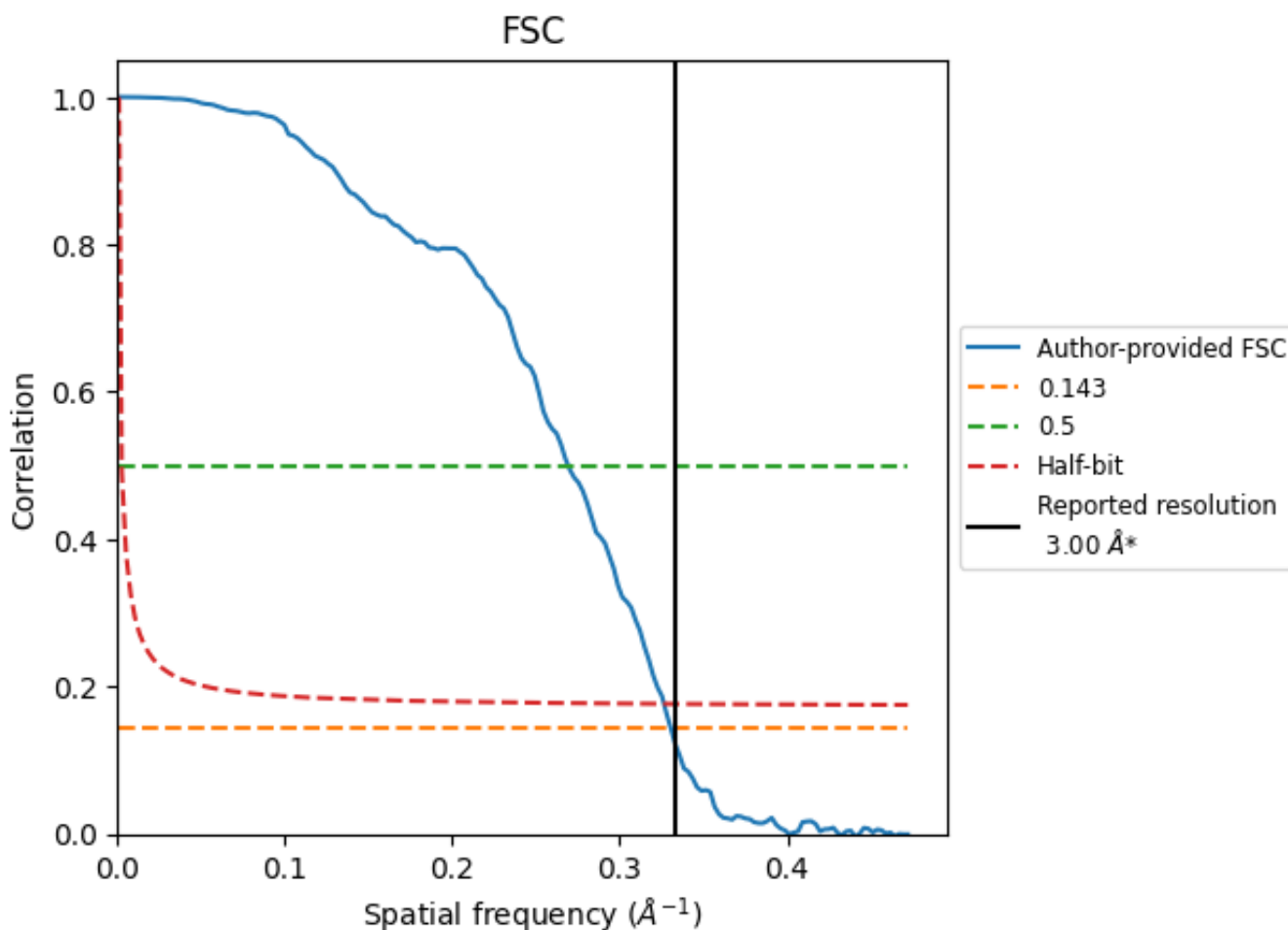


*Reported resolution corresponds to spatial frequency of 0.333 \AA^{-1}

8 Fourier-Shell correlation [\(i\)](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [\(i\)](#)



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

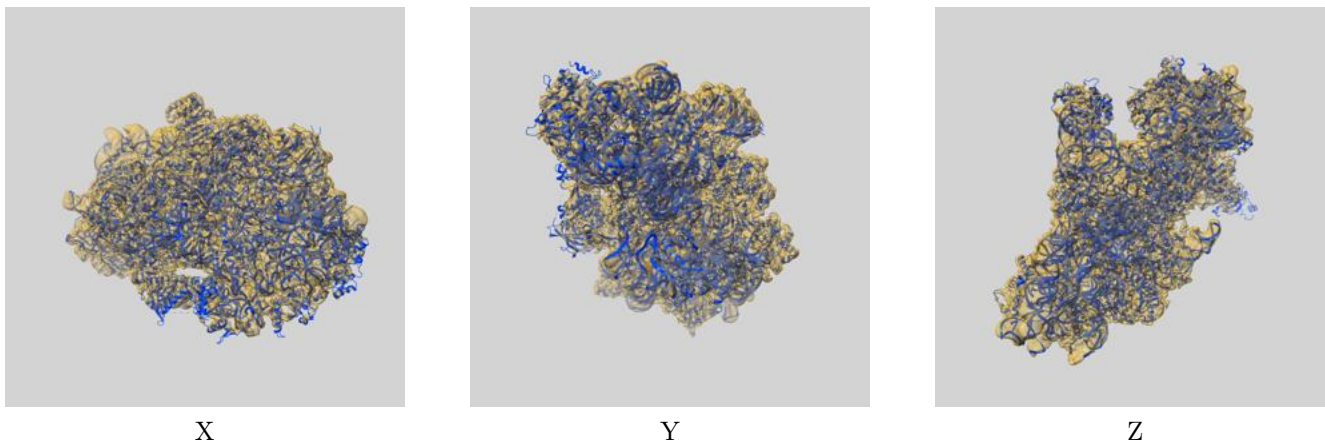
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.03	3.71	3.06
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

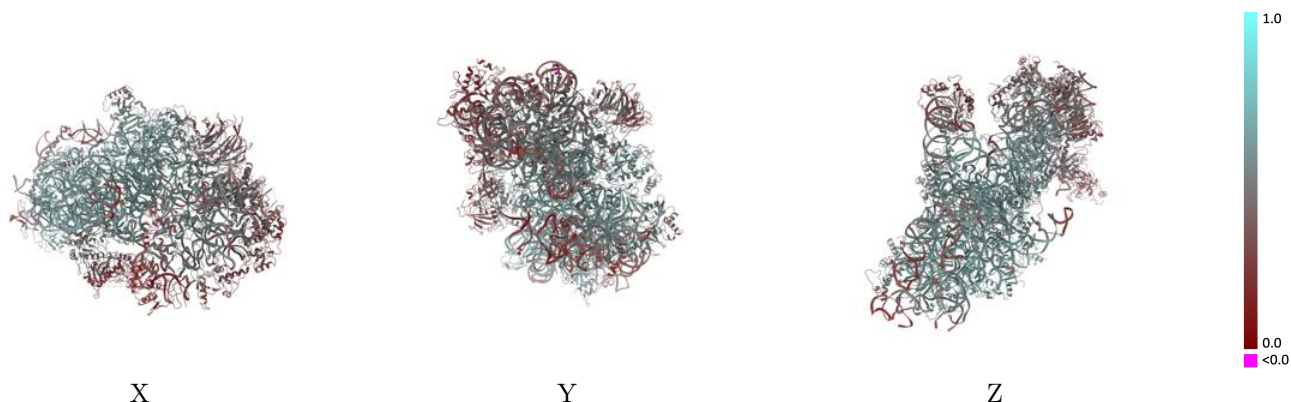
This section contains information regarding the fit between EMDB map EMD-11301 and PDB model 6ZMT. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



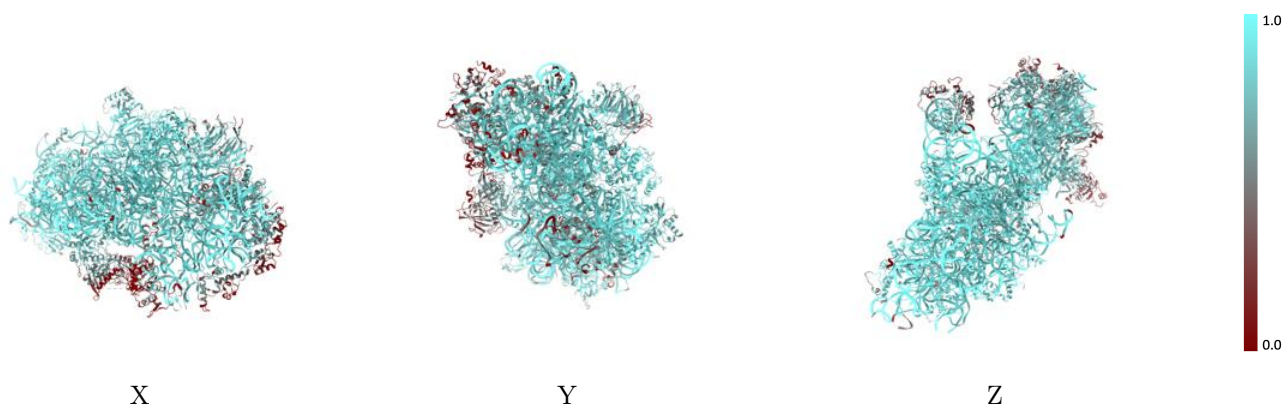
The images above show the 3D surface view of the map at the recommended contour level 0.038 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



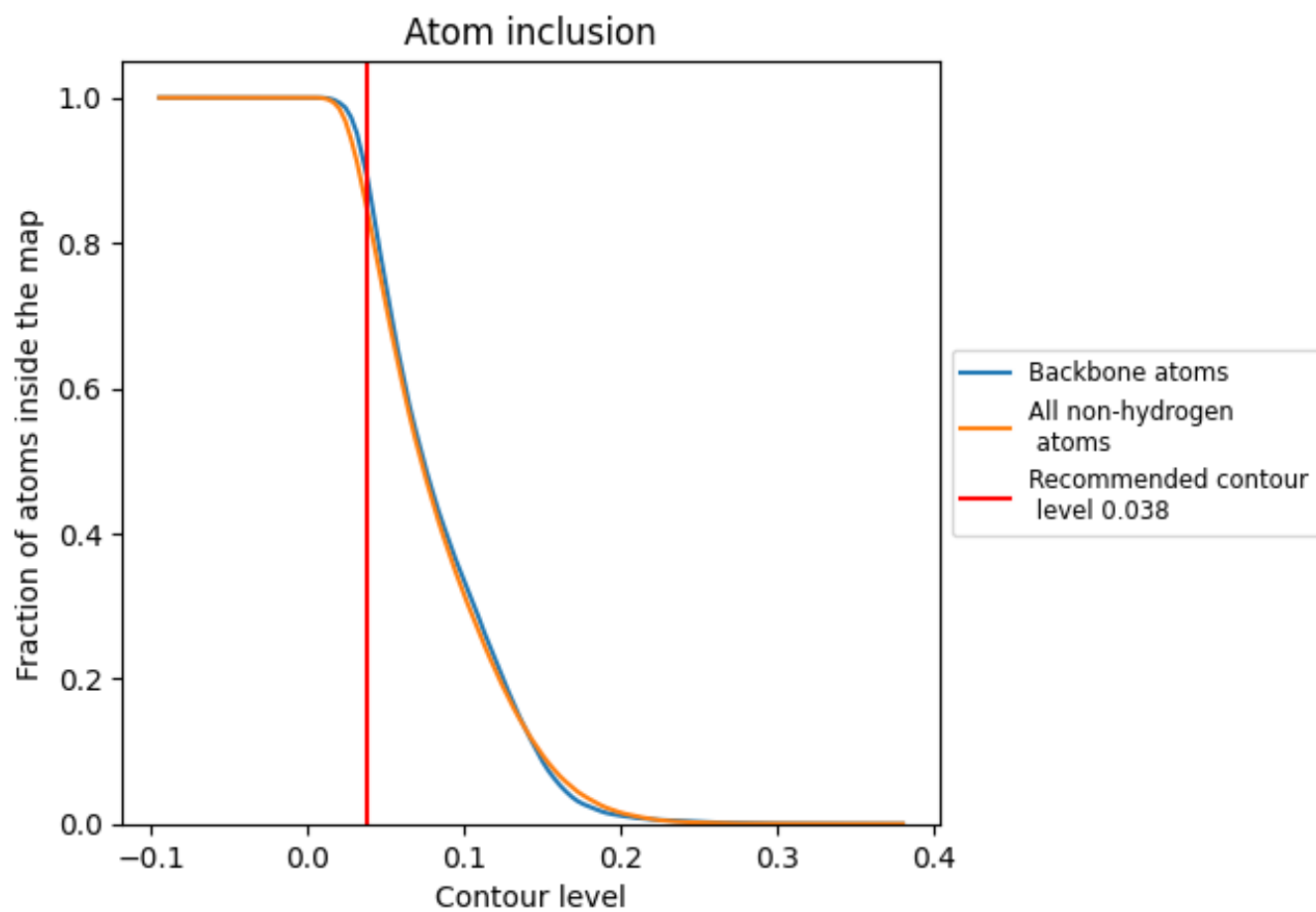
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.038).









































































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 85% 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 (0.038) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8470	 0.4890
2	 0.9591	 0.5170
B	 0.9615	 0.5790
C	 0.6398	 0.3920
D	 0.9648	 0.5980
E	 0.9570	 0.6030
F	 0.8029	 0.4600
G	 0.8939	 0.5250
H	 0.8499	 0.4860
I	 0.9026	 0.5490
J	 0.9618	 0.5990
K	 0.7146	 0.4200
L	 0.9154	 0.5880
M	 0.6795	 0.3540
N	 0.9220	 0.5390
O	 0.1970	 0.2250
P	 0.4398	 0.3160
Q	 0.5430	 0.3680
R	 0.8211	 0.4660
S	 0.8814	 0.5250
T	 0.4486	 0.3320
U	 0.6703	 0.3880
V	 0.6816	 0.4250
W	 0.9822	 0.6230
X	 0.9627	 0.5920
Y	 0.9563	 0.5910
Z	 0.9394	 0.5870
a	 0.3636	 0.3070
b	 0.8933	 0.5420
d	 0.6247	 0.3960
e	 0.8867	 0.5280
f	 0.9361	 0.5200
g	 0.4528	 0.2200
i	 0.9227	 0.5820
j	 0.7102	 0.3800
u	 0.4907	 0.3530

