



wwPDB EM Validation Summary Report ⓘ

Dec 10, 2022 – 08:20 pm GMT

PDB ID : 6QUL
EMDB ID : EMD-4638
Title : Structure of a bacterial 50S ribosomal subunit in complex with the novel quinoxolidinone antibiotic cadazolid
Authors : Scaiola, A.; Leibundgut, M.; Boehringer, D.; Ritz, D.
Deposited on : 2019-02-27
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:

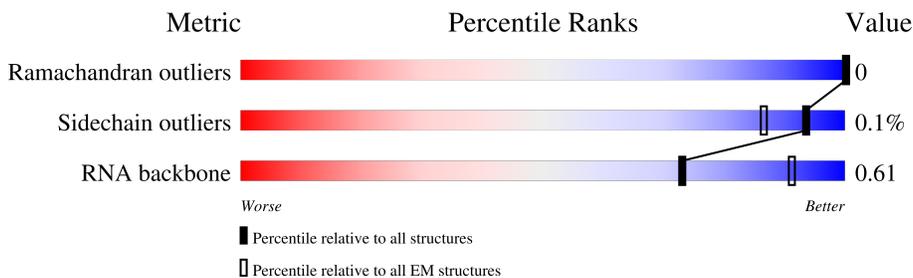
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 3.00 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)
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	1	4	
2	A	2795	
3	B	120	
4	C	273	
5	D	209	
6	E	201	
7	F	179	
8	G	177	

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Mol	Chain	Length	Quality of chain
9	H	149	
10	K	142	
11	L	123	
12	M	144	
13	N	136	
14	O	127	
15	P	117	
16	Q	115	
17	R	118	
18	S	103	
19	T	110	
20	U	100	
21	V	104	
22	W	94	
23	X	85	
24	Y	78	
25	Z	63	
26	a	59	
27	b	57	
28	c	55	
29	d	46	
30	e	65	
31	f	38	

2 Entry composition [i](#)

There are 36 unique types of molecules in this entry. The entry contains 87635 atoms, of which 28 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 P-site fMet-tRNA(fMet).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	4	84	38	16	26	4	0	0

- Molecule 2 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	A	2795	60085	26803	11076	19408	2798	3	0

- Molecule 3 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	B	120	2569	1144	468	837	120	0	0

- Molecule 4 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	271	2082	1288	423	364	7	0	0

- Molecule 5 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	D	209	1564	979	288	293	4	0	0

- Molecule 6 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	E	201	1551	974	283	289	5	0	0

- Molecule 7 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	F	177	1410	899	249	256	6	0	0

- Molecule 8 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	G	176	1322	832	243	245	2	0	0

- Molecule 9 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	H	50	384	247	68	68	1	0	0

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	K	142	1128	714	212	198	4	0	0

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	L	123	946	593	181	166	6	0	0

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	M	144	1052	654	207	189	2	0	0

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	N	136	1073	686	205	176	6	0	0

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	125	Total	C	N	O	S	0	0
			993	613	202	173	5		

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	117	Total	C	N	O	S	0	0
			899	557	179	162	1		

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	114	Total	C	N	O	S	0	0
			916	574	179	162	1		

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	R	117	Total	C	N	O	0	0
			946	604	192	150		

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	103	Total	C	N	O	S	0	0
			815	516	153	144	2		

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	110	Total	C	N	O	S	0	0
			856	532	166	155	3		

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	95	Total	C	N	O	S	0	0
			756	479	141	135	1		

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	V	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	94	Total	C	N	O	S	0	0
			752	479	137	133	3		

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	76	Total	C	N	O	S	0	0
			579	359	117	102	1		

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	77	Total	C	N	O	S	0	0
			624	388	129	105	2		

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	62	Total	C	N	O	S	0	0
			500	308	98	93	1		

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	58	Total	C	N	O	S	0	0
			448	281	87	78	2		

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	56	Total	C	N	O	S	0	0
			443	269	94	79	1		

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
28	c	51	414	266	76	72	0	0

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	d	46	376	228	90	56	2	0	0

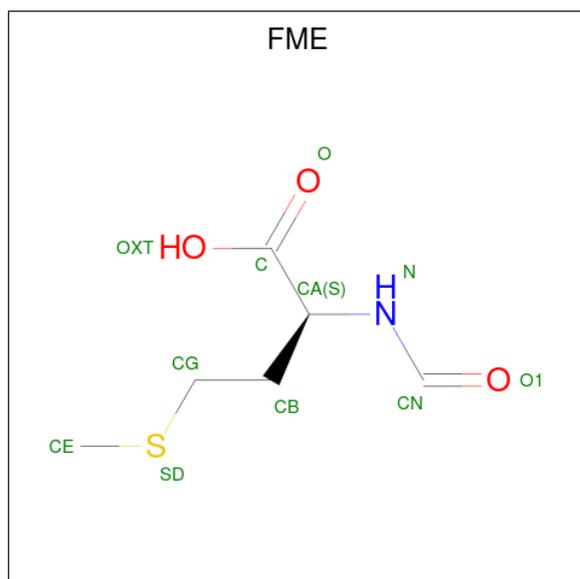
- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	e	64	503	323	105	73	2	0	0

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	f	38	301	185	65	47	4	0	0

- Molecule 32 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C₆H₁₁NO₃S).

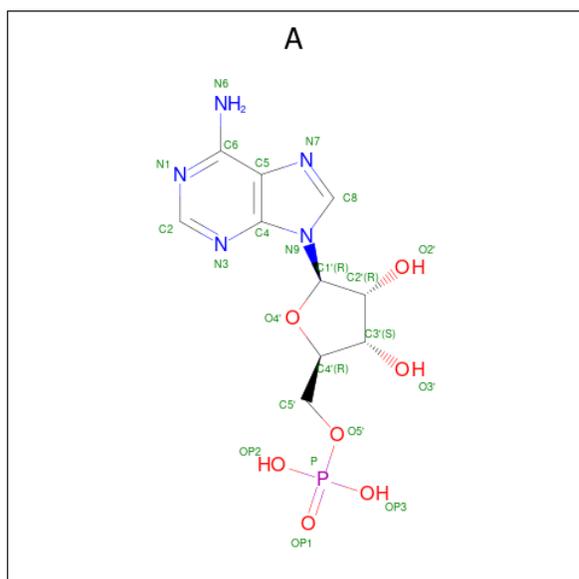


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
32	1	1	10	6	1	2	1	0

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
33	1	1	Total	Mg	0
			1	1	
33	A	369	Total	Mg	0
			369	369	
33	B	8	Total	Mg	0
			8	8	
33	C	1	Total	Mg	0
			1	1	
33	O	1	Total	Mg	0
			1	1	
33	R	1	Total	Mg	0
			1	1	
33	b	1	Total	Mg	0
			1	1	

- Molecule 34 is ADENOSINE-5'-MONOPHOSPHATE (three-letter code: A) (formula: C₁₀H₁₄N₅O₇P).



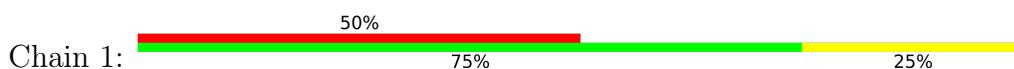
Mol	Chain	Residues	Atoms					AltConf
34	A	1	Total	C	N	O	P	0
			22	10	5	6	1	

- Molecule 35 is cadazolid (three-letter code: JJH) (formula: C₂₉H₂₉F₂N₃O₈) (labeled as "Ligand of Interest" by depositor).

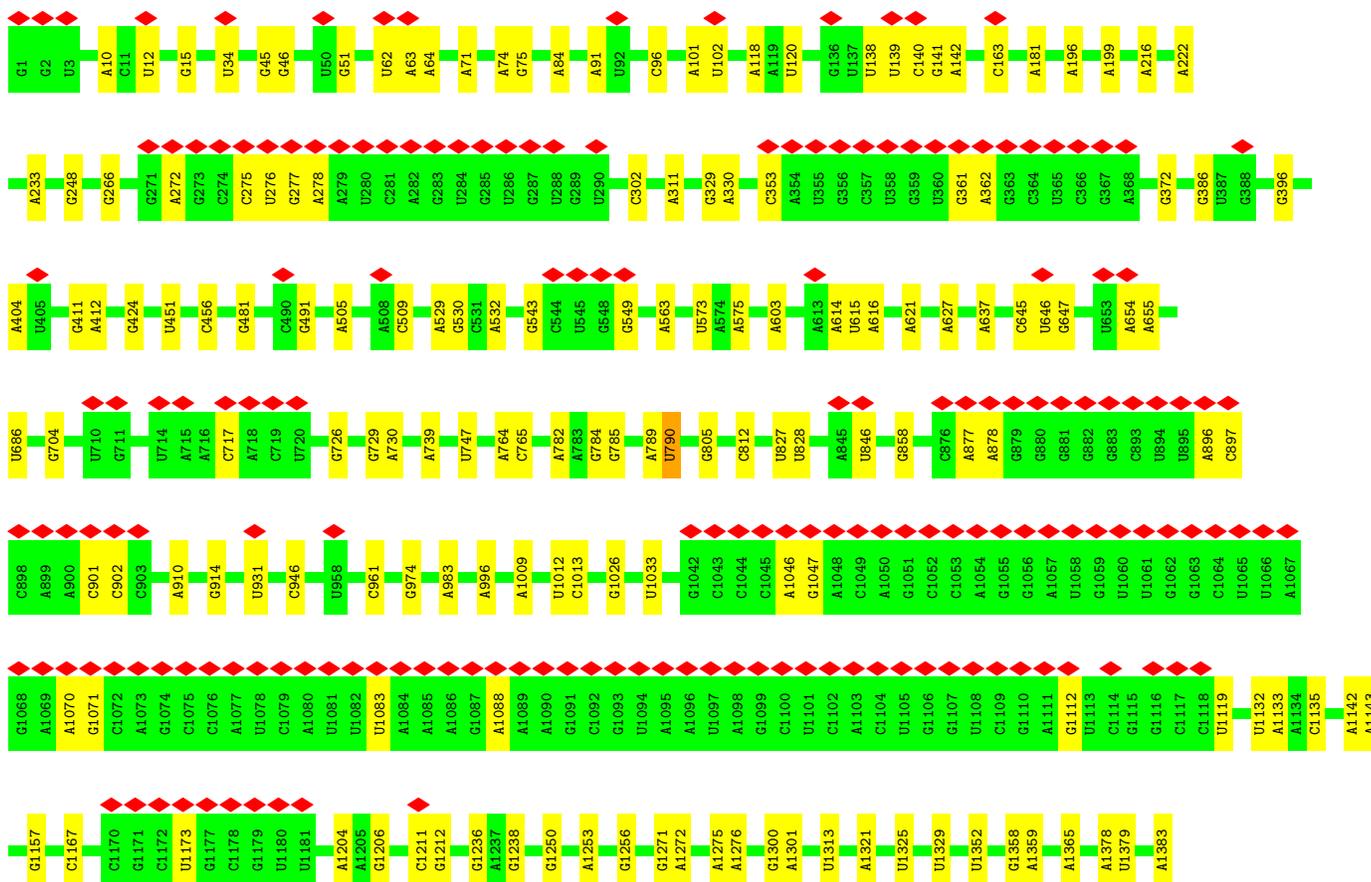
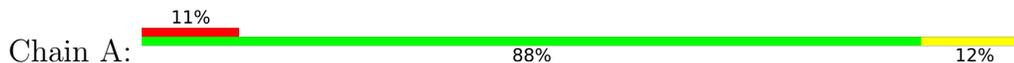
3 Residue-property plots

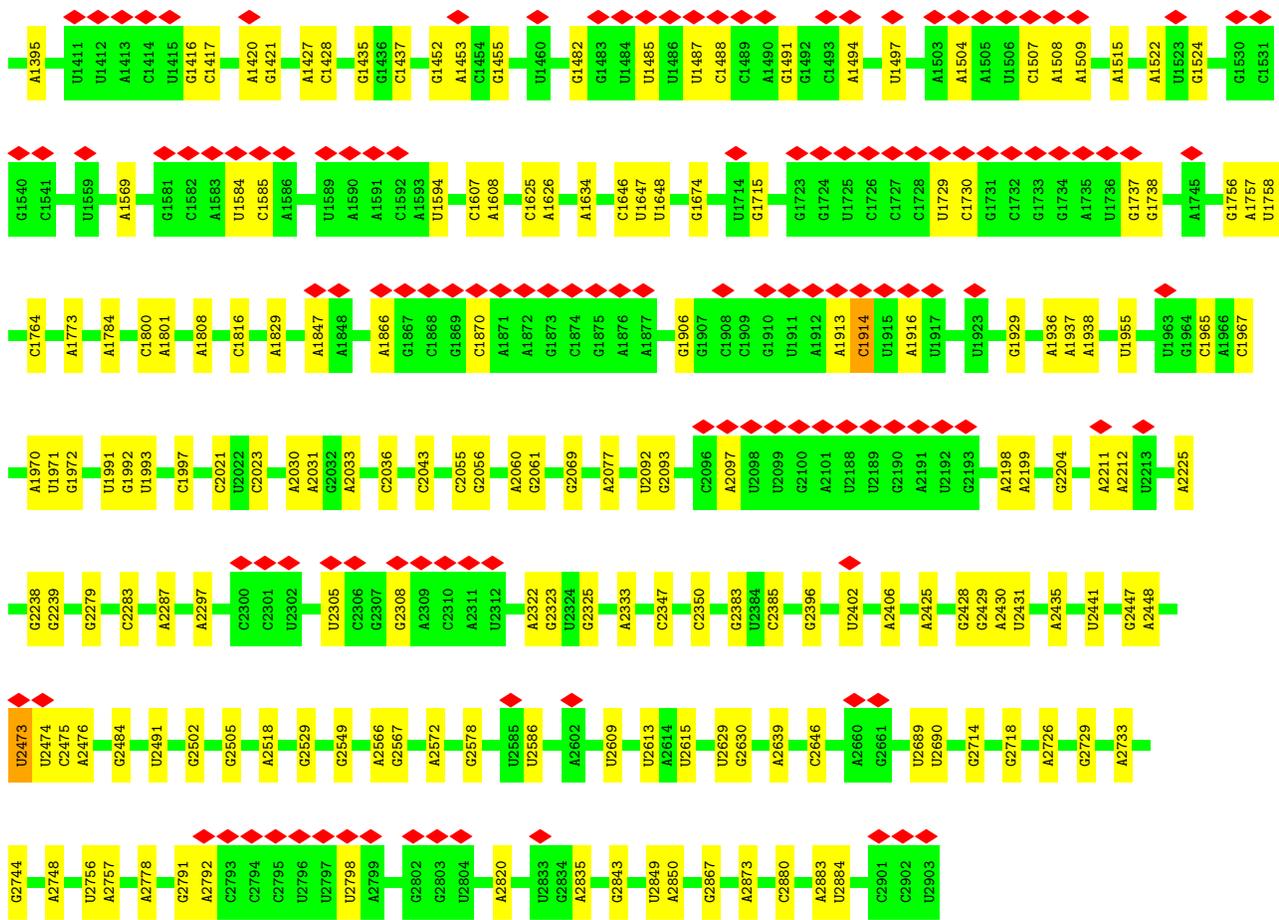
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: P-site fMet-tRNA(fMet)

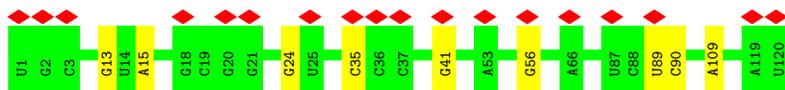
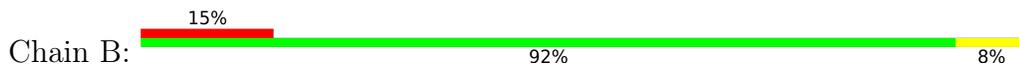


- Molecule 2: 23S rRNA





• Molecule 3: 5S rRNA



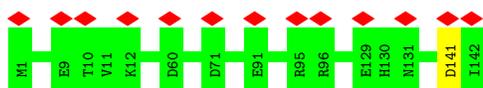
• Molecule 4: 50S ribosomal protein L2



• Molecule 5: 50S ribosomal protein L3



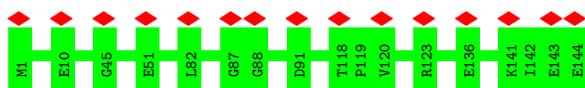
• Molecule 6: 50S ribosomal protein L4



- Molecule 11: 50S ribosomal protein L14



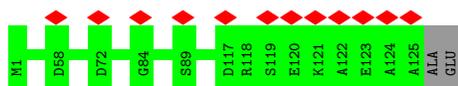
- Molecule 12: 50S ribosomal protein L15



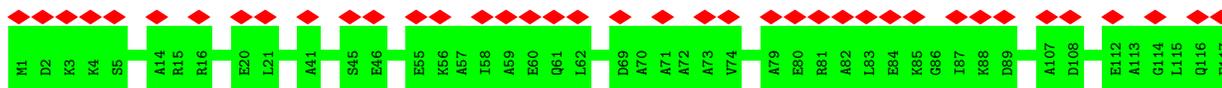
- Molecule 13: 50S ribosomal protein L16



- Molecule 14: 50S ribosomal protein L17



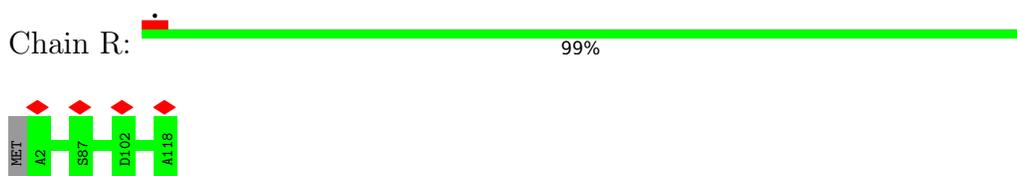
- Molecule 15: 50S ribosomal protein L18



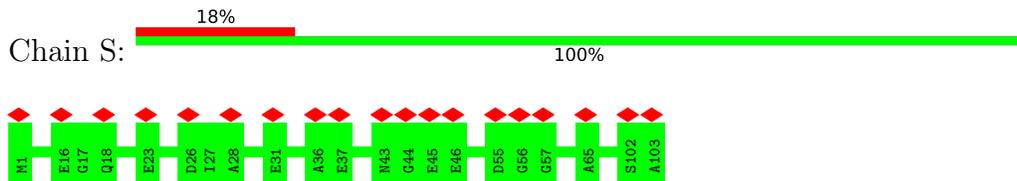
- Molecule 16: 50S ribosomal protein L19



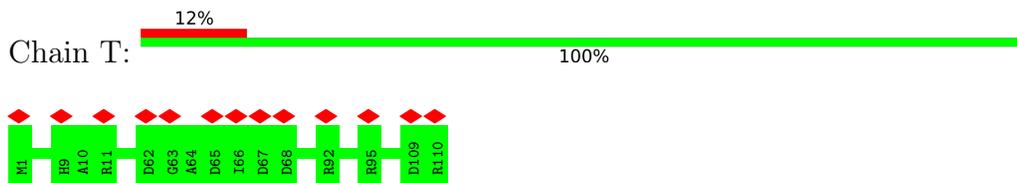
- Molecule 17: 50S ribosomal protein L20



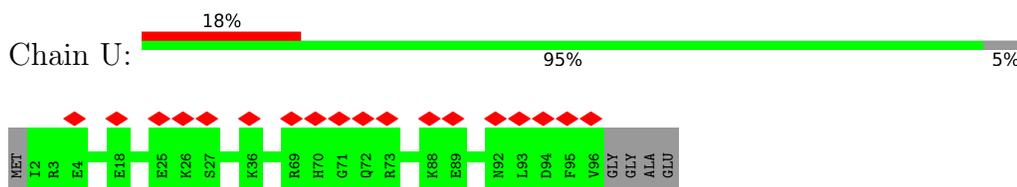
- Molecule 18: 50S ribosomal protein L21



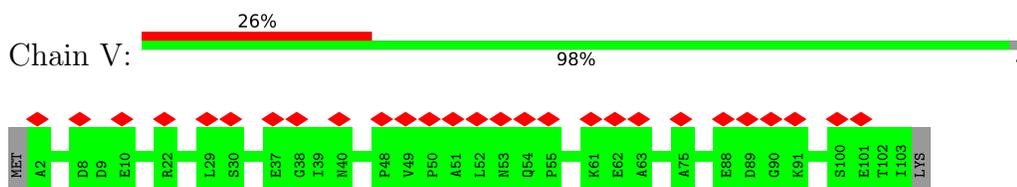
- Molecule 19: 50S ribosomal protein L22



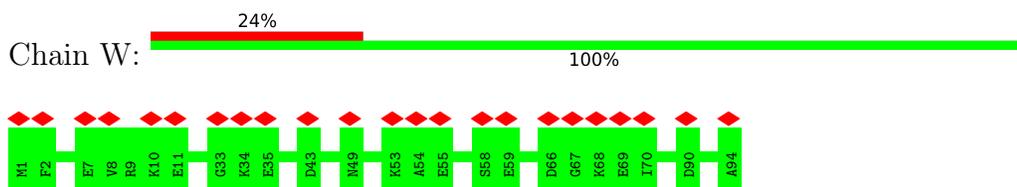
- Molecule 20: 50S ribosomal protein L23



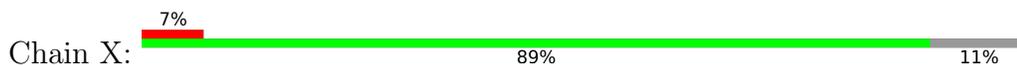
- Molecule 21: 50S ribosomal protein L24

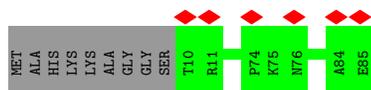


- Molecule 22: 50S ribosomal protein L25

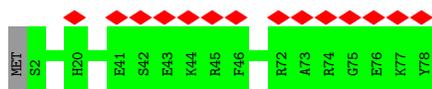


- Molecule 23: 50S ribosomal protein L27

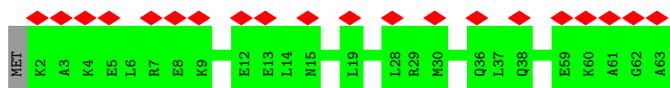




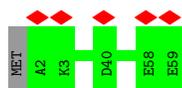
- Molecule 24: 50S ribosomal protein L28



- Molecule 25: 50S ribosomal protein L29



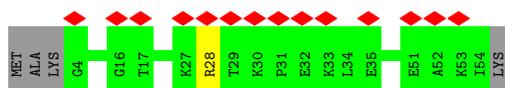
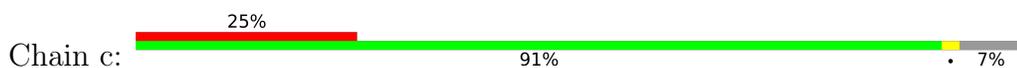
- Molecule 26: 50S ribosomal protein L30



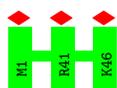
- Molecule 27: 50S ribosomal protein L32



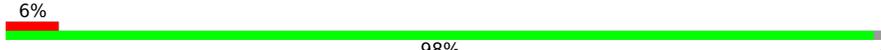
- Molecule 28: 50S ribosomal protein L33

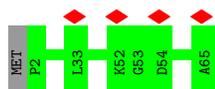


- Molecule 29: 50S ribosomal protein L34



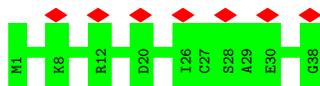
- Molecule 30: 50S ribosomal protein L35

Chain e:  6% 98%



- Molecule 31: 50S ribosomal protein L36

Chain f:  18% 100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	59148	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 ($e^-/\text{\AA}^2$)	1.14	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	0.616	Depositor
Minimum map value	-0.384	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	312.91, 312.91, 302.12	wwPDB
Map dimensions	290, 290, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.079, 1.079, 1.079	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: MG, FME, JJH, 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	1	0.18	0/93	0.73	0/142
2	A	0.21	0/67296	0.73	11/104979 (0.0%)
3	B	0.17	0/2872	0.71	0/4478
4	C	0.24	0/2121	0.41	0/2852
5	D	0.25	0/1585	0.43	0/2134
6	E	0.24	0/1570	0.40	0/2113
7	F	0.25	0/1434	0.40	0/1926
8	G	0.24	0/1342	0.42	0/1816
9	H	0.27	0/389	0.47	0/523
10	K	0.24	0/1151	0.40	0/1551
11	L	0.25	0/955	0.43	0/1279
12	M	0.25	0/1061	0.43	0/1413
13	N	0.25	0/1092	0.41	0/1460
14	O	0.23	0/1006	0.38	0/1345
15	P	0.24	0/909	0.39	0/1219
16	Q	0.24	0/928	0.40	0/1242
17	R	0.25	0/959	0.34	0/1278
18	S	0.25	0/828	0.43	0/1107
19	T	0.23	0/863	0.40	0/1156
20	U	0.23	0/763	0.40	0/1021
21	V	0.25	0/787	0.42	0/1051
22	W	0.25	0/765	0.40	0/1025
23	X	0.25	0/586	0.42	0/776
24	Y	0.23	0/634	0.41	0/848
25	Z	0.22	0/501	0.33	0/667
26	a	0.22	0/452	0.39	0/605
27	b	0.23	0/449	0.41	0/599
28	c	0.24	0/421	0.41	0/561
29	d	0.22	0/379	0.39	0/498
30	e	0.23	0/512	0.42	0/676
31	f	0.23	0/302	0.39	0/397
All	All	0.22	0/95005	0.67	11/142737 (0.0%)

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	790	U	C2-N1-C1'	7.03	126.14	117.70
2	A	1313	U	C2-N1-C1'	6.74	125.79	117.70
2	A	2473	U	C2-N1-C1'	6.56	125.58	117.70
2	A	1914	C	N1-C2-O2	6.17	122.60	118.90
2	A	2473	U	N1-C2-O2	5.91	126.94	122.80

There are no chirality outliers.

There are no planarity outliers.

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	
4	C	269/273 (98%)	258 (96%)	11 (4%)	0	100	100
5	D	207/209 (99%)	203 (98%)	4 (2%)	0	100	100
6	E	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
7	F	175/179 (98%)	172 (98%)	3 (2%)	0	100	100
8	G	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
9	H	48/149 (32%)	45 (94%)	3 (6%)	0	100	100
10	K	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
11	L	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
12	M	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
13	N	134/136 (98%)	134 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	O	123/127 (97%)	119 (97%)	4 (3%)	0	100	100
15	P	115/117 (98%)	115 (100%)	0	0	100	100
16	Q	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
17	R	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
18	S	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
19	T	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
20	U	93/100 (93%)	93 (100%)	0	0	100	100
21	V	100/104 (96%)	95 (95%)	5 (5%)	0	100	100
22	W	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
23	X	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
24	Y	75/78 (96%)	75 (100%)	0	0	100	100
25	Z	60/63 (95%)	60 (100%)	0	0	100	100
26	a	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
27	b	54/57 (95%)	54 (100%)	0	0	100	100
28	c	49/55 (89%)	49 (100%)	0	0	100	100
29	d	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
30	e	62/65 (95%)	56 (90%)	6 (10%)	0	100	100
31	f	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
All	All	3078/3267 (94%)	3010 (98%)	68 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	
4	C	216/218 (99%)	216 (100%)	0	100	100
5	D	164/164 (100%)	164 (100%)	0	100	100
6	E	165/165 (100%)	165 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	F	148/150 (99%)	148 (100%)	0	100	100
8	G	137/138 (99%)	137 (100%)	0	100	100
9	H	40/114 (35%)	40 (100%)	0	100	100
10	K	116/116 (100%)	115 (99%)	1 (1%)	78	92
11	L	104/104 (100%)	104 (100%)	0	100	100
12	M	103/103 (100%)	103 (100%)	0	100	100
13	N	109/109 (100%)	109 (100%)	0	100	100
14	O	102/103 (99%)	102 (100%)	0	100	100
15	P	87/87 (100%)	87 (100%)	0	100	100
16	Q	99/100 (99%)	98 (99%)	1 (1%)	76	91
17	R	89/90 (99%)	89 (100%)	0	100	100
18	S	84/84 (100%)	84 (100%)	0	100	100
19	T	93/93 (100%)	93 (100%)	0	100	100
20	U	82/84 (98%)	82 (100%)	0	100	100
21	V	83/85 (98%)	83 (100%)	0	100	100
22	W	78/78 (100%)	78 (100%)	0	100	100
23	X	57/63 (90%)	57 (100%)	0	100	100
24	Y	67/68 (98%)	67 (100%)	0	100	100
25	Z	54/55 (98%)	54 (100%)	0	100	100
26	a	48/49 (98%)	48 (100%)	0	100	100
27	b	47/48 (98%)	47 (100%)	0	100	100
28	c	45/49 (92%)	44 (98%)	1 (2%)	52	81
29	d	38/38 (100%)	38 (100%)	0	100	100
30	e	51/52 (98%)	51 (100%)	0	100	100
31	f	34/34 (100%)	34 (100%)	0	100	100
All	All	2540/2641 (96%)	2537 (100%)	3 (0%)	93	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	K	141	ASP
16	Q	37	LYS
28	c	28	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
10	K	136	GLN
29	d	26	ASN
14	O	62	ASN
24	Y	34	HIS
12	M	104	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3/4 (75%)	1 (33%)	0
2	A	2786/2795 (99%)	327 (11%)	8 (0%)
3	B	119/120 (99%)	9 (7%)	0
All	All	2908/2919 (99%)	337 (11%)	8 (0%)

5 of 337 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	76	A
2	A	10	A
2	A	12	U
2	A	15	G
2	A	34	U

5 of 8 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A	2756	U
2	A	2474	U
2	A	1757	A
2	A	1358	G
2	A	2211	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 386 ligands modelled in this entry, 383 are monoatomic - leaving 3 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	JJH	A	3370	-	46,47,47	1.93	10 (21%)	62,71,71	2.83	17 (27%)
32	FME	1	101	1	8,9,10	0.93	0	7,9,11	0.99	1 (14%)
34	A	A	3001	-	18,24,25	0.64	0	18,35,38	0.77	1 (5%)

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	JJH	A	3370	-	-	9/24/50/50	0/6/6/6
32	FME	1	101	1	-	2/7/9/11	-
34	A	A	3001	-	-	0/3/25/26	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	A	3370	JJH	CBB-CBF	-5.10	1.40	1.48
35	A	3370	JJH	CBJ-NAM	-4.73	1.33	1.43
35	A	3370	JJH	CBA-CBD	-4.58	1.39	1.48
35	A	3370	JJH	CAT-NAK	-4.18	1.35	1.40
35	A	3370	JJH	CAX-NAK	3.76	1.40	1.34

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	A	3370	JJH	CBL-OAH-CBO	-11.65	100.96	110.15
35	A	3370	JJH	CBK-NAM-CBO	-10.77	105.05	111.28
35	A	3370	JJH	OAJ-CBO-NAM	-6.81	123.50	128.91
35	A	3370	JJH	OAH-CBL-CBK	-5.27	99.26	104.57
35	A	3370	JJH	CBE-CBC-CAW	-4.23	119.84	123.34

There are no chirality outliers.

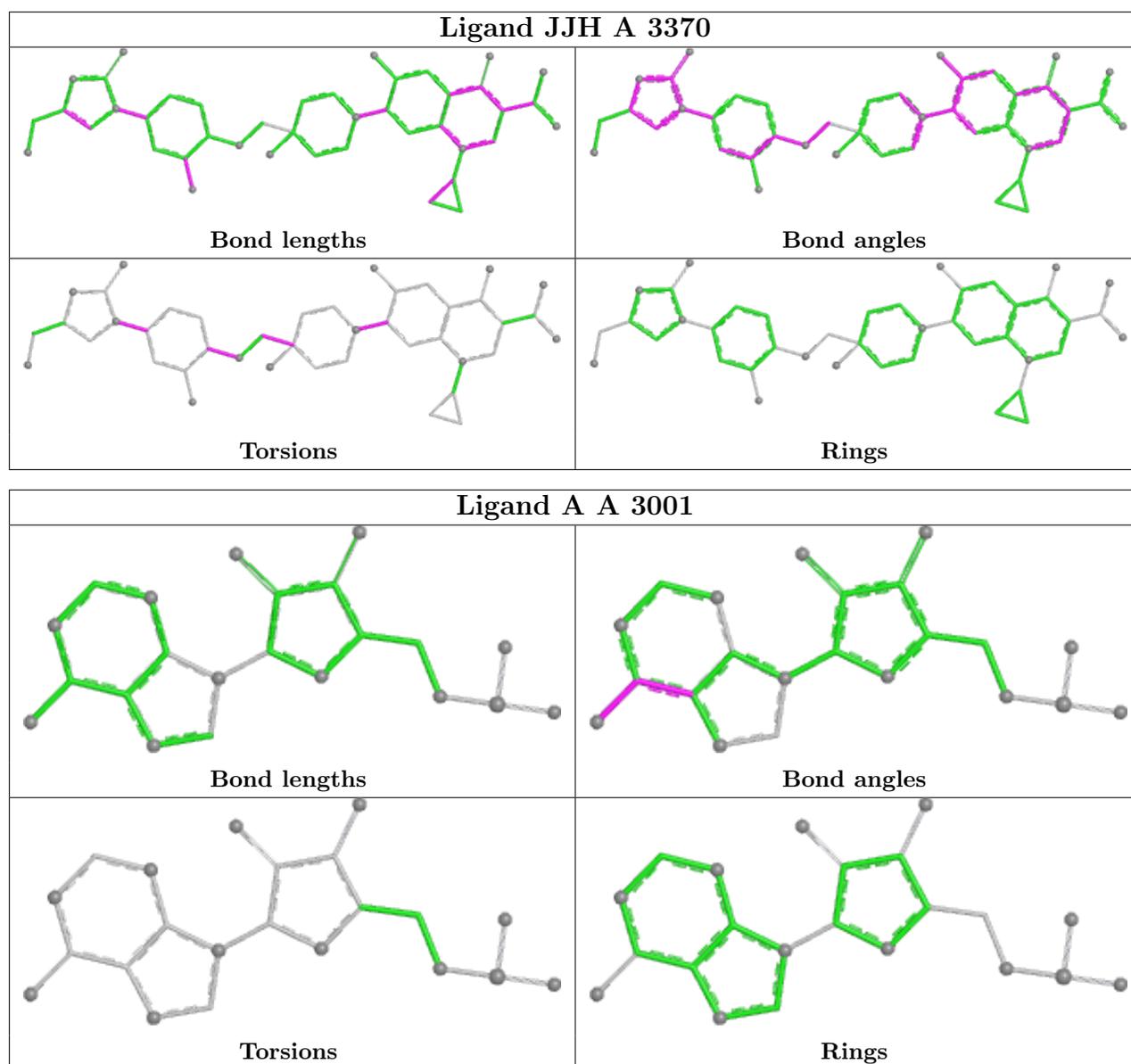
5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1	101	FME	O1-CN-N-CA
32	1	101	FME	CB-CA-N-CN
35	A	3370	JJH	CAR-CAQ-CAY-OAD
35	A	3370	JJH	CAS-CAQ-CAY-OAD
35	A	3370	JJH	OAC-CAQ-CAY-OAD

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	A	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1531:C	O3'	1540:G	P	18.12
1	A	883:G	O3'	893:C	P	17.33
1	A	2101:A	O3'	2188:U	P	16.18
1	A	545:U	O3'	548:G	P	15.10
1	A	1173:U	O3'	1177:G	P	12.82

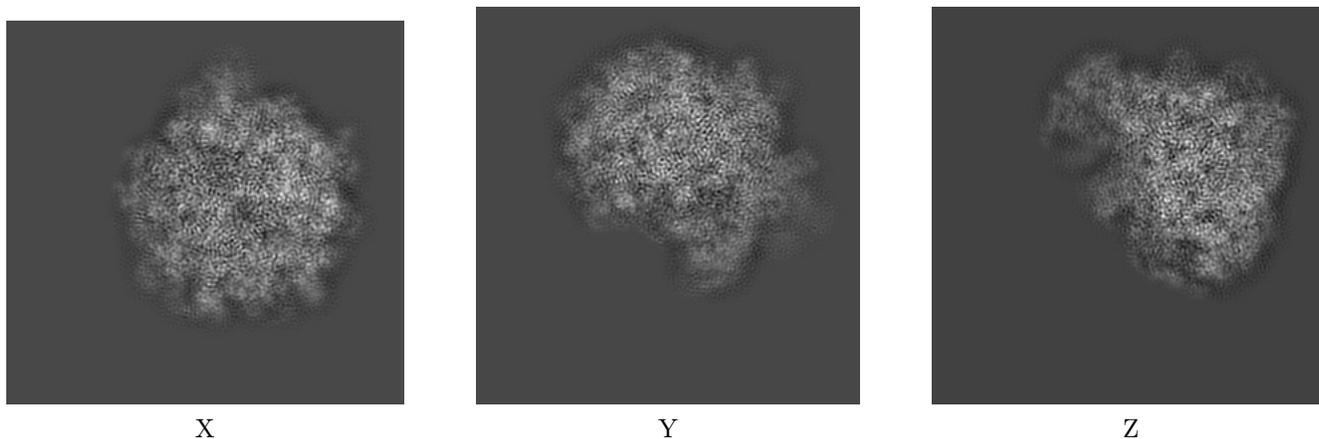
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4638. These allow visual inspection of the internal detail of the map and identification of artifacts.

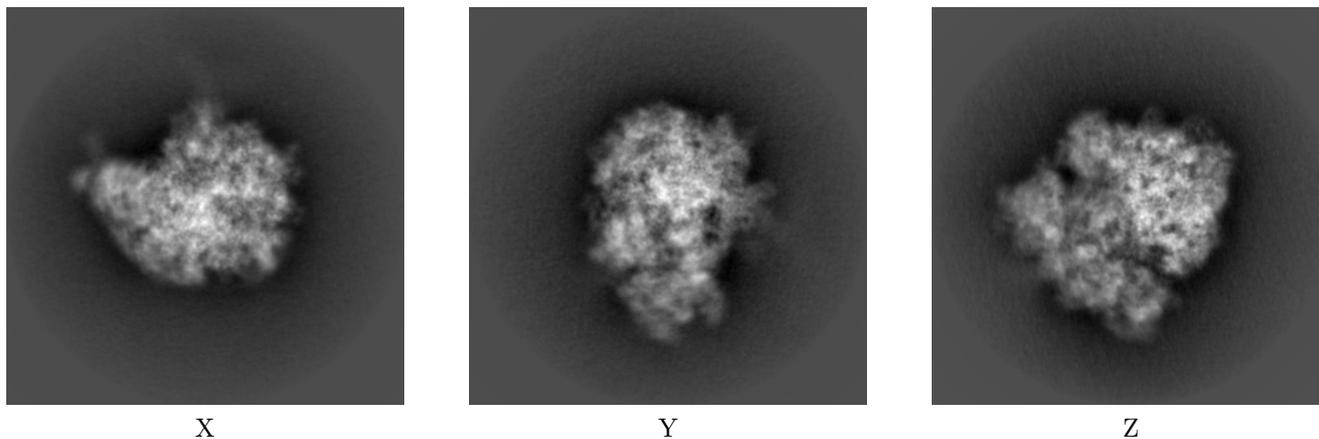
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



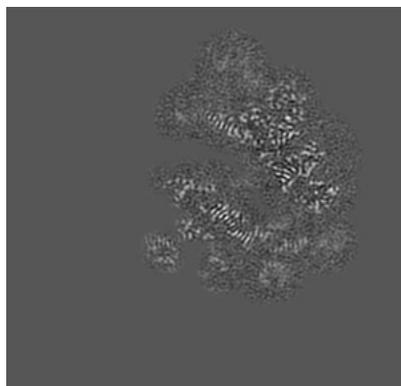
6.1.2 Raw map



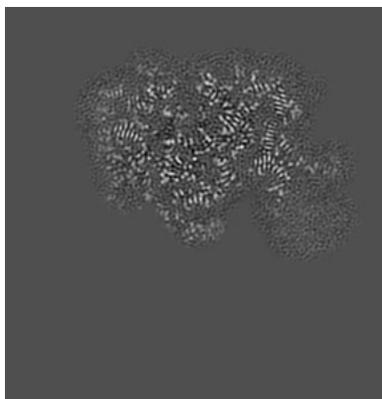
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

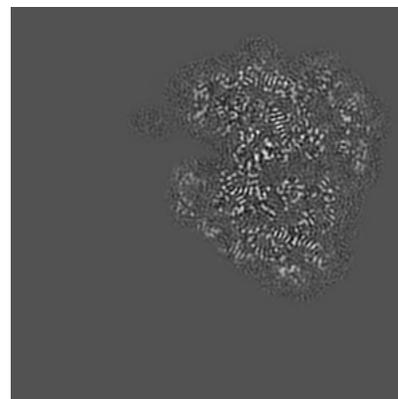
6.2.1 Primary map



X Index: 145

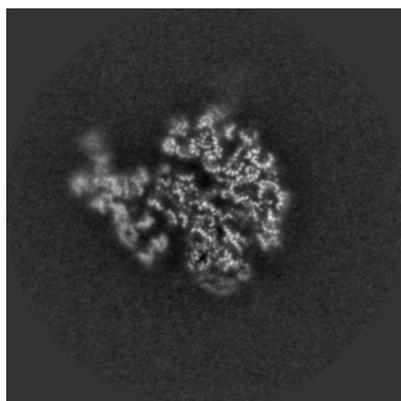


Y Index: 145

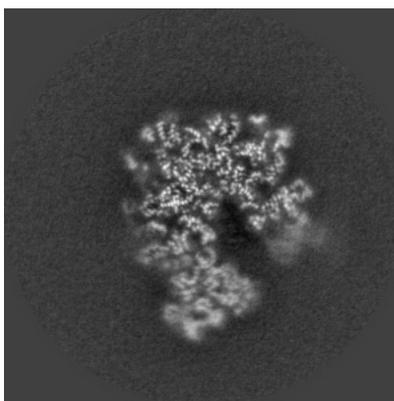


Z Index: 140

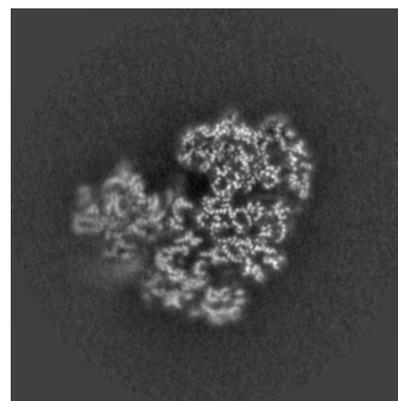
6.2.2 Raw map



X Index: 200



Y Index: 200

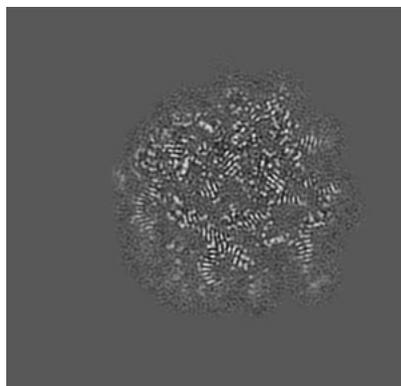


Z Index: 200

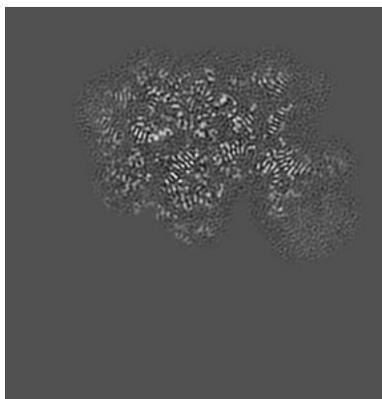
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

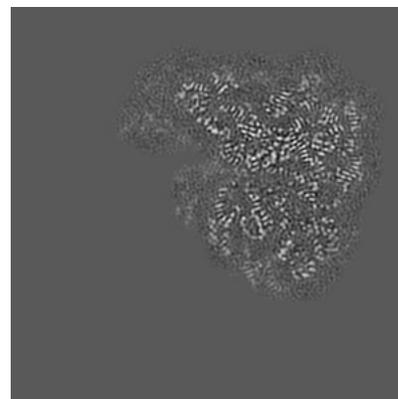
6.3.1 Primary map



X Index: 196

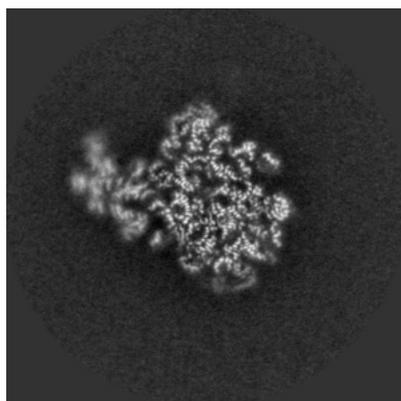


Y Index: 150

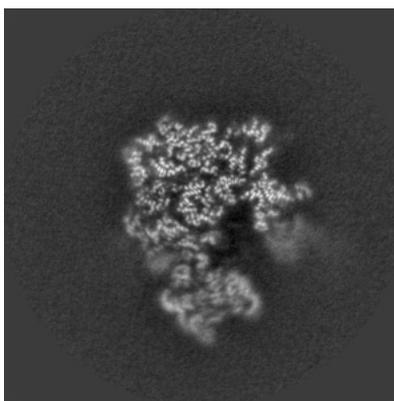


Z Index: 153

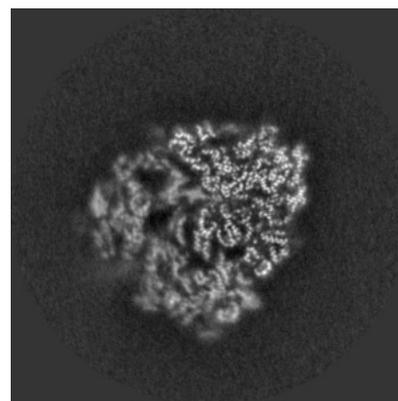
6.3.2 Raw map



X Index: 208



Y Index: 190

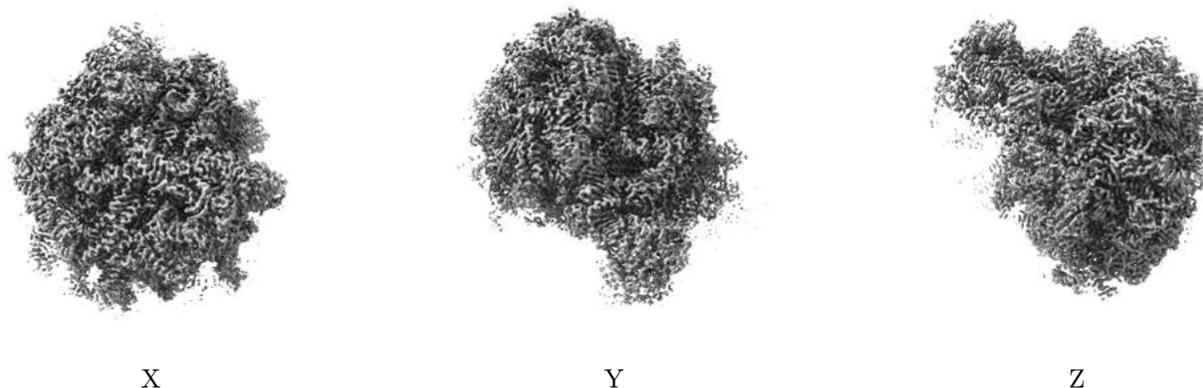


Z Index: 213

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

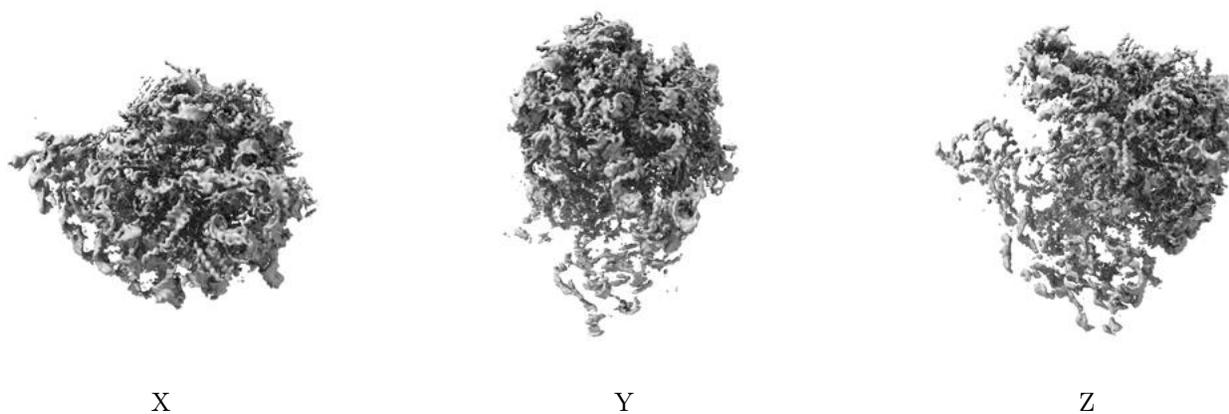
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

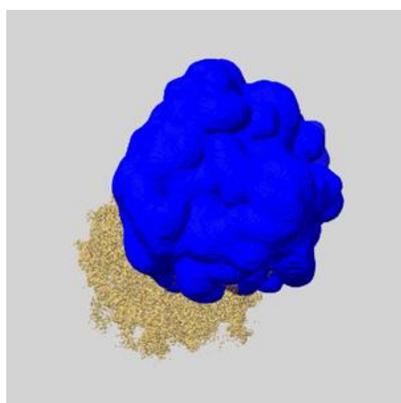
6.5 Mask visualisation [i](#)

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

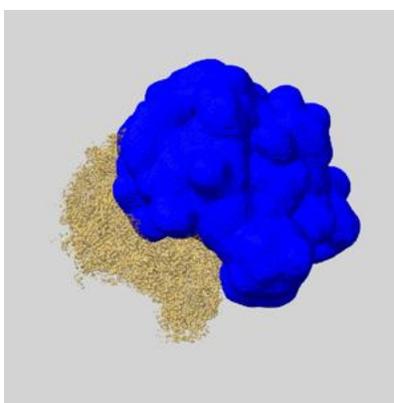
A mask typically either:

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

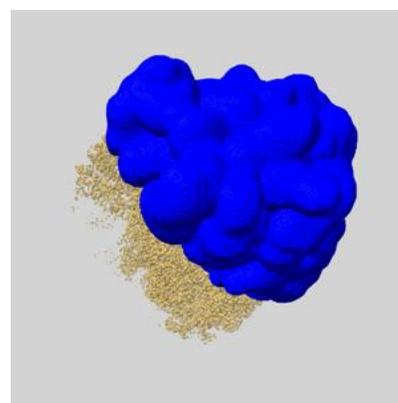
6.5.1 emd_4638_msk_1.map [i](#)



X



Y

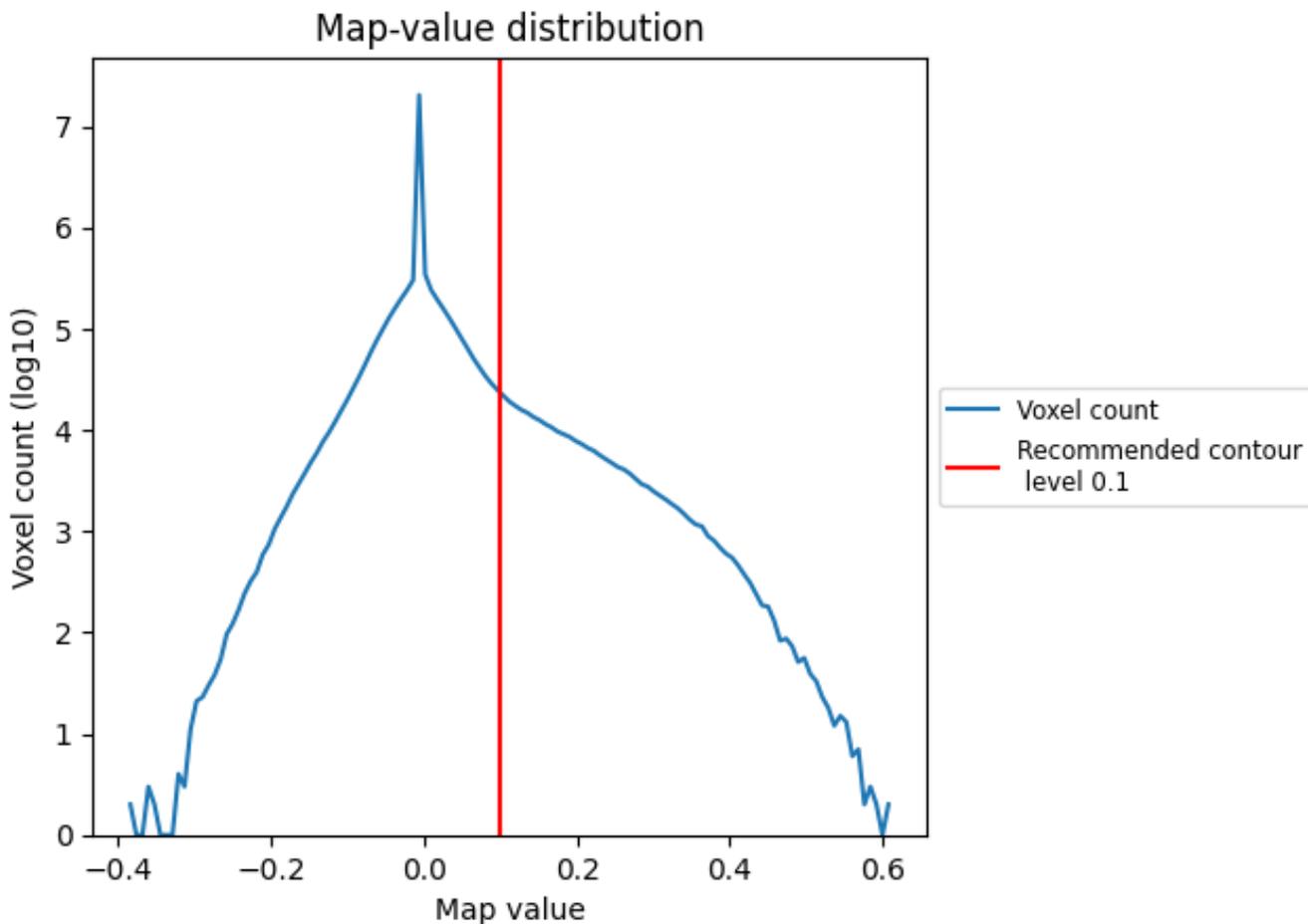


Z

7 Map analysis [i](#)

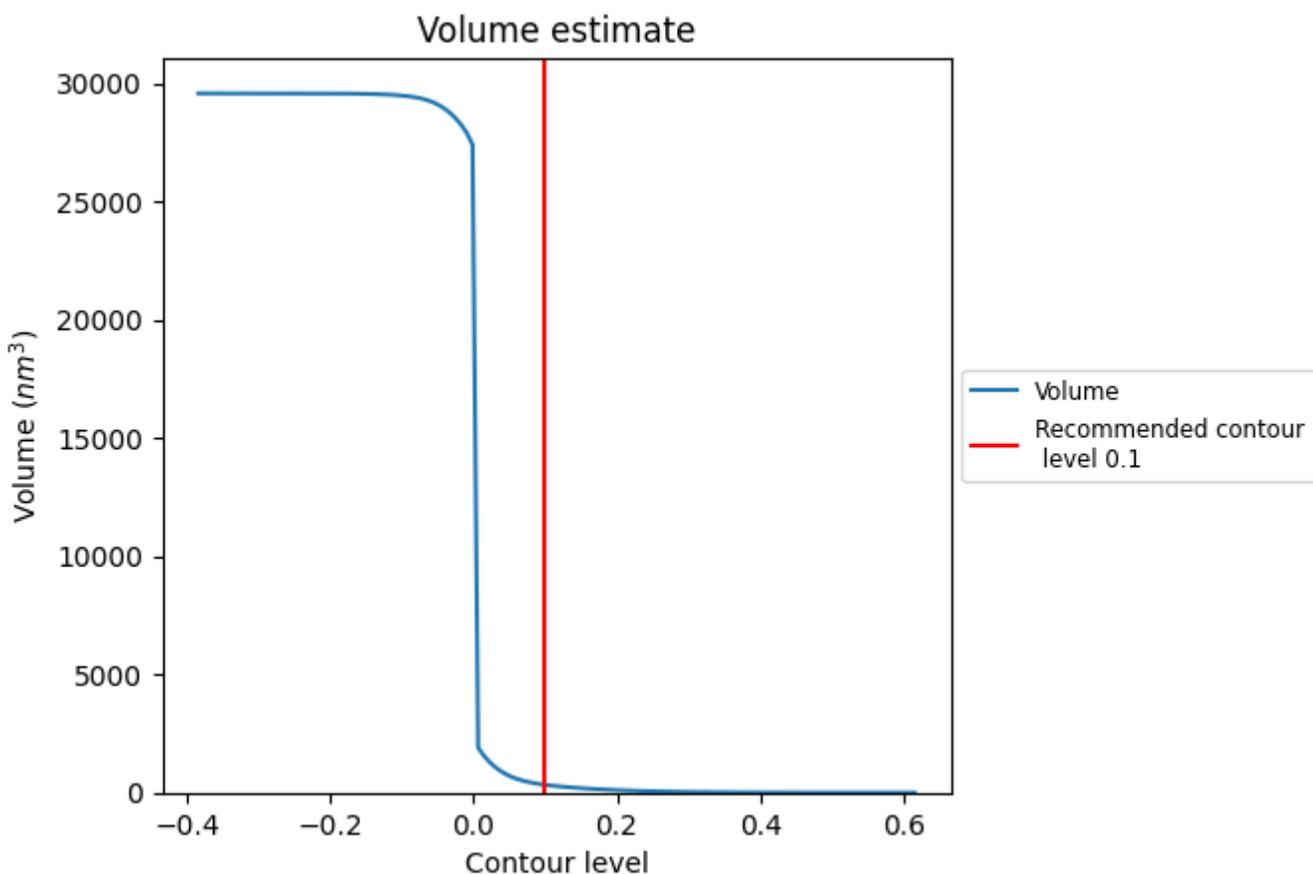
This section contains the results of statistical analysis of the map.

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 329 nm³; this corresponds to an approximate mass of 297 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.

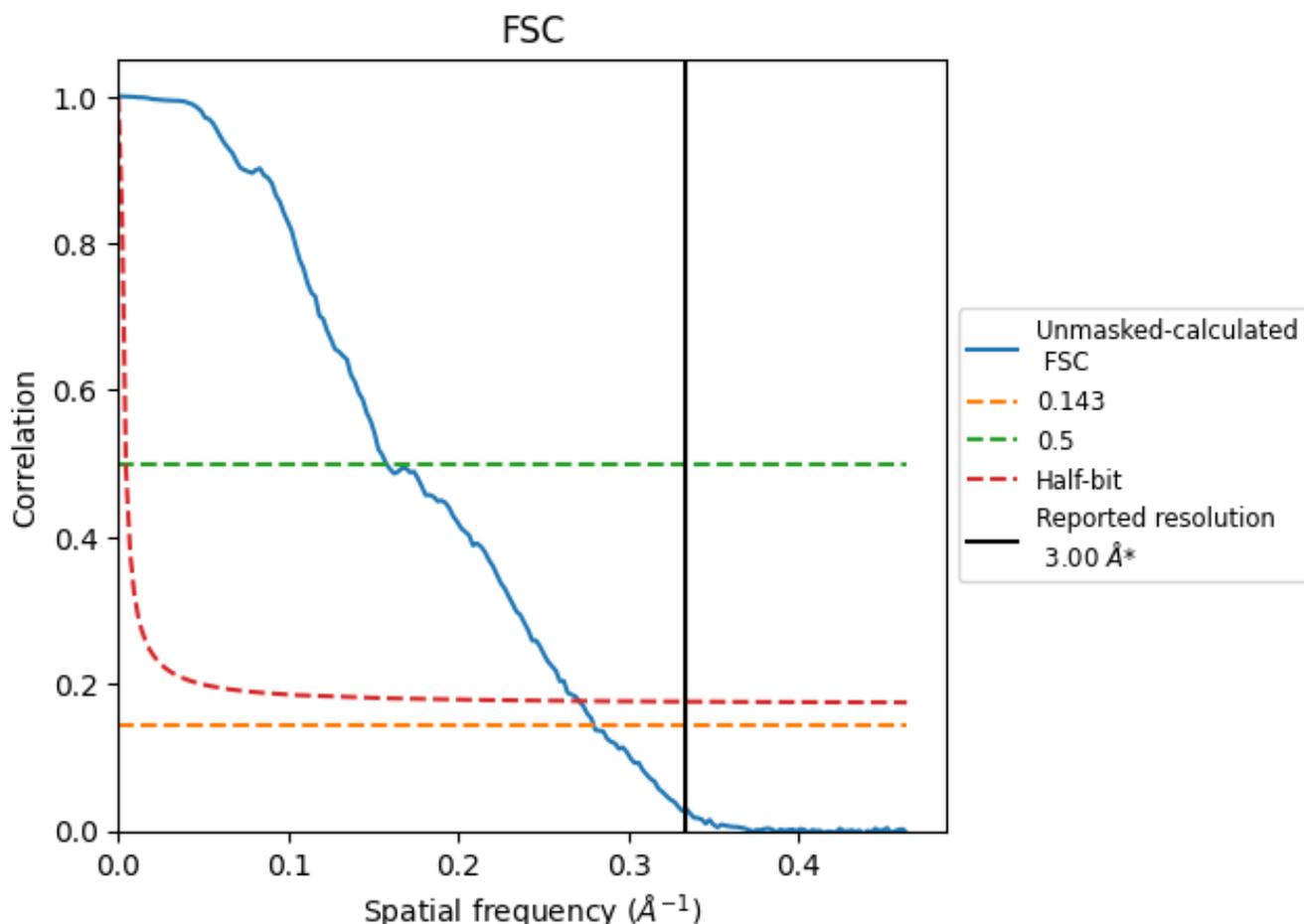
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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](#)

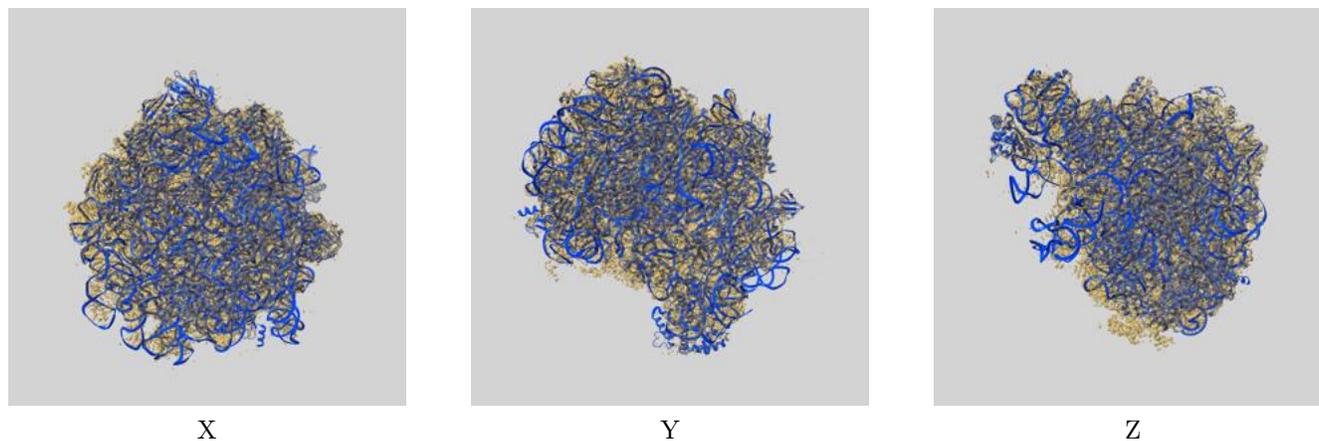
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.58	6.35	3.69

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.58 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

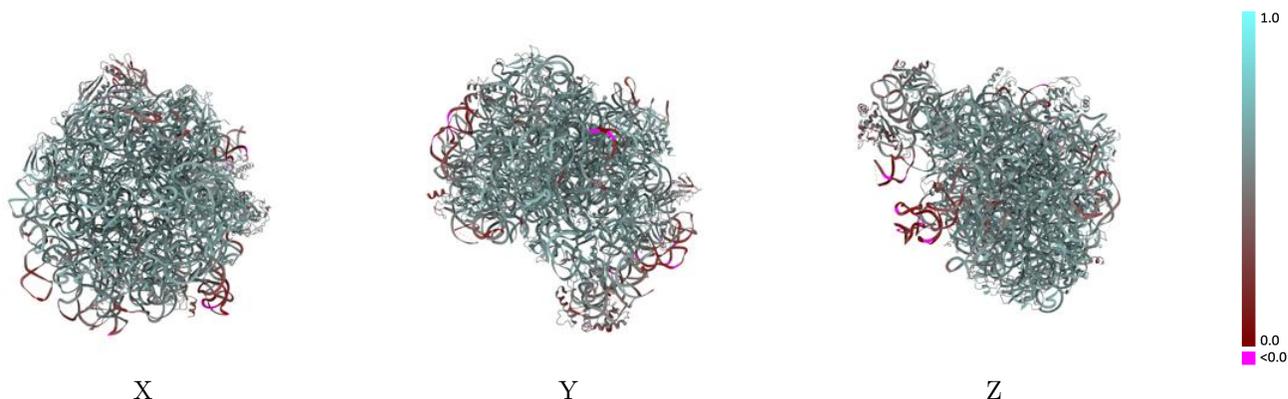
This section contains information regarding the fit between EMDB map EMD-4638 and PDB model 6QUL. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



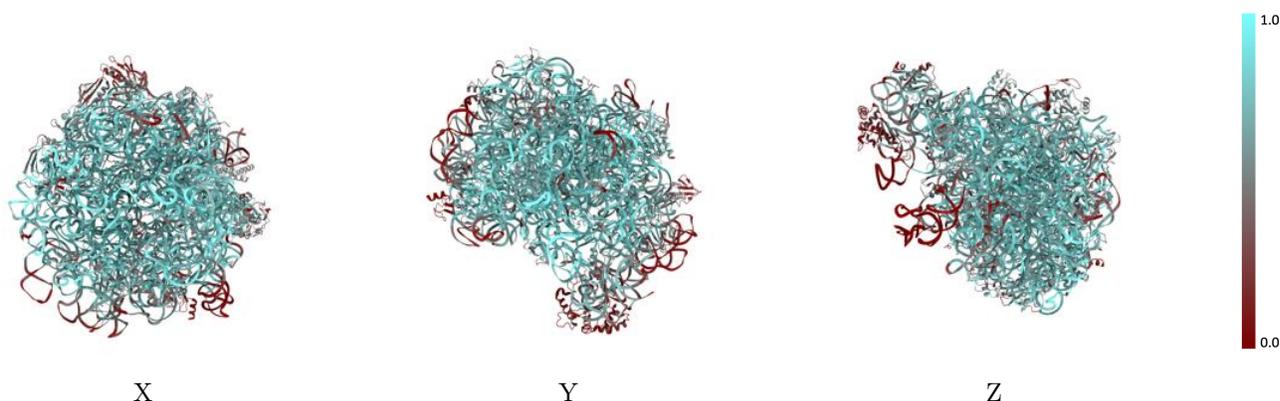
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



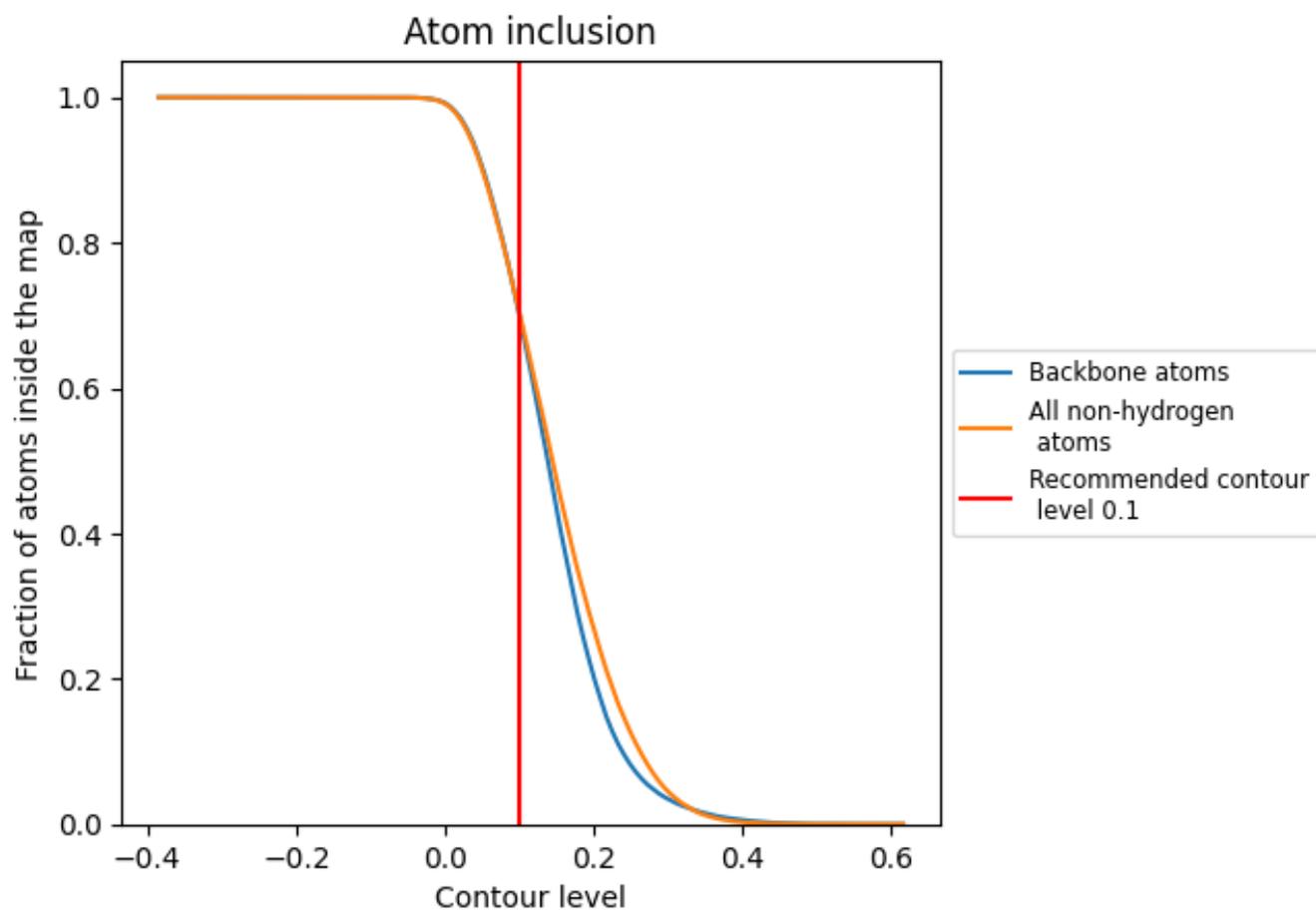
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 71% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7053	 0.5560
1	 0.3895	 0.4680
A	 0.7571	 0.5590
B	 0.6123	 0.5120
C	 0.7025	 0.5940
D	 0.6838	 0.5880
E	 0.5984	 0.5610
F	 0.1784	 0.4100
G	 0.3241	 0.4600
H	 0.2243	 0.4210
K	 0.7034	 0.5900
L	 0.6439	 0.5840
M	 0.6618	 0.5720
N	 0.6599	 0.5830
O	 0.7019	 0.5810
P	 0.5069	 0.5260
Q	 0.6077	 0.5710
R	 0.7379	 0.5940
S	 0.6495	 0.5750
T	 0.6575	 0.5800
U	 0.5649	 0.5500
V	 0.5346	 0.5300
W	 0.5482	 0.5390
X	 0.6980	 0.5910
Y	 0.6233	 0.5760
Z	 0.5082	 0.5210
a	 0.6651	 0.5750
b	 0.6449	 0.5610
c	 0.5862	 0.5550
d	 0.7514	 0.6080
e	 0.7306	 0.5940
f	 0.6027	 0.5590

