



wwPDB EM Validation Summary Report ⓘ

Oct 28, 2024 – 07:31 AM JST

PDB ID : 8HKU
EMDB ID : EMD-34860
Title : Cryo-EM Structures and Translocation Mechanism of Crenarchaeota Ribosome
Authors : Wang, Y.H.; Zhou, J.
Deposited on : 2022-11-28
Resolution : 2.72 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.dev113
MolProbity : 4.02b-467
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

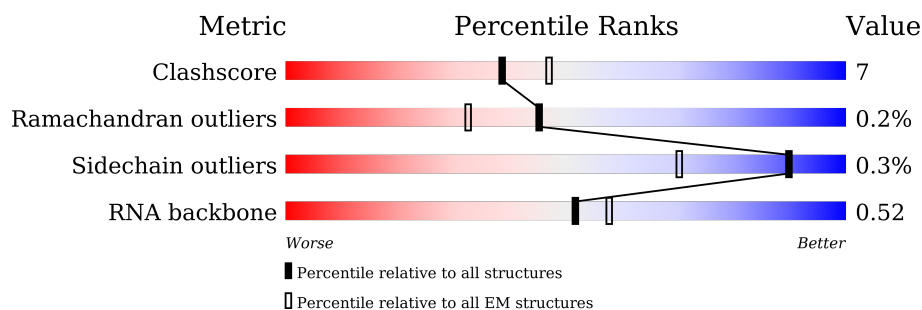
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.72 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.



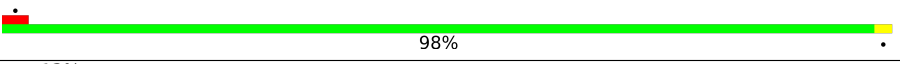
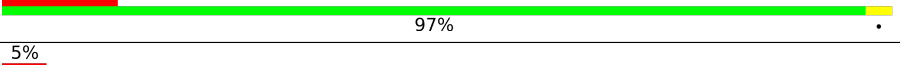
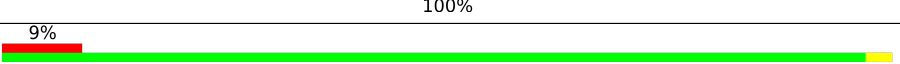
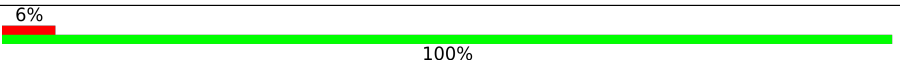
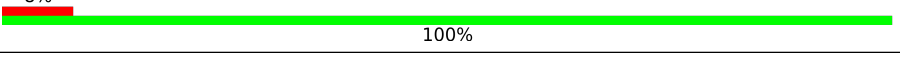
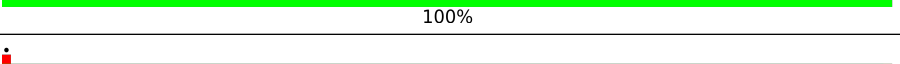
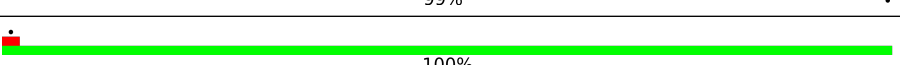
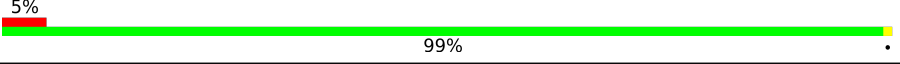
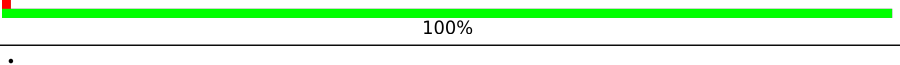
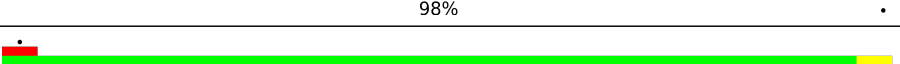
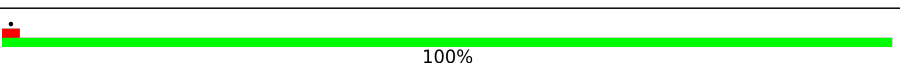
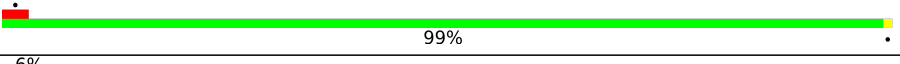
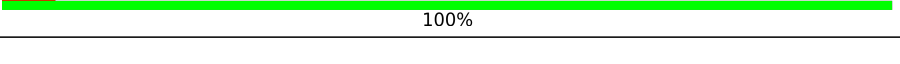
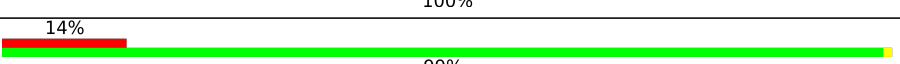
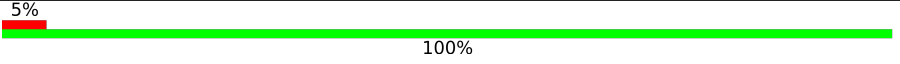
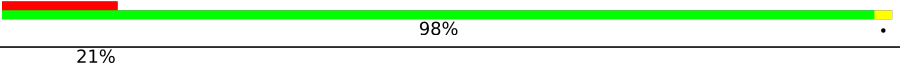
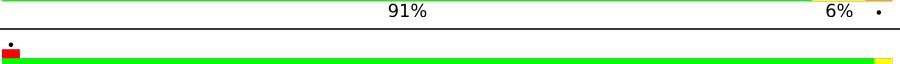
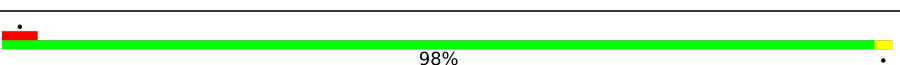
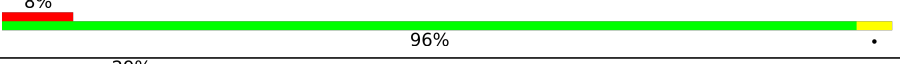
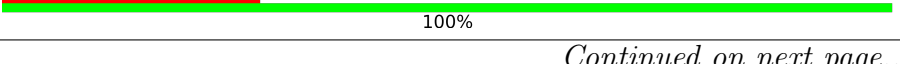



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 ≥ 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	A23S	3022	<div> <div>5%</div> <div>78%</div> <div>19%</div> <div>..</div> </div>
2	A5S	122	<div> <div>75%</div> <div>19%</div> <div>7%</div> </div>
3	AL1P	216	<div> <div>100%</div> <div>100%</div> </div>
4	AL2P	234	<div> <div>100%</div> </div>
5	AL3P	339	<div> <div>99%</div> <div>.</div> </div>
6	AL4P	251	<div> <div>100%</div> </div>
7	AL5P	168	<div> <div>6%</div> <div>100%</div> </div>











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Mol	Chain	Length	Quality of chain
8	AL6P	181	
9	ALX0	76	
10	L10E	164	
11	L13P	140	
12	L141	86	
12	L142	86	
13	L14P	134	
14	L15E	169	
15	L18E	112	
16	L18P	193	
17	L19E	144	
18	L22P	150	
19	L23P	81	
20	L24E	54	
21	L24P	122	
22	L29P	63	
23	L30E	94	
24	L30P	155	
25	L31E	75	
26	L32E	123	
27	L34E	77	
28	L37A	65	
29	L37E	54	
30	L39E	49	
31	L40E	55	

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Mol	Chain	Length	Quality of chain
32	L44E	92	 100%
33	L7A1	123	 100%
33	L7A2	123	 13% 98%
34	L15P	144	 65% 35%
35	L21E	97	 99%
36	ARF1	232	 51% 100%
37	L45A	101	 5% 96%
38	L46A	70	 7% 99%
39	L47A	80	 29% 100%
40	AETN	19	 37% 74% 16% 5% 5%

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 106630 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 23s rRNA (2996-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A23S	2995	Total	C	N	O	P	0	0
			64335	28663	11905	20772	2995		

- Molecule 2 is a RNA chain called 5s rRNA (122-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A5S	122	Total	C	N	O	P	0	0
			2609	1163	476	849	121		

- Molecule 3 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AL1P	216	Total	C	N	O	S	0	0
			1715	1096	303	312	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AL2P	234	Total	C	N	O	S	0	0
			1754	1101	344	307	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AL3P	339	Total	C	N	O	S	0	0
			2695	1730	484	477	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AL4P	251	Total	C	N	O	S	0	0
			1926	1223	356	345	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AL5P	168	Total	C	N	O	S	0	0
			1343	854	253	232	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AL6P	181	Total	C	N	O	S	0	0
			1431	920	246	264	1		

- Molecule 9 is a protein called 50S ribosomal protein L18Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	ALX0	76	Total	C	N	O	S	0	0
			629	403	110	115	1		

- Molecule 10 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L10E	164	Total	C	N	O	S	0	0
			1310	837	239	227	7		

- Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L13P	140	Total	C	N	O	S	0	0
			1109	707	208	190	4		

- Molecule 12 is a protein called 50S ribosomal protein L14e.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L141	86	Total	C	N	O	S	0	0
			669	417	123	127	2		
12	L142	86	Total	C	N	O	S	0	0
			669	417	123	127	2		

- Molecule 13 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L14P	134	Total	C	N	O	S	0	0
			1034	655	194	181	4		

- Molecule 14 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L15E	169	Total	C	N	O	S	0	0
			1423	899	283	236	5		

- Molecule 15 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L18E	112	Total	C	N	O	S	0	0
			895	576	163	153	3		

- Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L18P	193	Total	C	N	O	S	0	0
			1539	990	274	274	1		

- Molecule 17 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	L19E	144	Total	C	N	O	0	0
			1206	753	247	206		

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L22P	150	Total	C	N	O	S	0	0
			1223	782	225	213	3		

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L23P	81	Total	C	N	O	S	0	0
			650	419	109	121	1		

- Molecule 20 is a protein called 50S ribosomal protein L24e.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L24E	54	Total	C	N	O	S	0	0
			441	282	80	73	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	L24P	122	Total	C	N	O	S	0	0
			989	620	189	176	4		

- Molecule 22 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	L29P	63	Total	C	N	O	S	0	0
			513	319	95	96	3		

- Molecule 23 is a protein called 50S ribosomal protein L30e.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	L30E	94	Total	C	N	O	S	0	0
			729	474	116	136	3		

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	L30P	155	Total	C	N	O	S	0	0
			1254	804	222	223	5		

- Molecule 25 is a protein called 50S ribosomal protein L31e.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	L31E	75	Total	C	N	O	S	0	0
			625	398	126	97	4		

- Molecule 26 is a protein called 50S ribosomal protein L32e.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	L32E	123	Total	C	N	O	S	0	0
			1010	650	193	166	1		

- Molecule 27 is a protein called 50S ribosomal protein L34e.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	L34E	77	Total	C	N	O	S	0	0
			629	395	119	110	5		

- Molecule 28 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	L37A	65	Total	C	N	O	S	0	0
			527	335	99	87	6		

- Molecule 29 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	L37E	54	Total	C	N	O	S	0	0
			436	267	94	69	6		

- Molecule 30 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	L39E	49	Total	C	N	O	S	0	0
			414	265	88	61			

- Molecule 31 is a protein called 50S ribosomal protein L40E.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	L40E	55	Total	C	N	O	S	0	0
			439	273	89	72	5		

- Molecule 32 is a protein called 50S ribosomal protein L44e.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	L44E	92	Total	C	N	O	S	0	0
			753	474	144	129	6		

- Molecule 33 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	L7A1	123	Total	C	N	O	S	0	0
			935	593	155	184	3		
33	L7A2	123	Total	C	N	O	S	0	0
			935	593	155	184	3		

- Molecule 34 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	L15P	94	Total	C	N	O	S	0	0
			752	487	131	133	1		

- Molecule 35 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	L21E	97	Total	C	N	O	S	0	0
			785	502	152	129	2		

- Molecule 36 is a protein called Peptide chain release factor subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	ARF1	232	Total	C	N	O	S	0	0
			1869	1213	299	349	8		

- Molecule 37 is a protein called DUF2280 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	L45A	101	Total	C	N	O	S	0	0
			816	515	141	156	4		

- Molecule 38 is a protein called Conserved protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	L46A	70	Total	C	N	O	S	0	0
			586	382	101	102	1		

- Molecule 39 is a protein called 50S ribosomal protein L47A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	L47A	80	Total	C	N	O	S	0	0
			648	405	113	128	2		

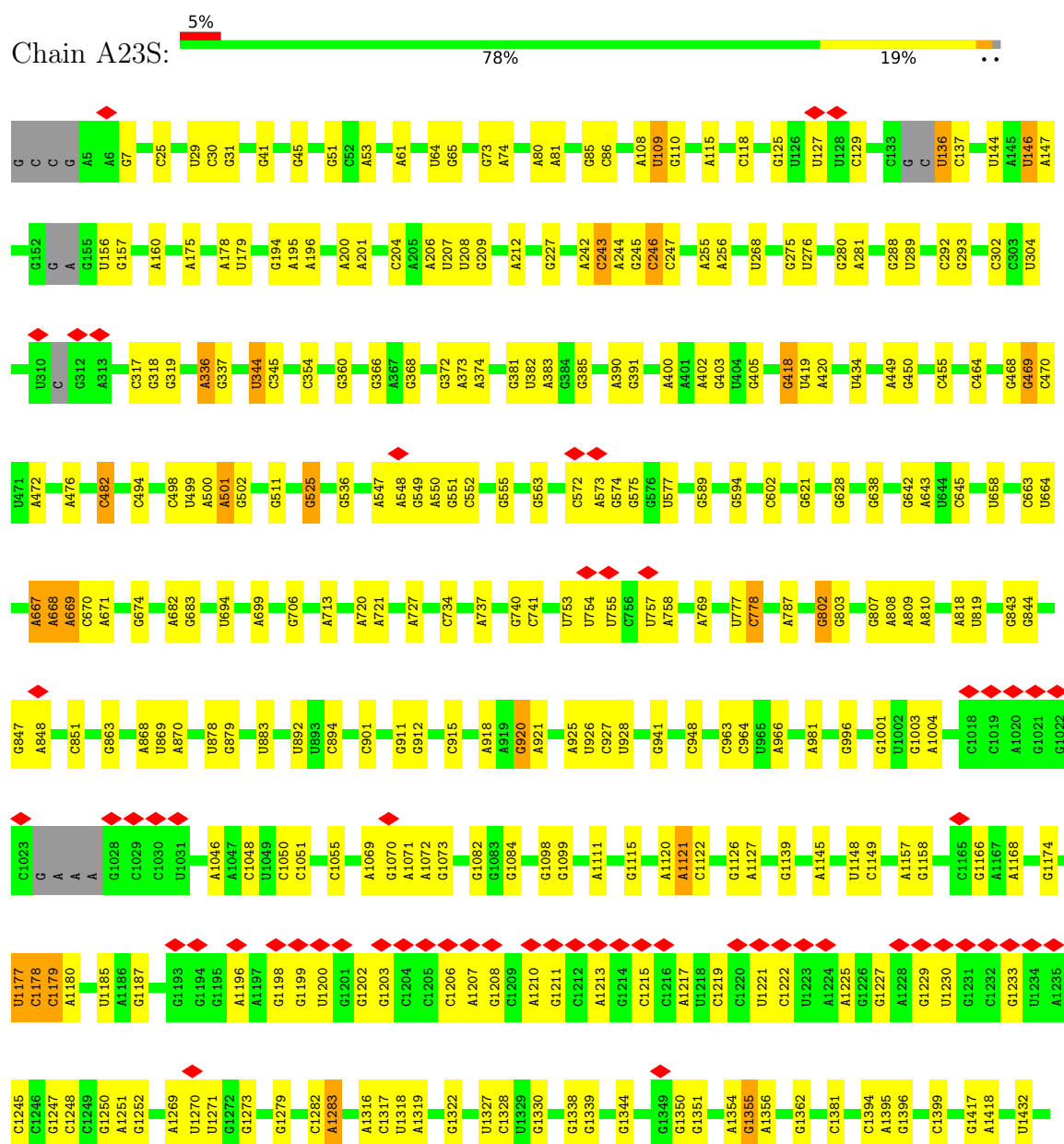
- Molecule 40 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	AETN	18	Total	C	N	O	P	0	0
			381	171	71	122	17		

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: 23s rRNA (2996-MER)





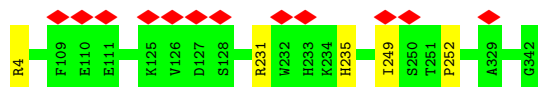
- Molecule 4: 50S ribosomal protein L2

Chain AL2P: 100%



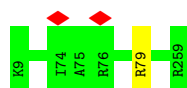
- Molecule 5: 50S ribosomal protein L3

Chain AL3P: 99%



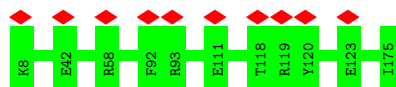
- Molecule 6: 50S ribosomal protein L4

Chain AL4P: 100%



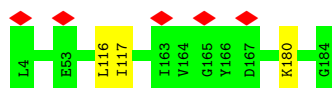
- Molecule 7: 50S ribosomal protein L5

Chain AL5P: 6% 100%



- Molecule 8: 50S ribosomal protein L6

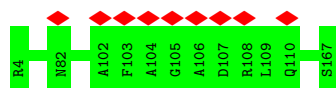
Chain AL6P: 98%



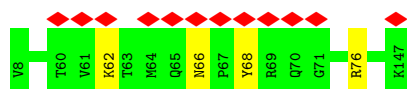
- Molecule 9: 50S ribosomal protein L18Ae



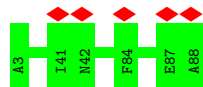
- Molecule 10: 50S ribosomal protein L10e



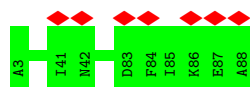
- Molecule 11: 50S ribosomal protein L13



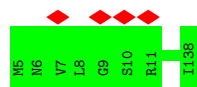
- Molecule 12: 50S ribosomal protein L14e



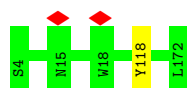
- Molecule 12: 50S ribosomal protein L14e



- Molecule 13: 50S ribosomal protein L14



- Molecule 14: 50S ribosomal protein L15e



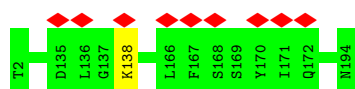
- Molecule 15: 50S ribosomal protein L18e

Chain L18E:  100%



- Molecule 16: 50S ribosomal protein L18

Chain L18P:  99%



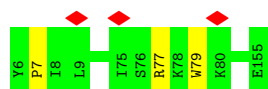
- Molecule 17: 50S ribosomal protein L19e

Chain L19E:  100%



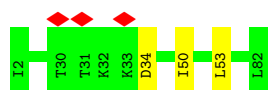
- Molecule 18: 50S ribosomal protein L22

Chain L22P:  98%



- Molecule 19: 50S ribosomal protein L23

Chain L23P:  96%



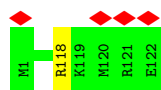
- Molecule 20: 50S ribosomal protein L24e

Chain L24E:  100%

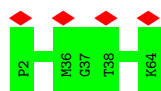


- Molecule 21: 50S ribosomal protein L24

Chain L24P:  99%



- Molecule 22: 50S ribosomal protein L29

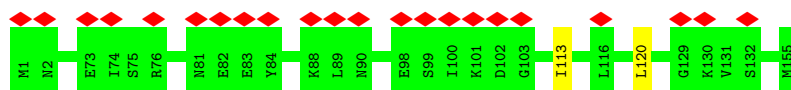


- Molecule 23: 50S ribosomal protein L30e

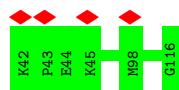


There are no outlier residues recorded for this chain.

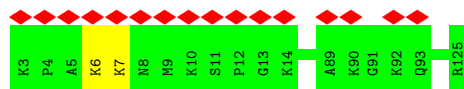
- Molecule 24: 50S ribosomal protein L30



- Molecule 25: 50S ribosomal protein L31e



- Molecule 26: 50S ribosomal protein L32e

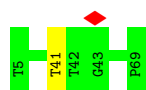


- Molecule 27: 50S ribosomal protein L34e

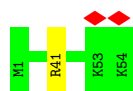


- Molecule 28: 50S ribosomal protein L37Ae

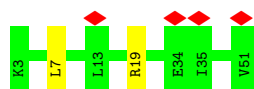




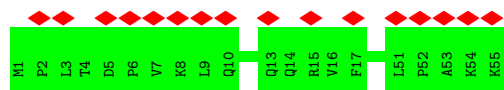
- Molecule 29: 50S ribosomal protein L37e



- Molecule 30: 50S ribosomal protein L39e



- Molecule 31: 50S ribosomal protein L40E

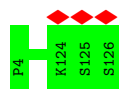


- Molecule 32: 50S ribosomal protein L44e

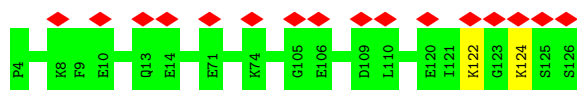


There are no outlier residues recorded for this chain.

- Molecule 33: 50S ribosomal protein L7Ae

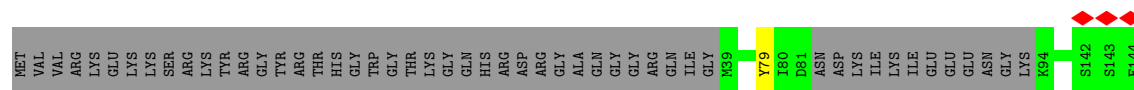


- Molecule 33: 50S ribosomal protein L7Ae



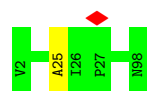
- Molecule 34: 50S ribosomal protein L15





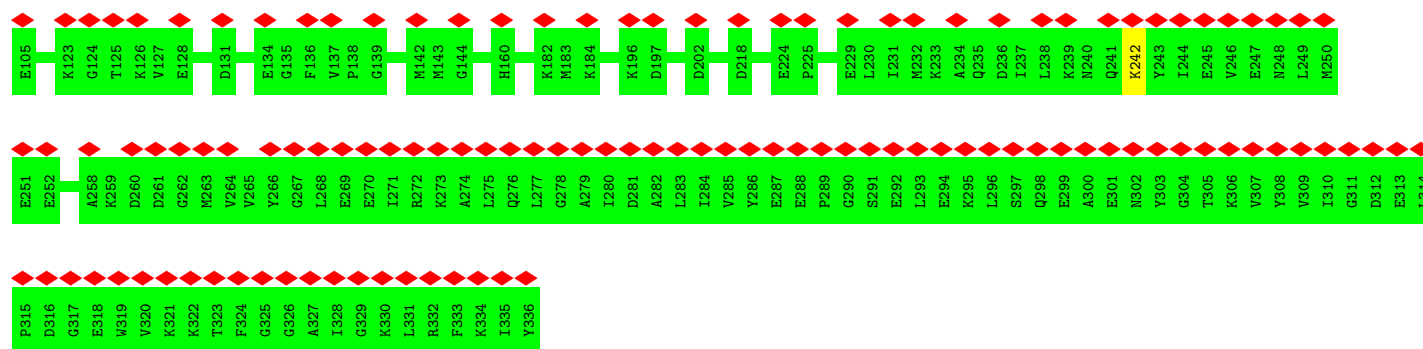
- Molecule 35: 50S ribosomal protein L21e

Chain L21E: 99%



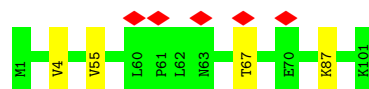
- Molecule 36: Peptide chain release factor subunit 1

Chain ARF1: 51%
100%



- Molecule 37: DUF2280 domain-containing protein

Chain L45A: 5%
96%



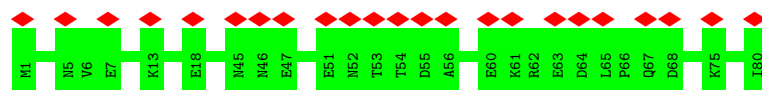
- Molecule 38: Conserved protein

Chain L46A: 7%
99%

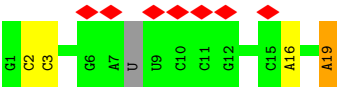
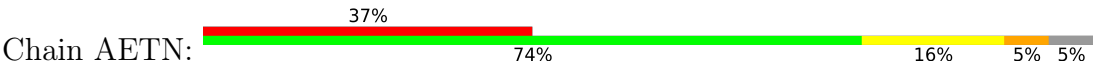


- Molecule 39: 50S ribosomal protein L47A

Chain L47A: 29%
100%



- Molecule 40: E-site tRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	772574	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 ($e^-/\text{\AA}^2$)	26.7	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	8.986	Depositor
Minimum map value	-4.723	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.259	Depositor
Recommended contour level	0.55	Depositor
Map size (Å)	391.32, 391.32, 391.32	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A23S	0.89	12/72025 (0.0%)	1.00	230/112376 (0.2%)
2	A5S	0.68	0/2917	0.77	0/4549
3	AL1P	0.24	0/1739	0.49	0/2338
4	AL2P	0.43	0/1787	0.62	1/2409 (0.0%)
5	AL3P	0.46	0/2758	0.62	0/3727
6	AL4P	0.41	0/1956	0.60	1/2635 (0.0%)
7	AL5P	0.31	0/1364	0.57	0/1827
8	AL6P	0.37	0/1450	0.54	0/1949
9	ALX0	0.44	0/638	0.66	0/851
10	L10E	0.41	0/1334	0.60	0/1787
11	L13P	0.45	1/1123 (0.1%)	0.68	1/1502 (0.1%)
12	L141	0.33	0/673	0.54	0/900
12	L142	0.30	0/673	0.52	0/900
13	L14P	0.41	0/1054	0.62	0/1425
14	L15E	0.56	3/1458 (0.2%)	0.67	0/1956
15	L18E	0.38	0/907	0.54	0/1214
16	L18P	0.37	0/1570	0.51	0/2115
17	L19E	0.40	0/1223	0.59	0/1622
18	L22P	0.45	0/1246	0.58	0/1671
19	L23P	0.41	0/655	0.57	1/874 (0.1%)
20	L24E	0.40	0/451	0.53	0/599
21	L24P	0.39	0/1000	0.59	0/1329
22	L29P	0.29	0/513	0.52	0/678
23	L30E	0.38	0/738	0.50	0/985
24	L30P	0.44	0/1278	0.66	1/1713 (0.1%)
25	L31E	0.41	0/632	0.66	0/837
26	L32E	0.48	0/1027	0.61	0/1366
27	L34E	0.51	0/642	0.95	3/854 (0.4%)
28	L37A	0.49	0/542	0.68	0/726
29	L37E	0.49	0/445	0.67	0/585
30	L39E	0.43	0/422	0.76	1/562 (0.2%)
31	L40E	0.32	0/443	0.68	0/587
32	L44E	0.44	0/763	0.61	0/1008
33	L7A1	0.32	0/946	0.44	0/1272

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	L7A2	0.26	0/946	0.44	0/1272
34	L15P	0.38	0/766	0.56	0/1023
35	L21E	0.48	0/800	0.56	0/1067
36	ARF1	0.27	0/1903	0.44	0/2553
37	L45A	0.34	0/824	0.56	0/1094
38	L46A	0.36	0/595	0.51	0/793
39	L47A	0.26	0/652	0.53	0/870
40	AETN	0.50	0/424	0.90	1/657 (0.2%)
All	All	0.75	16/115302 (0.0%)	0.88	240/171057 (0.1%)

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
5	AL3P	0	2
8	AL6P	0	1
9	ALX0	0	2
11	L13P	0	2
18	L22P	0	1
19	L23P	0	1
21	L24P	0	1
24	L30P	0	1
27	L34E	0	4
34	L15P	0	1
35	L21E	0	1
All	All	0	17

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A23S	1179	C	N1-C6	-8.64	1.31	1.37
1	A23S	1179	C	C4-C5	-7.43	1.37	1.43
1	A23S	469	G	C6-N1	-6.18	1.35	1.39
1	A23S	469	G	C8-N7	-6.12	1.27	1.30
1	A23S	1082	G	N9-C4	-5.94	1.33	1.38

The worst 5 of 240 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A23S	246	C	C2-N1-C1'	18.80	139.48	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A23S	246	C	C6-N1-C1'	-18.39	98.74	120.80
1	A23S	469	G	N3-C4-N9	18.33	137.00	126.00
1	A23S	1179	C	C6-N1-C2	-17.79	113.19	120.30
1	A23S	469	G	C8-N9-C1'	-16.41	105.66	127.00

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	AL3P	235	HIS	Peptide
5	AL3P	252	PRO	Peptide
8	AL6P	180	LYS	Peptide
9	ALX0	14	ILE	Peptide
9	ALX0	23	SER	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	A23S	64335	0	0	0	0
2	A5S	2609	0	1324	15	0
3	AL1P	1715	0	0	0	0
4	AL2P	1754	0	0	0	0
5	AL3P	2695	0	0	0	0
6	AL4P	1926	0	0	0	0
7	AL5P	1343	0	0	0	0
8	AL6P	1431	0	0	0	0
9	ALX0	629	0	0	0	0
10	L10E	1310	0	0	0	0
11	L13P	1109	0	0	0	0
12	L141	669	0	0	0	0
12	L142	669	0	0	0	0
13	L14P	1034	0	0	0	0
14	L15E	1423	0	0	0	0
15	L18E	895	0	0	0	0
16	L18P	1539	0	0	0	0
17	L19E	1206	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	L22P	1223	0	0	0	0
19	L23P	650	0	0	0	0
20	L24E	441	0	0	0	0
21	L24P	989	0	0	0	0
22	L29P	513	0	0	0	0
23	L30E	729	0	0	0	0
24	L30P	1254	0	0	0	0
25	L31E	625	0	0	0	0
26	L32E	1010	0	0	0	0
27	L34E	629	0	0	0	0
28	L37A	527	0	0	0	0
29	L37E	436	0	0	0	0
30	L39E	414	0	0	0	0
31	L40E	439	0	0	0	0
32	L44E	753	0	0	0	0
33	L7A1	935	0	0	0	0
33	L7A2	935	0	0	0	0
34	L15P	752	0	0	0	0
35	L21E	785	0	0	0	0
36	ARF1	1869	0	0	0	0
37	L45A	816	0	0	0	0
38	L46A	586	0	0	0	0
39	L47A	648	0	0	0	0
40	AETN	381	0	0	0	0
All	All	106630	0	1324	15	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 7.

The worst 5 of 15 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)
2:A5S:6:A:H61	2:A5S:119:A:H61	1.37	0.72
2:A5S:57:U:H4'	2:A5S:58:A:O5'	2.06	0.56
2:A5S:41:U:O2'	2:A5S:46:A:N6	2.39	0.54
2:A5S:6:A:H61	2:A5S:119:A:N6	2.05	0.53
2:A5S:6:A:N6	2:A5S:119:A:H61	2.08	0.50

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AL1P	214/216 (99%)	202 (94%)	12 (6%)	0	100	100
4	AL2P	232/234 (99%)	222 (96%)	10 (4%)	0	100	100
5	AL3P	337/339 (99%)	300 (89%)	36 (11%)	1 (0%)	37	60
6	AL4P	249/251 (99%)	235 (94%)	14 (6%)	0	100	100
7	AL5P	166/168 (99%)	152 (92%)	14 (8%)	0	100	100
8	AL6P	179/181 (99%)	167 (93%)	10 (6%)	2 (1%)	12	28
9	ALX0	74/76 (97%)	68 (92%)	6 (8%)	0	100	100
10	L10E	162/164 (99%)	146 (90%)	16 (10%)	0	100	100
11	L13P	138/140 (99%)	125 (91%)	13 (9%)	0	100	100
12	L141	84/86 (98%)	76 (90%)	8 (10%)	0	100	100
12	L142	84/86 (98%)	77 (92%)	7 (8%)	0	100	100
13	L14P	132/134 (98%)	124 (94%)	8 (6%)	0	100	100
14	L15E	167/169 (99%)	160 (96%)	7 (4%)	0	100	100
15	L18E	110/112 (98%)	106 (96%)	4 (4%)	0	100	100
16	L18P	191/193 (99%)	176 (92%)	15 (8%)	0	100	100
17	L19E	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
18	L22P	148/150 (99%)	135 (91%)	12 (8%)	1 (1%)	19	40
19	L23P	79/81 (98%)	75 (95%)	4 (5%)	0	100	100
20	L24E	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
21	L24P	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
22	L29P	61/63 (97%)	55 (90%)	6 (10%)	0	100	100
23	L30E	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
24	L30P	153/155 (99%)	126 (82%)	27 (18%)	0	100	100
25	L31E	73/75 (97%)	66 (90%)	7 (10%)	0	100	100
26	L32E	121/123 (98%)	110 (91%)	11 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	L34E	75/77 (97%)	47 (63%)	26 (35%)	2 (3%)	4	10
28	L37A	63/65 (97%)	56 (89%)	6 (10%)	1 (2%)	8	19
29	L37E	52/54 (96%)	48 (92%)	4 (8%)	0	100	100
30	L39E	47/49 (96%)	39 (83%)	7 (15%)	1 (2%)	5	14
31	L40E	53/55 (96%)	35 (66%)	18 (34%)	0	100	100
32	L44E	90/92 (98%)	85 (94%)	5 (6%)	0	100	100
33	L7A1	121/123 (98%)	120 (99%)	1 (1%)	0	100	100
33	L7A2	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
34	L15P	90/144 (62%)	85 (94%)	5 (6%)	0	100	100
35	L21E	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
36	ARF1	230/232 (99%)	224 (97%)	6 (3%)	0	100	100
37	L45A	99/101 (98%)	73 (74%)	23 (23%)	3 (3%)	3	8
38	L46A	68/70 (97%)	61 (90%)	7 (10%)	0	100	100
39	L47A	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
All	All	4842/4972 (97%)	4452 (92%)	379 (8%)	11 (0%)	45	67

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	AL3P	231	ARG
37	L45A	4	VAL
37	L45A	55	VAL
37	L45A	67	THR
8	AL6P	117	ILE

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	
3	AL1P	189/190 (100%)	188 (100%)	1 (0%)	86	95
4	AL2P	181/181 (100%)	181 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	AL3P	297/297 (100%)	295 (99%)	2 (1%)	81	92
6	AL4P	212/212 (100%)	212 (100%)	0	100	100
7	AL5P	144/144 (100%)	144 (100%)	0	100	100
8	AL6P	157/157 (100%)	157 (100%)	0	100	100
9	ALX0	68/68 (100%)	68 (100%)	0	100	100
10	L10E	137/137 (100%)	137 (100%)	0	100	100
11	L13P	121/121 (100%)	121 (100%)	0	100	100
12	L141	74/74 (100%)	74 (100%)	0	100	100
12	L142	74/74 (100%)	74 (100%)	0	100	100
13	L14P	110/110 (100%)	110 (100%)	0	100	100
14	L15E	146/146 (100%)	146 (100%)	0	100	100
15	L18E	98/98 (100%)	98 (100%)	0	100	100
16	L18P	162/162 (100%)	161 (99%)	1 (1%)	84	93
17	L19E	126/126 (100%)	126 (100%)	0	100	100
18	L22P	131/131 (100%)	130 (99%)	1 (1%)	79	91
19	L23P	74/74 (100%)	73 (99%)	1 (1%)	62	83
20	L24E	50/50 (100%)	50 (100%)	0	100	100
21	L24P	108/108 (100%)	108 (100%)	0	100	100
22	L29P	59/59 (100%)	59 (100%)	0	100	100
23	L30E	83/83 (100%)	83 (100%)	0	100	100
24	L30P	136/136 (100%)	136 (100%)	0	100	100
25	L31E	66/66 (100%)	66 (100%)	0	100	100
26	L32E	106/106 (100%)	104 (98%)	2 (2%)	52	77
27	L34E	70/70 (100%)	70 (100%)	0	100	100
28	L37A	53/53 (100%)	53 (100%)	0	100	100
29	L37E	45/45 (100%)	44 (98%)	1 (2%)	47	74
30	L39E	44/44 (100%)	44 (100%)	0	100	100
31	L40E	50/50 (100%)	50 (100%)	0	100	100
32	L44E	84/84 (100%)	84 (100%)	0	100	100
33	L7A1	104/104 (100%)	104 (100%)	0	100	100
33	L7A2	104/104 (100%)	102 (98%)	2 (2%)	52	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	L15P	78/118 (66%)	78 (100%)	0	100	100
35	L21E	85/85 (100%)	85 (100%)	0	100	100
36	ARF1	199/199 (100%)	198 (100%)	1 (0%)	86	95
37	L45A	91/91 (100%)	90 (99%)	1 (1%)	70	87
38	L46A	66/66 (100%)	65 (98%)	1 (2%)	60	82
39	L47A	74/74 (100%)	74 (100%)	0	100	100
All	All	4256/4297 (99%)	4242 (100%)	14 (0%)	90	97

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	L32E	7	LYS
29	L37E	41	ARG
38	L46A	67	LYS
36	ARF1	242	LYS
37	L45A	87	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A23S	2988/3022 (98%)	561 (18%)	42 (1%)
2	A5S	121/122 (99%)	19 (15%)	2 (1%)
40	AETN	16/19 (84%)	4 (25%)	1 (6%)
All	All	3125/3163 (98%)	584 (18%)	45 (1%)

5 of 584 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A23S	7	G
1	A23S	25	C
1	A23S	29	U
1	A23S	30	C
1	A23S	31	G

5 of 45 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A23S	1689	C
1	A23S	2429	A
1	A23S	1706	U
1	A23S	1776	G
1	A23S	2598	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](#)

There are no ligands in this entry.

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.

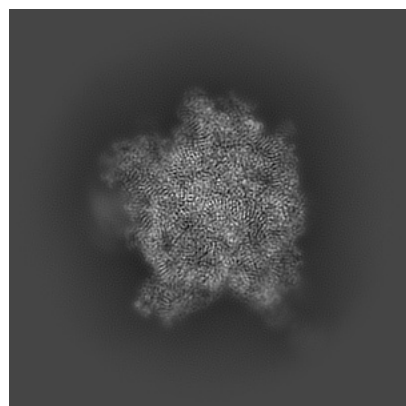
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34860. These allow visual inspection of the internal detail of the map and identification of artifacts.

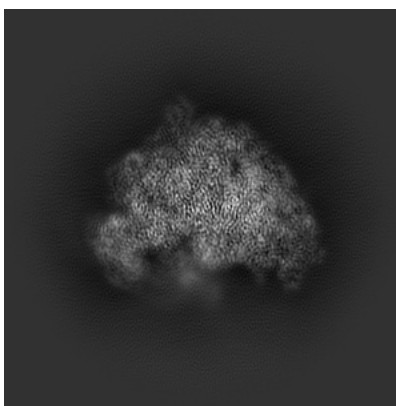
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

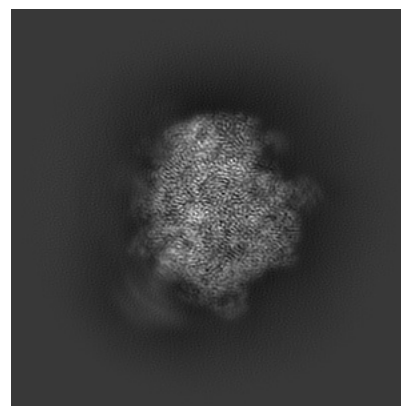
6.1.1 Primary map



X

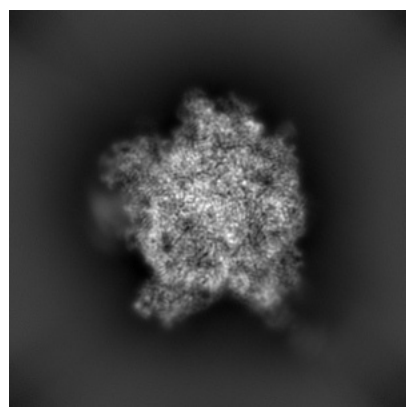


Y

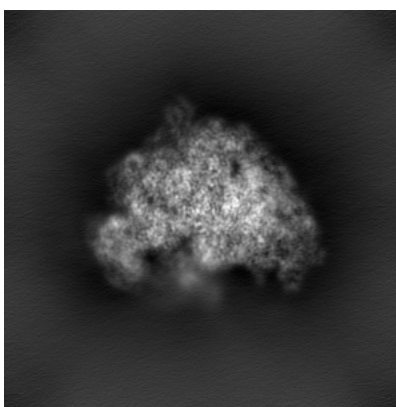


Z

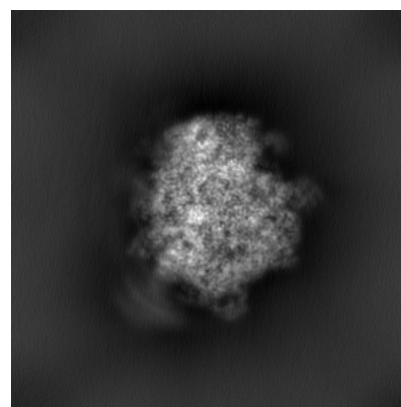
6.1.2 Raw map



X



Y

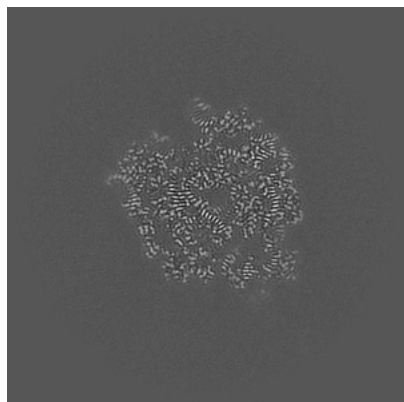


Z

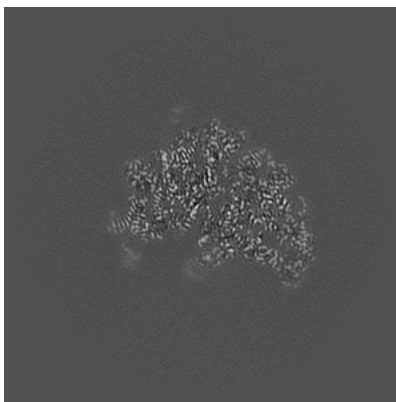
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

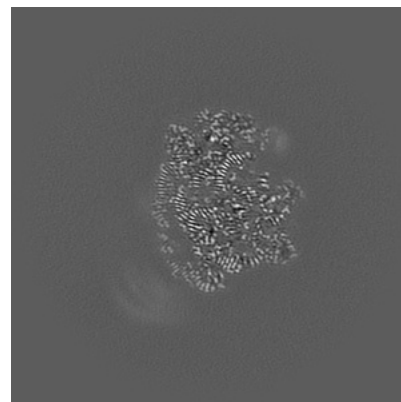
6.2.1 Primary map



X Index: 180

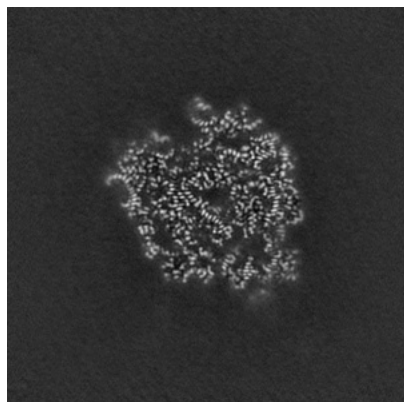


Y Index: 180

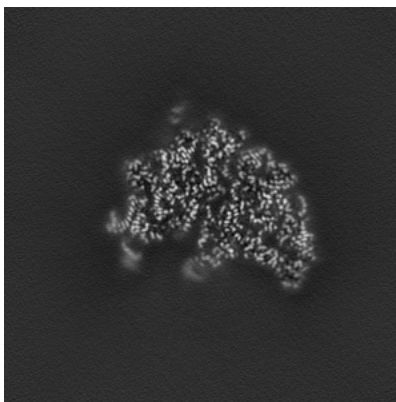


Z Index: 180

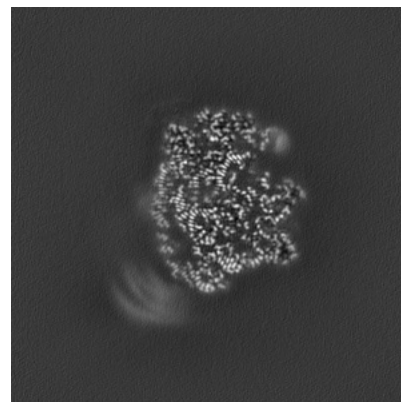
6.2.2 Raw map



X Index: 180



Y Index: 180

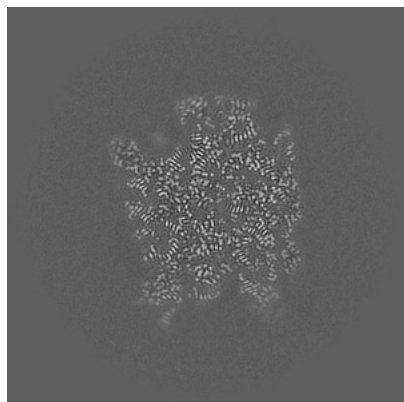


Z Index: 180

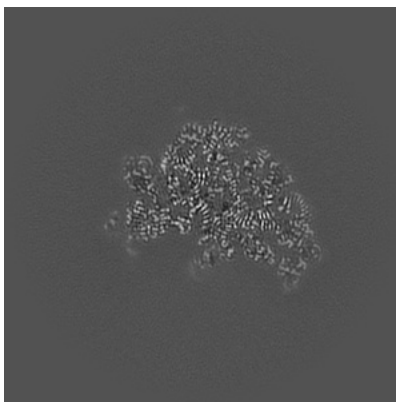
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

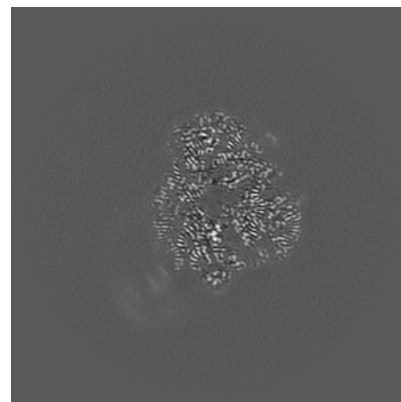
6.3.1 Primary map



X Index: 169

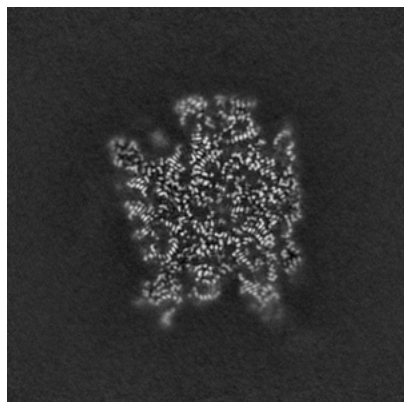


Y Index: 176

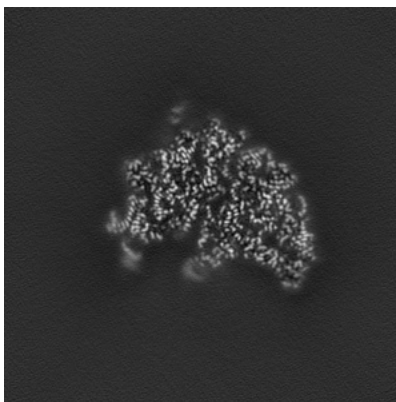


Z Index: 191

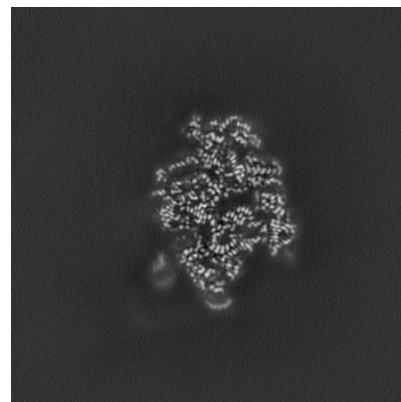
6.3.2 Raw map



X Index: 169



Y Index: 180

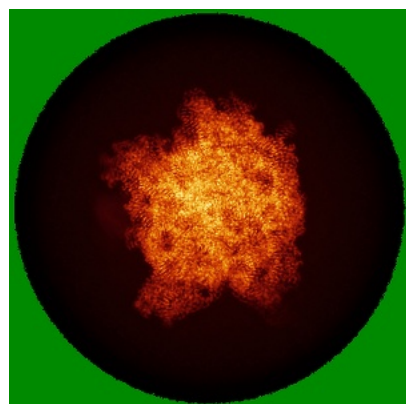


Z Index: 202

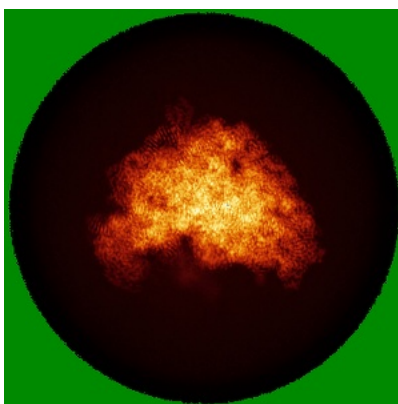
The images above show the largest variance slices of the map in three orthogonal directions.

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

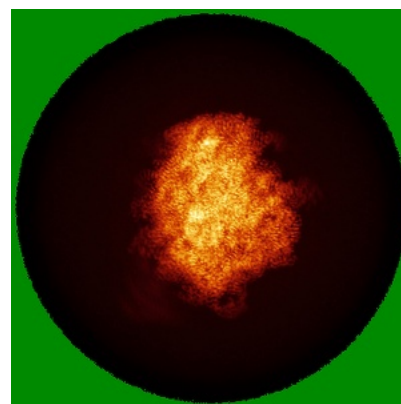
6.4.1 Primary map



X

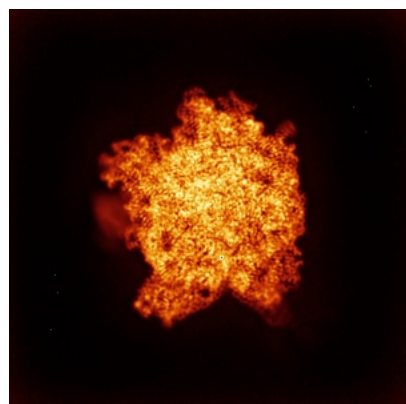


Y

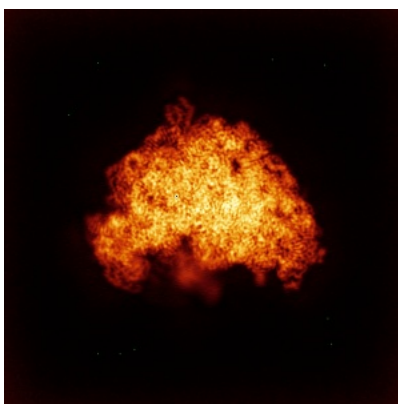


Z

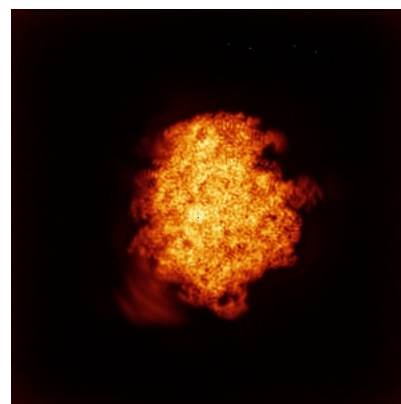
6.4.2 Raw map



X



Y

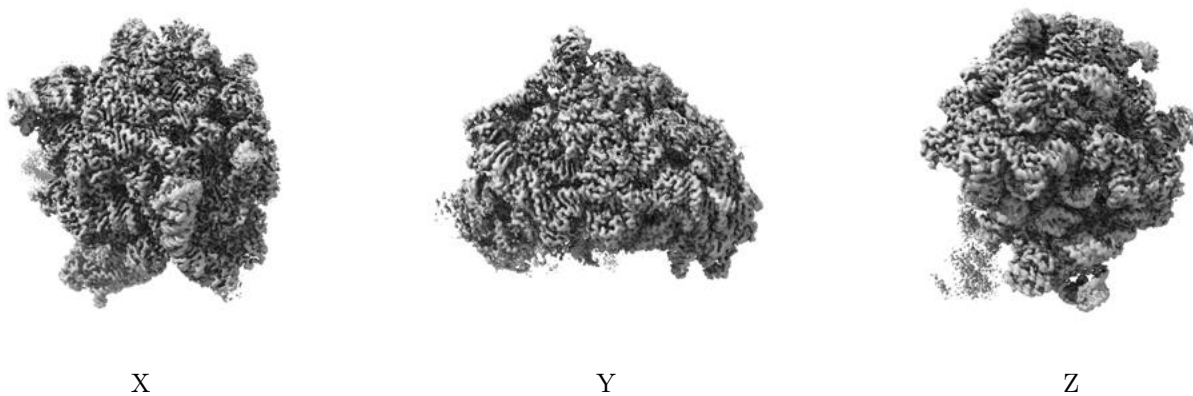


Z

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

6.5.2 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.

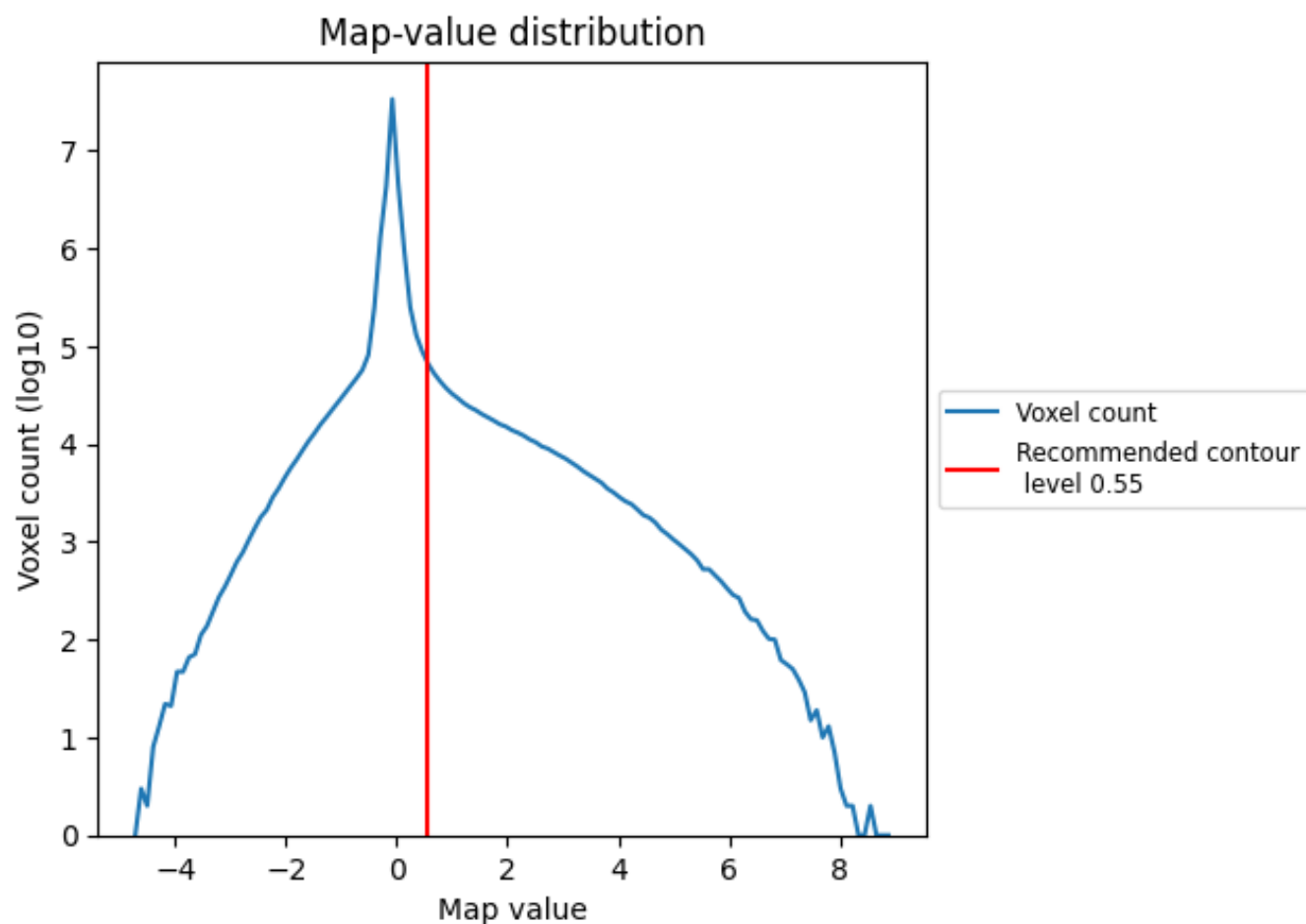
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

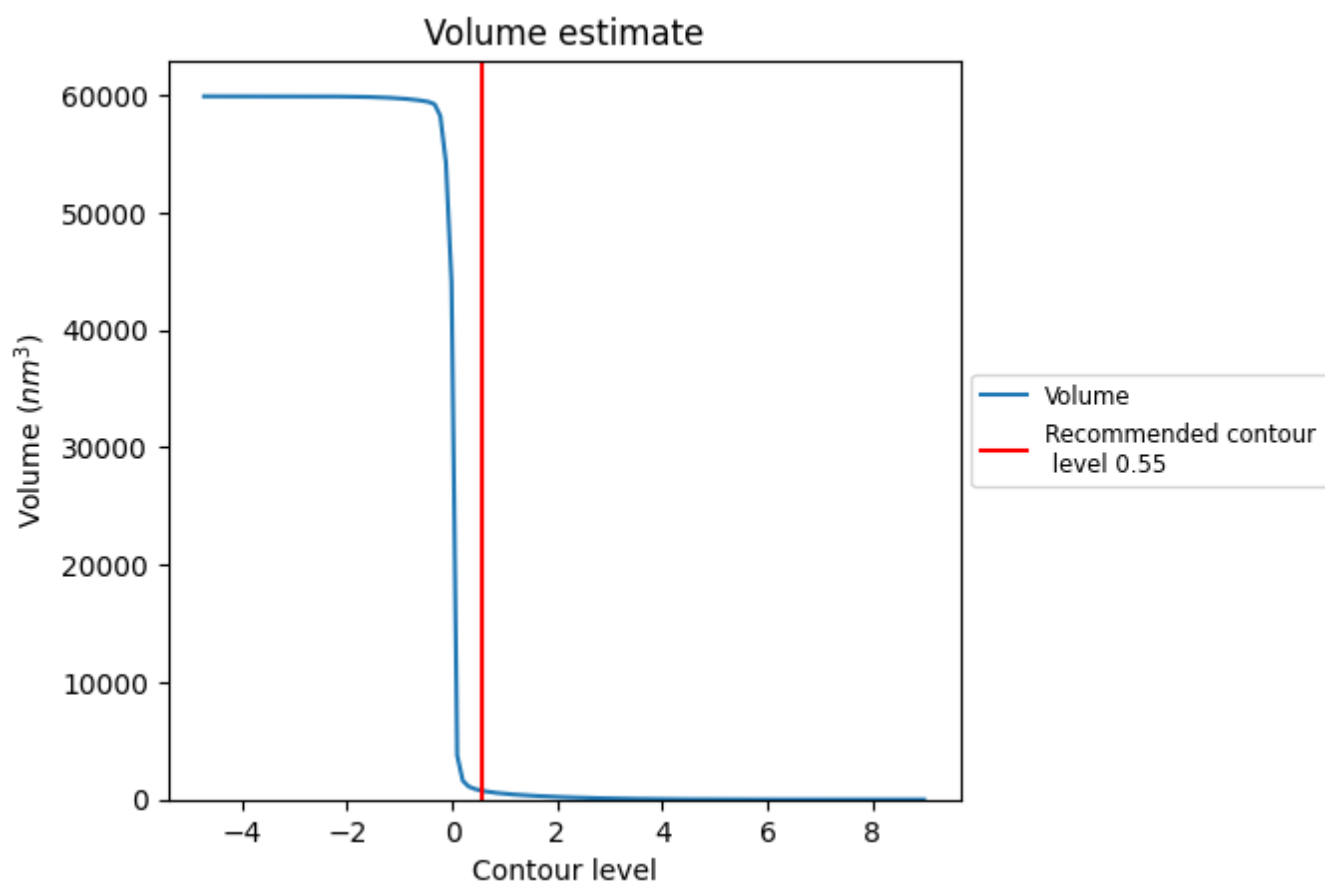
This section contains the results of statistical analysis of the map.

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.

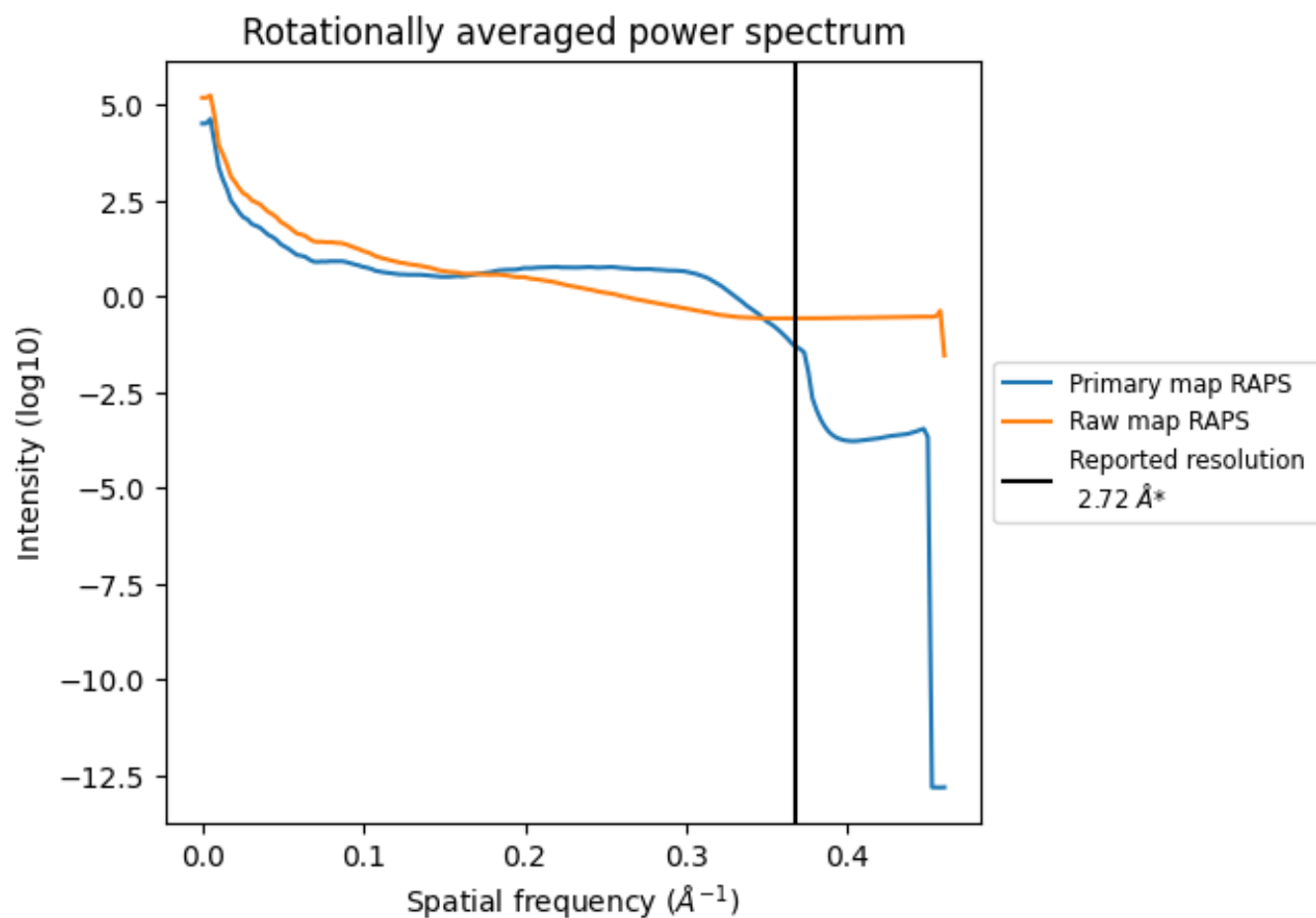
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 772 nm³; this corresponds to an approximate mass of 698 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 ⓘ

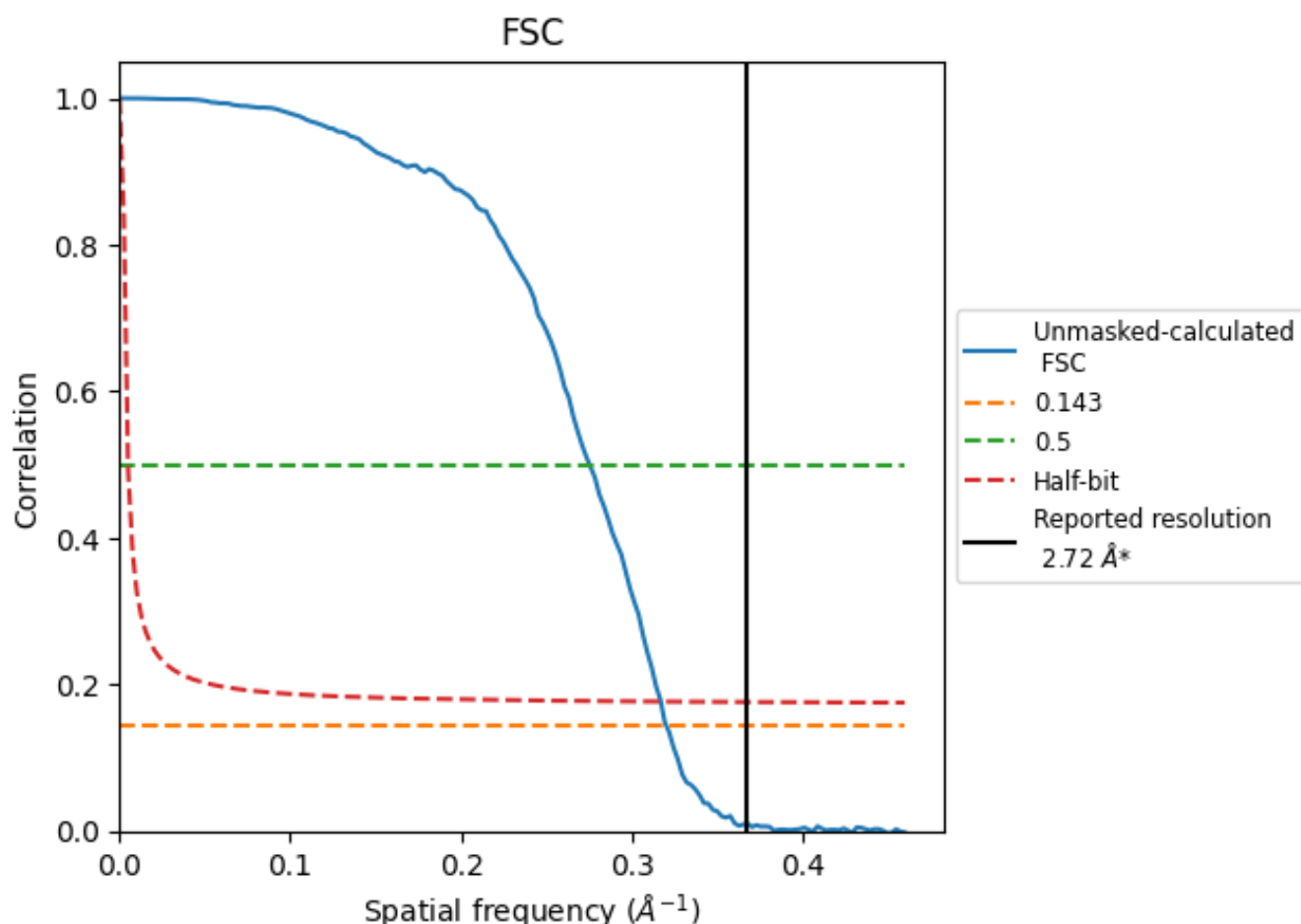


*Reported resolution corresponds to spatial frequency of 0.368 \AA^{-1}

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 0.368 \AA^{-1}

8.2 Resolution estimates [i](#)

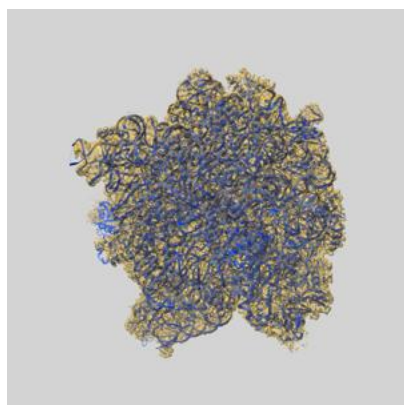
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.72	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.12	3.63	3.15

*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 3.12 differs from the reported value 2.72 by more than 10 %

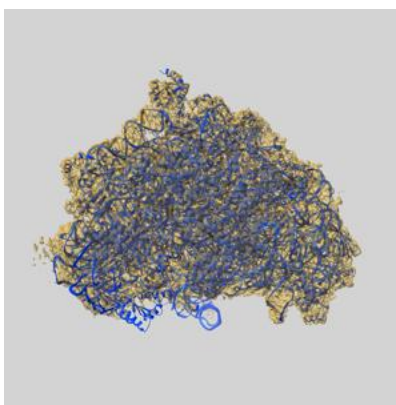
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-34860 and PDB model 8HKU. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

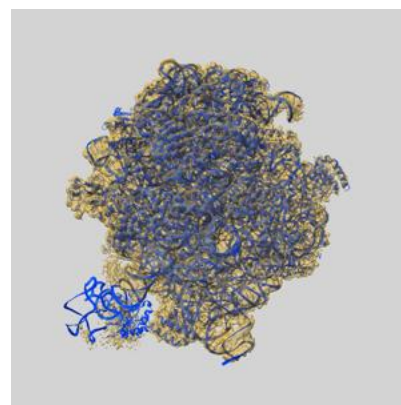
9.1 Map-model overlay [i](#)



X



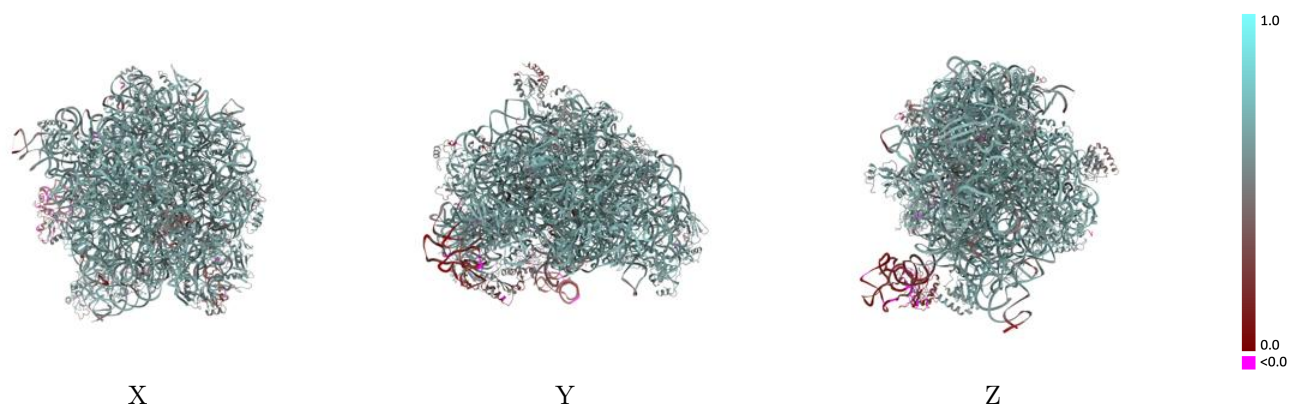
Y



Z

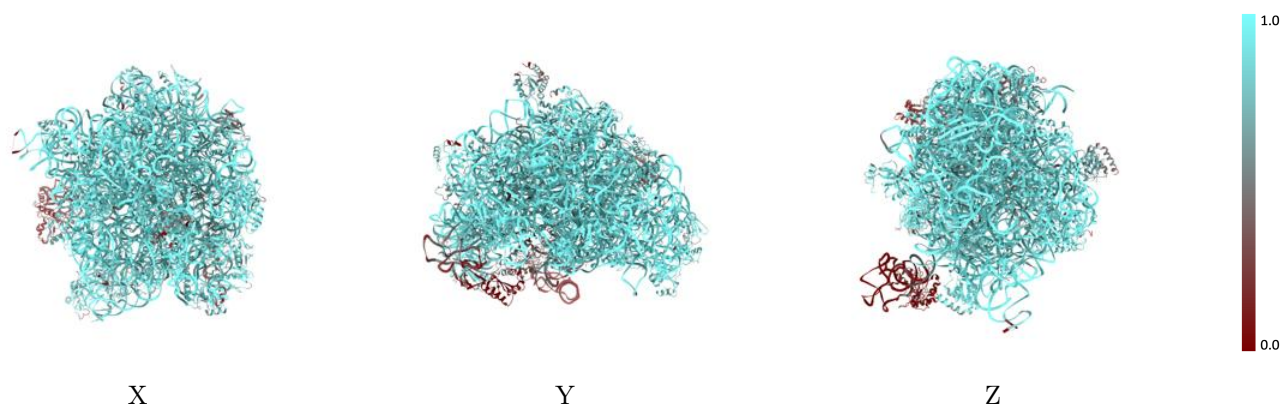
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



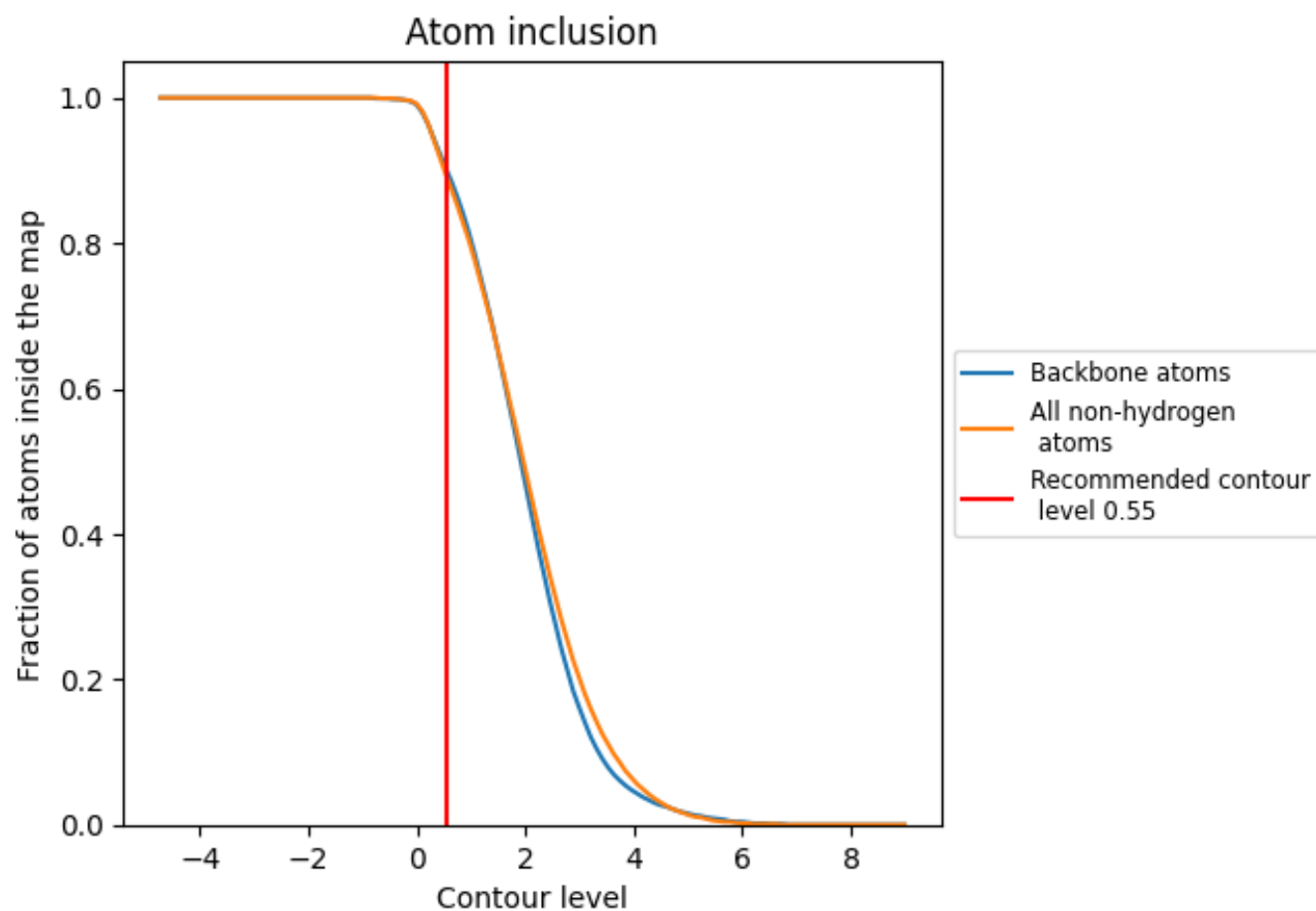
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.55).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 89% 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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8910	 0.5770
A23S	 0.9360	 0.5940
A5S	 0.9820	 0.6060
AETN	 0.5040	 0.4280
AL1P	 0.0250	 0.1530
AL2P	 0.9510	 0.6200
AL3P	 0.9220	 0.5930
AL4P	 0.9460	 0.6100
AL5P	 0.7910	 0.5180
AL6P	 0.8820	 0.5680
ALX0	 0.7660	 0.4840
ARF1	 0.3960	 0.4770
L10E	 0.8870	 0.5850
L13P	 0.8760	 0.5720
L141	 0.8480	 0.5320
L142	 0.8020	 0.5170
L14P	 0.9270	 0.6070
L15E	 0.9570	 0.6260
L15P	 0.9040	 0.5890
L18E	 0.9230	 0.5960
L18P	 0.8840	 0.5550
L19E	 0.9470	 0.6210
L21E	 0.9550	 0.6240
L22P	 0.9400	 0.6160
L23P	 0.8880	 0.5850
L24E	 0.9670	 0.6360
L24P	 0.9150	 0.5910
L29P	 0.8500	 0.5520
L30E	 0.8810	 0.5790
L30P	 0.7830	 0.4880
L31E	 0.9110	 0.5830
L32E	 0.8260	 0.5650
L34E	 0.7230	 0.4090
L37A	 0.9580	 0.6190
L37E	 0.9330	 0.6160



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
L39E	 0.8340	 0.5290
L40E	 0.6600	 0.4210
L44E	 0.9450	 0.6210
L45A	 0.8090	 0.5390
L46A	 0.8110	 0.5590
L47A	 0.5310	 0.5420
L7A1	 0.8740	 0.5770
L7A2	 0.6380	 0.4730