



wwPDB EM Validation Summary Report ⓘ

Jan 2, 2025 – 01:02 AM EST

PDB ID : 9FIA
EMDB ID : EMD-50470
Title : SSU(body) structure derived from the SSU sample of the mitoribosome from *T. gondii*.
Authors : Rocha, R.E.O.; Barua, S.; Boissier, F.; Nguyen, T.T.; Hashem, Y.
Deposited on : 2024-05-28
Resolution : 3.29 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:

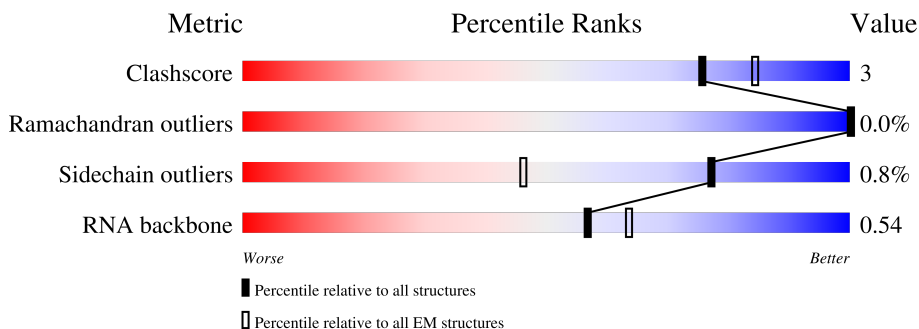
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

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 3.29 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	B0	680	
2	B1	17	
3	B2	738	
4	B3	377	
5	B4	138	
6	B5	393	
7	B6	163	



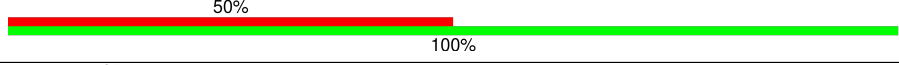
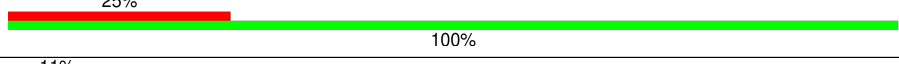
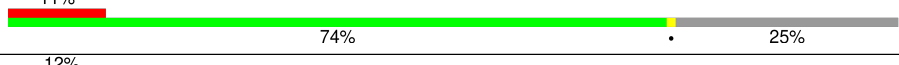
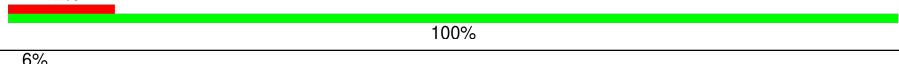
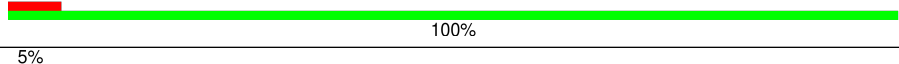
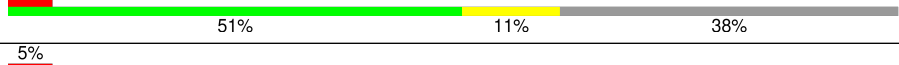
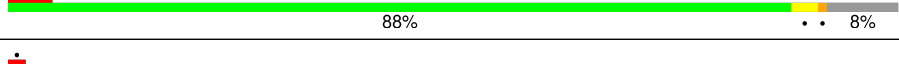

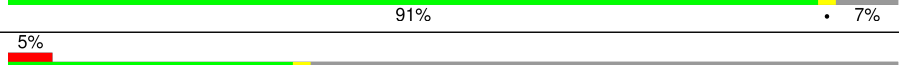


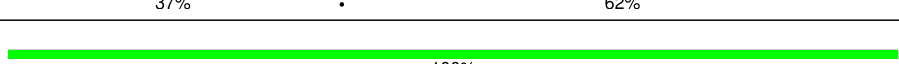
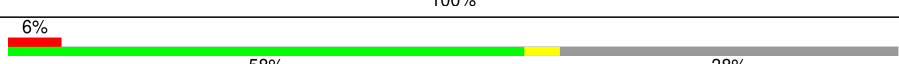
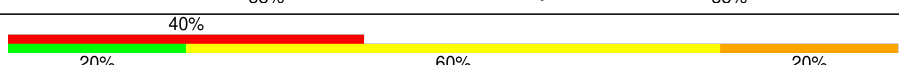
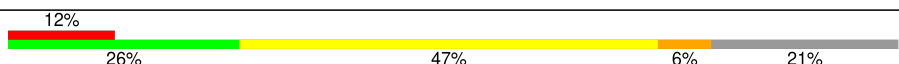
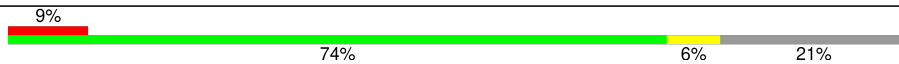
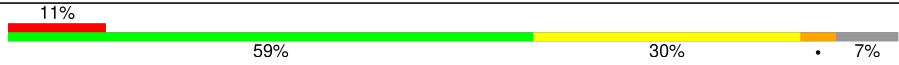

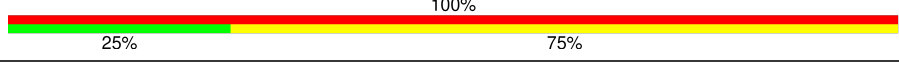
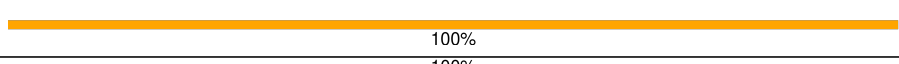
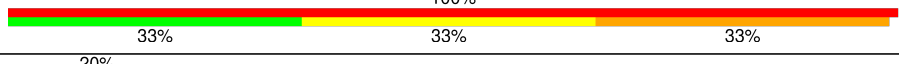


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Mol	Chain	Length	Quality of chain
8	B7	12	67% 100%
9	B8	21	24% 100%
9	Bj	21	100%
10	B9	233	25% 73%
11	BA	939	10% 53% 44%
12	BB	1547	13% 30% 6%
13	BC	421	9% 46% 52%
14	BD	686	16% 41% 8%
15	BE	1053	20% 50% 8%
16	BF	304	17% 77% 12% 11%
17	BG	160	14% 89% 8%
18	BH	129	88% 9%
19	BI	13	100%
19	BN	13	15% 100%
19	BX	13	8% 100%
20	BJ	26	27% 100%
21	BK	530	35% 63%
22	BL	116	79% 9% 11%
23	BO	395	63% 35%
24	BP	47	9% 100%
25	BQ	698	8% 59% 6% 35%
26	BS	243	24% 60% 5% 36%
27	BT	280	32% 64%
28	BU	14	29% 100%
29	BV	597	5% 43% 56%

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Mol	Chain	Length	Quality of chain
30	BW	547	
31	BY	11	
32	Ba	10	
33	Bb	8	
34	Bc	716	
35	Bd	33	
36	Be	18	
37	Bg	302	
38	Bh	167	
39	Bi	268	
40	Bk	447	
41	Bl	593	
42	HJ	1140	
43	HS	235	
44	b1	8	
45	b2	48	
46	b3	5	
47	b4	34	
48	bA	34	
49	bD	27	
50	bE	107	
51	bG	4	
52	bH	2	
53	bI	3	
54	bJ	71	

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Mol	Chain	Length	Quality of chain
55	bK	83	
56	bL	48	
57	bN	122	
58	bO	115	
59	bP	15	
60	bQ	14	
61	bR	31	
62	bS	31	
63	bT	60	
64	bU	25	
65	bV	6	
66	bY	11	

2 Entry composition [i](#)

There are 66 unique types of molecules in this entry. The entry contains 80775 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Mitochondrial ribosomal protein, mS145.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B0	278	2311	1461	428	414	8	0	0

- Molecule 2 is a protein called unidentified peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	B1	17	68	34	17	17	0	0

- Molecule 3 is a protein called Ribosomal protein S18, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B2	335	2790	1755	522	502	11	0	0

- Molecule 4 is a protein called Mitochondrial ribosomal protein, mS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	B3	218	1735	1092	329	303	11	0	0

- Molecule 5 is a protein called CHCH domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B4	80	663	434	120	106	3	0	0

- Molecule 6 is a protein called Ribosomal protein S11, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	B5	140	1109	692	229	184	4	0	0

- Molecule 7 is a protein called Putative mitochondrial ribosomal protein s6-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	B6	113	943	606	183	150	4	0	0

- Molecule 8 is a protein called unidentified peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	B7	12	48	24	12	12	0	0

- Molecule 9 is a protein called unidentified peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	B8	21	84	42	21	21	0	0
9	Bj	21	84	42	21	21	0	0

- Molecule 10 is a protein called DnaJ domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	B9	62	531	340	99	91	1	0	0

- Molecule 11 is a protein called Mitochondrial ribosomal protein, mS137.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	BA	526	4093	2596	723	759	15	0	0

- Molecule 12 is a protein called RAP domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	BB	546	4313	2744	793	755	21	0	0

- Molecule 13 is a protein called Mitochondrial ribosomal protein, mS47.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	BC	204	1581	1014	292	269	6	0	0

- Molecule 14 is a protein called Pentatricopeptide repeat domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	BD	341	Total	C	N	O	S	0	0
			2682	1693	498	484	7		

- Molecule 15 is a protein called Mitochondrial ribosomal protein, mS140.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	BE	624	Total	C	N	O	S	0	0
			5085	3236	940	887	22		

- Molecule 16 is a protein called Mitochondrial ribosomal protein, mS147.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	BF	271	Total	C	N	O	S	0	0
			2195	1391	428	370	6		

- Molecule 17 is a protein called Ribosomal protein, uS2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	BG	148	Total	C	N	O	S	0	0
			1187	765	210	204	8		

- Molecule 18 is a protein called Putative ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	BH	125	Total	C	N	O	S	0	0
			998	636	188	166	8		

- Molecule 19 is a protein called unidentified peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
19	BI	13	Total	C	N	O	0	0
			52	26	13	13		
19	BN	13	Total	C	N	O	0	0
			52	26	13	13		
19	BX	13	Total	C	N	O	0	0
			52	26	13	13		

- Molecule 20 is a protein called unidentified peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	BJ	26	Total	C	N	O	0	0
			104	52	26	26		

- Molecule 21 is a protein called Mitochondrial ribosomal protein, mS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BK	198	Total	C	N	O	S	0	0
			1673	1068	307	292	6		

- Molecule 22 is a protein called Putative ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BL	103	Total	C	N	O	S	0	0
			887	570	168	144	5		

- Molecule 23 is a protein called Putative 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BO	257	Total	C	N	O	S	0	0
			2150	1371	419	350	10		

- Molecule 24 is a protein called unidentified peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	BP	47	Total	C	N	O	0	0
			188	94	47	47		

- Molecule 25 is a protein called Macro domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BQ	455	Total	C	N	O	S	0	0
			3588	2295	657	628	8		

- Molecule 26 is a protein called Ribosomal protein, bS21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BS	156	Total	C	N	O	S	0	0
			1305	825	253	225	2		

- Molecule 27 is a protein called Mitochondrial ribosomal protein, mS156.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	BT	100	801	519	148	132	2	0	0

- Molecule 28 is a protein called unidentified peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O			
28	BU	14	56	28	14	14		0	0

- Molecule 29 is a protein called Putative homeodomain containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	BV	262	2181	1410	370	395	6	0	0

- Molecule 30 is a protein called Mitochondrial ribosomal protein, mS144.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	BW	339	2716	1714	489	503	10	0	0

- Molecule 31 is a protein called unidentified peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O			
31	BY	11	44	22	11	11		0	0

- Molecule 32 is a protein called unidentified peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O			
32	Ba	10	40	20	10	10		0	0

- Molecule 33 is a protein called unidentified peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O			
33	Bb	8	32	16	8	8		0	0

- Molecule 34 is a protein called Enoyl-CoA hydratase/isomerase family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	Bc	537	4276	2717	763	779	17	0	0

- Molecule 35 is a protein called unidentified peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
35	Bd	33	132	66	33	33	0	0

- Molecule 36 is a protein called unidentified peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
36	Be	18	72	36	18	18	0	0

- Molecule 37 is a protein called Ribosomal protein, uS2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	Bg	187	1543	997	294	249	3	0	0

- Molecule 38 is a protein called Putative 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	Bh	153	1242	791	229	215	7	0	0

- Molecule 39 is a protein called Mitochondrial ribosomal protein, mS153.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	Bi	119	928	595	163	167	3	0	0

- Molecule 40 is a protein called Mitochondrial ribosomal protein, mS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	Bk	415	3394	2130	645	612	7	0	0

- Molecule 41 is a protein called 30S ribosomal protein S12, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Bl	200	Total	C	N	O	S	0	0
			1660	1044	334	276	6		

- Molecule 42 is a protein called 30S ribosomal protein S5, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	HJ	355	Total	C	N	O	S	0	0
			2916	1851	550	505	10		

- Molecule 43 is a protein called Acylphosphatase-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	HS	90	Total	C	N	O	S	0	0
			720	450	141	127	2		

- Molecule 44 is a RNA chain called ulr11.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	b1	8	Total	C	N	O	P	0	0
			160	72	16	64	8		

- Molecule 45 is a RNA chain called SSUE.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	b2	30	Total	C	N	O	P	0	0
			632	284	112	206	30		

- Molecule 46 is a RNA chain called ulr12.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	b3	5	Total	C	N	O	P	0	0
			100	45	10	40	5		

- Molecule 47 is a RNA chain called RNA13.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	b4	27	Total	C	N	O	P	0	0
			585	260	108	190	27		

- Molecule 48 is a RNA chain called RNA19.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	bA	27	Total	C	N	O	P	0	0
			571	255	93	196	27		

- Molecule 49 is a RNA chain called RNA15.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	bD	25	Total	C	N	O	P	0	0
			546	243	106	172	25		

- Molecule 50 is a RNA chain called RNA8.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	bE	92	Total	C	N	O	P	0	0
			1965	879	355	639	92		

- Molecule 51 is a RNA chain called ulr13.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	bG	4	Total	C	N	O	P	0	0
			80	36	8	32	4		

- Molecule 52 is a RNA chain called ulr14.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	bH	2	Total	C	N	O	P	0	0
			40	18	4	16	2		

- Molecule 53 is a RNA chain called ulr15.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	bI	3	Total	C	N	O	P	0	0
			60	27	6	24	3		

- Molecule 54 is a RNA chain called RNA33.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	bJ	58	Total	C	N	O	P	0	0
			1220	548	203	411	58		

- Molecule 55 is a RNA chain called RNA5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
55	bK	66	1397	628	246	457	66	0	0

- Molecule 56 is a RNA chain called RNA17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
56	bL	48	1019	456	176	339	48	0	0

- Molecule 57 is a RNA chain called SSUB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
57	bN	50	1069	477	187	355	50	0	0

- Molecule 58 is a RNA chain called SSUA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
58	bO	115	2451	1099	445	792	115	0	0

- Molecule 59 is a RNA chain called ulr16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
59	bP	15	300	135	30	120	15	0	0

- Molecule 60 is a RNA chain called ulr17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
60	bQ	14	280	126	28	112	14	0	0

- Molecule 61 is a RNA chain called RNA30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
61	bR	19	408	183	77	129	19	0	0

- Molecule 62 is a RNA chain called url18.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	bS	31	Total	C	N	O	P	0	0
			620	279	62	248	31		

- Molecule 63 is a RNA chain called SSUF.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	bT	52	Total	C	N	O	P	0	0
			1128	504	219	353	52		

- Molecule 64 is a RNA chain called ulr19.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	bU	25	Total	C	N	O	P	0	0
			500	225	50	200	25		

- Molecule 65 is a RNA chain called ulr20.

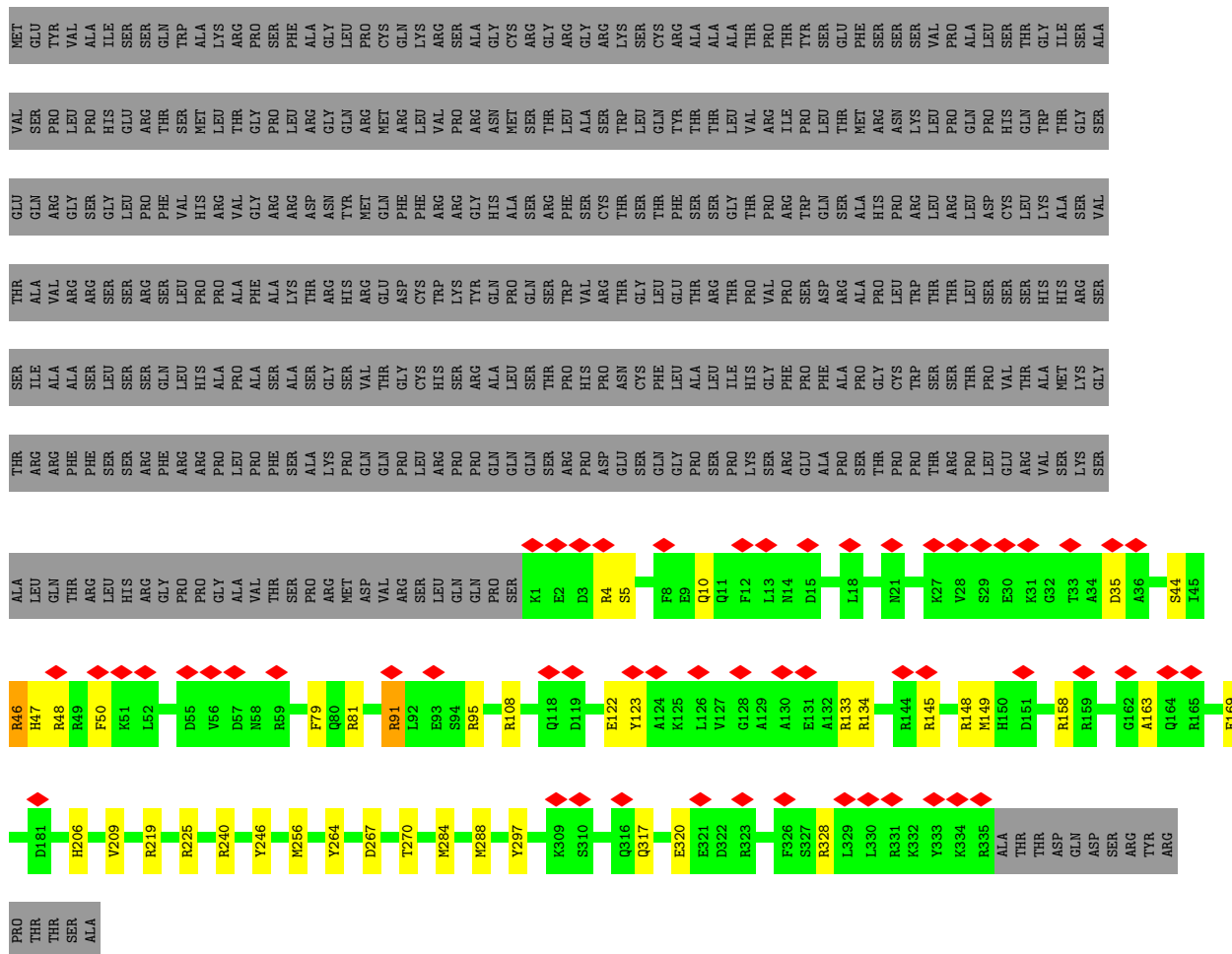
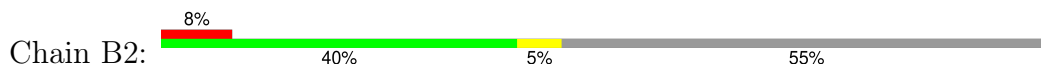
Mol	Chain	Residues	Atoms					AltConf	Trace
65	bV	6	Total	C	N	O	P	0	0
			120	54	12	48	6		

- Molecule 66 is a RNA chain called ulr21.

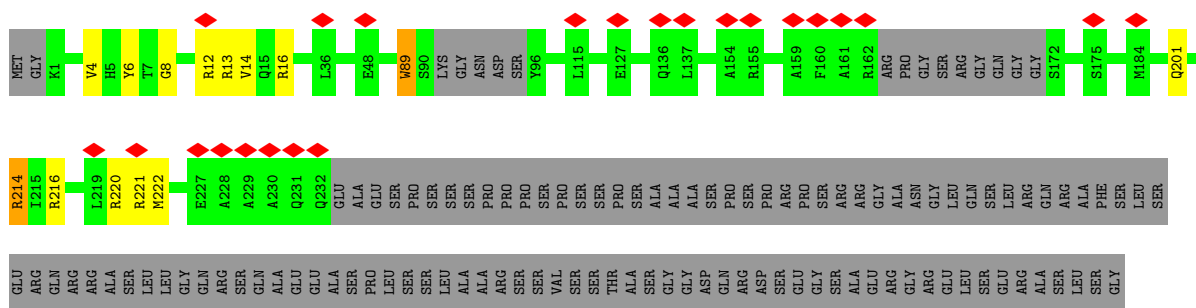
Mol	Chain	Residues	Atoms					AltConf	Trace
66	bY	11	Total	C	N	O	P	0	0
			220	99	22	88	11		

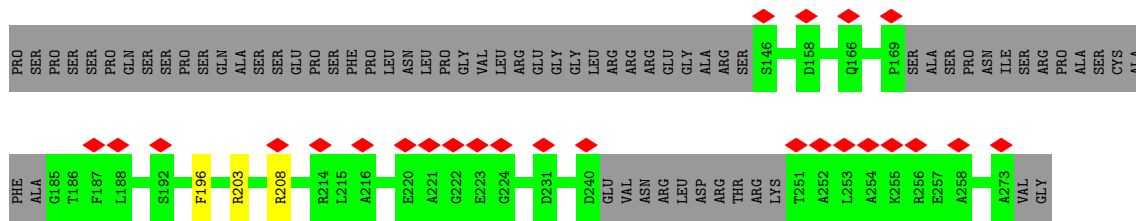


• Molecule 3: Ribosomal protein S18, putative

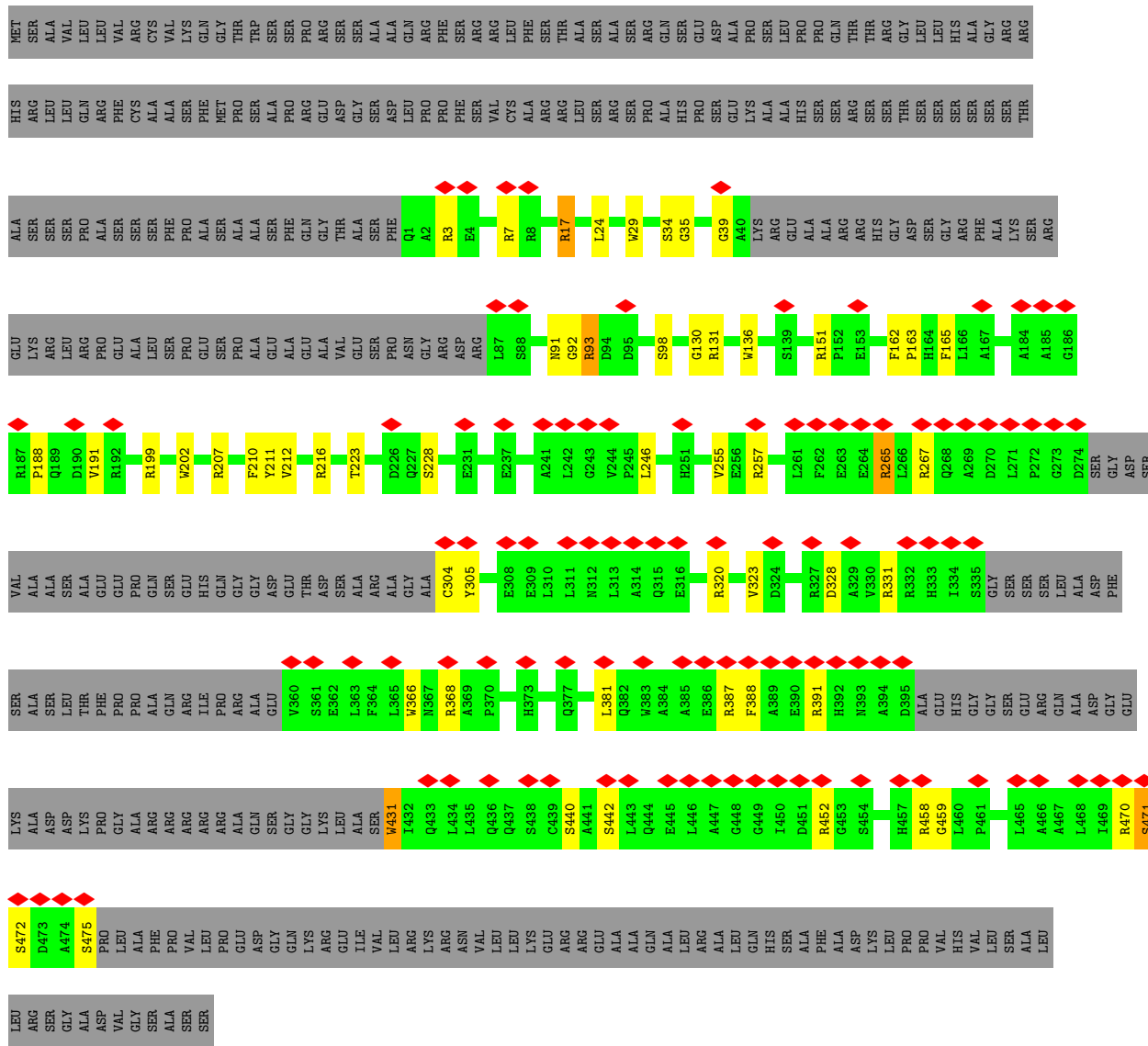


• Molecule 4: Mitochondrial ribosomal protein, mS23

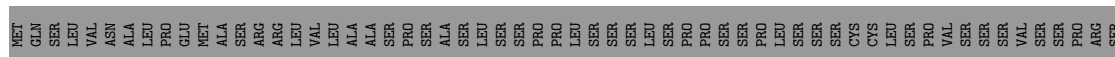


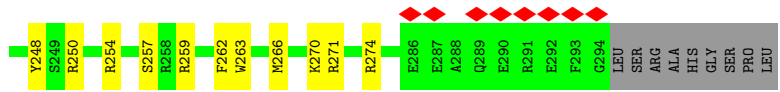
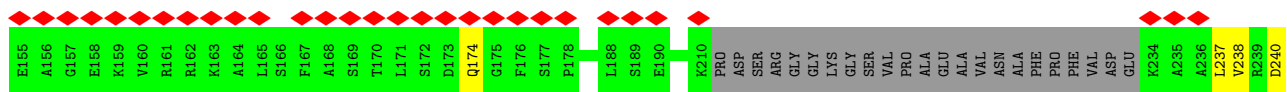


• Molecule 14: Pentatricopeptide repeat domain-containing protein

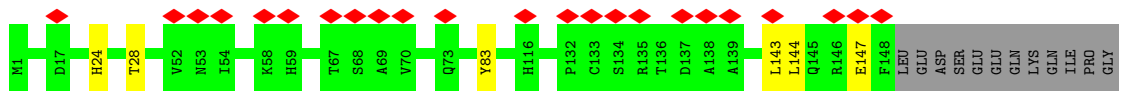
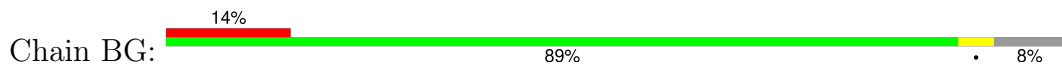


• Molecule 15: Mitochondrial ribosomal protein, mS140

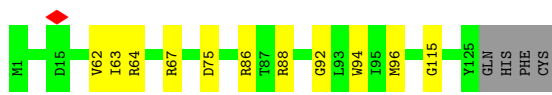
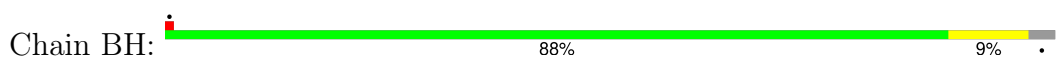




• Molecule 17: Ribosomal protein, uS2m



• Molecule 18: Putative ribosomal protein S8

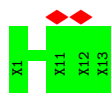


• Molecule 19: unidentified peptide

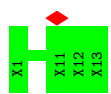


There are no outlier residues recorded for this chain.

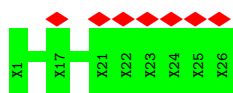
• Molecule 19: unidentified peptide

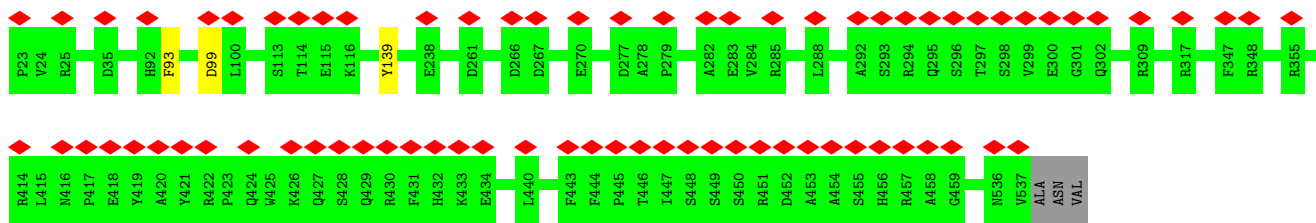


• Molecule 19: unidentified peptide

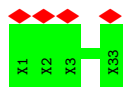


• Molecule 20: unidentified peptide





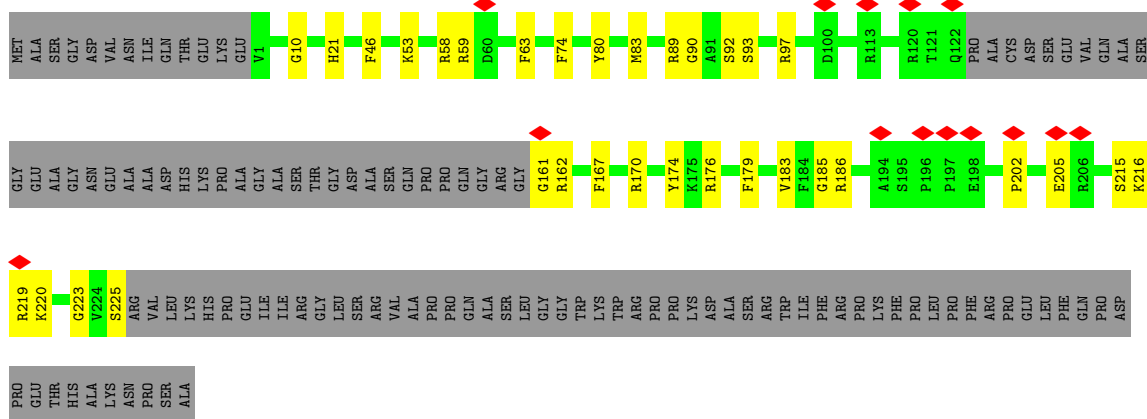
• Molecule 35: unidentified peptide



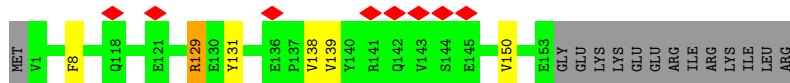
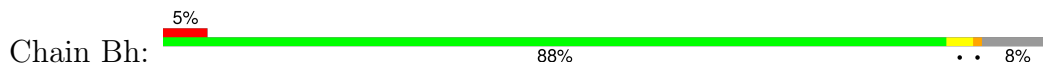
• Molecule 36: unidentified peptide



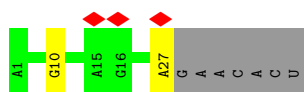
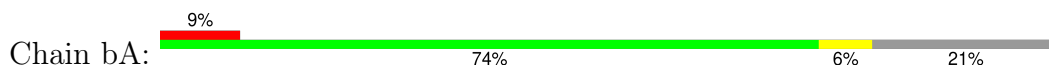
• Molecule 37: Ribosomal protein, uS2m



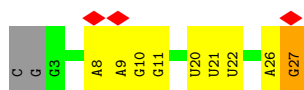
• Molecule 38: Putative 30S ribosomal protein S16



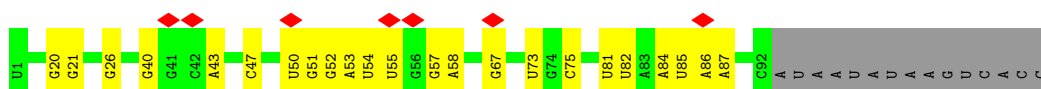
• Molecule 39: Mitochondrial ribosomal protein, mS153



• Molecule 49: RNA15



• Molecule 50: RNA8



• Molecule 51: ulr13



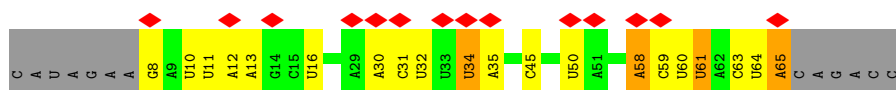
• Molecule 52: ulr14



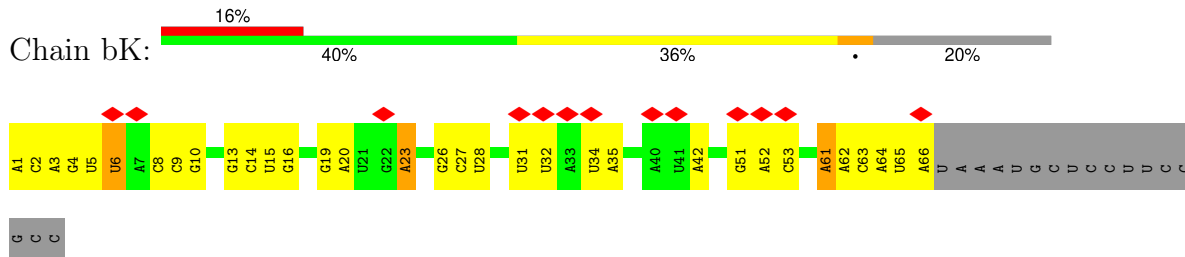
• Molecule 53: ulr15



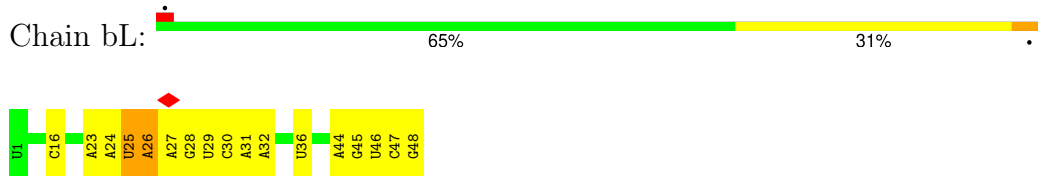
• Molecule 54: RNA33



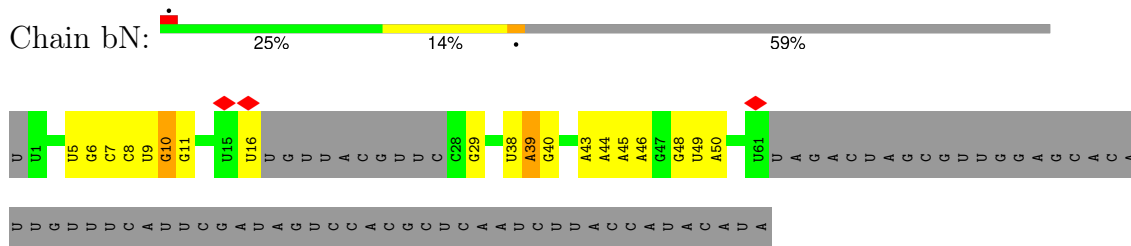
• Molecule 55: RNA5



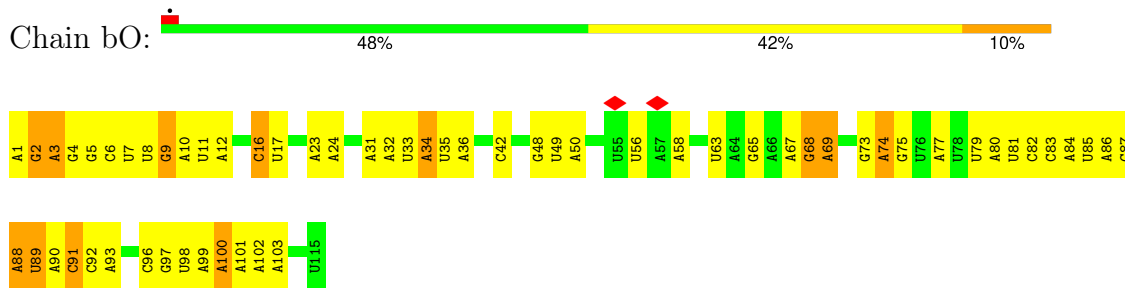
• Molecule 56: RNA17



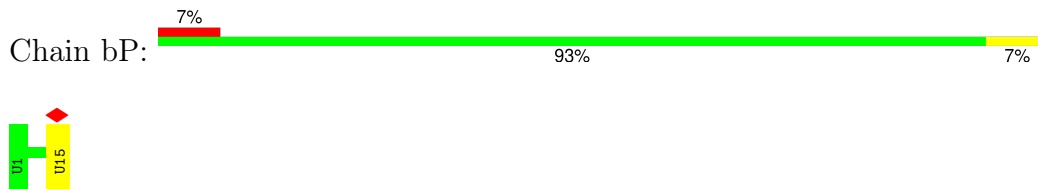
• Molecule 57: SSUB



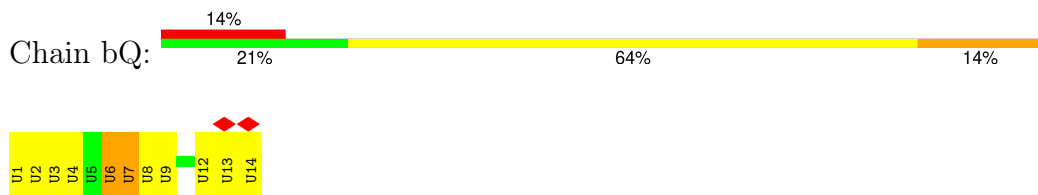
• Molecule 58: SSUA



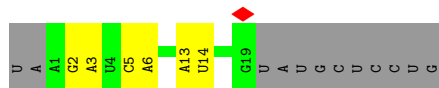
• Molecule 59: ulr16



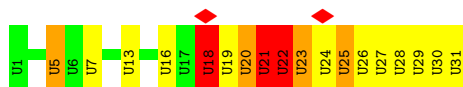
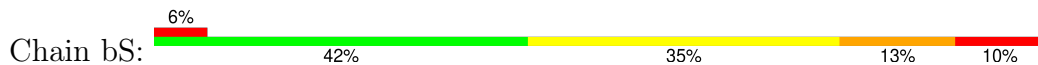
• Molecule 60: ulr17



• Molecule 61: RNA30



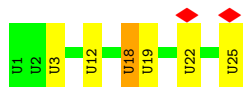
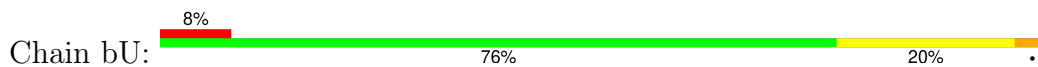
• Molecule 62: url18



• Molecule 63: SSUF



• Molecule 64: ulr19



• Molecule 65: ulr20



• Molecule 66: ulr21



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22169	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	59000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.159	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	632.394, 632.394, 632.394	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.5057, 1.5057, 1.5057	Depositor

5 Model quality i

5.1 Standard geometry i

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	B0	1.81	67/2369 (2.8%)	1.51	16/3204 (0.5%)
3	B2	1.19	23/2853 (0.8%)	1.13	14/3844 (0.4%)
4	B3	1.10	16/1767 (0.9%)	0.98	3/2381 (0.1%)
5	B4	0.56	0/682	0.60	1/914 (0.1%)
6	B5	0.30	0/1129	0.56	0/1513
7	B6	1.71	14/967 (1.4%)	1.52	7/1298 (0.5%)
10	B9	0.78	4/546 (0.7%)	0.68	2/730 (0.3%)
11	BA	0.74	2/4190 (0.0%)	0.71	4/5693 (0.1%)
12	BB	1.63	74/4388 (1.7%)	1.35	24/5925 (0.4%)
13	BC	0.81	11/1617 (0.7%)	0.75	7/2196 (0.3%)
14	BD	1.88	50/2738 (1.8%)	1.55	20/3720 (0.5%)
15	BE	1.35	41/5196 (0.8%)	1.26	23/7021 (0.3%)
16	BF	1.23	23/2259 (1.0%)	1.06	9/3058 (0.3%)
17	BG	0.40	0/1217	0.52	0/1657
18	BH	1.19	10/1015 (1.0%)	0.99	2/1365 (0.1%)
21	BK	0.87	6/1713 (0.4%)	0.87	3/2311 (0.1%)
22	BL	1.33	13/912 (1.4%)	1.22	3/1228 (0.2%)
23	BO	0.39	2/2206 (0.1%)	0.55	0/2975
25	BQ	1.24	32/3683 (0.9%)	1.06	6/5001 (0.1%)
26	BS	0.54	0/1334	0.67	0/1796
27	BT	1.60	11/830 (1.3%)	1.36	5/1131 (0.4%)
29	BV	0.57	3/2242 (0.1%)	0.63	2/3045 (0.1%)
30	BW	1.54	44/2773 (1.6%)	1.29	18/3752 (0.5%)
34	Bc	0.32	0/4386	0.49	0/5958
37	Bg	1.67	35/1602 (2.2%)	1.38	11/2164 (0.5%)
38	Bh	0.93	10/1272 (0.8%)	0.85	3/1710 (0.2%)
39	Bi	1.05	9/947 (1.0%)	0.94	4/1278 (0.3%)
40	Bk	1.06	13/3445 (0.4%)	1.00	5/4624 (0.1%)
41	Bl	0.94	19/1696 (1.1%)	0.85	3/2277 (0.1%)
42	HJ	1.31	45/2987 (1.5%)	1.16	15/4027 (0.4%)
43	HS	0.70	0/733	0.75	0/986
44	b1	1.07	0/175	1.31	0/268
45	b2	0.26	0/705	0.74	0/1094
46	b3	1.30	2/109 (1.8%)	1.52	4/166 (2.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
47	b4	2.73	56/655 (8.5%)	2.68	78/1021 (7.6%)
48	bA	0.35	0/636	0.79	0/988
49	bD	1.36	8/613 (1.3%)	1.55	20/956 (2.1%)
50	bE	0.26	0/2199	0.75	3/3425 (0.1%)
51	bG	1.05	1/87 (1.1%)	1.47	1/132 (0.8%)
52	bH	1.43	0/43	2.22	3/64 (4.7%)
53	bI	0.85	0/65	1.58	2/98 (2.0%)
54	bJ	0.66	3/1361 (0.2%)	1.24	21/2114 (1.0%)
55	bK	2.14	72/1562 (4.6%)	2.09	102/2428 (4.2%)
56	bL	1.59	32/1138 (2.8%)	1.68	47/1770 (2.7%)
57	bN	1.76	38/1194 (3.2%)	1.77	55/1857 (3.0%)
58	bO	2.27	143/2744 (5.2%)	2.19	202/4272 (4.7%)
59	bP	0.80	0/329	1.19	0/506
60	bQ	1.88	10/307 (3.3%)	1.43	0/472
61	bR	1.02	5/457 (1.1%)	1.26	9/710 (1.3%)
62	bS	1.13	0/681	1.97	32/1050 (3.0%)
63	bT	0.61	0/1267	1.12	13/1976 (0.7%)
64	bU	1.05	0/549	1.44	2/846 (0.2%)
65	bV	1.55	4/131 (3.1%)	1.51	3/200 (1.5%)
66	bY	1.19	2/241 (0.8%)	1.26	0/370
All	All	1.27	953/82942 (1.1%)	1.22	807/115565 (0.7%)

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
15	BE	0	1
42	HJ	0	1
52	bH	0	1
62	bS	0	4
63	bT	0	2
All	All	0	9

The worst 5 of 953 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	BE	935	PRO	N-CD	-13.11	1.29	1.47
55	bK	3	A	C6-N6	-12.84	1.23	1.33
56	bL	27	A	C6-N6	-12.63	1.23	1.33
56	bL	26	A	C6-N6	-12.60	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	b4	5	A	C6-N6	-12.57	1.23	1.33

The worst 5 of 807 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	bJ	63	C	O4'-C1'-N1	22.53	126.22	108.20
54	bJ	64	U	O4'-C1'-N1	13.24	118.79	108.20
58	bO	4	G	N7-C8-N9	12.30	119.25	113.10
55	bK	16	G	N7-C8-N9	12.24	119.22	113.10
47	b4	18	A	N1-C2-N3	12.23	135.41	129.30

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	BE	931	TYR	Sidechain
42	HJ	745	ARG	Sidechain
52	bH	1	U	Sidechain
62	bS	18	U	Sidechain
62	bS	5	U	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B0	2311	0	2283	6	0
2	B1	68	0	3	0	0
3	B2	2790	0	2770	12	0
4	B3	1735	0	1758	3	0
5	B4	663	0	684	3	0
6	B5	1109	0	1144	7	0
7	B6	943	0	963	2	0
8	B7	48	0	2	0	0
9	B8	84	0	2	0	0
9	Bj	84	0	3	0	0
10	B9	531	0	533	1	0
11	BA	4093	0	4060	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	BB	4313	0	4430	15	0
13	BC	1581	0	1643	4	0
14	BD	2682	0	2667	13	0
15	BE	5085	0	5150	47	0
16	BF	2195	0	2198	14	0
17	BG	1187	0	1220	4	0
18	BH	998	0	1050	3	0
19	BI	52	0	3	0	0
19	BN	52	0	2	0	0
19	BX	52	0	3	0	0
20	BJ	104	0	3	0	0
21	BK	1673	0	1689	5	0
22	BL	887	0	901	3	0
23	BO	2150	0	2220	8	0
24	BP	188	0	3	0	0
25	BQ	3588	0	3626	15	0
26	BS	1305	0	1320	6	0
27	BT	801	0	804	14	0
28	BU	56	0	2	0	0
29	BV	2181	0	2158	3	0
30	BW	2716	0	2681	22	0
31	BY	44	0	4	3	0
32	Ba	40	0	3	0	0
33	Bb	32	0	2	0	0
34	Bc	4276	0	4207	0	0
35	Bd	132	0	5	0	0
36	Be	72	0	2	0	0
37	Bg	1543	0	1534	0	0
38	Bh	1242	0	1259	0	0
39	Bi	928	0	936	0	0
40	Bk	3394	0	3540	0	0
41	Bl	1660	0	1739	0	0
42	HJ	2916	0	2948	16	0
43	HS	720	0	753	1	0
44	b1	160	0	81	0	0
45	b2	632	0	325	0	0
46	b3	100	0	51	0	0
47	b4	585	0	254	0	0
48	bA	571	0	286	0	0
49	bD	546	0	263	0	0
50	bE	1965	0	990	0	0
51	bG	80	0	41	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	bH	40	0	21	0	0
53	bI	60	0	31	0	0
54	bJ	1220	0	614	0	0
55	bK	1397	0	665	0	0
56	bL	1019	0	493	0	0
57	bN	1069	0	510	0	0
58	bO	2451	0	1152	0	0
59	bP	300	0	151	0	0
60	bQ	280	0	141	0	0
61	bR	408	0	202	0	0
62	bS	620	0	311	0	0
63	bT	1128	0	564	0	0
64	bU	500	0	251	0	0
65	bV	120	0	61	0	0
66	bY	220	0	111	0	0
All	All	80775	0	72479	212	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 3.

The worst 5 of 212 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)
27:BT:45:ARG:HG3	27:BT:51:HIS:CE1	1.46	1.50
27:BT:45:ARG:CG	27:BT:51:HIS:CE1	2.26	1.17
15:BE:971:THR:HG22	15:BE:1010:VAL:CG2	1.81	1.11
15:BE:971:THR:CG2	15:BE:1010:VAL:CG2	2.32	1.07
14:BD:246:LEU:HD12	14:BD:246:LEU:O	1.60	1.00

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B0	274/680 (40%)	259 (94%)	15 (6%)	0	100	100
3	B2	333/738 (45%)	321 (96%)	12 (4%)	0	100	100
4	B3	212/377 (56%)	208 (98%)	4 (2%)	0	100	100
5	B4	76/138 (55%)	75 (99%)	1 (1%)	0	100	100
6	B5	138/393 (35%)	133 (96%)	5 (4%)	0	100	100
7	B6	111/163 (68%)	105 (95%)	6 (5%)	0	100	100
10	B9	60/233 (26%)	60 (100%)	0	0	100	100
11	BA	516/939 (55%)	503 (98%)	13 (2%)	0	100	100
12	BB	518/1547 (34%)	490 (95%)	28 (5%)	0	100	100
13	BC	196/421 (47%)	191 (97%)	5 (3%)	0	100	100
14	BD	331/686 (48%)	312 (94%)	19 (6%)	0	100	100
15	BE	612/1053 (58%)	580 (95%)	30 (5%)	2 (0%)	37	66
16	BF	267/304 (88%)	262 (98%)	5 (2%)	0	100	100
17	BG	146/160 (91%)	141 (97%)	5 (3%)	0	100	100
18	BH	123/129 (95%)	122 (99%)	1 (1%)	0	100	100
21	BK	196/530 (37%)	190 (97%)	6 (3%)	0	100	100
22	BL	101/116 (87%)	101 (100%)	0	0	100	100
23	BO	255/395 (65%)	248 (97%)	7 (3%)	0	100	100
25	BQ	447/698 (64%)	433 (97%)	14 (3%)	0	100	100
26	BS	152/243 (63%)	144 (95%)	8 (5%)	0	100	100
27	BT	98/280 (35%)	88 (90%)	10 (10%)	0	100	100
29	BV	260/597 (44%)	248 (95%)	12 (5%)	0	100	100
30	BW	335/547 (61%)	307 (92%)	28 (8%)	0	100	100
34	Bc	535/716 (75%)	522 (98%)	13 (2%)	0	100	100
37	Bg	183/302 (61%)	164 (90%)	18 (10%)	1 (0%)	25	56
38	Bh	151/167 (90%)	149 (99%)	2 (1%)	0	100	100
39	Bi	111/268 (41%)	109 (98%)	2 (2%)	0	100	100
40	Bk	413/447 (92%)	404 (98%)	9 (2%)	0	100	100
41	Bl	198/593 (33%)	184 (93%)	14 (7%)	0	100	100
42	HJ	349/1140 (31%)	325 (93%)	24 (7%)	0	100	100
43	HS	86/235 (37%)	83 (96%)	3 (4%)	0	100	100
All	All	7783/15235 (51%)	7461 (96%)	319 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	BE	915	PRO
37	Bg	202	PRO
15	BE	935	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B0	238/558 (43%)	234 (98%)	4 (2%)	56	74
3	B2	297/648 (46%)	293 (99%)	4 (1%)	65	79
4	B3	177/302 (59%)	174 (98%)	3 (2%)	56	74
5	B4	72/123 (58%)	71 (99%)	1 (1%)	62	78
6	B5	114/328 (35%)	114 (100%)	0	100	100
7	B6	98/142 (69%)	98 (100%)	0	100	100
10	B9	55/197 (28%)	55 (100%)	0	100	100
11	BA	429/769 (56%)	421 (98%)	8 (2%)	52	72
12	BB	465/1261 (37%)	459 (99%)	6 (1%)	65	79
13	BC	166/351 (47%)	166 (100%)	0	100	100
14	BD	276/548 (50%)	273 (99%)	3 (1%)	70	82
15	BE	541/908 (60%)	539 (100%)	2 (0%)	89	93
16	BF	227/252 (90%)	227 (100%)	0	100	100
17	BG	134/145 (92%)	134 (100%)	0	100	100
18	BH	109/115 (95%)	109 (100%)	0	100	100
21	BK	183/456 (40%)	182 (100%)	1 (0%)	86	91
22	BL	94/106 (89%)	94 (100%)	0	100	100
23	BO	230/346 (66%)	229 (100%)	1 (0%)	89	93
25	BQ	376/572 (66%)	373 (99%)	3 (1%)	79	87
26	BS	137/207 (66%)	134 (98%)	3 (2%)	47	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	BT	86/249 (34%)	84 (98%)	2 (2%)	45	68
29	BV	238/525 (45%)	237 (100%)	1 (0%)	89	93
30	BW	296/475 (62%)	292 (99%)	4 (1%)	62	78
34	Bc	458/620 (74%)	454 (99%)	4 (1%)	75	85
37	Bg	160/251 (64%)	158 (99%)	2 (1%)	65	79
38	Bh	130/143 (91%)	129 (99%)	1 (1%)	79	87
39	Bi	99/221 (45%)	98 (99%)	1 (1%)	73	84
40	Bk	360/385 (94%)	360 (100%)	0	100	100
41	Bl	181/534 (34%)	181 (100%)	0	100	100
42	HJ	307/968 (32%)	305 (99%)	2 (1%)	81	88
43	HS	78/207 (38%)	78 (100%)	0	100	100
All	All	6811/12912 (53%)	6755 (99%)	56 (1%)	77	87

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	BD	452	ARG
42	HJ	862	PHE
25	BQ	433	LYS
42	HJ	812	ARG
34	Bc	139	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
37	Bg	49	HIS
34	Bc	45	ASN
15	BE	929	ASN
12	BB	846	GLN
16	BF	77	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
44	b1	7/8 (87%)	0	0
45	b2	29/48 (60%)	2 (6%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
46	b3	4/5 (80%)	2 (50%)	0
47	b4	26/34 (76%)	3 (11%)	0
48	bA	26/34 (76%)	2 (7%)	0
49	bD	24/27 (88%)	5 (20%)	0
50	bE	90/107 (84%)	22 (24%)	0
51	bG	3/4 (75%)	2 (66%)	0
52	bH	1/2 (50%)	1 (100%)	0
53	bI	2/3 (66%)	2 (100%)	0
54	bJ	57/71 (80%)	16 (28%)	0
55	bK	63/83 (75%)	12 (19%)	0
56	bL	47/48 (97%)	9 (19%)	0
57	bN	48/122 (39%)	7 (14%)	0
58	bO	114/115 (99%)	24 (21%)	0
59	bP	14/15 (93%)	1 (7%)	0
60	bQ	13/14 (92%)	3 (23%)	0
61	bR	18/31 (58%)	4 (22%)	0
62	bS	30/31 (96%)	11 (36%)	0
63	bT	51/60 (85%)	11 (21%)	0
64	bU	24/25 (96%)	6 (25%)	0
65	bV	5/6 (83%)	1 (20%)	0
66	bY	10/11 (90%)	2 (20%)	0
All	All	706/904 (78%)	148 (20%)	0

5 of 148 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
45	b2	31	A
45	b2	48	A
46	b3	4	U
46	b3	5	U
47	b4	2	G

There are no RNA pucker outliers to report.

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.

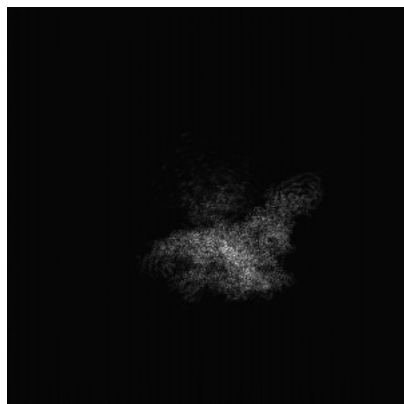
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50470. These allow visual inspection of the internal detail of the map and identification of artifacts.

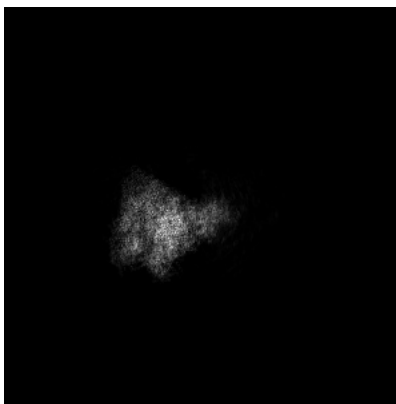
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

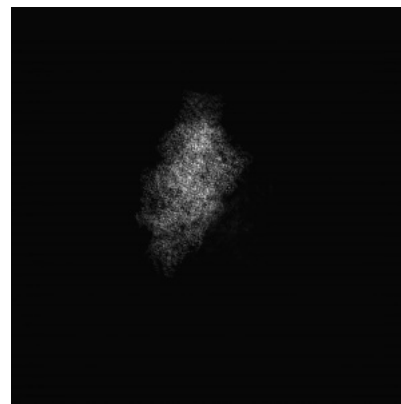
6.1.1 Primary map



X

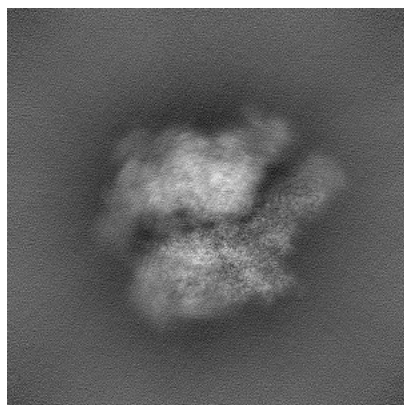


Y

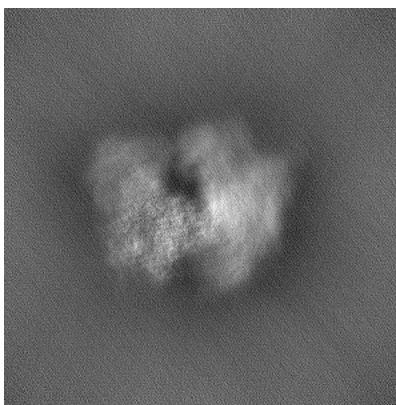


Z

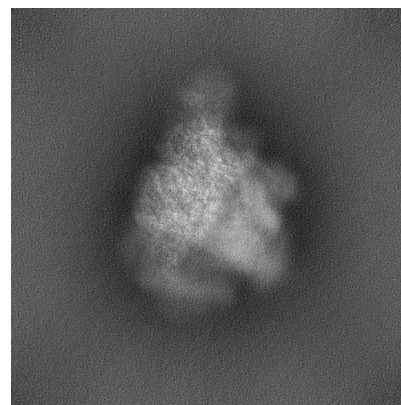
6.1.2 Raw map



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: 210

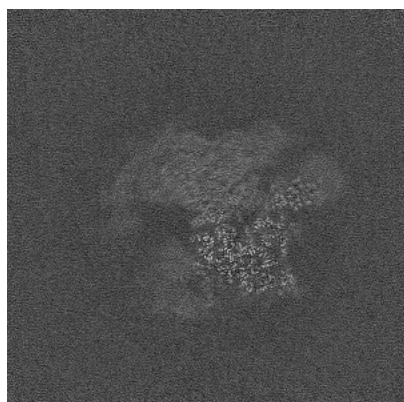


Y Index: 210

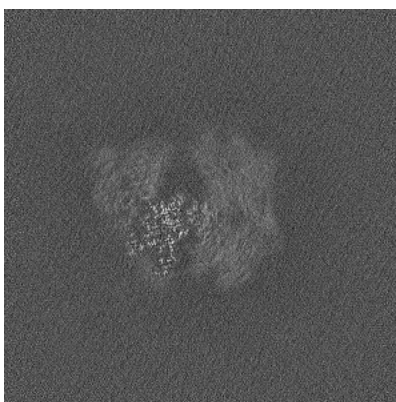


Z Index: 210

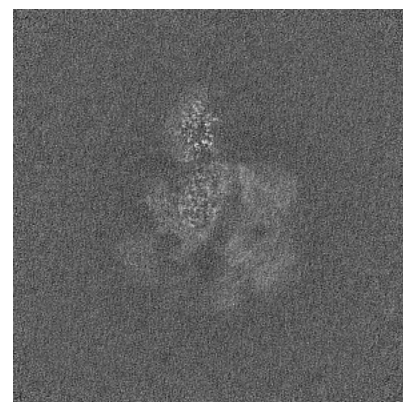
6.2.2 Raw map



X Index: 210



Y Index: 210



Z Index: 210

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

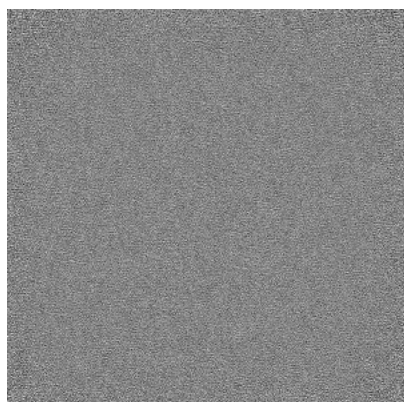


Y Index: 241

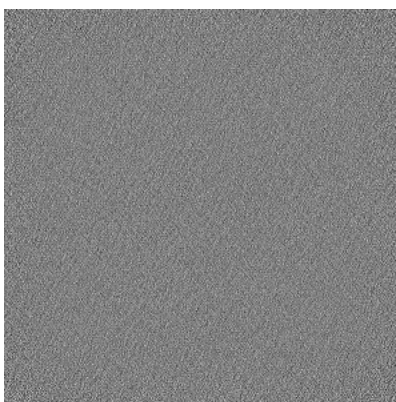


Z Index: 165

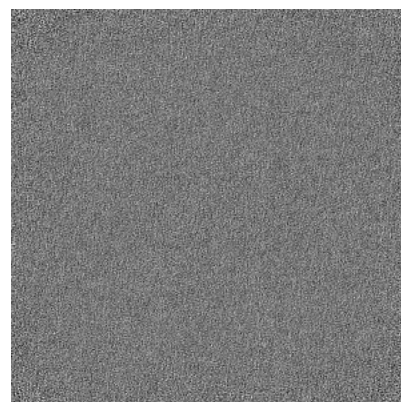
6.3.2 Raw map



X Index: 0



Y Index: 0

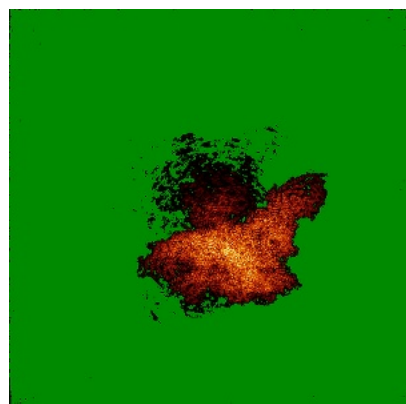


Z Index: 419

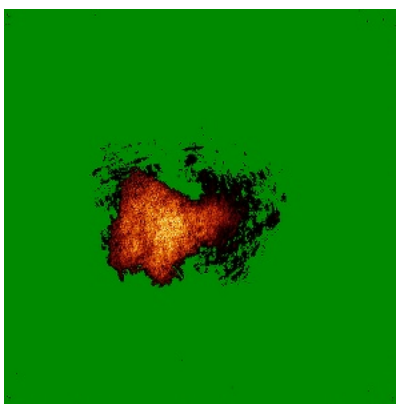
The images above show the largest variance slices of the map in three orthogonal directions.

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

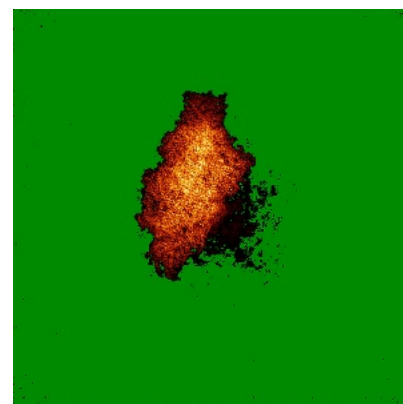
6.4.1 Primary map



X

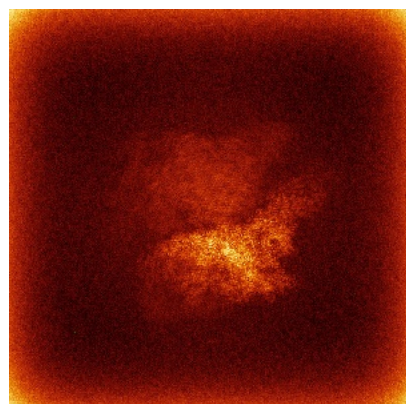


Y

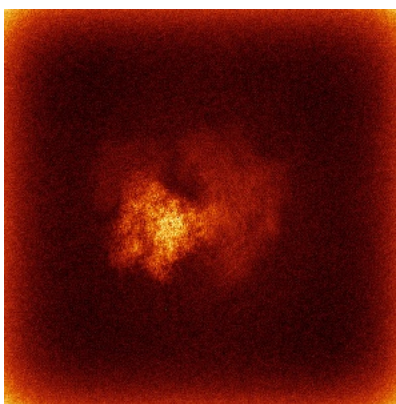


Z

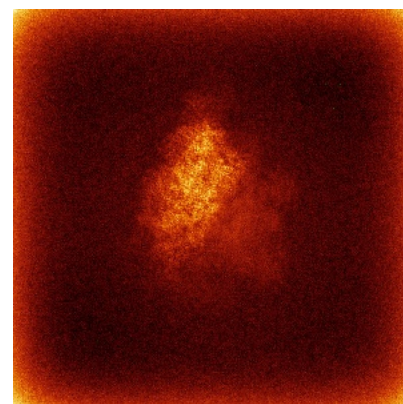
6.4.2 Raw map



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.

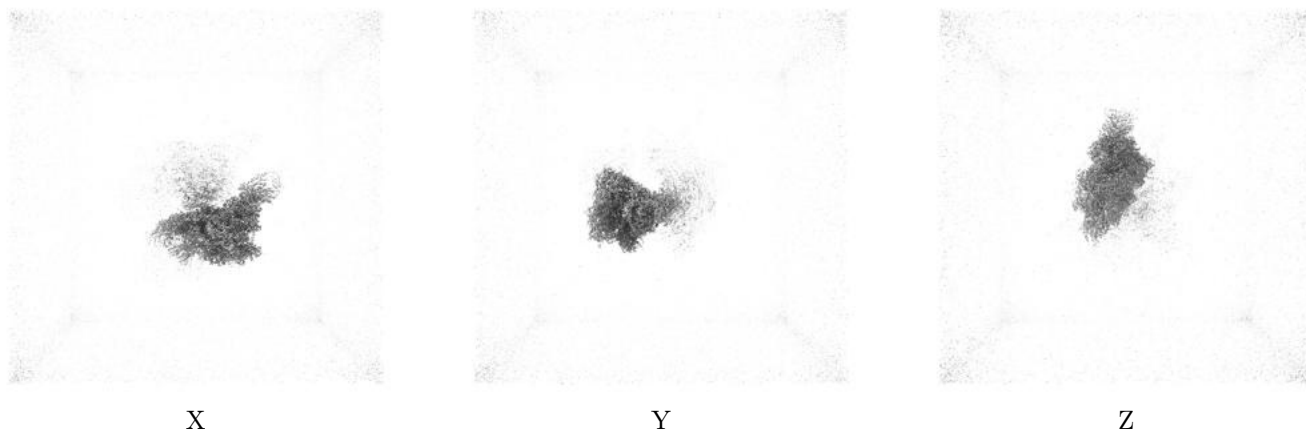
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

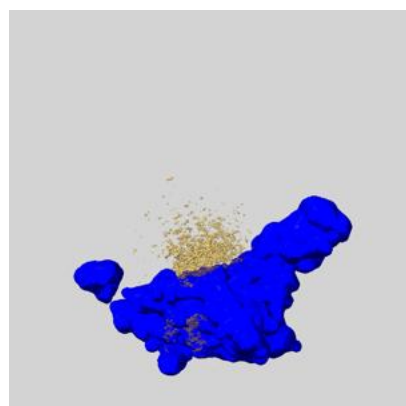
6.6 Mask visualisation [i](#)

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

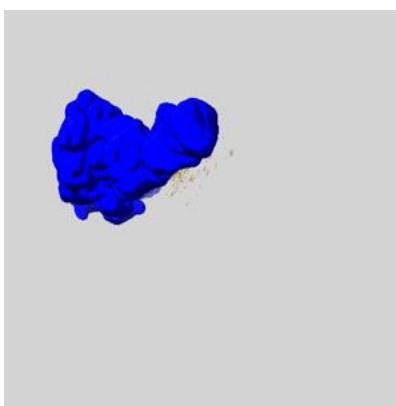
A mask typically either:

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

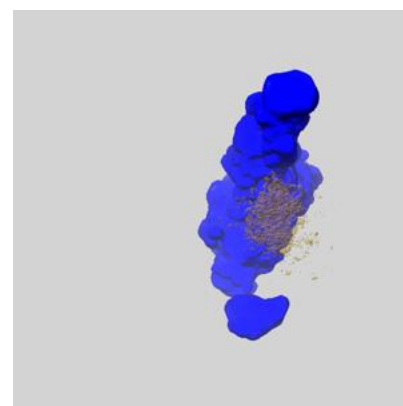
6.6.1 emd_50470_msk_1.map [i](#)



X



Y

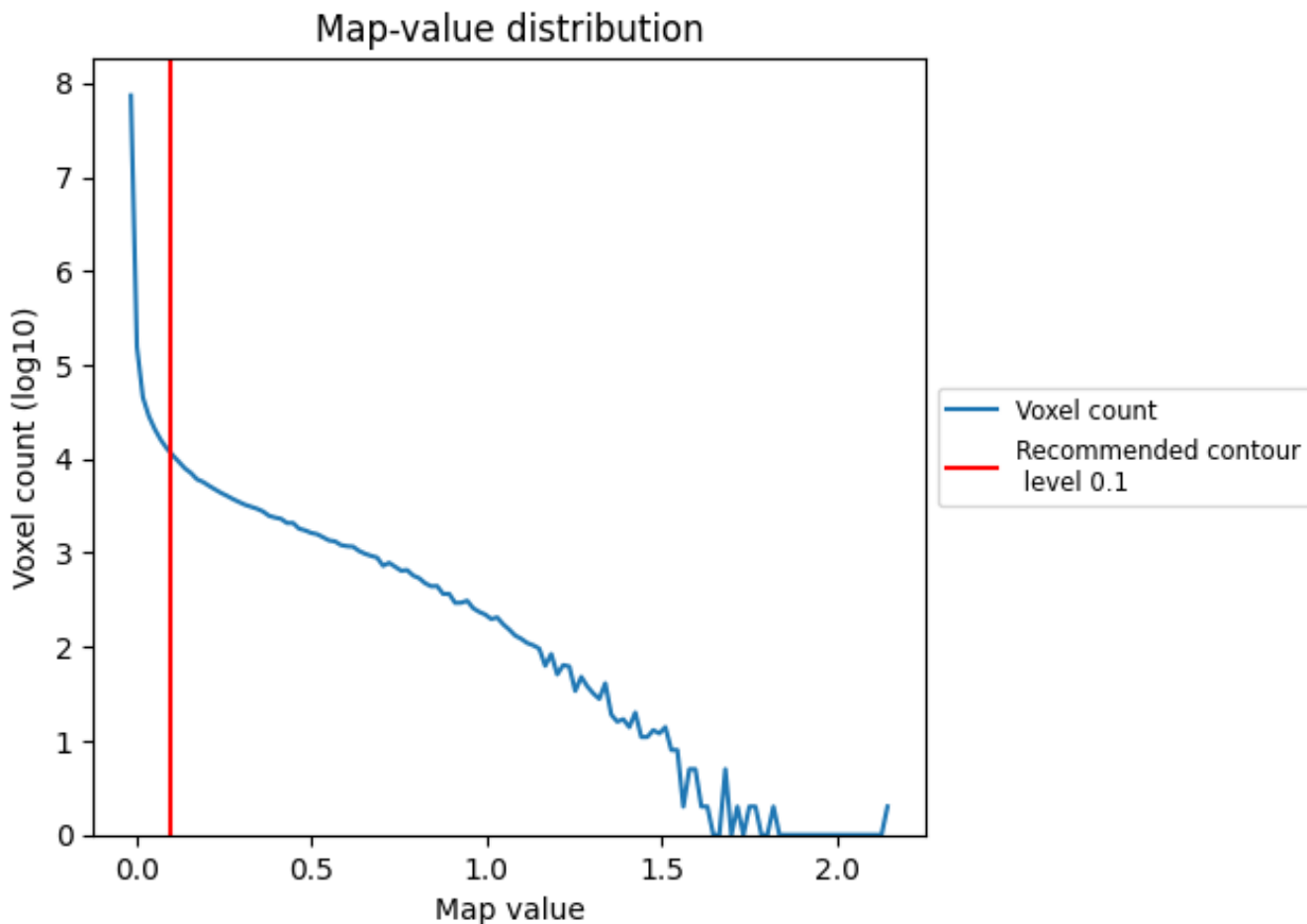


Z

7 Map analysis [i](#)

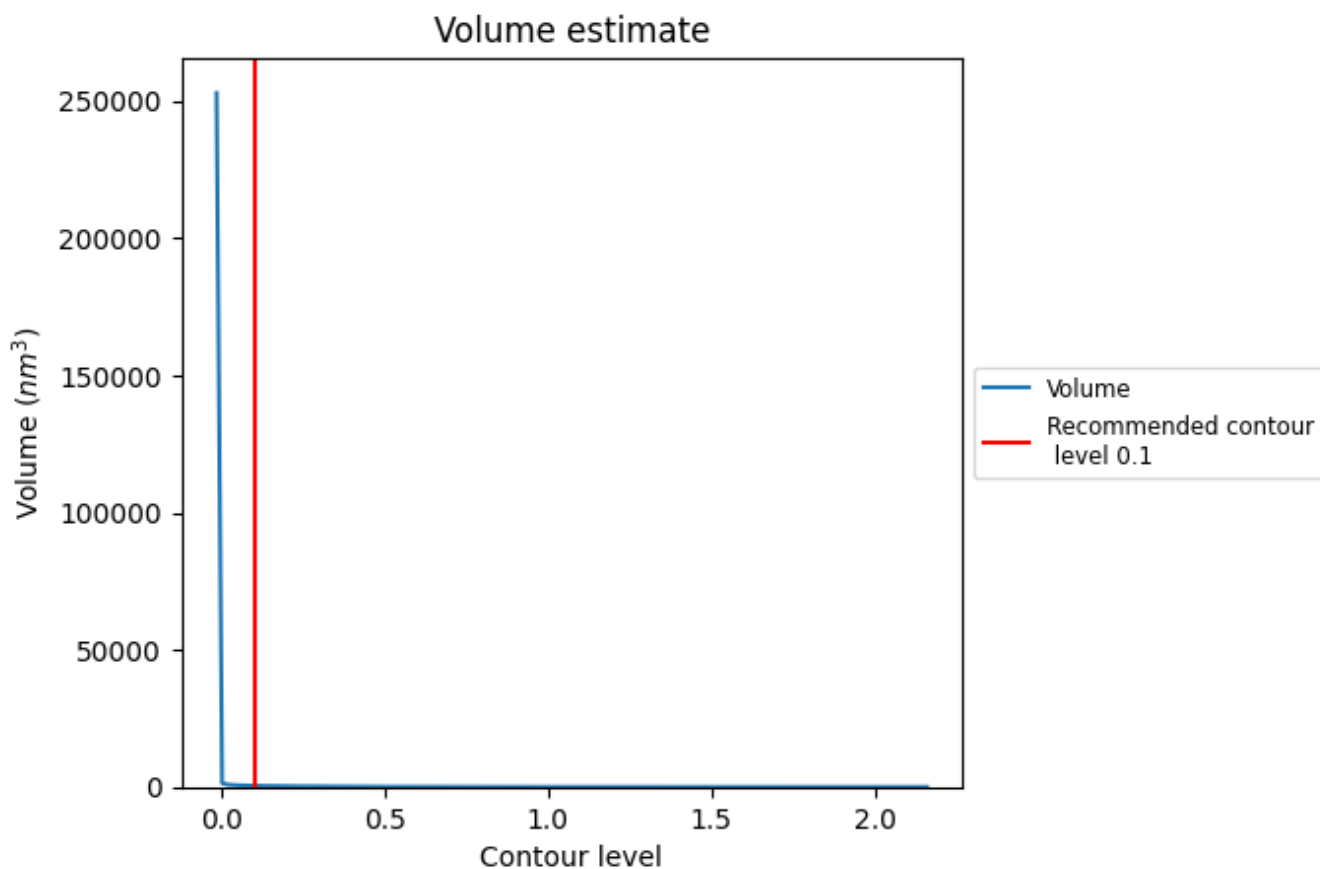
This section contains the results of statistical analysis of the map.

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.

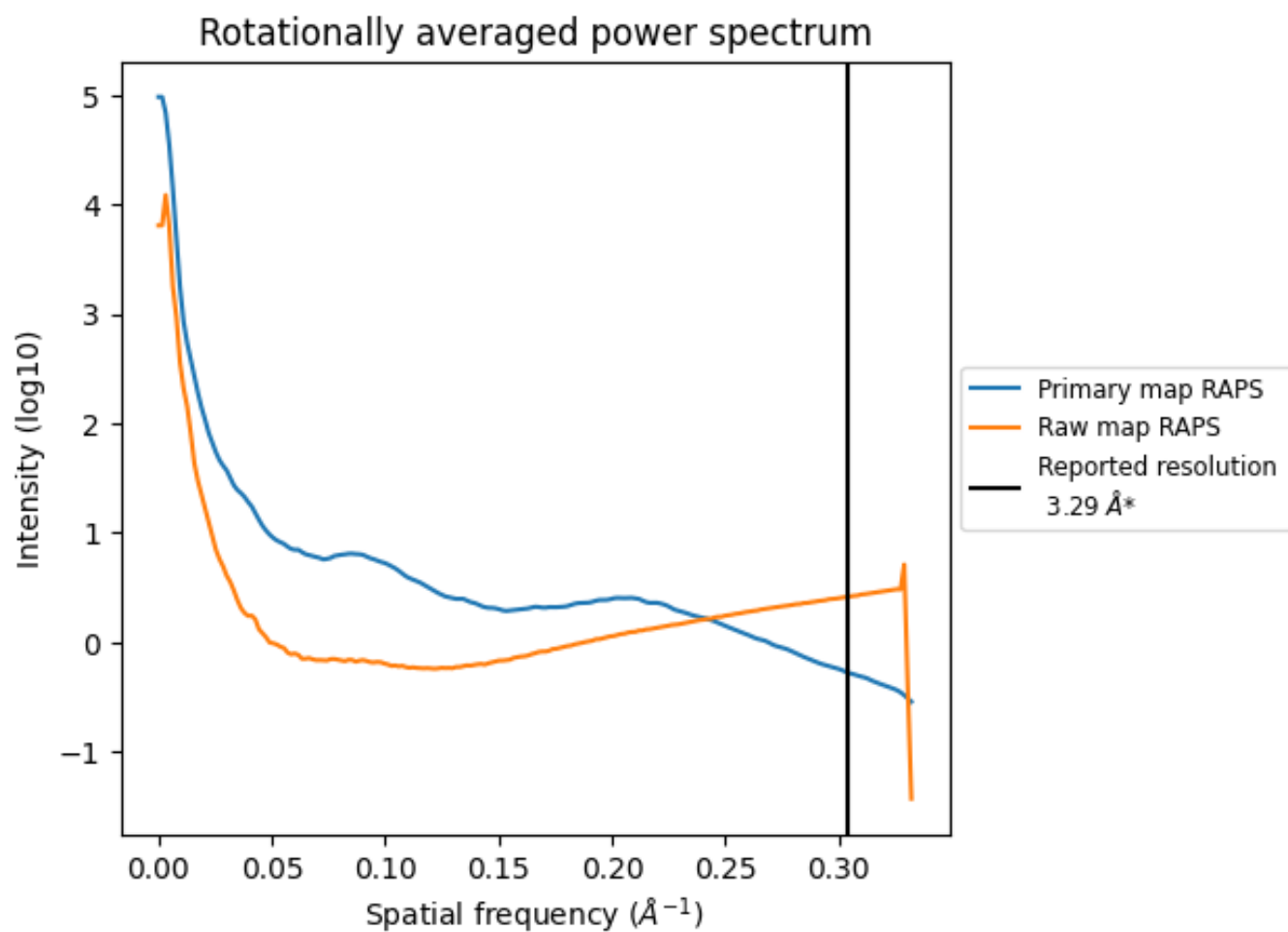
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 439 nm^3 ; this corresponds to an approximate mass of 397 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum i

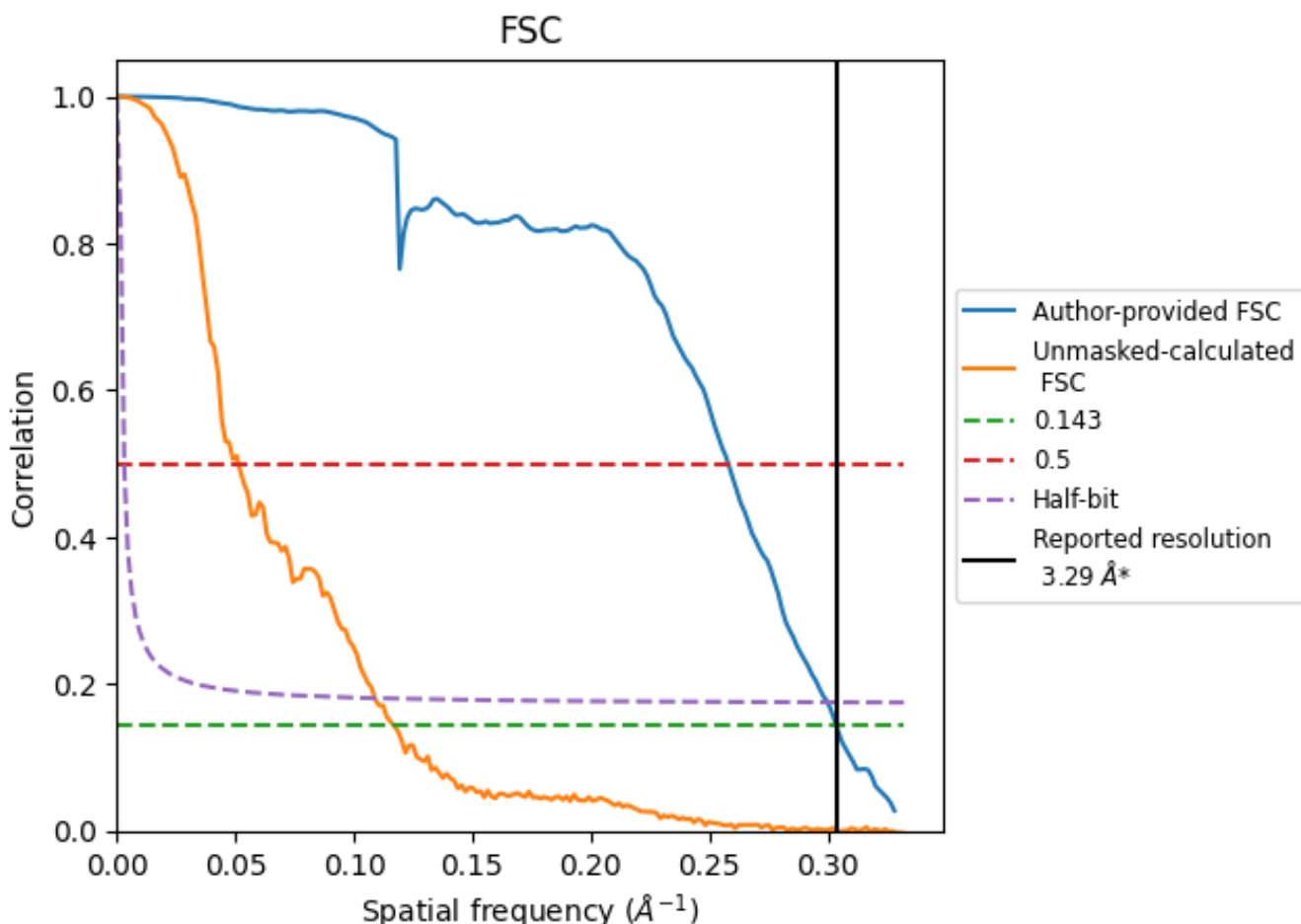


*Reported resolution corresponds to spatial frequency of 0.304 Å⁻¹

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 0.304 Å⁻¹

8.2 Resolution estimates [i](#)

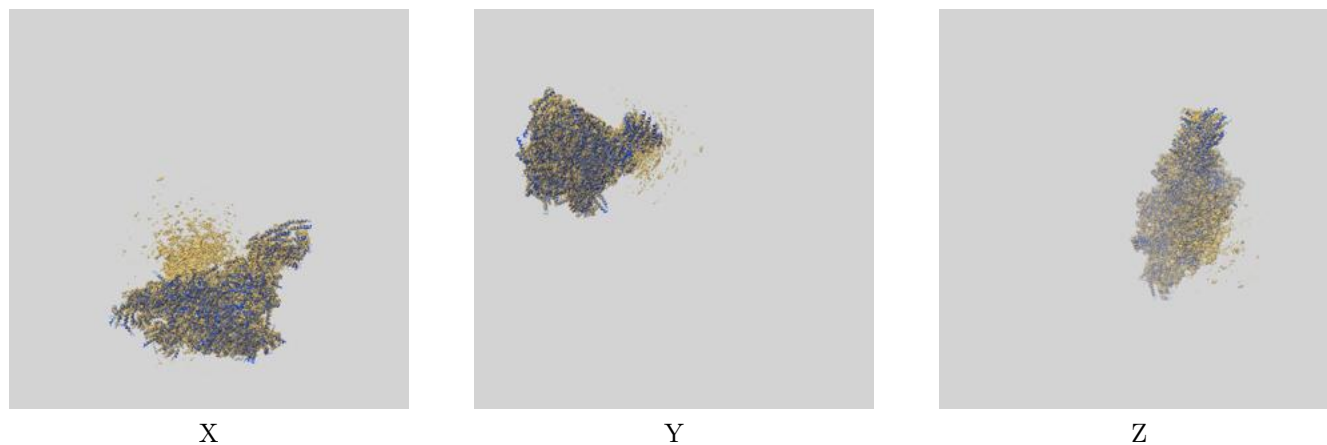
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.29	-	-
Author-provided FSC curve	3.29	3.88	3.33
Unmasked-calculated*	8.55	19.46	9.18

*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 8.55 differs from the reported value 3.29 by more than 10 %

9 Map-model fit [i](#)

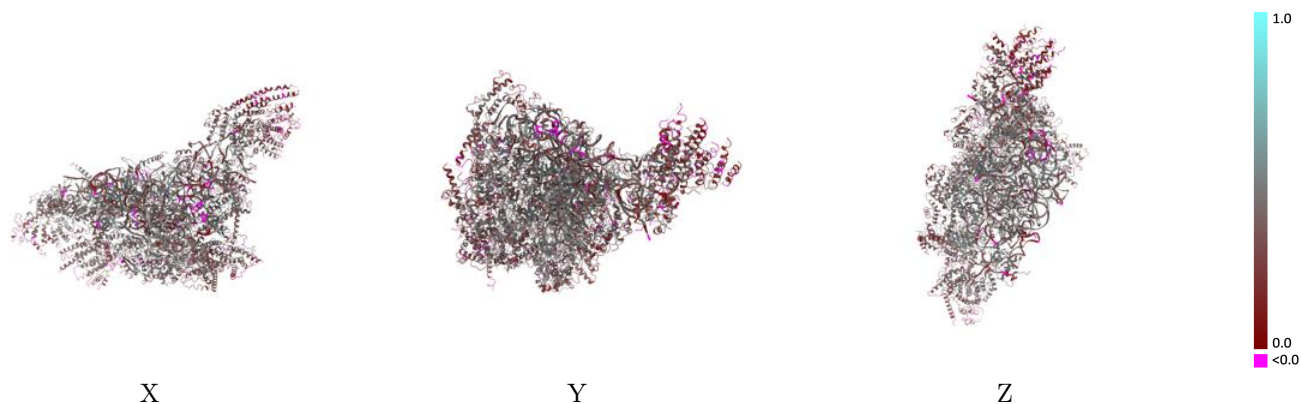
This section contains information regarding the fit between EMDB map EMD-50470 and PDB model 9FIA. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



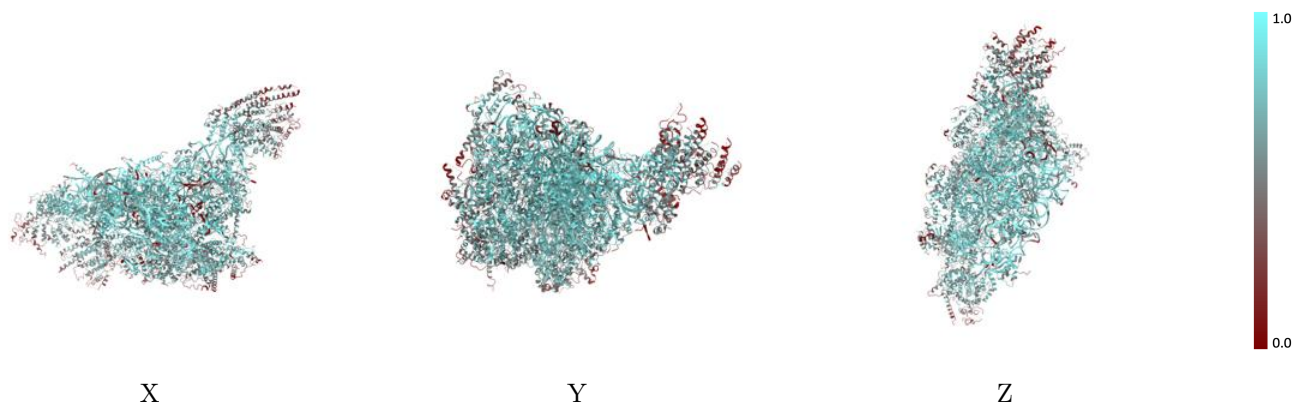
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



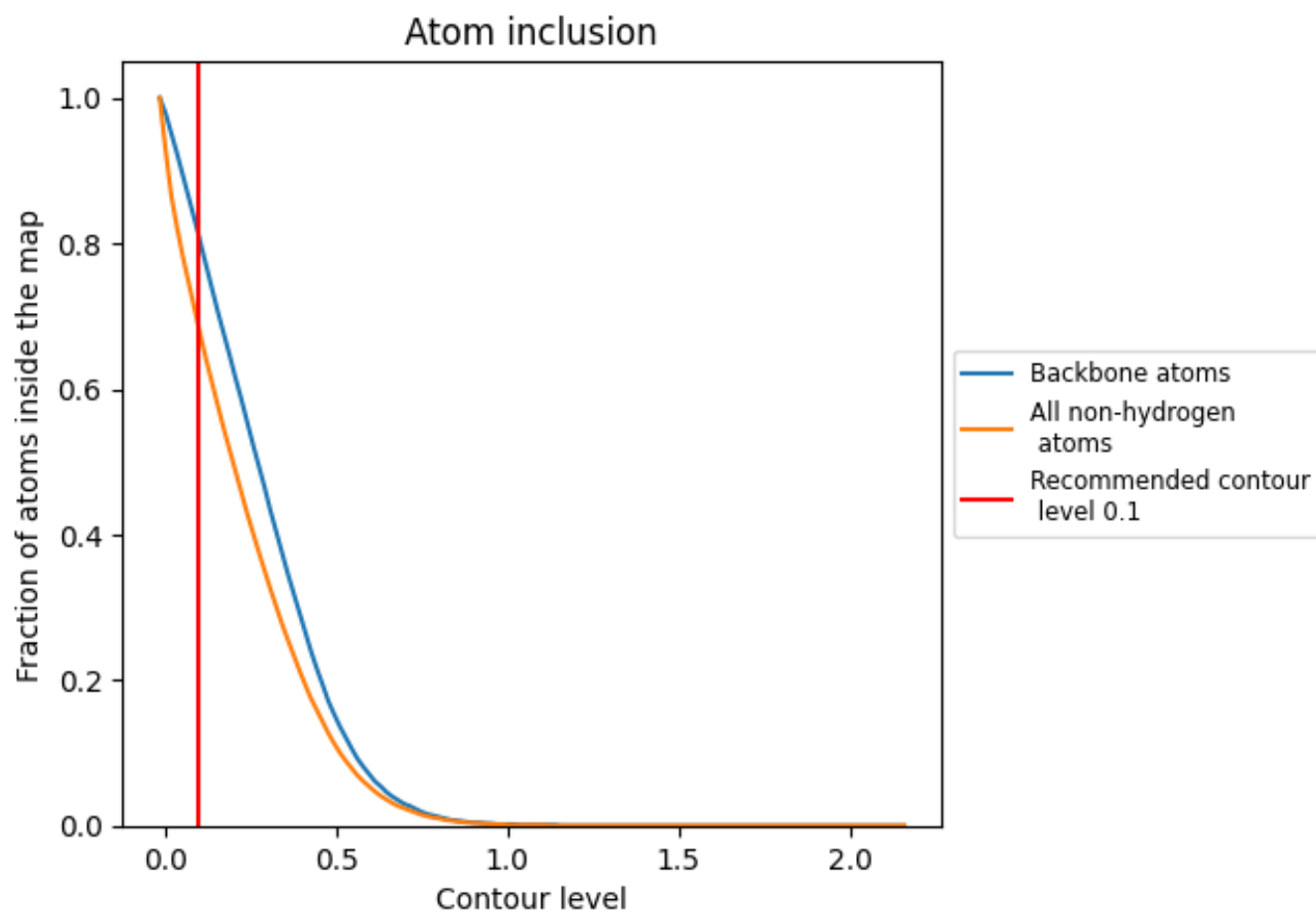
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 81% of all backbone atoms, 68% 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	 0.6830	 0.3530
B0	 0.5680	 0.3020
B1	 0.7500	 0.4160
B2	 0.6760	 0.3560
B3	 0.7200	 0.3910
B4	 0.7010	 0.4030
B5	 0.7510	 0.3930
B6	 0.8290	 0.4550
B7	 0.2500	 0.2890
B8	 0.6550	 0.4170
B9	 0.7440	 0.3960
BA	 0.6590	 0.3660
BB	 0.5020	 0.2630
BC	 0.6700	 0.3640
BD	 0.5540	 0.2860
BE	 0.5270	 0.3000
BF	 0.6900	 0.3860
BG	 0.6830	 0.3790
BH	 0.8530	 0.4580
BI	 0.8460	 0.4210
BJ	 0.6250	 0.4180
BK	 0.8060	 0.4230
BL	 0.8630	 0.4570
BN	 0.6150	 0.3530
BO	 0.8030	 0.4380
BP	 0.8080	 0.4020
BQ	 0.7070	 0.3770
BS	 0.5640	 0.3120
BT	 0.7310	 0.3420
BU	 0.5890	 0.3880
BV	 0.6830	 0.3720
BW	 0.6510	 0.3050
BX	 0.7880	 0.5010
BY	 0.2270	 0.1740
Ba	 0.4000	 0.3490



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Chain	Atom inclusion	Q-score
Bb	 0.5940	 0.3650
Bc	 0.6780	 0.3710
Bd	 0.7880	 0.3780
Be	 0.7920	 0.4840
Bg	 0.7550	 0.3820
Bh	 0.7780	 0.4300
Bi	 0.7450	 0.4040
Bj	 0.9290	 0.5160
Bk	 0.6500	 0.3530
Bl	 0.6760	 0.3490
HJ	 0.6470	 0.3320
HS	 0.5180	 0.2740
b1	 0.8500	 0.3990
b2	 0.7780	 0.3900
b3	 0.5000	 0.2460
b4	 0.7280	 0.3060
bA	 0.7850	 0.3670
bD	 0.7970	 0.3800
bE	 0.7840	 0.3460
bG	 0.1630	 -0.1460
bH	 0.6500	 0.1360
bI	 0.1330	 -0.1050
bJ	 0.6640	 0.2890
bK	 0.6900	 0.3040
bL	 0.8390	 0.3670
bN	 0.7830	 0.3630
bO	 0.8280	 0.3940
bP	 0.7730	 0.3660
bQ	 0.7040	 0.3080
bR	 0.8140	 0.3820
bS	 0.7660	 0.3670
bT	 0.8130	 0.3740
bU	 0.7760	 0.3190
bV	 0.8830	 0.4030
bY	 0.7680	 0.3110