



wwPDB EM Validation Summary Report ⓘ

Mar 27, 2026 – 05:54 AM UTC

PDB ID : 9N5T / pdb_00009n5t
EMDB ID : EMD-49038
Title : Mycobacterium smegmatis 70S ribosome with small molecule drug MK-7762
Authors : Zhu, J.
Deposited on : 2025-02-04
Resolution : 2.01 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:

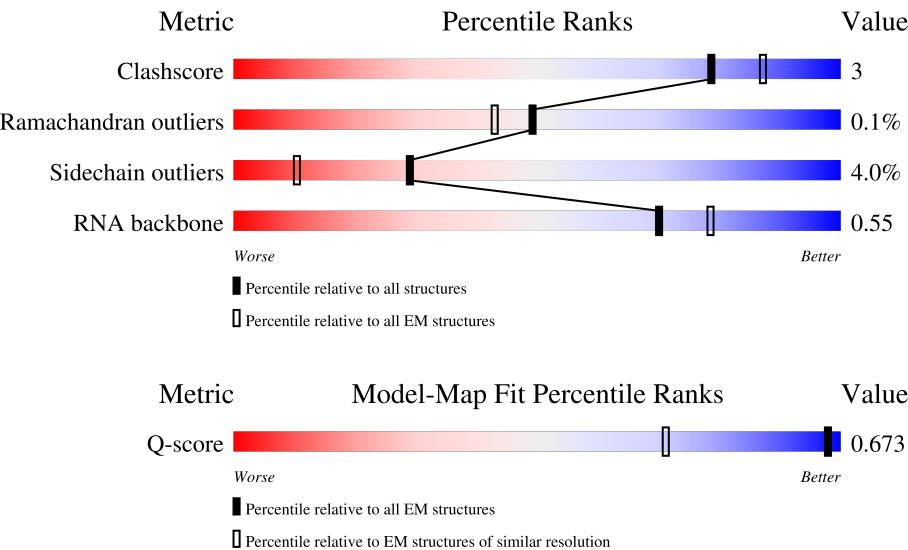
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.01 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	1691 (1.52 - 2.51)

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	3	24	79%12% . .
2	A	3120	10% 75%20% . .
3	B	118	. 84%14% .

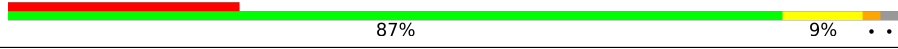
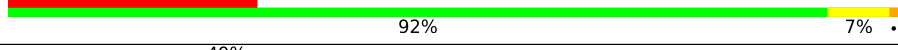
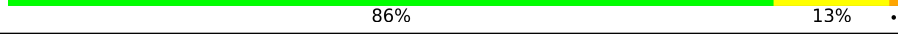
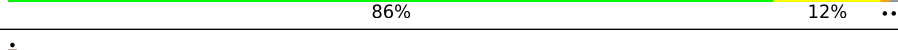
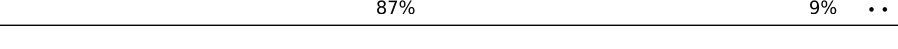
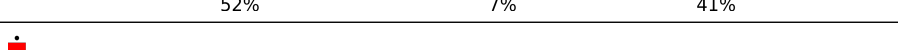
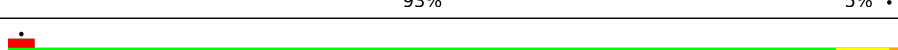
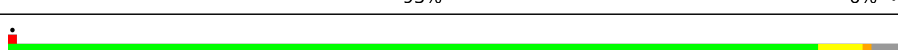
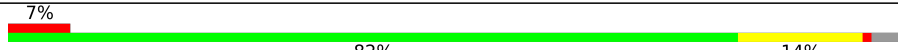
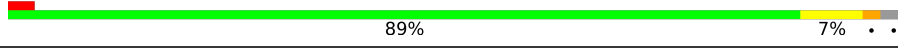
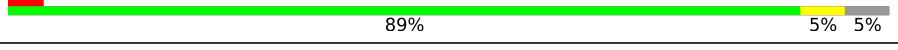
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Mol	Chain	Length	Quality of chain
4	BA	1528	
5	BB	33	
6	BC	275	
7	BD	201	
8	BE	214	
9	BF	96	
10	BG	156	
11	BH	132	
12	BI	150	
13	BJ	101	
14	BK	138	
15	BL	124	
16	BM	124	
17	BN	61	
18	BO	89	
19	BP	156	
20	BQ	98	
21	BR	84	
22	BS	93	
23	BT	86	
24	BV	277	
25	BW	76	
26	I	15	
27	C	278	
28	D	217	

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Mol	Chain	Length	Quality of chain
29	E	215	
30	F	187	
31	G	179	
32	H	151	
33	J	142	
34	K	147	
35	L	122	
36	M	147	
37	N	138	
38	O	199	
39	P	127	
40	Q	113	
41	R	129	
42	S	103	
43	T	153	
44	U	100	
45	V	105	
46	W	215	
47	X	88	
48	Y	64	
49	Z	77	
50	a	61	
51	b	57	
52	c	55	
53	d	47	

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Mol	Chain	Length	Quality of chain
54	e	64	 77% 19%
55	f	37	 86% 14%
56	g	75	 9% 68% 11% 21%
57	s	5	 40% 20% 20% 60%

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 156393 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 50S Ribosomal Protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	3	23	Total	C	N	O	0	0
			190	111	50	29		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	3085	Total	C	N	O	P	0	0
			66255	29532	12188	21450	3085		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	118	Total	C	N	O	P	0	0
			2522	1126	468	810	118		

- Molecule 4 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	BA	1512	Total	C	N	O	P	0	0
			32462	14458	5935	10557	1512		

- Molecule 5 is a protein called Conserved domain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	BB	32	Total	C	N	O	S	0	0
			281	172	71	37	1		

- Molecule 6 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	BC	208	Total	C	N	O	S	0	0
			1660	1036	322	298	4		

- Molecule 7 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BD	200	Total	C	N	O	S	0	0
			1642	1028	316	296	2		

- Molecule 8 is a protein called 30S Ribosomal Protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	BE	180	Total	C	N	O	S	0	0
			1297	812	245	236	4		

- Molecule 9 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	BF	96	Total	C	N	O	S	0	0
			772	486	138	146	2		

- Molecule 10 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	BG	155	Total	C	N	O	S	0	0
			1233	768	241	222	2		

- Molecule 11 is a protein called 30S Ribosomal Protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	BH	131	Total	C	N	O	S	0	0
			1011	633	189	188	1		

- Molecule 12 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BI	126	Total	C	N	O	S	0	0
			995	630	194	171			

- Molecule 13 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BJ	99	Total	C	N	O	S	0	0
			789	495	146	145	3		

- Molecule 14 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BK	115	Total	C	N	O	S	0	0
			855	528	170	156	1		

- Molecule 15 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BL	122	Total	C	N	O	S	0	0
			958	594	197	165	2		

- Molecule 16 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BM	116	Total	C	N	O	S	0	0
			935	572	191	169	3		

- Molecule 17 is a protein called 30S Ribosomal Protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	BN	60	Total	C	N	O	S	0	0
			478	302	97	74	5		

- Molecule 18 is a protein called 30S Ribosomal Protein S15.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	BO	88	Total	C	N	O	0	0
			721	449	147	125		

- Molecule 19 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	BP	113	Total	C	N	O	0	0
			891	570	162	159		

- Molecule 20 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	BQ	94	Total	C	N	O	S	0	0
			748	469	142	135	2		

- Molecule 21 is a protein called 30S Ribosomal Protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BR	65	Total	C	N	O	S	0	0
			513	318	102	90	3		

- Molecule 22 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BS	82	Total	C	N	O	S	0	0
			662	425	124	112	1		

- Molecule 23 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BT	85	Total	C	N	O		0	0
			661	402	139	120			

- Molecule 24 is a protein called 30S Ribosomal Protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BV	228	Total	C	N	O	S	0	0
			1793	1132	322	330	9		

- Molecule 25 is a RNA chain called P/P-site Phe-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BW	76	Total	C	N	O	P	0	0
			1622	723	290	533	76		

- Molecule 26 is a RNA chain called mRNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	I	6	Total	C	N	O	P	0	0
			125	56	20	43	6		

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	C	275	Total	C	N	O	S	0	0
			2110	1298	438	370	4		

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	D	214	Total	C	N	O	S	0	0
			1587	982	310	290	5		

- Molecule 29 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	E	209	Total	C	N	O	S	0	0
			1569	969	295	303	2		

- Molecule 30 is a protein called 50S Ribosomal Protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	F	182	Total	C	N	O	S	0	0
			1446	907	271	262	6		

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	G	176	Total	C	N	O	S	0	0
			1348	845	249	253	1		

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	H	151	Total	C	N	O	S	0	0
			1120	695	209	215	1		

- Molecule 33 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	J	69	Total	C	N	O	S	0	0
			505	315	91	98	1		

- Molecule 34 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	K	146	Total	C	N	O	S	0	0
			1131	722	207	201	1		

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	L	122	Total	C	N	O	S	0	0
			939	586	179	171	3		

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	M	145	Total	C	N	O	S	0	0
			1079	676	205	195	3		

- Molecule 37 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	N	136	Total	C	N	O	S	0	0
			1092	690	213	187	2		

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	O	118	Total	C	N	O	S	0	0
			928	583	180	163	2		

- Molecule 39 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	P	126	Total	C	N	O	S	0	0
			956	586	199	171			

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Q	113	Total	C	N	O	S	0	0
			908	570	171	166	1		

- Molecule 41 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	R	124	Total	C	N	O	S	0	0
			988	613	203	172			

- Molecule 42 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	S	100	Total	C	N	O	0	0
			754	478	137	139		

- Molecule 43 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	T	114	Total	C	N	O	0	0
			873	543	171	159		

- Molecule 44 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	U	97	Total	C	N	O	0	0
			756	479	138	139		

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	V	97	Total	C	N	O	S	0	0
			732	456	137	137	2		

- Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	W	192	Total	C	N	O	0	0
			1428	881	255	292		

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	X	79	Total	C	N	O	0	0
			586	361	123	102		

- Molecule 48 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Y	63	Total	C	N	O	S	0	0
			471	283	103	81	4		

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Z	66	Total	C	N	O	S	0	0
			544	333	105	105	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
50	a	59	Total	C	N	O	0	0
			474	292	95	87		

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	b	54	Total	C	N	O	S	0	0
			423	260	93	69	1		

- Molecule 52 is a protein called 50S Ribosomal Protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	c	49	Total	C	N	O	S	0	0
			405	248	82	71	4		

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	d	46	Total	C	N	O	S	0	0
			378	225	97	55	1		

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	e	63	Total	C	N	O	0	0
			503	302	115	86		

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	f	37	Total	C	N	O	S	0	0
			299	181	66	47	5		

- Molecule 56 is a protein called 50S Ribosomal Protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	g	59	Total	C	N	O	S	0	0
			458	284	84	85	5		

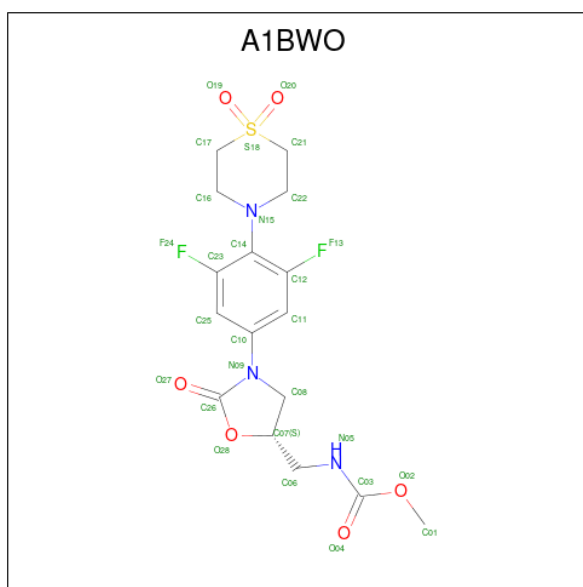
- Molecule 57 is a protein called Nascent peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	s	2	Total	C	N	O	0	0
			16	12	2	2		

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
58	A	250	Total	Mg	0
			250	250	
58	B	5	Total	Mg	0
			5	5	
58	BA	85	Total	Mg	0
			85	85	
58	BM	1	Total	Mg	0
			1	1	
58	BR	1	Total	Mg	0
			1	1	
58	BW	1	Total	Mg	0
			1	1	
58	C	2	Total	Mg	0
			2	2	
58	D	1	Total	Mg	0
			1	1	
58	M	1	Total	Mg	0
			1	1	

- Molecule 59 is methyl ({(5S)-3-[4-(1,1-dioxo-1λ⁶-thiomorpholin-4-yl)-3,5-difluorophenyl]-2-oxo-1,3-oxazolidin-5-yl}methyl)carbamate (CCD ID: A1BWO) (formula: C₁₆H₁₉F₂N₃O₆S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
59	A	1	Total	C	F	N	O	S	0
			28	16	2	3	6	1	

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
60	BN	1	Total	Zn	0
			1	1	
60	BR	1	Total	Zn	0
			1	1	
60	Y	1	Total	Zn	0
			1	1	
60	c	1	Total	Zn	0
			1	1	
60	f	1	Total	Zn	0
			1	1	
60	g	1	Total	Zn	0
			1	1	

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		AltConf
61	3	3	Total	O	0
			3	3	
61	A	5185	Total	O	0
			5185	5185	

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Mol	Chain	Residues	Atoms		AltConf
61	B	55	Total 55	O 55	0
61	BA	1204	Total 1204	O 1204	0
61	BB	2	Total 2	O 2	0
61	BC	1	Total 1	O 1	0
61	BD	1	Total 1	O 1	0
61	BE	2	Total 2	O 2	0
61	BG	1	Total 1	O 1	0
61	BH	5	Total 5	O 5	0
61	BI	10	Total 10	O 10	0
61	BJ	4	Total 4	O 4	0
61	BK	10	Total 10	O 10	0
61	BL	7	Total 7	O 7	0
61	BN	4	Total 4	O 4	0
61	BO	4	Total 4	O 4	0
61	BP	4	Total 4	O 4	0
61	BR	5	Total 5	O 5	0
61	BT	4	Total 4	O 4	0
61	BW	9	Total 9	O 9	0
61	I	7	Total 7	O 7	0
61	C	100	Total 100	O 100	0
61	D	53	Total 53	O 53	0

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Mol	Chain	Residues	Atoms		AltConf
61	E	43	Total 43	O 43	0
61	F	2	Total 2	O 2	0
61	G	1	Total 1	O 1	0
61	H	3	Total 3	O 3	0
61	K	14	Total 14	O 14	0
61	L	9	Total 9	O 9	0
61	M	39	Total 39	O 39	0
61	N	33	Total 33	O 33	0
61	O	26	Total 26	O 26	0
61	P	11	Total 11	O 11	0
61	Q	15	Total 15	O 15	0
61	R	46	Total 46	O 46	0
61	S	19	Total 19	O 19	0
61	T	29	Total 29	O 29	0
61	U	20	Total 20	O 20	0
61	V	5	Total 5	O 5	0
61	W	3	Total 3	O 3	0
61	X	25	Total 25	O 25	0
61	Y	23	Total 23	O 23	0
61	Z	2	Total 2	O 2	0
61	a	10	Total 10	O 10	0

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Mol	Chain	Residues	Atoms		AltConf
61	b	12	Total 12	O 12	0
61	c	8	Total 8	O 8	0
61	d	22	Total 22	O 22	0
61	e	32	Total 32	O 32	0
61	f	3	Total 3	O 3	0

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.

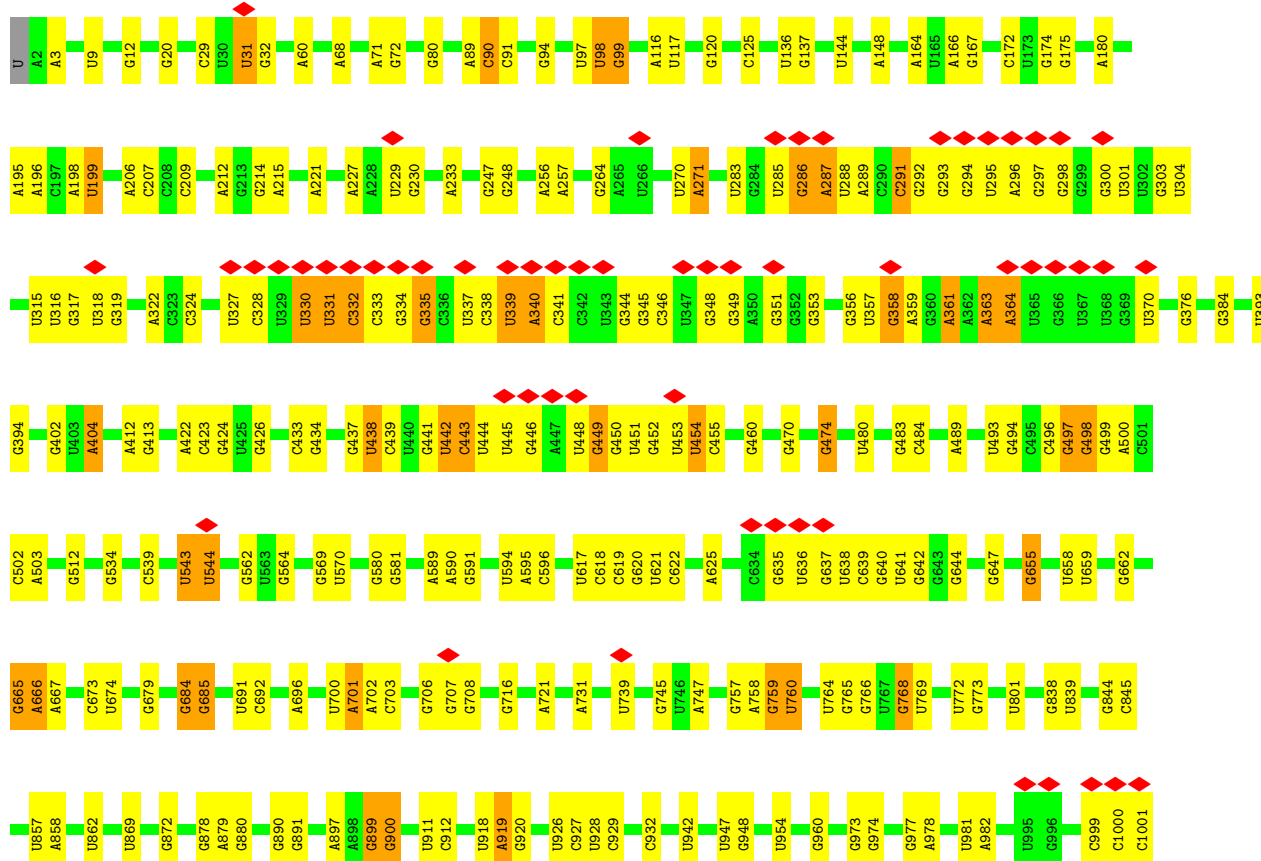
• Molecule 1: 50S Ribosomal Protein L27

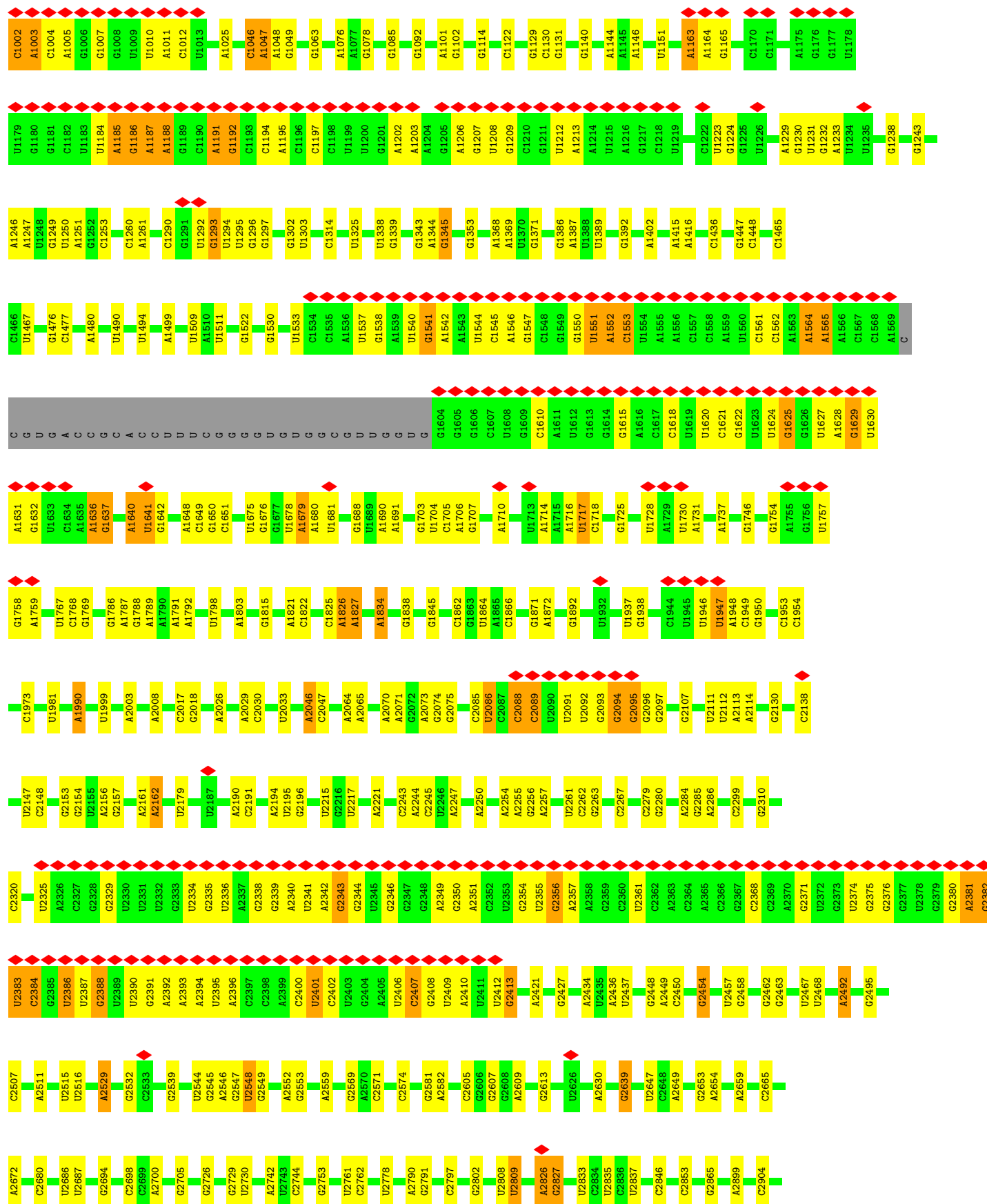
Chain 3: 

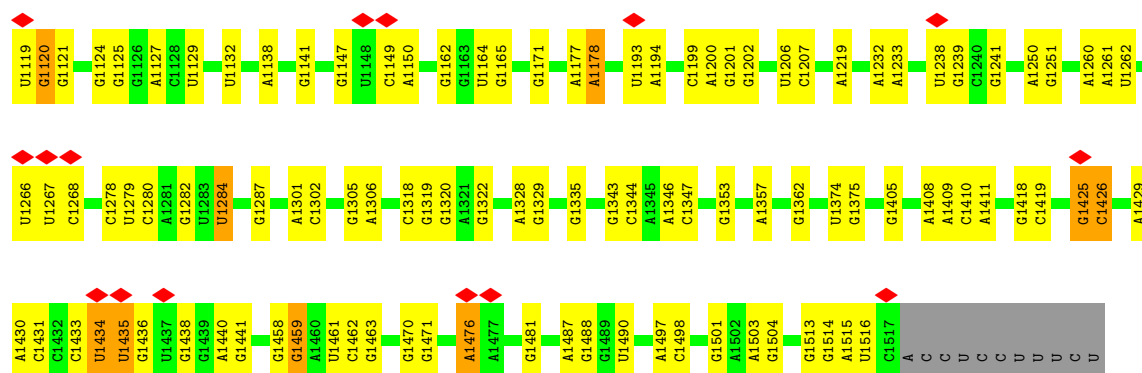


• Molecule 2: 23S rRNA

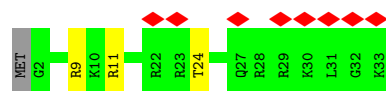
Chain A: 



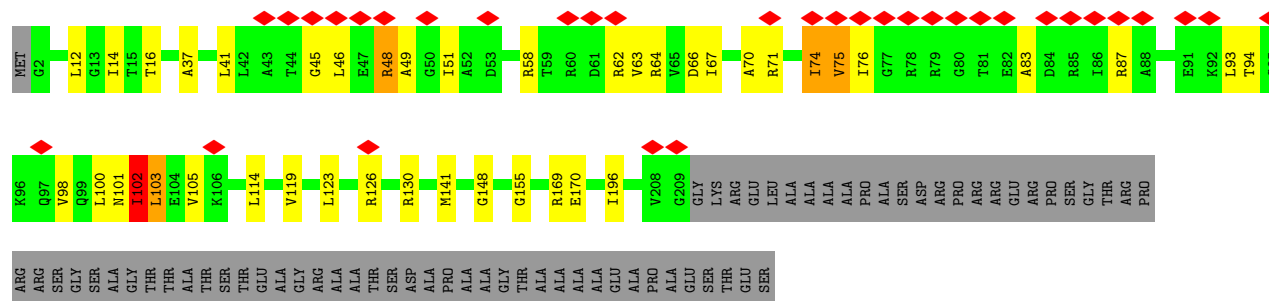




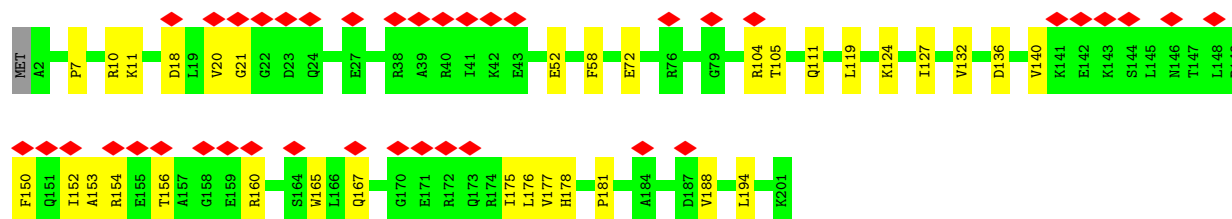
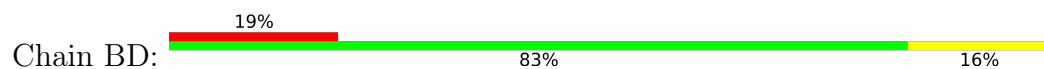
• Molecule 5: Conserved domain protein



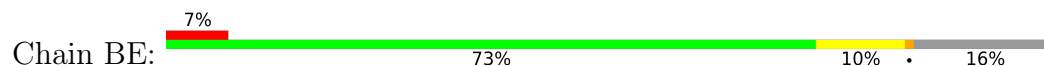
• Molecule 6: 30S ribosomal protein S3

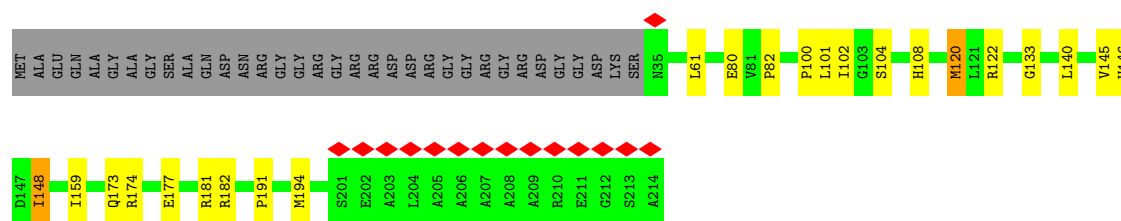


• Molecule 7: 30S ribosomal protein S4

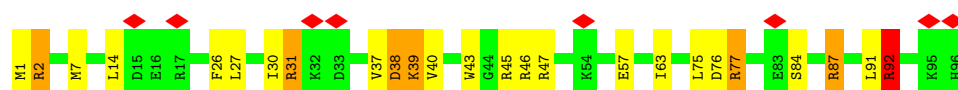
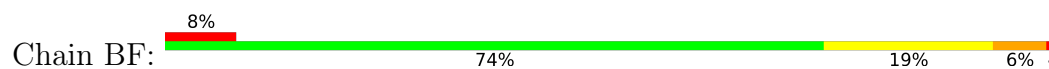


• Molecule 8: 30S Ribosomal Protein S5

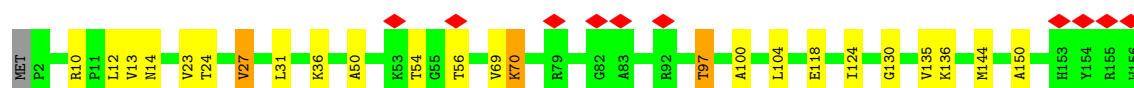
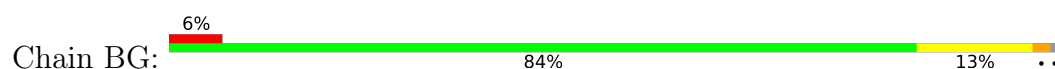




• Molecule 9: 30S ribosomal protein S6



• Molecule 10: 30S ribosomal protein S7



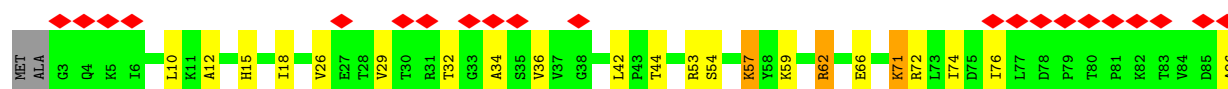
• Molecule 11: 30S Ribosomal Protein S8

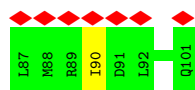


• Molecule 12: 30S ribosomal protein S9

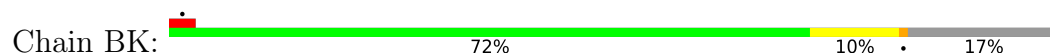


• Molecule 13: 30S ribosomal protein S10

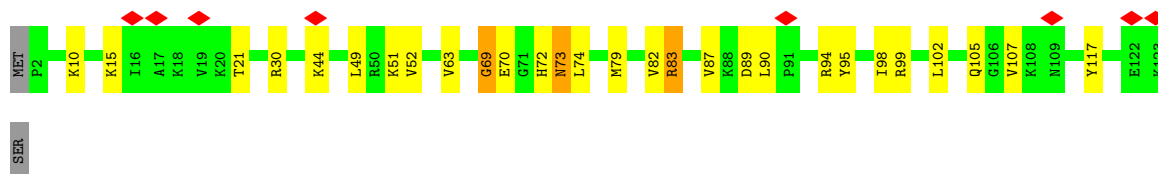
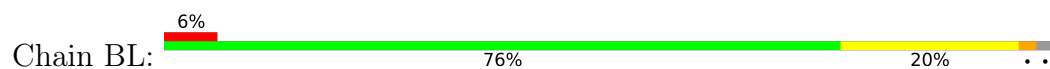




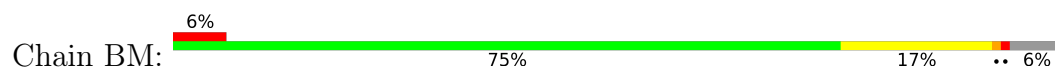
- Molecule 14: 30S ribosomal protein S11



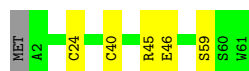
- Molecule 15: 30S ribosomal protein S12



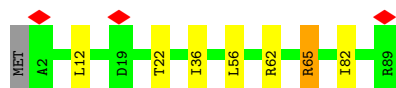
- Molecule 16: 30S ribosomal protein S13



- Molecule 17: 30S Ribosomal Protein S14



- Molecule 18: 30S Ribosomal Protein S15



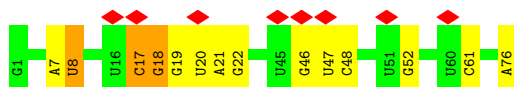
- Molecule 19: 30S ribosomal protein S16



ALA
PRO
GLU
SER
SER
THR
ASP
ALA
SER

- Molecule 25: P/P-site Phe-tRNA

Chain BW: 



- Molecule 26: mRNA fragment

Chain I: 



- Molecule 27: 50S ribosomal protein L2

Chain C: 



- Molecule 28: 50S ribosomal protein L3

Chain D: 



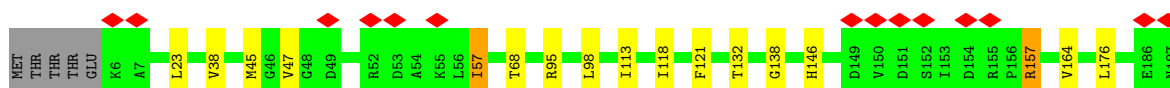
- Molecule 29: Large ribosomal subunit protein uL4

Chain E: 



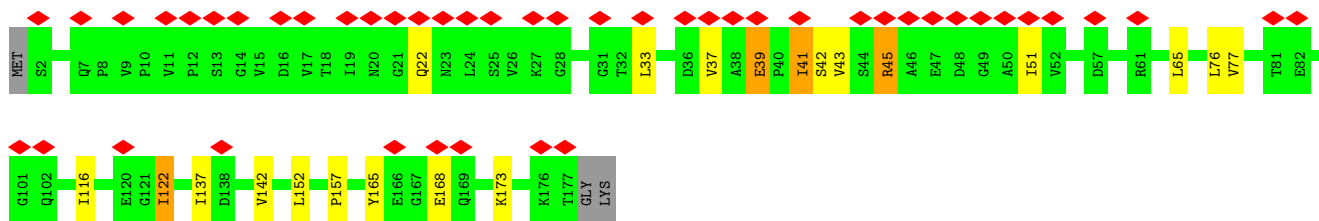
- Molecule 30: 50S Ribosomal Protein L5

Chain F: 

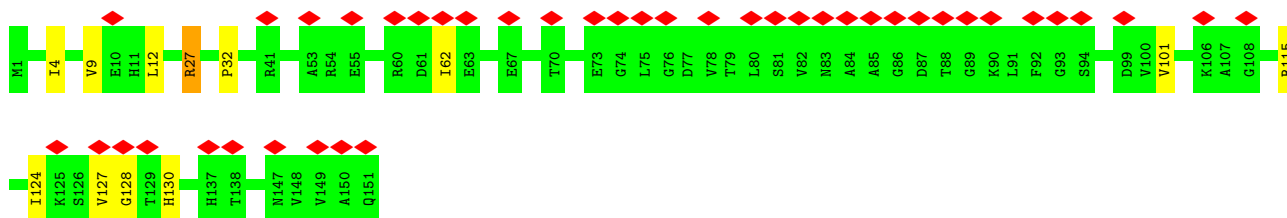
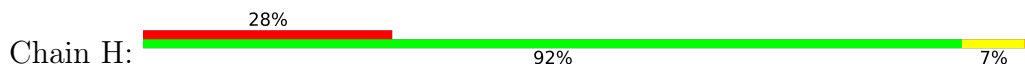


- Molecule 31: 50S ribosomal protein L6

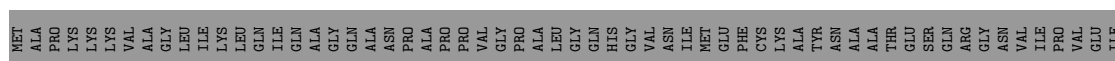
Chain G: 



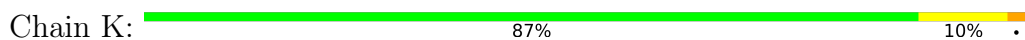
• Molecule 32: 50S ribosomal protein L9



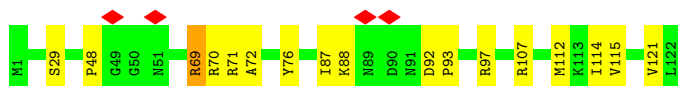
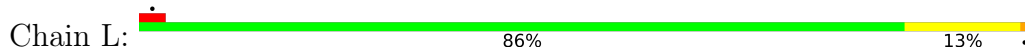
• Molecule 33: 50S ribosomal protein L11



• Molecule 34: Large ribosomal subunit protein uL13

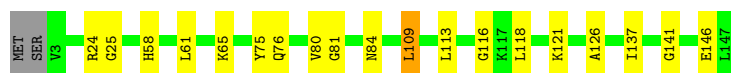


• Molecule 35: 50S ribosomal protein L14

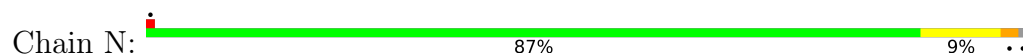


• Molecule 36: 50S ribosomal protein L15





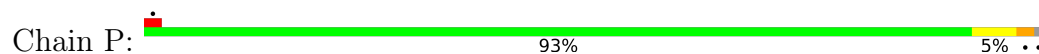
- Molecule 37: Large ribosomal subunit protein uL16



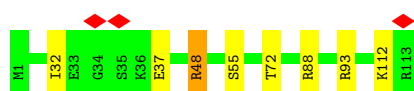
- Molecule 38: 50S ribosomal protein L17



- Molecule 39: Large ribosomal subunit protein uL18



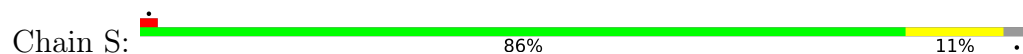
- Molecule 40: 50S ribosomal protein L19



- Molecule 41: Large ribosomal subunit protein bL20

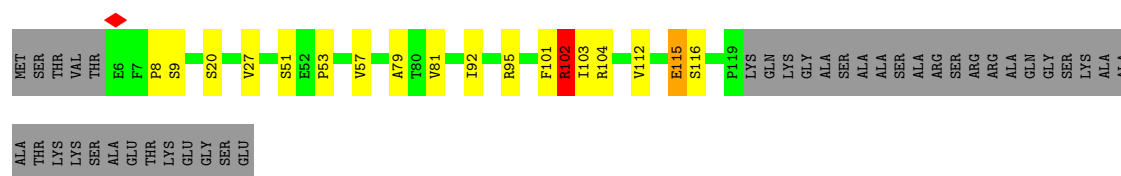


- Molecule 42: Large ribosomal subunit protein bL21



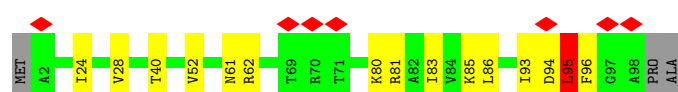
- Molecule 43: Large ribosomal subunit protein uL22

Chain T: 



- Molecule 44: Large ribosomal subunit protein uL23

Chain U: 



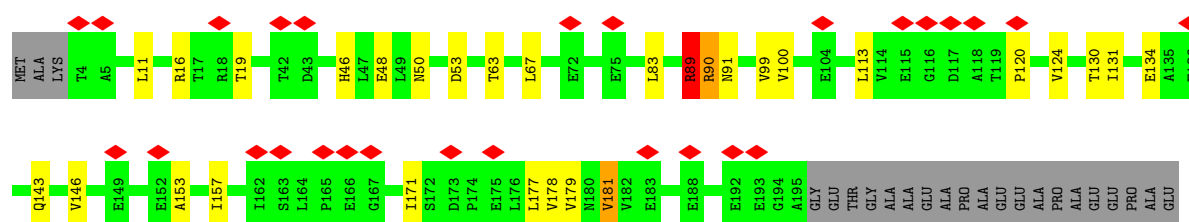
- Molecule 45: 50S ribosomal protein L24

Chain V: 



- Molecule 46: 50S ribosomal protein L25

Chain W: 



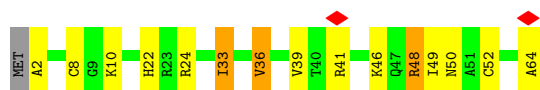
- Molecule 47: 50S ribosomal protein L27

Chain X: 

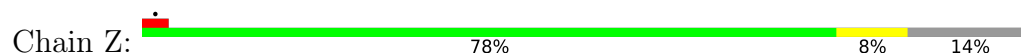


- Molecule 48: Large ribosomal subunit protein bL28

Chain Y: 



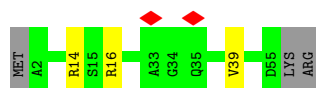
- Molecule 49: 50S ribosomal protein L29



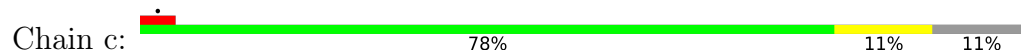
- Molecule 50: 50S ribosomal protein L30



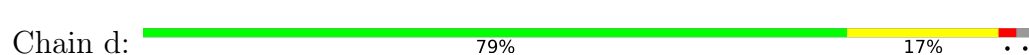
- Molecule 51: 50S ribosomal protein L32



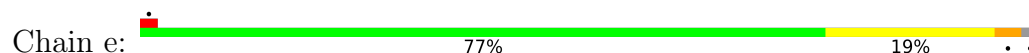
- Molecule 52: 50S Ribosomal Protein L33



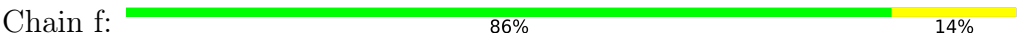
- Molecule 53: 50S ribosomal protein L34



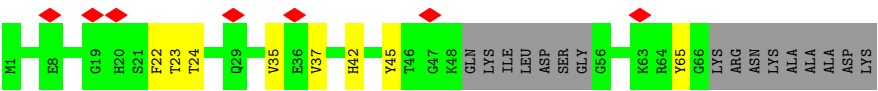
- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36



• Molecule 56: 50S Ribosomal Protein L31



• Molecule 57: Nascent peptide



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	638803	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	1.131	Depositor
Minimum map value	-0.407	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	528.768, 528.768, 528.768	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8262, 0.8262, 0.8262	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, A1BWO

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	3	0.47	0/192	0.60	0/247
2	A	0.17	0/74190	0.40	0/115759
3	B	0.15	0/2821	0.35	0/4396
4	BA	0.17	0/36335	0.39	3/56698 (0.0%)
5	BB	0.11	0/281	0.37	0/359
6	BC	0.31	0/1684	0.47	0/2261
7	BD	0.19	0/1673	0.42	0/2251
8	BE	0.25	0/1313	0.45	0/1772
9	BF	0.27	0/783	0.45	0/1059
10	BG	0.10	0/1253	0.32	0/1690
11	BH	0.10	0/1026	0.35	0/1385
12	BI	0.30	0/1013	0.47	0/1362
13	BJ	0.28	0/803	0.52	1/1086 (0.1%)
14	BK	0.32	0/873	0.46	0/1180
15	BL	0.32	0/969	0.53	1/1294 (0.1%)
16	BM	0.43	0/942	0.64	0/1260
17	BN	0.12	0/489	0.33	0/650
18	BO	0.11	0/730	0.32	0/977
19	BP	0.39	0/908	0.58	0/1226
20	BQ	0.40	0/759	0.57	1/1016 (0.1%)
21	BR	0.09	0/518	0.33	0/693
22	BS	0.28	0/680	0.49	0/915
23	BT	0.10	0/664	0.30	0/882
24	BV	0.32	0/1822	0.47	1/2457 (0.0%)
25	BW	0.18	0/1812	0.37	0/2823
26	I	0.13	0/138	0.34	0/212
27	C	0.28	0/2153	0.48	0/2895
28	D	0.37	0/1609	0.56	0/2165
29	E	0.12	0/1592	0.35	0/2153
30	F	0.23	0/1468	0.39	0/1973
31	G	0.31	0/1369	0.45	0/1848
32	H	0.38	0/1130	0.50	1/1524 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
33	J	0.10	0/510	0.30	0/687
34	K	0.22	0/1158	0.39	0/1567
35	L	0.12	0/947	0.36	0/1268
36	M	0.35	0/1092	0.56	1/1457 (0.1%)
37	N	0.34	0/1118	0.47	0/1506
38	O	0.12	0/945	0.36	0/1267
39	P	0.11	0/966	0.35	0/1298
40	Q	0.23	0/922	0.39	0/1236
41	R	0.21	0/1000	0.39	0/1341
42	S	0.23	0/764	0.41	0/1030
43	T	0.12	0/887	0.37	0/1204
44	U	0.23	0/766	0.39	0/1030
45	V	0.11	0/738	0.35	0/987
46	W	0.10	0/1443	0.32	0/1970
47	X	0.44	0/595	0.65	1/798 (0.1%)
48	Y	0.15	0/479	0.45	0/641
49	Z	0.10	0/547	0.27	0/731
50	a	0.10	0/477	0.34	0/640
51	b	0.14	0/427	0.42	0/572
52	c	0.10	0/413	0.34	0/553
53	d	0.12	0/381	0.40	0/500
54	e	0.38	0/508	0.53	0/672
55	f	0.13	0/303	0.41	0/401
56	g	0.08	0/467	0.30	0/626
57	s	0.07	0/16	0.15	0/20
All	All	0.20	0/161861	0.41	10/242470 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	3	0	1
5	BB	0	2
6	BC	0	7
7	BD	0	3
8	BE	0	2
9	BF	0	7
11	BH	0	3
12	BI	0	7
13	BJ	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
15	BL	0	3
16	BM	0	5
17	BN	0	1
18	BO	0	2
19	BP	0	3
20	BQ	0	1
21	BR	0	1
23	BT	0	1
24	BV	0	5
27	C	0	7
28	D	0	3
29	E	0	2
30	F	0	1
31	G	0	1
32	H	0	2
34	K	0	3
35	L	0	3
37	N	0	2
38	O	0	2
39	P	0	2
40	Q	0	2
41	R	0	1
43	T	0	1
44	U	0	2
45	V	0	1
46	W	0	2
47	X	0	3
48	Y	0	3
50	a	0	2
51	b	0	2
52	c	0	1
53	d	0	2
54	e	0	4
All	All	0	111

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	BA	457	A	C2'-C3'-O3'	6.17	118.75	109.50
36	M	25	GLY	CA-C-O	-5.64	118.56	122.22
4	BA	429	U	C2'-C3'-O3'	5.61	117.92	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BV	155	GLN	N-CA-C	-5.60	107.45	114.56
47	X	44	HIS	N-CA-C	-5.33	104.88	111.33

There are no chirality outliers.

5 of 111 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	3	11	ARG	Sidechain
5	BB	11	ARG	Sidechain
5	BB	9	ARG	Sidechain
6	BC	48	ARG	Sidechain
6	BC	58	ARG	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	3	190	0	205	3	0
2	A	66255	0	33335	215	0
3	B	2522	0	1285	5	0
4	BA	32462	0	16331	141	0
5	BB	281	0	342	0	0
6	BC	1660	0	1707	18	0
7	BD	1642	0	1668	15	0
8	BE	1297	0	1360	15	0
9	BF	772	0	797	8	0
10	BG	1233	0	1282	13	0
11	BH	1011	0	1046	3	0
12	BI	995	0	1050	10	0
13	BJ	789	0	819	10	0
14	BK	855	0	863	14	0
15	BL	958	0	1045	17	0
16	BM	935	0	986	12	0
17	BN	478	0	499	2	0
18	BO	721	0	760	2	0
19	BP	891	0	935	13	0
20	BQ	748	0	795	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	BR	513	0	537	3	0
22	BS	662	0	677	11	0
23	BT	661	0	712	3	0
24	BV	1793	0	1839	34	0
25	BW	1622	0	820	2	0
26	I	125	0	65	0	0
27	C	2110	0	2165	11	0
28	D	1587	0	1630	13	0
29	E	1569	0	1607	8	0
30	F	1446	0	1476	9	0
31	G	1348	0	1399	9	0
32	H	1120	0	1170	3	0
33	J	505	0	533	5	0
34	K	1131	0	1167	9	0
35	L	939	0	1000	8	0
36	M	1079	0	1151	14	0
37	N	1092	0	1128	6	0
38	O	928	0	972	7	0
39	P	956	0	991	3	0
40	Q	908	0	938	4	0
41	R	988	0	1038	6	0
42	S	754	0	802	6	0
43	T	873	0	909	9	0
44	U	756	0	802	6	0
45	V	732	0	782	9	0
46	W	1428	0	1443	14	0
47	X	586	0	601	6	0
48	Y	471	0	480	8	0
49	Z	544	0	557	3	0
50	a	474	0	500	2	0
51	b	423	0	463	0	0
52	c	405	0	407	2	0
53	d	378	0	411	5	0
54	e	503	0	541	7	0
55	f	299	0	321	2	0
56	g	458	0	443	4	0
57	s	16	0	13	0	0
58	A	250	0	0	0	0
58	B	5	0	0	0	0
58	BA	85	0	0	0	0
58	BM	1	0	0	0	0
58	BR	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	BW	1	0	0	0	0
58	C	2	0	0	0	0
58	D	1	0	0	0	0
58	M	1	0	0	0	0
59	A	28	0	0	0	0
60	BN	1	0	0	0	0
60	BR	1	0	0	0	0
60	Y	1	0	0	0	0
60	c	1	0	0	0	0
60	f	1	0	0	0	0
60	g	1	0	0	0	0
61	3	3	0	0	0	0
61	A	5185	0	0	3	0
61	B	55	0	0	0	0
61	BA	1204	0	0	1	0
61	BB	2	0	0	0	0
61	BC	1	0	0	0	0
61	BD	1	0	0	0	0
61	BE	2	0	0	0	0
61	BG	1	0	0	0	0
61	BH	5	0	0	0	0
61	BI	10	0	0	0	0
61	BJ	4	0	0	0	0
61	BK	10	0	0	0	0
61	BL	7	0	0	0	0
61	BN	4	0	0	0	0
61	BO	4	0	0	0	0
61	BP	4	0	0	0	0
61	BR	5	0	0	0	0
61	BT	4	0	0	0	0
61	BW	9	0	0	0	0
61	C	100	0	0	0	0
61	D	53	0	0	0	0
61	E	43	0	0	0	0
61	F	2	0	0	0	0
61	G	1	0	0	0	0
61	H	3	0	0	0	0
61	I	7	0	0	0	0
61	K	14	0	0	1	0
61	L	9	0	0	0	0
61	M	39	0	0	0	0
61	N	33	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	O	26	0	0	0	0
61	P	11	0	0	0	0
61	Q	15	0	0	0	0
61	R	46	0	0	0	0
61	S	19	0	0	0	0
61	T	29	0	0	0	0
61	U	20	0	0	0	0
61	V	5	0	0	0	0
61	W	3	0	0	0	0
61	X	25	0	0	0	0
61	Y	23	0	0	0	0
61	Z	2	0	0	0	0
61	a	10	0	0	0	0
61	b	12	0	0	0	0
61	c	8	0	0	0	0
61	d	22	0	0	0	0
61	e	32	0	0	0	0
61	f	3	0	0	0	0
All	All	156393	0	99600	691	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 691 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)
4:BA:697:C:C4'	14:BK:128:ASN:HD22	1.27	1.44
4:BA:697:C:H4'	14:BK:128:ASN:ND2	1.38	1.39
24:BV:73:LYS:HE2	24:BV:205:ASP:HA	1.33	1.05
16:BM:65:LYS:NZ	16:BM:73:GLU:OE1	1.94	1.01
24:BV:90:PRO:HG2	24:BV:154:MET:SD	2.01	1.01

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	
1	3	21/24 (88%)	21 (100%)	0	0	100	100
5	BB	30/33 (91%)	30 (100%)	0	0	100	100
6	BC	206/275 (75%)	190 (92%)	14 (7%)	2 (1%)	12	8
7	BD	198/201 (98%)	197 (100%)	1 (0%)	0	100	100
8	BE	178/214 (83%)	175 (98%)	3 (2%)	0	100	100
9	BF	94/96 (98%)	89 (95%)	4 (4%)	1 (1%)	11	7
10	BG	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
11	BH	129/132 (98%)	127 (98%)	2 (2%)	0	100	100
12	BI	124/150 (83%)	117 (94%)	7 (6%)	0	100	100
13	BJ	97/101 (96%)	93 (96%)	4 (4%)	0	100	100
14	BK	113/138 (82%)	107 (95%)	5 (4%)	1 (1%)	14	9
15	BL	120/124 (97%)	118 (98%)	2 (2%)	0	100	100
16	BM	114/124 (92%)	106 (93%)	7 (6%)	1 (1%)	14	9
17	BN	58/61 (95%)	58 (100%)	0	0	100	100
18	BO	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
19	BP	111/156 (71%)	109 (98%)	2 (2%)	0	100	100
20	BQ	92/98 (94%)	88 (96%)	4 (4%)	0	100	100
21	BR	63/84 (75%)	61 (97%)	2 (3%)	0	100	100
22	BS	80/93 (86%)	76 (95%)	4 (5%)	0	100	100
23	BT	83/86 (96%)	83 (100%)	0	0	100	100
24	BV	226/277 (82%)	213 (94%)	12 (5%)	1 (0%)	30	27
27	C	273/278 (98%)	269 (98%)	4 (2%)	0	100	100
28	D	212/217 (98%)	205 (97%)	7 (3%)	0	100	100
29	E	207/215 (96%)	205 (99%)	2 (1%)	0	100	100
30	F	180/187 (96%)	170 (94%)	10 (6%)	0	100	100
31	G	174/179 (97%)	169 (97%)	5 (3%)	0	100	100
32	H	149/151 (99%)	141 (95%)	8 (5%)	0	100	100
33	J	67/142 (47%)	64 (96%)	3 (4%)	0	100	100
34	K	144/147 (98%)	144 (100%)	0	0	100	100
35	L	120/122 (98%)	117 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	M	143/147 (97%)	139 (97%)	4 (3%)	0	100	100
37	N	134/138 (97%)	132 (98%)	2 (2%)	0	100	100
38	O	116/199 (58%)	112 (97%)	4 (3%)	0	100	100
39	P	124/127 (98%)	123 (99%)	1 (1%)	0	100	100
40	Q	111/113 (98%)	109 (98%)	2 (2%)	0	100	100
41	R	122/129 (95%)	122 (100%)	0	0	100	100
42	S	98/103 (95%)	97 (99%)	1 (1%)	0	100	100
43	T	112/153 (73%)	111 (99%)	1 (1%)	0	100	100
44	U	95/100 (95%)	94 (99%)	0	1 (1%)	11	7
45	V	93/105 (89%)	89 (96%)	4 (4%)	0	100	100
46	W	190/215 (88%)	189 (100%)	1 (0%)	0	100	100
47	X	77/88 (88%)	75 (97%)	2 (3%)	0	100	100
48	Y	61/64 (95%)	60 (98%)	1 (2%)	0	100	100
49	Z	64/77 (83%)	64 (100%)	0	0	100	100
50	a	57/61 (93%)	56 (98%)	1 (2%)	0	100	100
51	b	52/57 (91%)	52 (100%)	0	0	100	100
52	c	47/55 (86%)	47 (100%)	0	0	100	100
53	d	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
54	e	61/64 (95%)	60 (98%)	1 (2%)	0	100	100
55	f	35/37 (95%)	35 (100%)	0	0	100	100
56	g	55/75 (73%)	54 (98%)	1 (2%)	0	100	100
All	All	5793/6504 (89%)	5640 (97%)	146 (2%)	7 (0%)	49	46

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	BC	102	ILE
16	BM	11	ARG
24	BV	124	GLY
44	U	95	LEU
9	BF	39	LYS

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	
1	3	18/19 (95%)	18 (100%)	0	100	100
5	BB	30/31 (97%)	29 (97%)	1 (3%)	33	34
6	BC	170/212 (80%)	162 (95%)	8 (5%)	23	22
7	BD	175/176 (99%)	170 (97%)	5 (3%)	37	40
8	BE	127/147 (86%)	124 (98%)	3 (2%)	43	47
9	BF	85/85 (100%)	74 (87%)	11 (13%)	4	2
10	BG	131/132 (99%)	124 (95%)	7 (5%)	20	18
11	BH	107/108 (99%)	105 (98%)	2 (2%)	50	56
12	BI	102/125 (82%)	93 (91%)	9 (9%)	9	6
13	BJ	89/90 (99%)	83 (93%)	6 (7%)	15	11
14	BK	89/105 (85%)	85 (96%)	4 (4%)	24	23
15	BL	103/105 (98%)	97 (94%)	6 (6%)	18	15
16	BM	99/104 (95%)	95 (96%)	4 (4%)	28	27
17	BN	49/50 (98%)	48 (98%)	1 (2%)	48	54
18	BO	76/77 (99%)	74 (97%)	2 (3%)	40	44
19	BP	92/118 (78%)	90 (98%)	2 (2%)	45	50
20	BQ	80/83 (96%)	75 (94%)	5 (6%)	16	13
21	BR	55/72 (76%)	55 (100%)	0	100	100
22	BS	73/84 (87%)	71 (97%)	2 (3%)	39	42
23	BT	69/70 (99%)	65 (94%)	4 (6%)	18	15
24	BV	191/218 (88%)	184 (96%)	7 (4%)	30	30
27	C	215/218 (99%)	207 (96%)	8 (4%)	30	30
28	D	160/163 (98%)	155 (97%)	5 (3%)	35	37
29	E	169/173 (98%)	164 (97%)	5 (3%)	36	38
30	F	151/156 (97%)	146 (97%)	5 (3%)	33	34
31	G	148/150 (99%)	140 (95%)	8 (5%)	20	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	H	116/116 (100%)	111 (96%)	5 (4%)	26	25
33	J	51/108 (47%)	51 (100%)	0	100	100
34	K	119/120 (99%)	116 (98%)	3 (2%)	42	45
35	L	100/100 (100%)	97 (97%)	3 (3%)	36	38
36	M	112/114 (98%)	110 (98%)	2 (2%)	51	58
37	N	114/116 (98%)	108 (95%)	6 (5%)	20	18
38	O	97/158 (61%)	95 (98%)	2 (2%)	47	52
39	P	93/94 (99%)	90 (97%)	3 (3%)	34	35
40	Q	100/100 (100%)	99 (99%)	1 (1%)	68	75
41	R	97/99 (98%)	96 (99%)	1 (1%)	68	75
42	S	81/83 (98%)	79 (98%)	2 (2%)	42	45
43	T	90/117 (77%)	86 (96%)	4 (4%)	25	24
44	U	83/85 (98%)	79 (95%)	4 (5%)	23	21
45	V	81/86 (94%)	74 (91%)	7 (9%)	10	6
46	W	155/168 (92%)	147 (95%)	8 (5%)	21	18
47	X	58/63 (92%)	56 (97%)	2 (3%)	32	33
48	Y	50/51 (98%)	47 (94%)	3 (6%)	17	14
49	Z	59/66 (89%)	59 (100%)	0	100	100
50	a	52/54 (96%)	51 (98%)	1 (2%)	50	56
51	b	43/46 (94%)	42 (98%)	1 (2%)	44	49
52	c	47/52 (90%)	46 (98%)	1 (2%)	47	52
53	d	35/36 (97%)	33 (94%)	2 (6%)	18	15
54	e	53/54 (98%)	48 (91%)	5 (9%)	8	5
55	f	35/35 (100%)	34 (97%)	1 (3%)	37	40
56	g	51/63 (81%)	48 (94%)	3 (6%)	18	14
57	s	1/4 (25%)	0	1 (100%)	0	0
All	All	4826/5259 (92%)	4635 (96%)	191 (4%)	29	27

5 of 191 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
31	G	45	ARG
39	P	104	ARG

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Mol	Chain	Res	Type
31	G	137	ILE
35	L	87	ILE
43	T	102	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 101 such sidechains are listed below:

Mol	Chain	Res	Type
32	H	64	HIS
38	O	17	GLN
55	f	20	HIS
32	H	130	HIS
36	M	45	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	A	3083/3120 (98%)	499 (16%)	63 (2%)
25	BW	75/76 (98%)	13 (17%)	2 (2%)
26	I	5/15 (33%)	0	0
3	B	117/118 (99%)	12 (10%)	5 (4%)
4	BA	1511/1528 (98%)	271 (17%)	27 (1%)
All	All	4791/4857 (98%)	795 (16%)	97 (2%)

5 of 795 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	A	9	U
2	A	12	G
2	A	20	G
2	A	29	C
2	A	31	U

5 of 97 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A	2381	A
4	BA	350	G
2	A	2548	U
3	B	87	U
4	BA	485	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 354 ligands modelled in this entry, 353 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
59	A1BWO	A	4251	58	30,30,30	2.66	15 (50%)	40,44,44	2.99	13 (32%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	A1BWO	A	4251	58	-	0/15/39/39	0/2/3/3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	A	4251	A1BWO	C06-C07	5.61	1.59	1.51
59	A	4251	A1BWO	C26-N09	5.31	1.42	1.36
59	A	4251	A1BWO	C21-S18	-4.50	1.72	1.76
59	A	4251	A1BWO	C03-N05	3.73	1.42	1.34
59	A	4251	A1BWO	C17-S18	-3.55	1.73	1.76

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	A	4251	A1BWO	O02-C03-N05	9.18	120.62	110.91
59	A	4251	A1BWO	C08-N09-C26	-8.64	104.78	111.17
59	A	4251	A1BWO	C07-C08-N09	7.38	108.82	101.85
59	A	4251	A1BWO	C10-N09-C26	5.04	131.26	125.98
59	A	4251	A1BWO	O02-C03-O04	-4.70	117.77	124.62

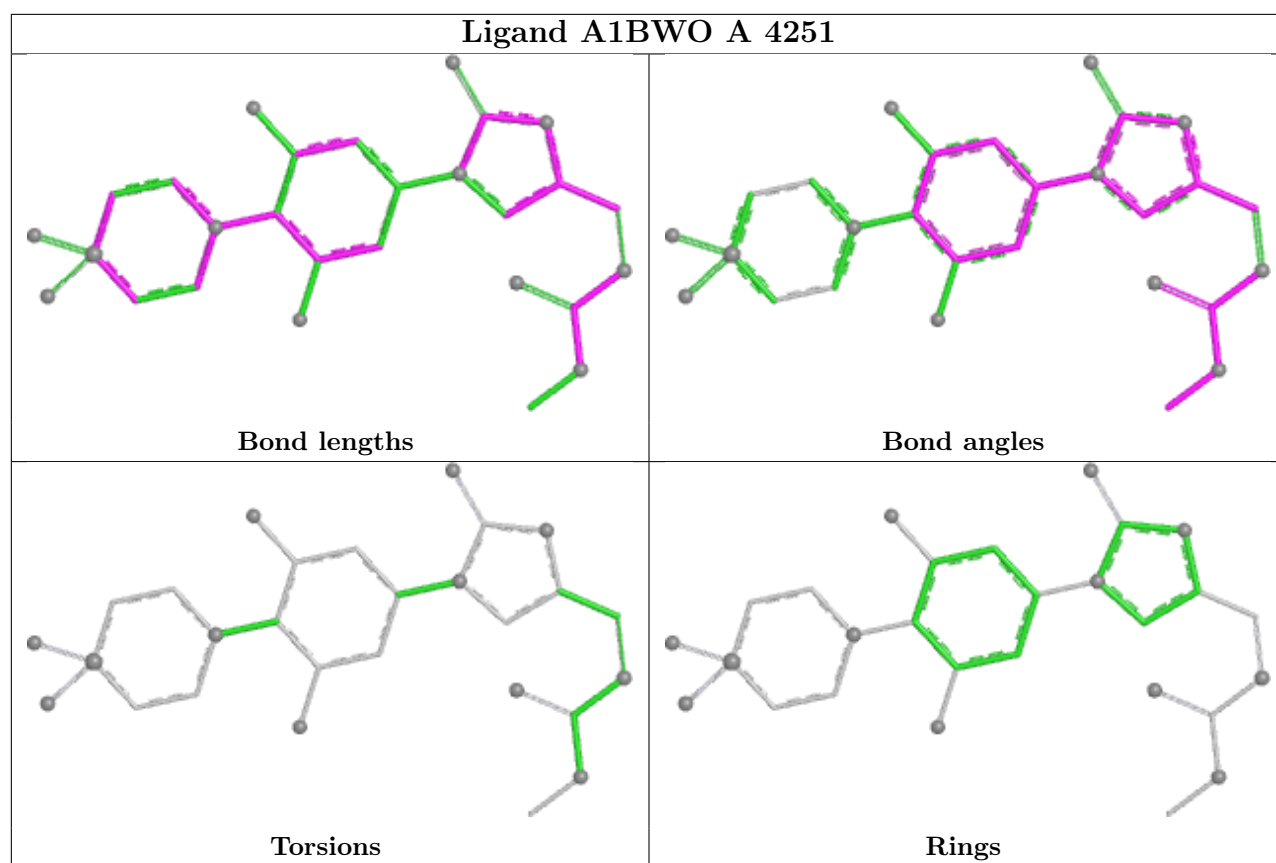
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

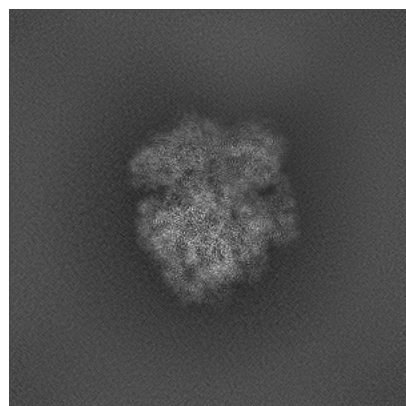
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49038. These allow visual inspection of the internal detail of the map and identification of artifacts.

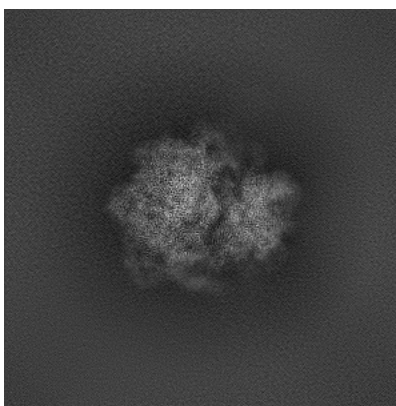
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

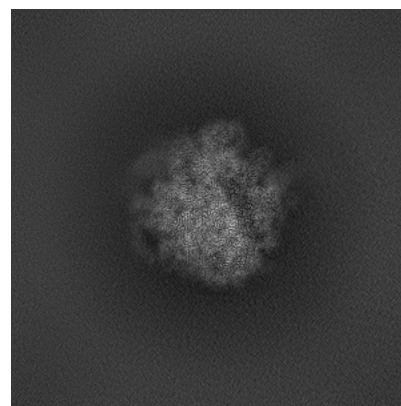
6.1.1 Primary map



X

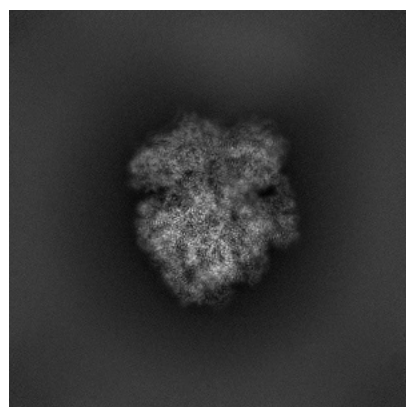


Y

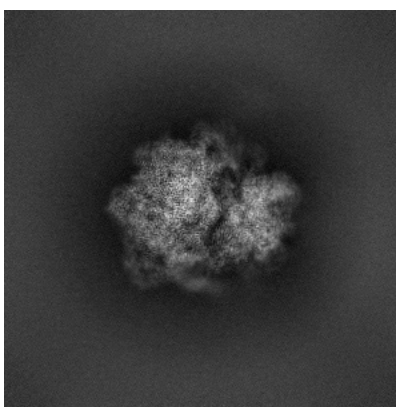


Z

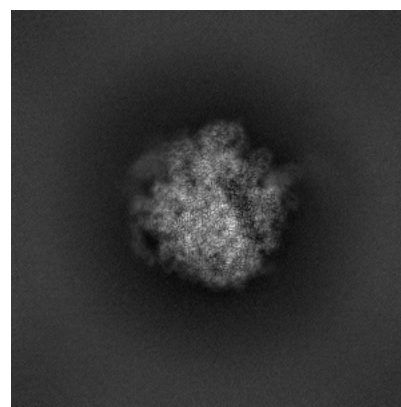
6.1.2 Raw map



X



Y

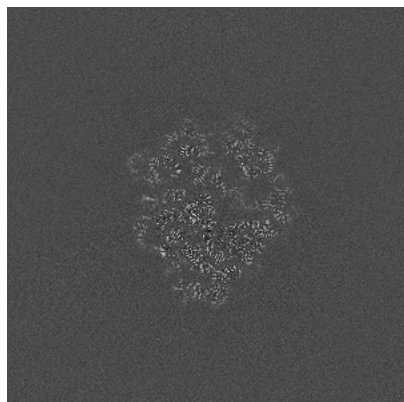


Z

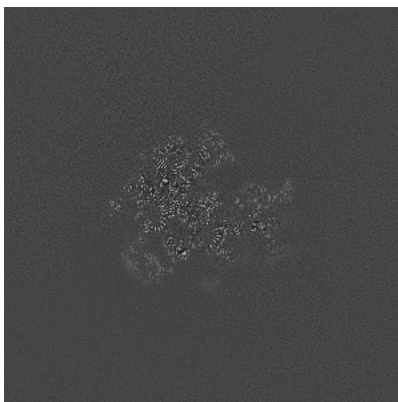
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

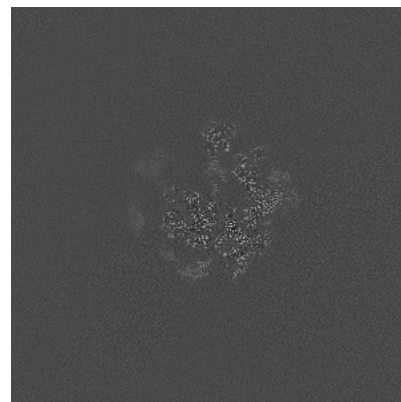
6.2.1 Primary map



X Index: 320

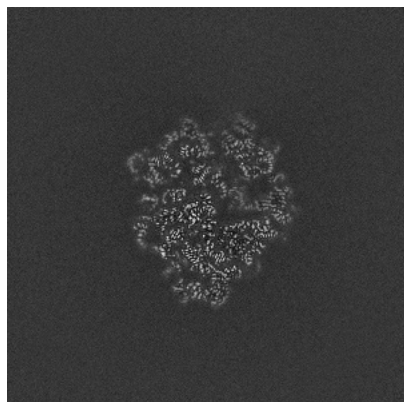


Y Index: 320

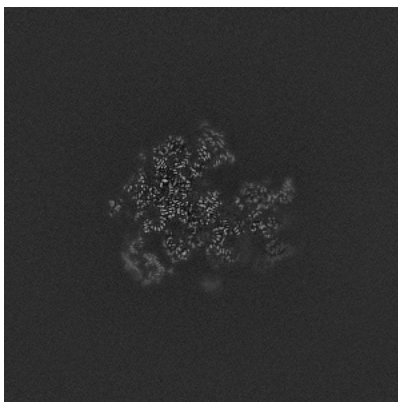


Z Index: 320

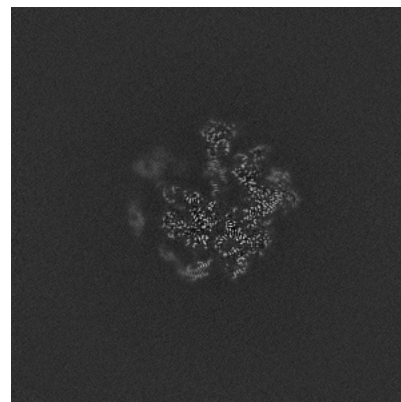
6.2.2 Raw map



X Index: 320



Y Index: 320

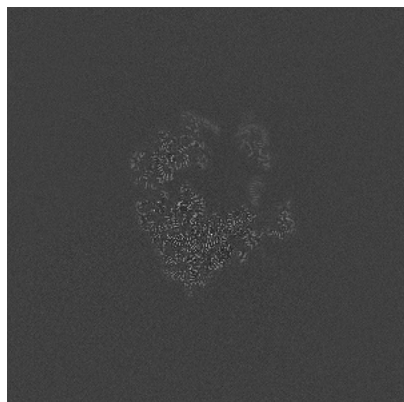


Z Index: 320

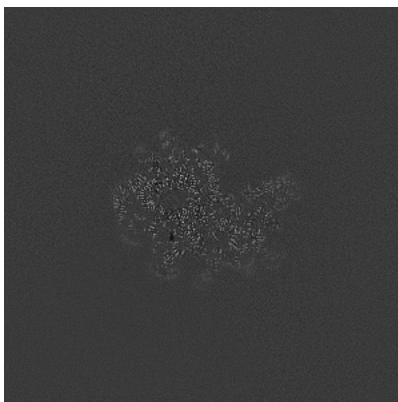
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

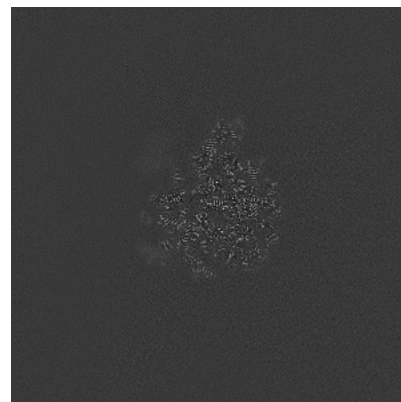
6.3.1 Primary map



X Index: 356

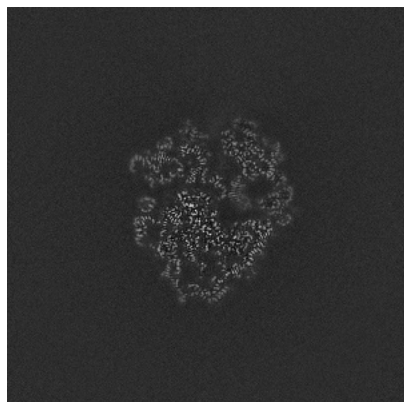


Y Index: 300

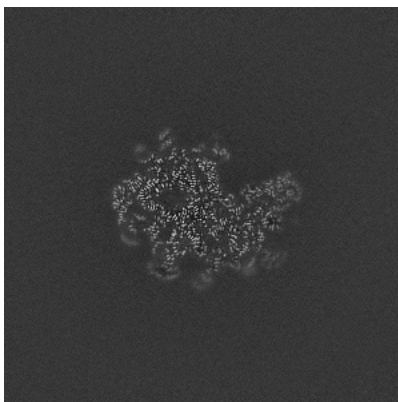


Z Index: 275

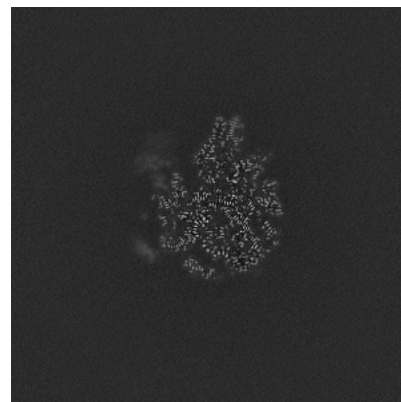
6.3.2 Raw map



X Index: 315



Y Index: 299

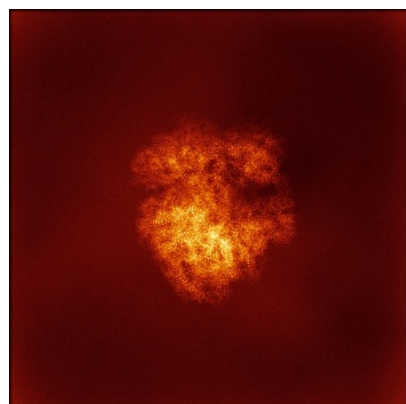


Z Index: 281

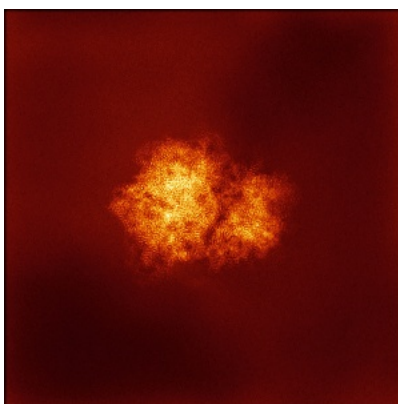
The images above show the largest variance slices of the map in three orthogonal directions.

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

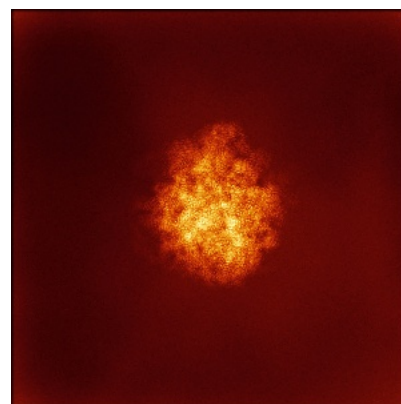
6.4.1 Primary map



X

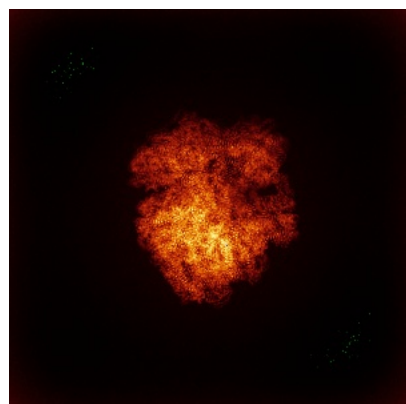


Y

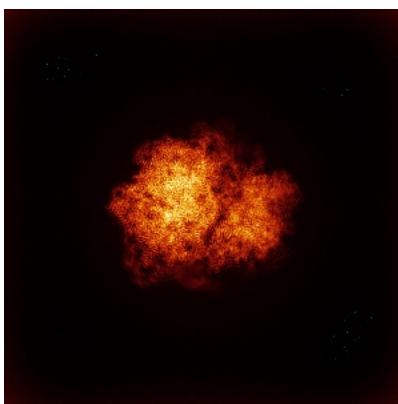


Z

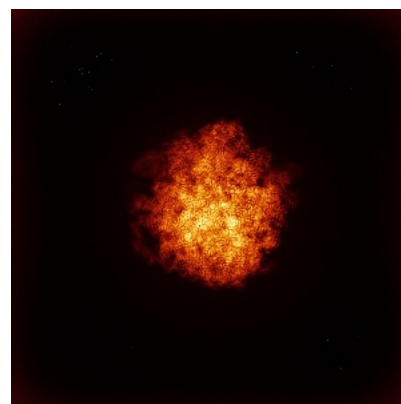
6.4.2 Raw map



X



Y

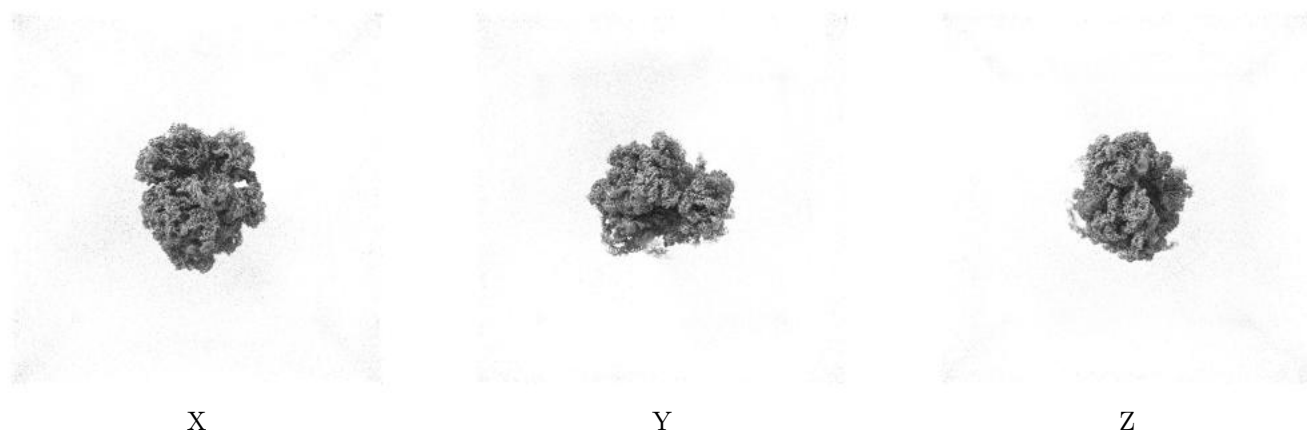


Z

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.

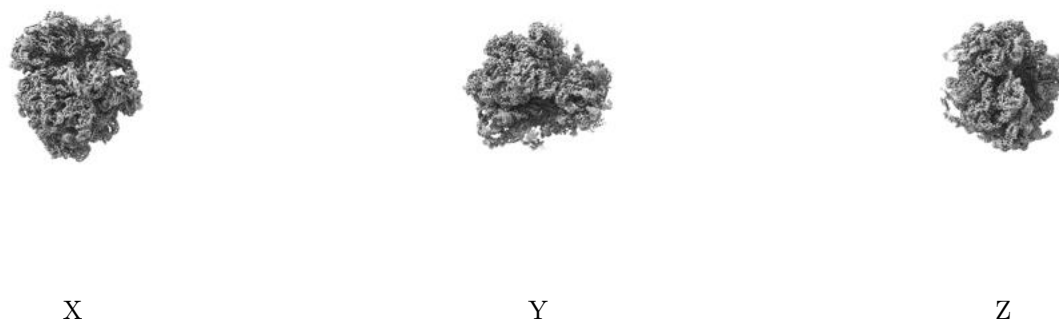
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. 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.

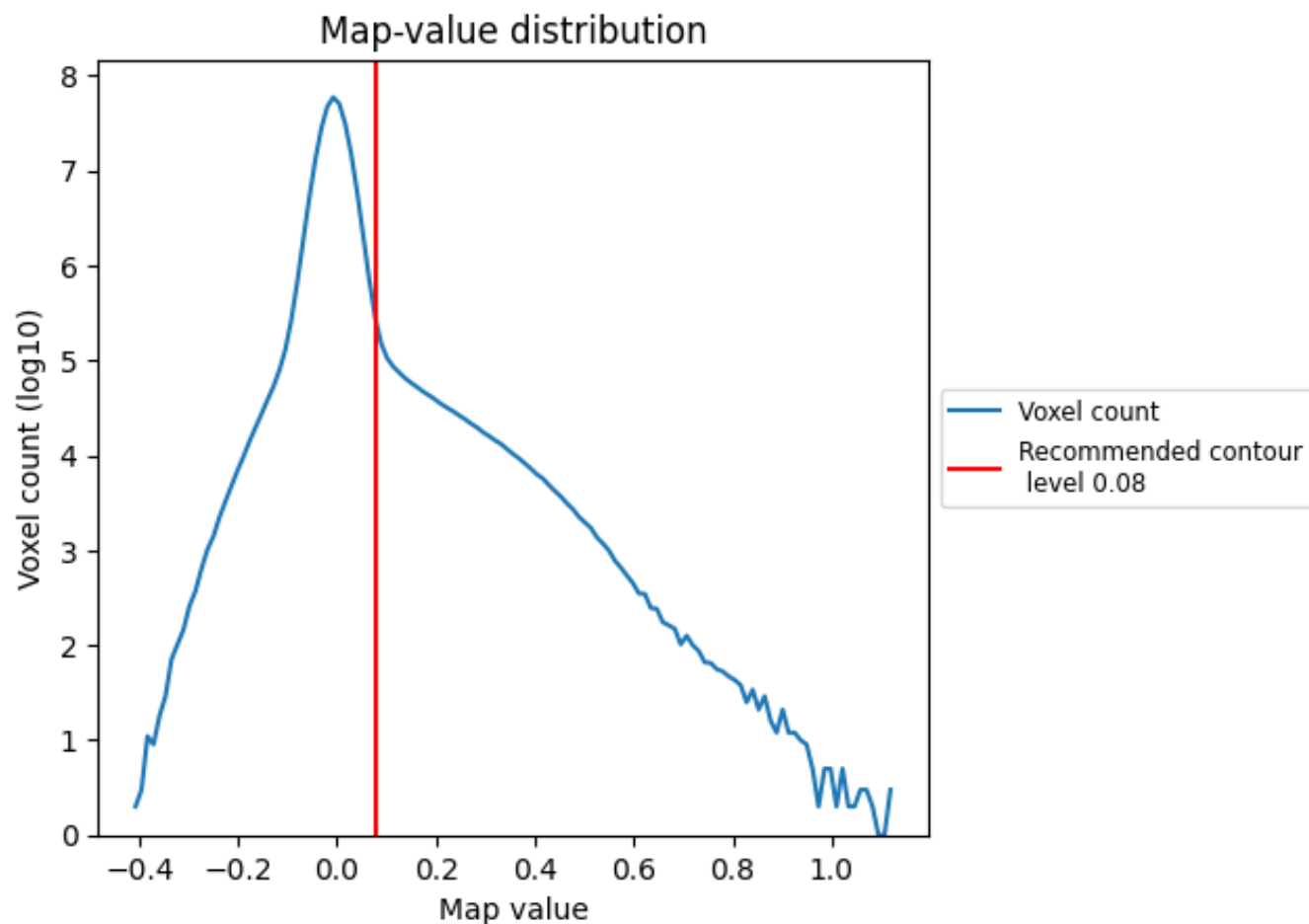
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

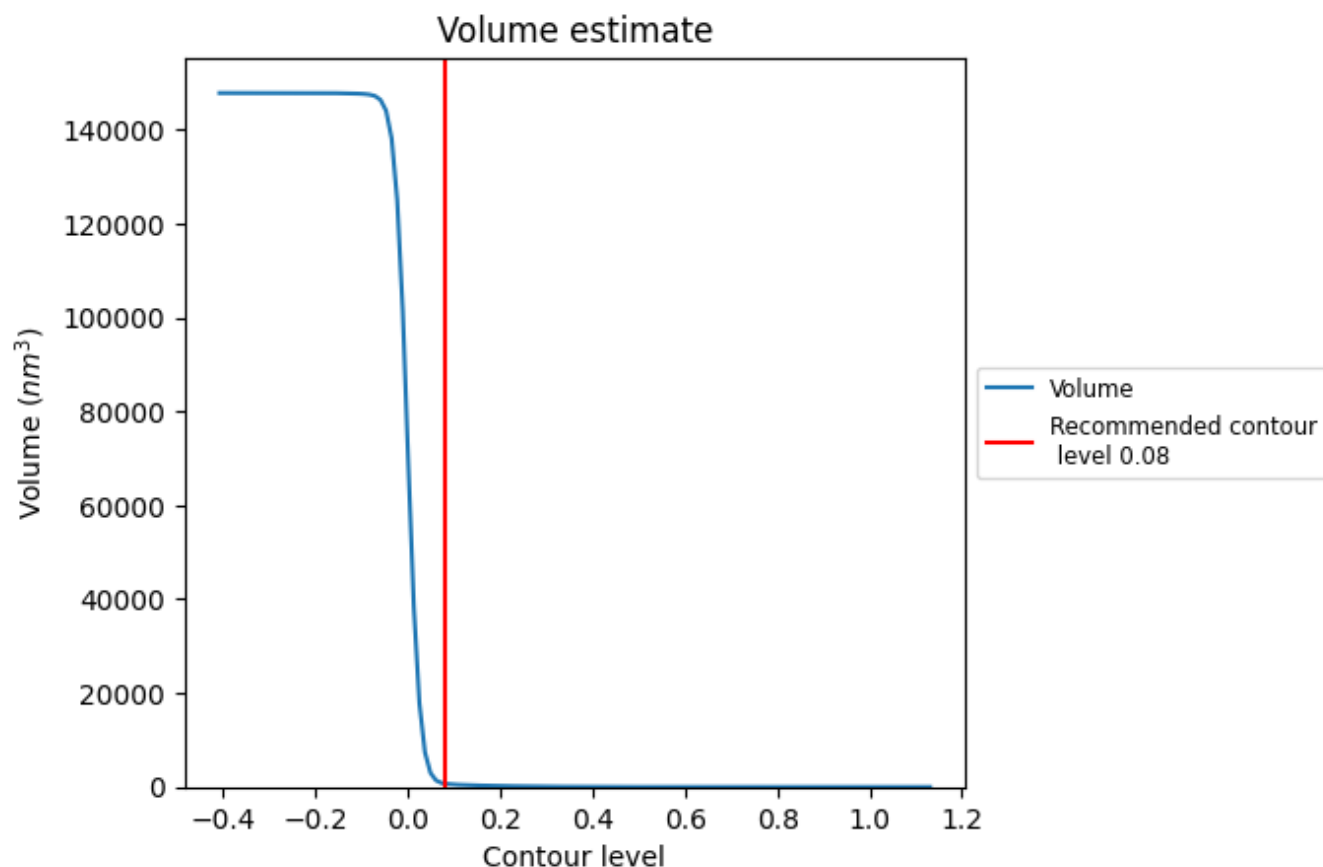
This section contains the results of statistical analysis of the map.

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.

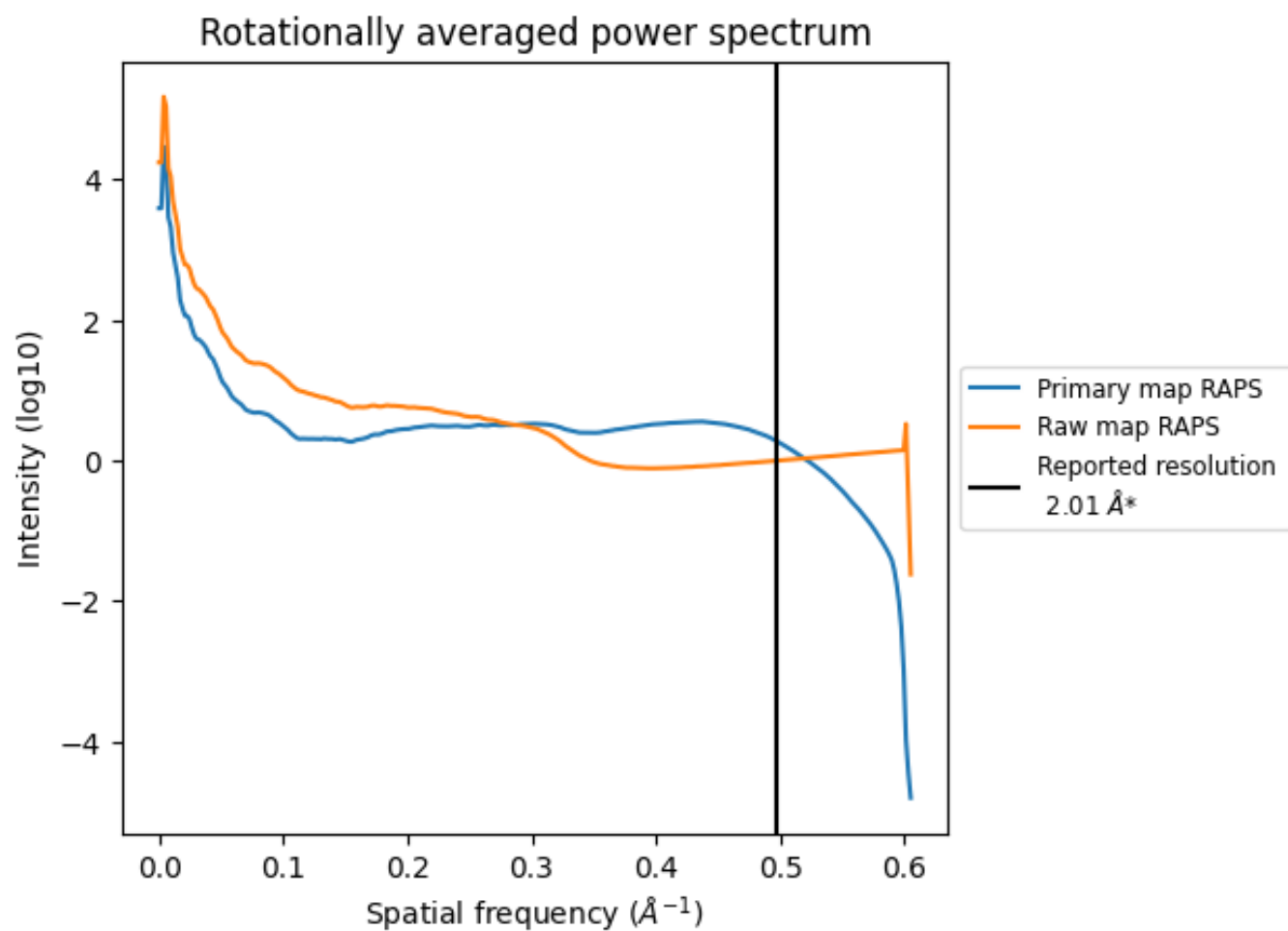
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 733 nm^3 ; this corresponds to an approximate mass of 662 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 ⓘ

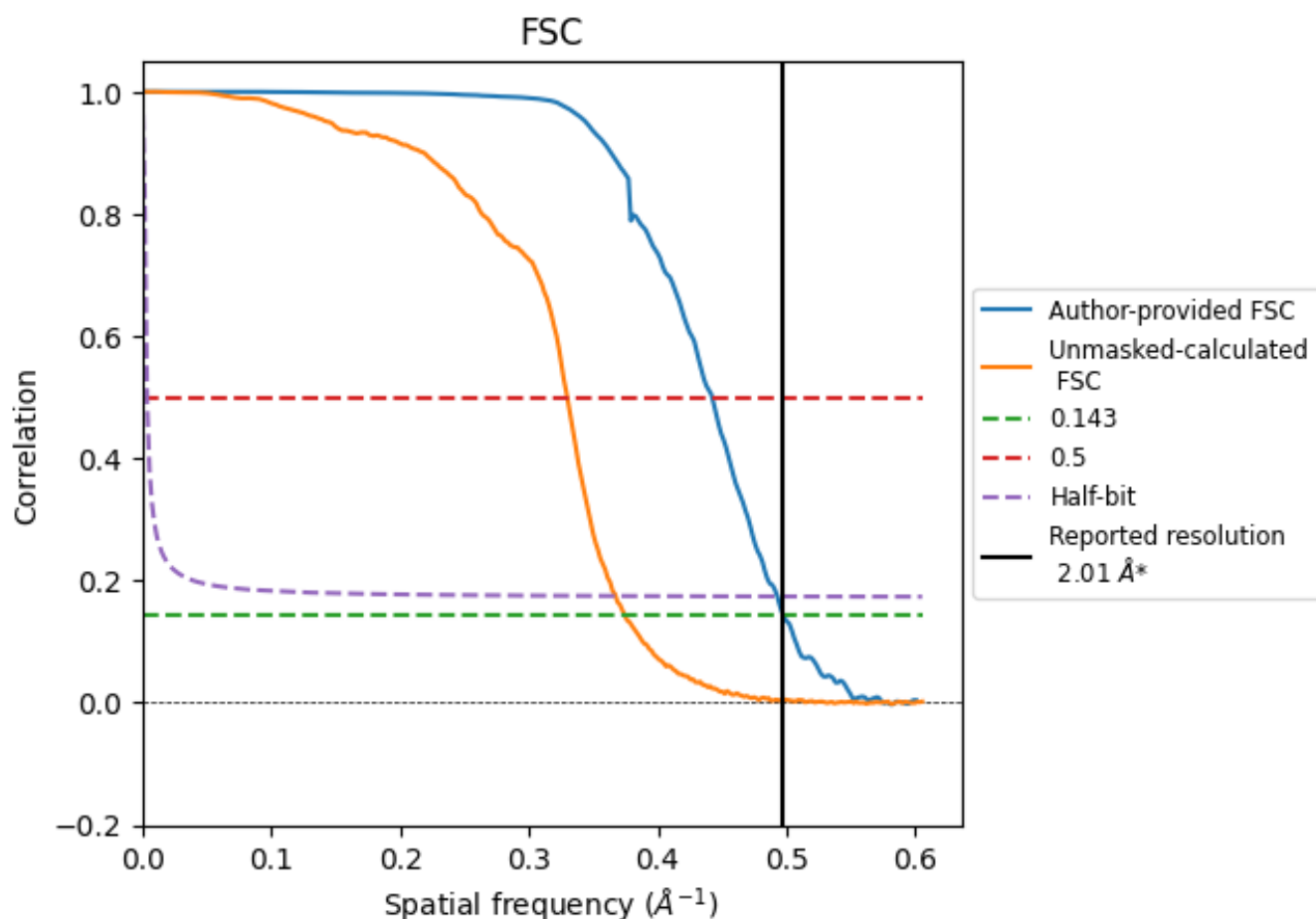


*Reported resolution corresponds to spatial frequency of $0.498 \text{ \AA}^{-1}$

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 0.498 Å⁻¹

8.2 Resolution estimates [i](#)

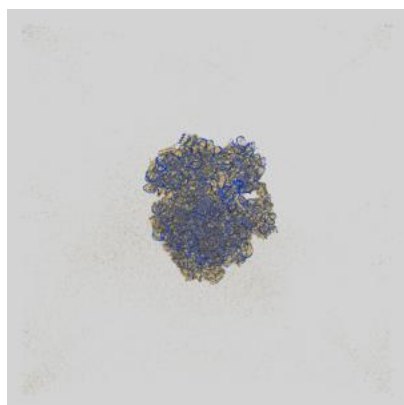
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.01	-	-
Author-provided FSC curve	2.01	2.26	2.03
Unmasked-calculated*	2.67	3.03	2.72

*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 2.67 differs from the reported value 2.01 by more than 10 %

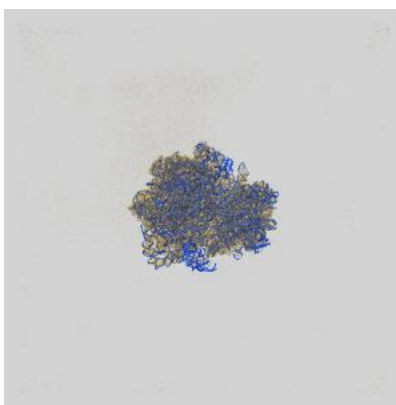
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-49038 and PDB model 9N5T. Per-residue inclusion information can be found in [section 3](#) on [page 19](#).

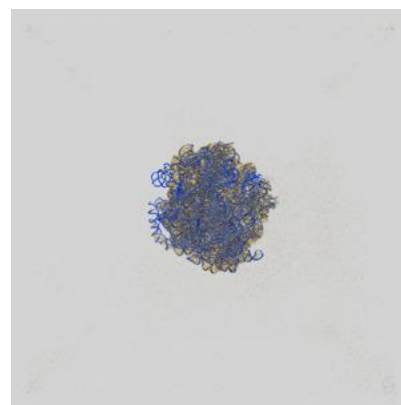
9.1 Map-model overlay [i](#)



X



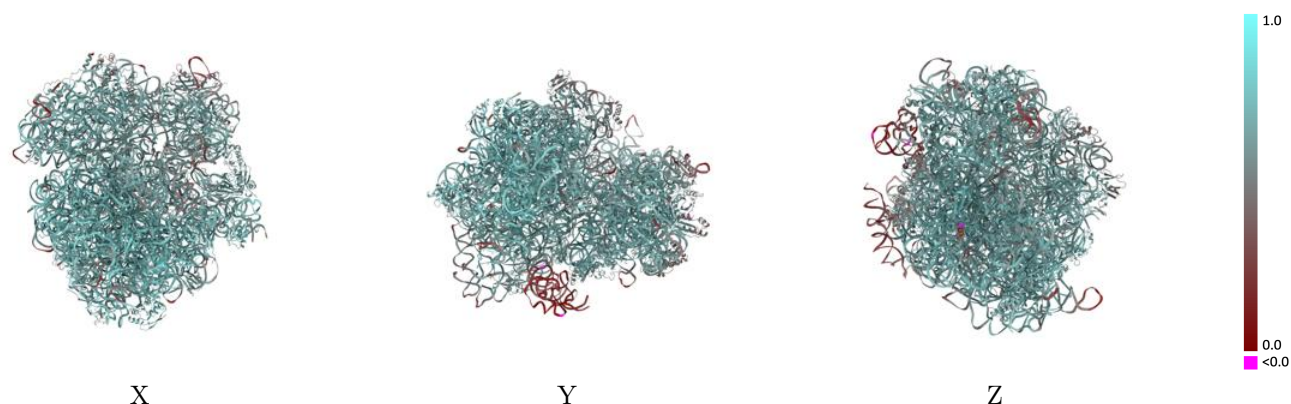
Y



Z

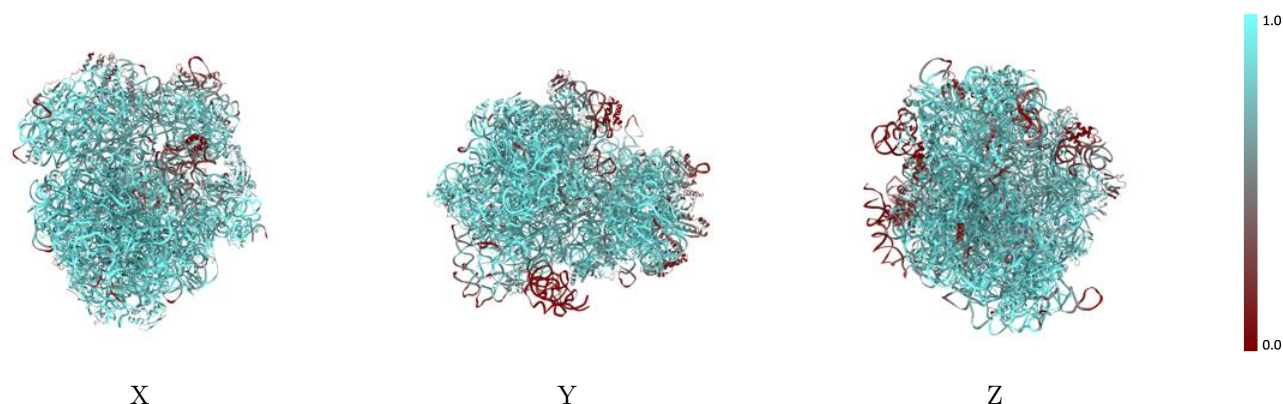
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



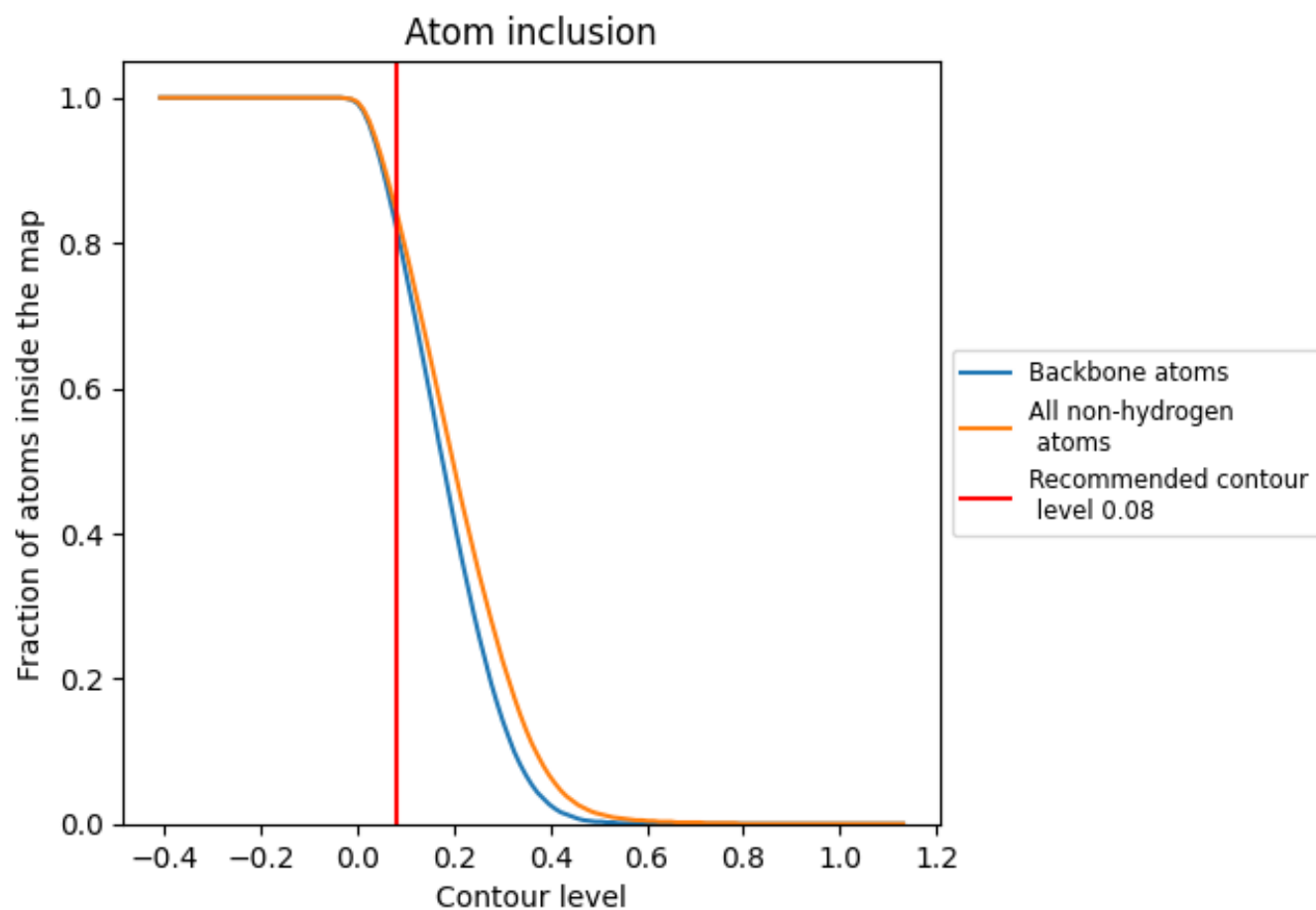
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8470	 0.6730
3	 0.9220	 0.7530
A	 0.8720	 0.6870
B	 0.9110	 0.6770
BA	 0.9000	 0.6700
BB	 0.5970	 0.6240
BC	 0.6980	 0.5980
BD	 0.6600	 0.5880
BE	 0.7940	 0.6440
BF	 0.7170	 0.6160
BG	 0.7470	 0.6250
BH	 0.8690	 0.6860
BI	 0.8010	 0.6410
BJ	 0.6380	 0.5670
BK	 0.8250	 0.6460
BL	 0.7680	 0.6390
BM	 0.7900	 0.6310
BN	 0.9090	 0.6890
BO	 0.8200	 0.6650
BP	 0.7680	 0.6410
BQ	 0.7260	 0.6140
BR	 0.7670	 0.6220
BS	 0.7470	 0.6140
BT	 0.8100	 0.6530
BV	 0.2740	 0.4890
BW	 0.6800	 0.5830
C	 0.9330	 0.7450
D	 0.9130	 0.7350
E	 0.8930	 0.7230
F	 0.7990	 0.6370
G	 0.5800	 0.5480
H	 0.5870	 0.5660
I	 0.8560	 0.6690
J	 0.0140	 0.4800
K	 0.9280	 0.7320



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Chain	Atom inclusion	Q-score
L	 0.8690	 0.7180
M	 0.8910	 0.7080
N	 0.9000	 0.7210
O	 0.9390	 0.7560
P	 0.8850	 0.6840
Q	 0.8510	 0.7000
R	 0.9480	 0.7680
S	 0.9030	 0.7160
T	 0.9170	 0.7470
U	 0.8230	 0.6790
V	 0.7080	 0.6010
W	 0.6560	 0.5990
X	 0.9240	 0.7450
Y	 0.8920	 0.7170
Z	 0.8180	 0.6610
a	 0.9130	 0.7440
b	 0.8860	 0.7200
c	 0.9040	 0.7270
d	 0.9400	 0.7580
e	 0.9610	 0.7670
f	 0.8960	 0.6970
g	 0.6720	 0.5950
s	 0.2500	 0.4800