



wwPDB EM Validation Summary Report ⓘ

Feb 23, 2025 – 01:05 AM JST

PDB ID : 8XI2
EMDB ID : EMD-38362
Title : Cryo-EM structure of the Chlamydomonas C* complex
Authors : Lu, Y.; Zhan, X.
Deposited on : 2023-12-19
Resolution : 2.60 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:

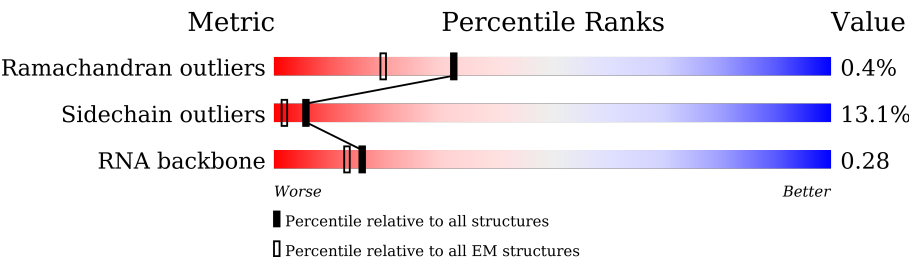
EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.2

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 2.60 Å.

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








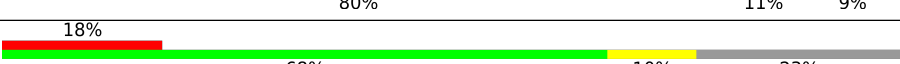
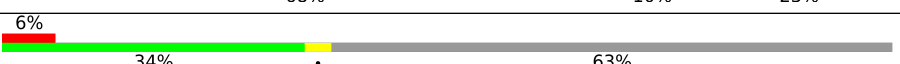
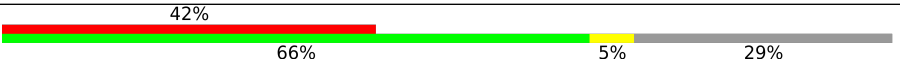


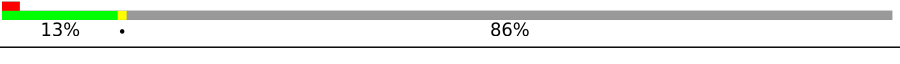
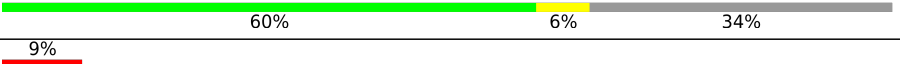


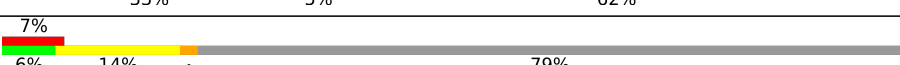
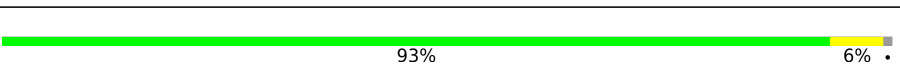

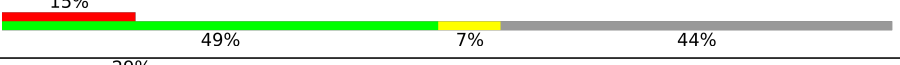

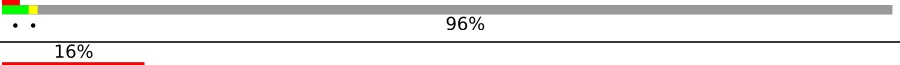





Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	A	2398	<div><div>10%</div><div>71%</div><div>9%</div><div>19%</div></div>
2	B	111	<div><div>5%</div><div>29%</div><div>46%</div><div>23%</div></div>
3	C	989	<div><div>8%</div><div>80%</div><div>11%</div><div>9%</div></div>
4	E	362	<div><div>78%</div><div>10%</div><div>12%</div></div>
5	F	101	<div><div>27%</div><div>58%</div><div>6%</div><div>9%</div></div>
6	q	503	<div><div>8%</div><div>18%</div><div>79%</div></div>
6	r	503	<div><div>6%</div><div>22%</div><div>74%</div></div>
6	s	503	<div><div>13%</div><div>86%</div></div>

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Mol	Chain	Length	Quality of chain
6	t	503	
7	a	127	
8	g	77	
9	e	87	
10	f	85	
11	d	110	
12	c	114	
13	b	265	
14	I	925	
15	J	835	
16	P	235	
17	M	563	
18	T	518	
19	O	417	
20	N	233	
21	R	684	
22	H	192	
23	S	157	
24	W	576	
25	L	833	
26	K	303	
27	U	721	
28	V	928	
29	Q	1844	
30	5	7	

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Mol	Chain	Length	Quality of chain
31	3	173	<p>6% 8% 9% 80%</p>

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 73326 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 MPN domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1931	Total	C	N	O	S	0	0
			15194	9743	2699	2682	70		

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	86	Total	C	N	O	P	0	0
			1817	812	307	612	86		

- Molecule 3 is a protein called Elongation factor Tu, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	897	Total	C	N	O	S	0	0
			6973	4431	1203	1297	42		

- Molecule 4 is a protein called U5-40K.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	318	Total	C	N	O	S	0	0
			2441	1524	436	465	16		

- Molecule 5 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	92	Total	C	N	O	P	0	0
			1985	885	369	637	94		

- Molecule 6 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	q	106	Total	C	N	O	S	0	0
			831	522	145	160	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	r	131	Total	C	N	O	S	0	0
			1021	638	183	196	4		
6	s	70	Total	C	N	O	S	0	0
			570	353	108	107	2		
6	t	62	Total	C	N	O	S	0	0
			504	312	95	96	1		

- Molecule 7 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	a	90	Total	C	N	O	S	0	0
			705	444	129	126	6		

- Molecule 8 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	g	65	Total	C	N	O	S	0	0
			512	323	90	96	3		

- Molecule 9 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	e	80	Total	C	N	O	S	0	0
			660	420	117	119	4		

- Molecule 10 is a protein called Sm protein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	f	71	Total	C	N	O	S	0	0
			559	358	91	106	4		

- Molecule 11 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	d	100	Total	C	N	O	S	0	0
			810	505	152	147	6		

- Molecule 12 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	c	88	Total	C	N	O	S	0	0
			684	435	121	124	4		

- Molecule 13 is a protein called Sm domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	b	99	Total	C	N	O	S	0	0
			780	489	149	138	4		

- Molecule 14 is a protein called Syf1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	661	Total	C	N	O	S	0	0
			4629	2900	855	861	13		

- Molecule 15 is a protein called Crooked neck protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	595	Total	C	N	O	S	0	0
			4033	2511	759	753	10		

- Molecule 16 is a protein called Cwf15/Cwc15 cell cycle control protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	P	104	Total	C	N	O	0	0
			867	536	175	156		

- Molecule 17 is a protein called PPIase cyclophilin-type domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	80	Total	C	N	O	S	0	0
			644	402	121	120	1		

- Molecule 18 is a protein called PLRG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	344	Total	C	N	O	S	0	0
			2700	1705	488	490	17		

- Molecule 19 is a protein called Rbm22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	273	Total	C	N	O	S	0	0
			2136	1337	376	405	18		

- Molecule 20 is a protein called G10 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	171	Total	C	N	O	S	0	0
			1412	897	260	248	7		

- Molecule 21 is a protein called SKI-interacting protein SKIP SNW domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	R	260	Total	C	N	O	P	S	0	0
			1994	1251	361	377	2	3		

- Molecule 22 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	H	40	Total	C	N	O	P	0	0
			838	375	134	289	40		

- Molecule 23 is a protein called Peptidyl-prolyl cis-trans isomerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	155	Total	C	N	O	S	0	0
			1198	754	213	225	6		

- Molecule 24 is a protein called Prp17.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	487	Total	C	N	O	S	0	0
			2826	1721	553	549	3		

- Molecule 25 is a protein called Cdc5L.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	L	468	Total	C	N	O	S	0	0
			3795	2349	722	712	12		

- Molecule 26 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	K	210	Total	C	N	O	S	0	0
			1688	1045	318	321	4		

- Molecule 27 is a protein called CWF21 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	26	Total	C	N	O	S	0	0
			191	119	34	36	2		

- Molecule 28 is a protein called MI domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	186	Total	C	N	O	S	0	0
			1020	621	198	200	1		

- Molecule 29 is a protein called Intron-binding protein aquarius.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Q	1299	Total	C	N	O		0	0
			6423	3825	1299	1299			

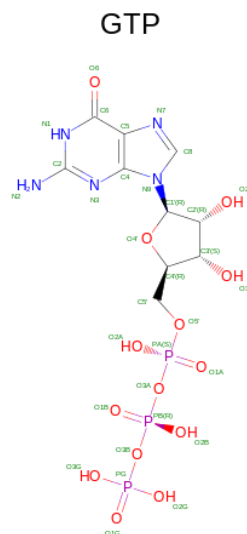
- Molecule 30 is a RNA chain called RNA (5'-R(P*CP*CP*GP*AP*AP*CP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
30	5	7	Total	C	N	O	P	0	0
			150	67	29	47	7		

- Molecule 31 is a RNA chain called RNA (173-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
31	3	34	Total	C	N	O	P	0	0
			694	311	111	238	34		

- Molecule 32 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



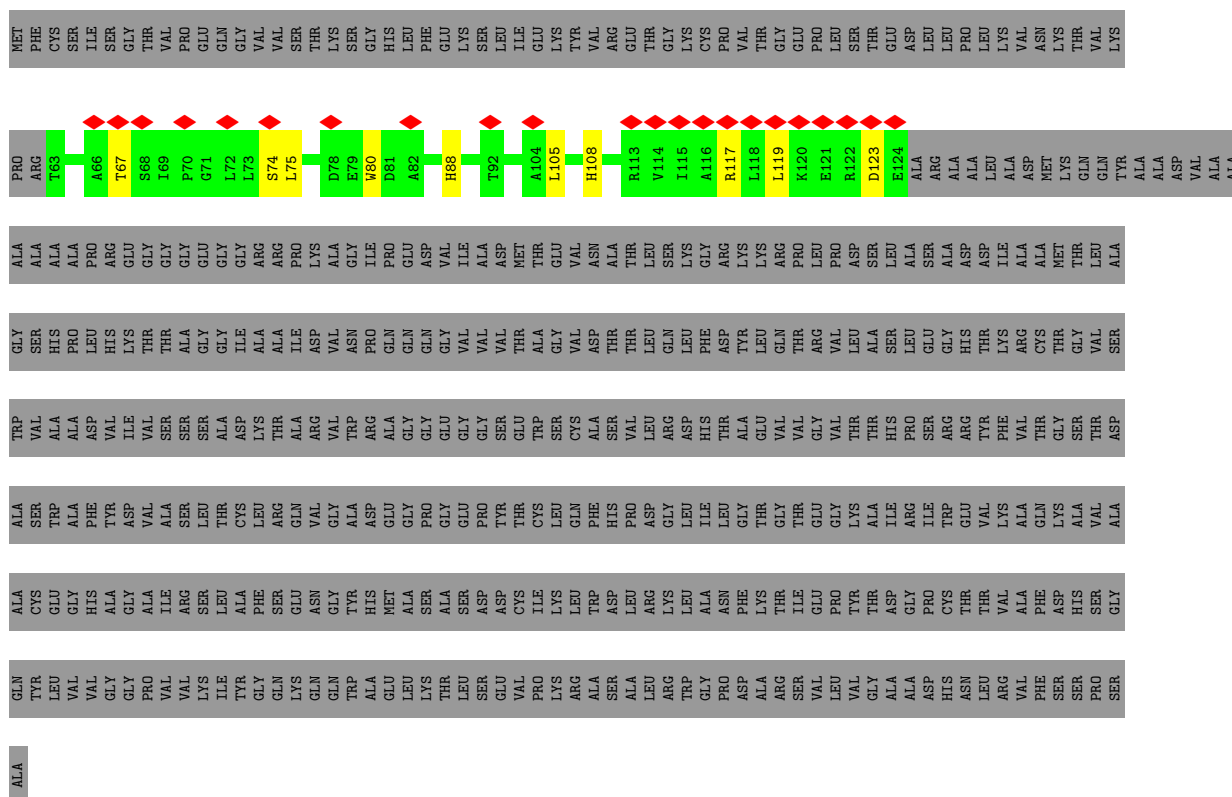
Mol	Chain	Residues	Atoms					AltConf
32	C	1	Total	C	N	O	P	0
			32	10	5	14	3	

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

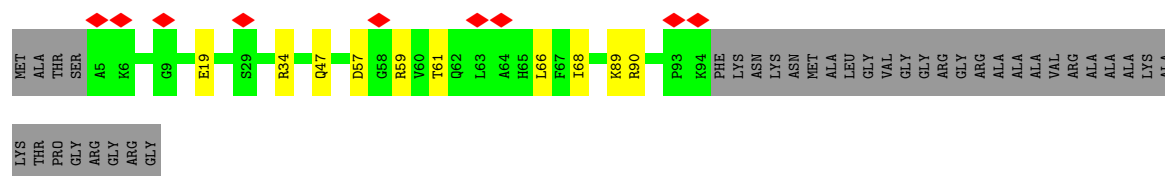
Mol	Chain	Residues	Atoms	AltConf
33	C	1	Total Mg 1 1	0
33	F	6	Total Mg 6 6	0

- Molecule 34 is ZINC ION (three-letter code: ZN) (formula: Zn).

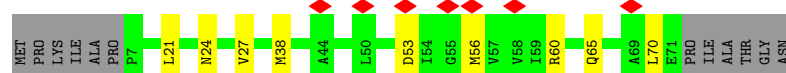
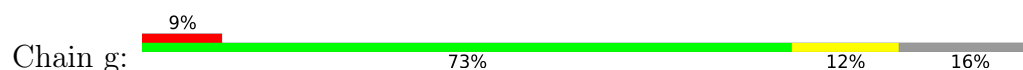
Mol	Chain	Residues	Atoms	AltConf
34	O	2	Total Zn 2 2	0
34	N	1	Total Zn 1 1	0

[illegible]

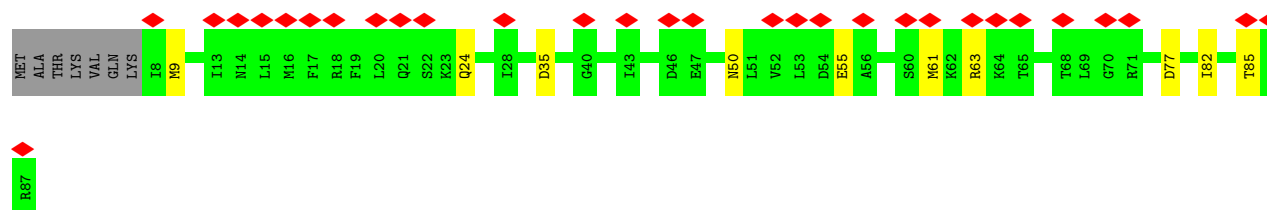
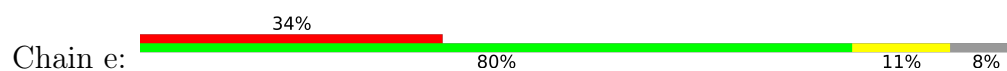
- Molecule 7: Small nuclear ribonucleoprotein Sm D3



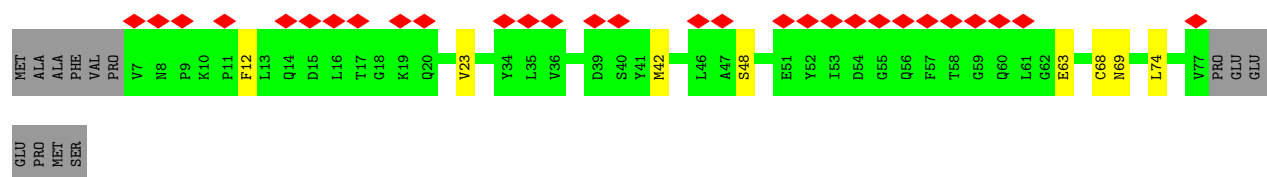
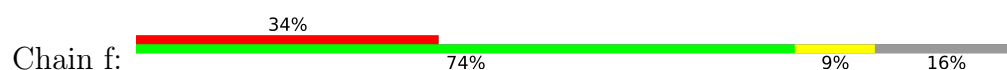
- Molecule 8: Small nuclear ribonucleoprotein G



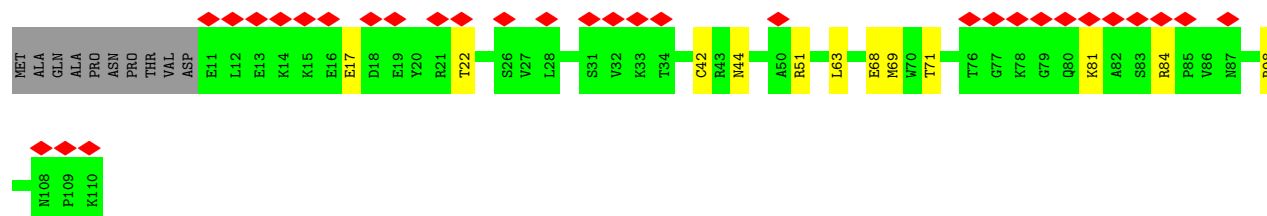
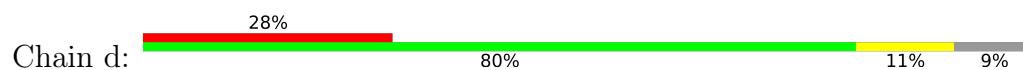
- Molecule 9: Small nuclear ribonucleoprotein E



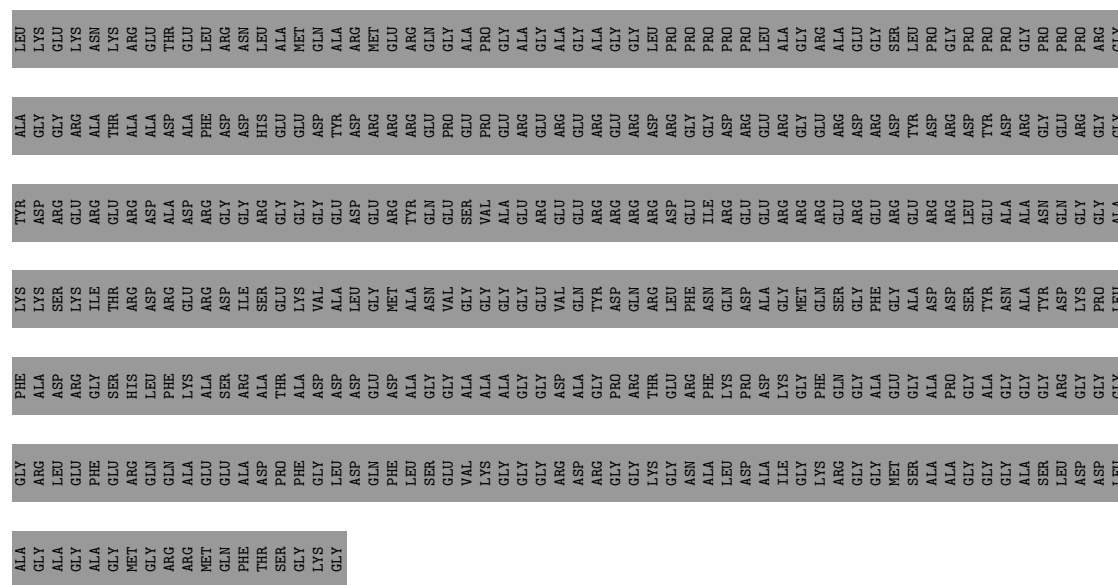
- Molecule 10: Sm protein F



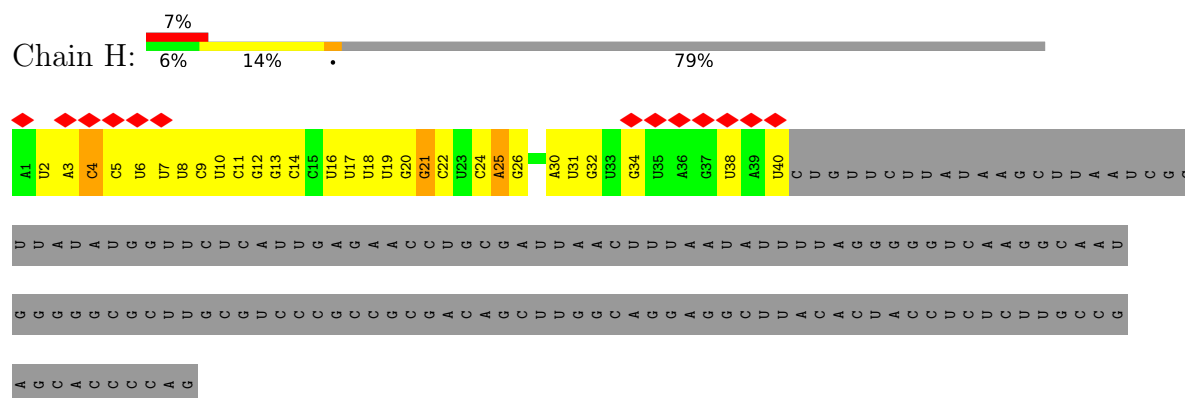
- Molecule 11: Small nuclear ribonucleoprotein Sm D2







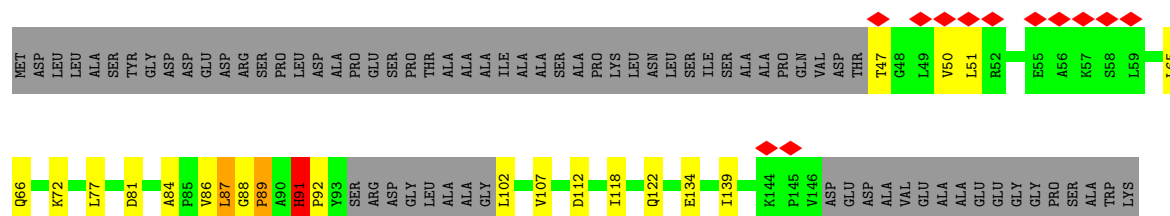
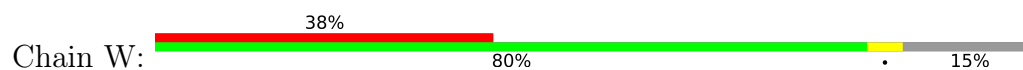
- Molecule 22: U2 snRNA



- Molecule 23: Peptidyl-prolyl cis-trans isomerase

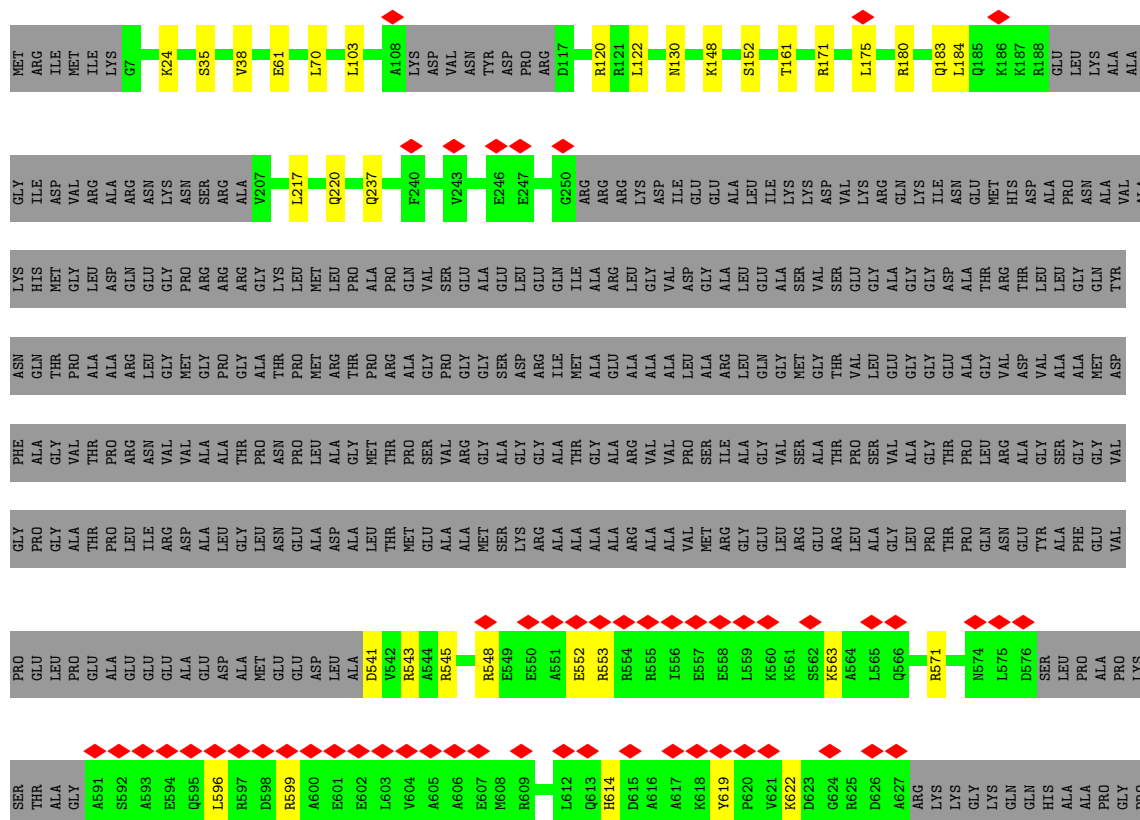


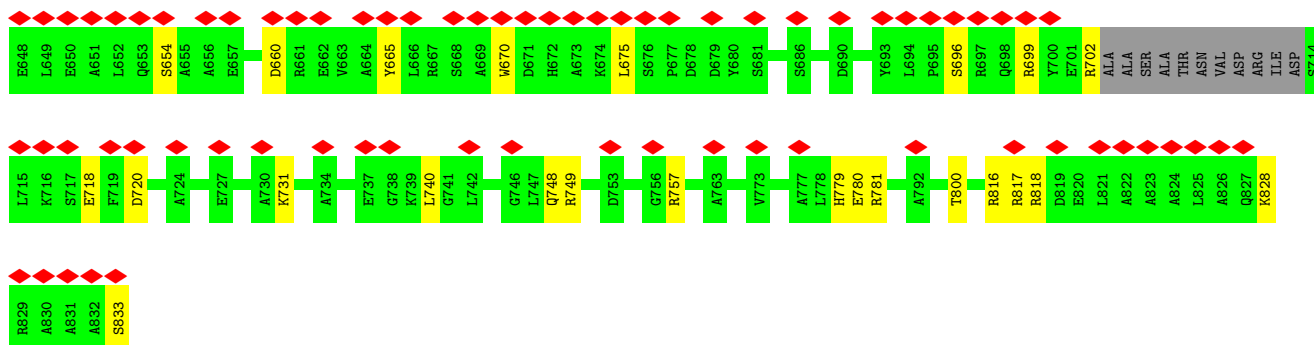
- Molecule 24: Prp17



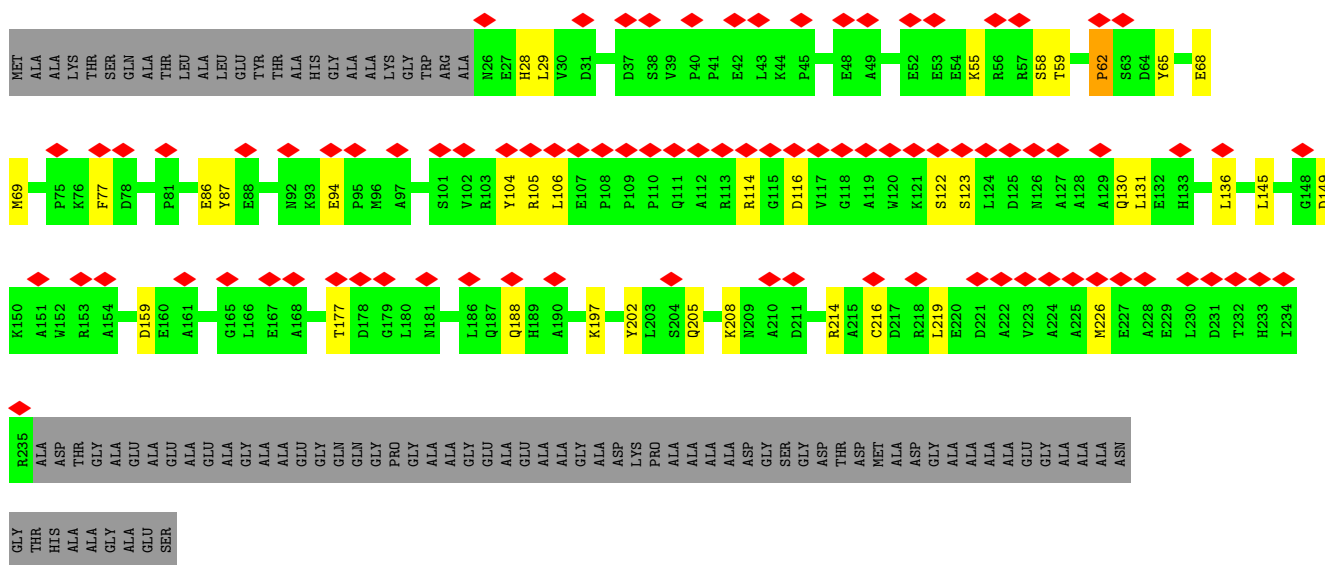


● Molecule 25: Cdc5L

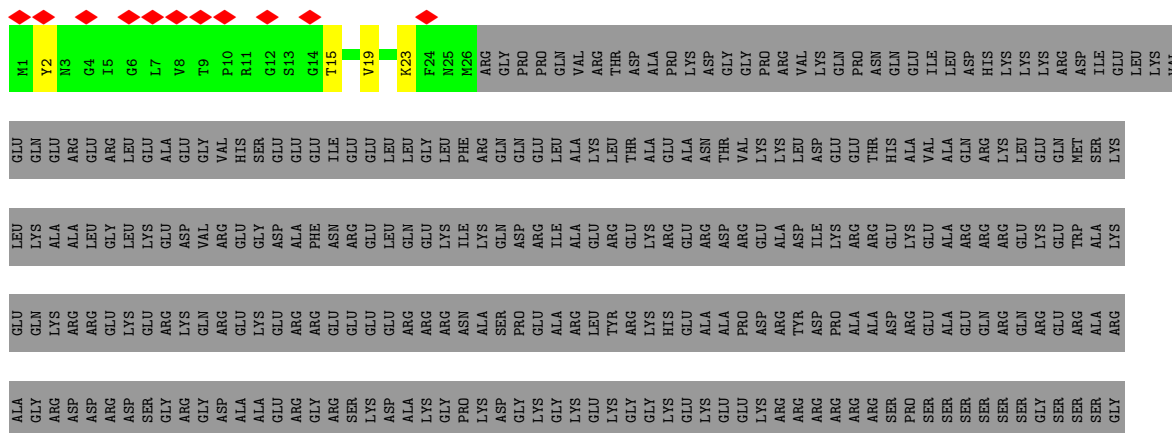




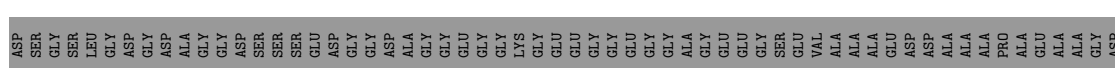
- Molecule 26: Pre-mRNA-splicing factor SPF27



- Molecule 27: CWF21 domain-containing protein









G G D D G A C G A C A A A C D C D D C G C G G D C D D D C C A G D G G G G A D C C G A D A D C C G

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	518369	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.00	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.593	Depositor
Minimum map value	-1.565	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.08	Depositor
Map size (\AA)	404.80002, 404.80002, 404.80002	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.92, 0.92, 0.92	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SEP, GTP, G5J, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.86	19/15581 (0.1%)	0.67	7/21167 (0.0%)
2	B	1.22	6/2024 (0.3%)	1.16	5/3144 (0.2%)
3	C	0.41	0/7126	0.57	1/9683 (0.0%)
4	E	0.40	0/2496	0.58	1/3382 (0.0%)
5	F	1.60	43/2188 (2.0%)	1.31	17/3409 (0.5%)
6	q	0.30	0/847	0.57	0/1148
6	r	0.31	0/1040	0.58	0/1411
6	s	0.30	0/580	0.59	0/784
6	t	0.33	0/514	0.62	0/698
7	a	0.30	0/716	0.53	0/960
8	g	0.31	0/516	0.56	0/691
9	e	0.28	0/667	0.52	0/891
10	f	0.29	0/567	0.56	0/764
11	d	0.28	0/821	0.50	0/1097
12	c	0.29	0/691	0.61	0/933
13	b	0.30	0/792	0.60	0/1059
14	I	0.28	0/4712	0.48	0/6427
15	J	0.65	0/4092	0.52	1/5574 (0.0%)
16	P	0.74	1/882 (0.1%)	0.60	0/1173
17	M	0.39	0/654	0.56	0/874
18	T	1.14	5/2773 (0.2%)	0.81	0/3765
19	O	0.54	0/2179	0.59	0/2944
20	N	0.82	0/1446	0.64	2/1944 (0.1%)
21	R	0.64	0/2020	0.59	0/2736
22	H	1.25	4/932 (0.4%)	1.29	4/1447 (0.3%)
23	S	0.43	0/1224	0.56	0/1652
24	W	0.44	2/2852 (0.1%)	0.57	2/3908 (0.1%)
25	L	0.46	0/3847	0.57	1/5158 (0.0%)
26	K	0.29	0/1717	0.55	3/2320 (0.1%)
27	U	0.32	0/194	0.60	0/259
28	V	0.28	0/1023	0.42	0/1413
29	Q	0.28	0/6411	0.48	1/8913 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	5	1.29	0/167	1.52	4/258 (1.6%)
31	3	0.55	0/771	1.19	4/1193 (0.3%)
All	All	0.69	80/75062 (0.1%)	0.68	53/103179 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	11
3	C	0	1
6	s	0	1
6	t	0	1
25	L	0	1
28	V	0	1
All	All	0	16

The worst 5 of 80 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	W	89	PRO	N-CA	13.08	1.69	1.47
5	F	58	G	C8-N7	-7.87	1.26	1.30
5	F	58	G	C5-C4	-7.64	1.33	1.38
5	F	60	G	C8-N7	-7.22	1.26	1.30
5	F	57	U	C2-N3	-7.16	1.32	1.37

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	H	22	C	O5'-P-OP1	-18.02	89.07	110.70
20	N	46	LEU	CA-CB-CG	7.61	132.81	115.30
1	A	843	LEU	CA-CB-CG	7.12	131.67	115.30
5	F	39	G	C5-C6-O6	-6.80	124.52	128.60
5	F	68	G	N9-C4-C5	-6.78	102.69	105.40

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1004	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	A	1005	LYS	Peptide
1	A	1045	PHE	Peptide
1	A	532	LYS	Peptide
1	A	686	GLY	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1923/2398 (80%)	1730 (90%)	182 (10%)	11 (1%)	22	43
3	C	895/989 (90%)	816 (91%)	78 (9%)	1 (0%)	48	71
4	E	316/362 (87%)	289 (92%)	26 (8%)	1 (0%)	37	59
6	q	102/503 (20%)	102 (100%)	0	0	100	100
6	r	129/503 (26%)	120 (93%)	8 (6%)	1 (1%)	16	34
6	s	68/503 (14%)	65 (96%)	3 (4%)	0	100	100
6	t	60/503 (12%)	56 (93%)	4 (7%)	0	100	100
7	a	88/127 (69%)	86 (98%)	2 (2%)	0	100	100
8	g	63/77 (82%)	60 (95%)	3 (5%)	0	100	100
9	e	78/87 (90%)	74 (95%)	4 (5%)	0	100	100
10	f	69/85 (81%)	68 (99%)	1 (1%)	0	100	100
11	d	98/110 (89%)	97 (99%)	1 (1%)	0	100	100
12	c	86/114 (75%)	82 (95%)	4 (5%)	0	100	100
13	b	95/265 (36%)	89 (94%)	6 (6%)	0	100	100
14	I	657/925 (71%)	641 (98%)	16 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	J	587/835 (70%)	551 (94%)	30 (5%)	6 (1%)	13	29
16	P	98/235 (42%)	90 (92%)	8 (8%)	0	100	100
17	M	74/563 (13%)	68 (92%)	6 (8%)	0	100	100
18	T	342/518 (66%)	326 (95%)	15 (4%)	1 (0%)	37	59
19	O	269/417 (64%)	245 (91%)	24 (9%)	0	100	100
20	N	167/233 (72%)	154 (92%)	13 (8%)	0	100	100
21	R	254/684 (37%)	240 (94%)	14 (6%)	0	100	100
23	S	153/157 (98%)	137 (90%)	16 (10%)	0	100	100
24	W	475/576 (82%)	431 (91%)	38 (8%)	6 (1%)	10	21
25	L	454/833 (54%)	429 (94%)	25 (6%)	0	100	100
26	K	208/303 (69%)	191 (92%)	16 (8%)	1 (0%)	25	47
27	U	24/721 (3%)	23 (96%)	1 (4%)	0	100	100
28	V	184/928 (20%)	177 (96%)	7 (4%)	0	100	100
29	Q	1275/1844 (69%)	1217 (96%)	49 (4%)	9 (1%)	19	38
All	All	9291/16398 (57%)	8654 (93%)	600 (6%)	37 (0%)	32	52

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	389	VAL
1	A	449	GLU
15	J	26	ALA
15	J	27	GLU
29	Q	893	ARG

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	A	1505/2124 (71%)	1306 (87%)	199 (13%)	3	6
3	C	753/825 (91%)	647 (86%)	106 (14%)	3	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	264/300 (88%)	231 (88%)	33 (12%)	3	7
6	q	94/398 (24%)	79 (84%)	15 (16%)	2	3
6	r	113/398 (28%)	93 (82%)	20 (18%)	1	2
6	s	59/398 (15%)	54 (92%)	5 (8%)	8	18
6	t	54/398 (14%)	45 (83%)	9 (17%)	2	3
7	a	76/97 (78%)	66 (87%)	10 (13%)	3	6
8	g	58/67 (87%)	49 (84%)	9 (16%)	2	3
9	e	73/79 (92%)	63 (86%)	10 (14%)	3	5
10	f	62/75 (83%)	54 (87%)	8 (13%)	3	6
11	d	92/100 (92%)	80 (87%)	12 (13%)	3	6
12	c	78/95 (82%)	67 (86%)	11 (14%)	3	5
13	b	84/211 (40%)	76 (90%)	8 (10%)	7	14
14	I	357/743 (48%)	308 (86%)	49 (14%)	3	5
15	J	260/676 (38%)	228 (88%)	32 (12%)	4	8
16	P	88/188 (47%)	77 (88%)	11 (12%)	3	7
17	M	63/424 (15%)	56 (89%)	7 (11%)	5	10
18	T	291/416 (70%)	263 (90%)	28 (10%)	7	14
19	O	228/318 (72%)	210 (92%)	18 (8%)	10	21
20	N	148/193 (77%)	137 (93%)	11 (7%)	11	24
21	R	209/507 (41%)	179 (86%)	30 (14%)	2	5
23	S	128/130 (98%)	119 (93%)	9 (7%)	12	27
24	W	118/474 (25%)	95 (80%)	23 (20%)	1	2
25	L	388/648 (60%)	333 (86%)	55 (14%)	2	5
26	K	177/221 (80%)	144 (81%)	33 (19%)	1	2
27	U	20/572 (4%)	16 (80%)	4 (20%)	1	2
28	V	28/746 (4%)	24 (86%)	4 (14%)	2	5
All	All	5868/11821 (50%)	5099 (87%)	769 (13%)	6	6

5 of 769 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	I	392	LYS
18	T	462	SER

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Mol	Chain	Res	Type
14	I	487	ARG
14	I	384	LYS
15	J	202	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 156 such sidechains are listed below:

Mol	Chain	Res	Type
17	M	495	ASN
24	W	125	HIS
18	T	353	HIS
20	N	138	GLN
26	K	26	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	83/111 (74%)	48 (57%)	2 (2%)
22	H	39/192 (20%)	28 (71%)	3 (7%)
30	5	6/7 (85%)	1 (16%)	0
31	3	33/173 (19%)	16 (48%)	6 (18%)
5	F	90/101 (89%)	48 (53%)	5 (5%)
All	All	251/584 (42%)	141 (56%)	16 (6%)

5 of 141 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	8	A
2	B	9	C
2	B	10	G
2	B	11	A
2	B	15	G

5 of 16 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
31	3	95	U
31	3	90	C
22	H	30	A
31	3	21	C
22	H	6	U

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
21	SEP	R	225	21	8,9,10	1.19	1 (12%)	8,12,14	1.31	2 (25%)
21	SEP	R	217	21	8,9,10	1.16	1 (12%)	8,12,14	1.38	1 (12%)

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
21	SEP	R	225	21	-	0/5/8/10	-
21	SEP	R	217	21	-	1/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	R	217	SEP	P-O1P	2.38	1.58	1.50
21	R	225	SEP	P-O1P	2.18	1.57	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	R	217	SEP	O2P-P-OG	3.08	114.92	106.73
21	R	225	SEP	OG-CB-CA	2.72	110.79	108.14
21	R	225	SEP	O3P-P-OG	2.09	112.30	106.73

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	R	217	SEP	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 10 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
32	GTP	C	1001	33	26,34,34	1.11	3 (11%)	32,54,54	0.89	1 (3%)

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
32	GTP	C	1001	33	-	5/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	C	1001	GTP	C5-C6	-2.67	1.42	1.47
32	C	1001	GTP	C8-N7	-2.23	1.31	1.35
32	C	1001	GTP	C5-C4	-2.16	1.37	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	C	1001	GTP	C3'-C2'-C1'	2.08	104.11	100.98

There are no chirality outliers.

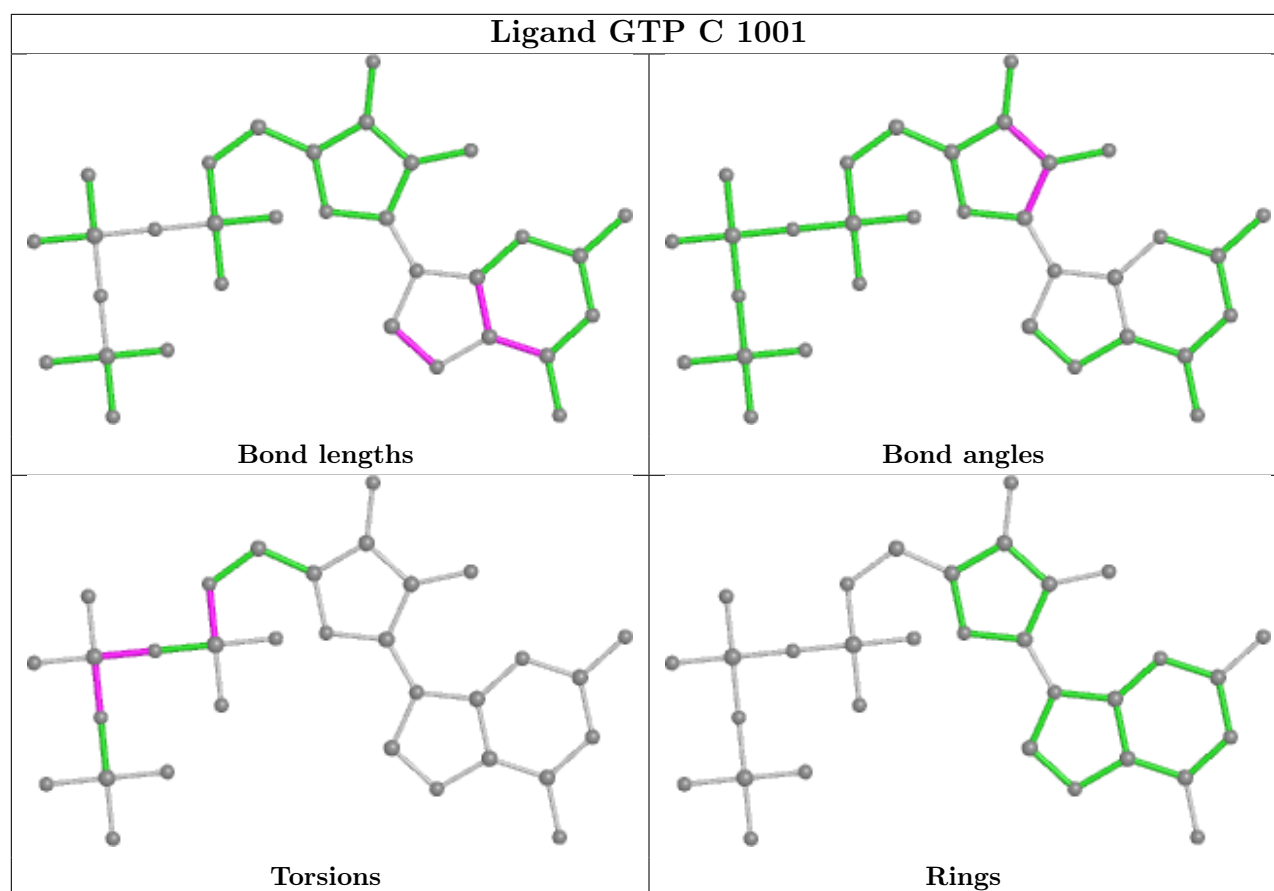
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	C	1001	GTP	C5'-O5'-PA-O1A
32	C	1001	GTP	C5'-O5'-PA-O2A
32	C	1001	GTP	PA-O3A-PB-O3B
32	C	1001	GTP	PG-O3B-PB-O2B
32	C	1001	GTP	C5'-O5'-PA-O3A

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.

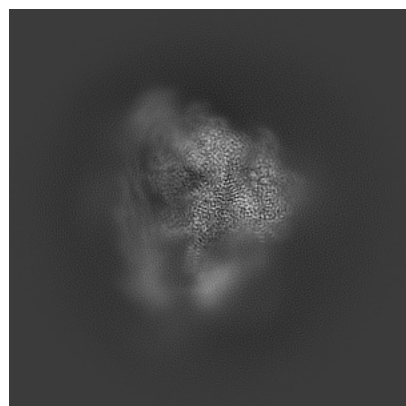
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38362. These allow visual inspection of the internal detail of the map and identification of artifacts.

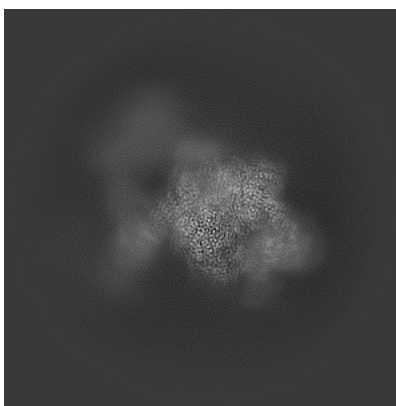
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

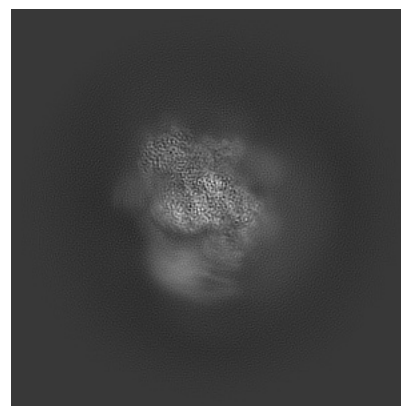
6.1.1 Primary map



X

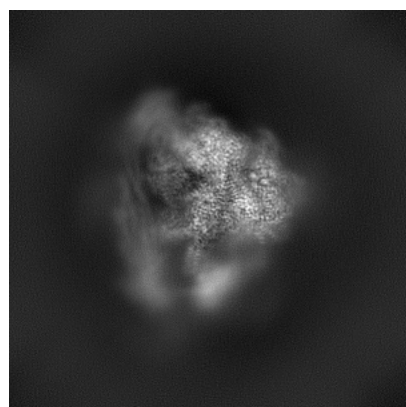


Y

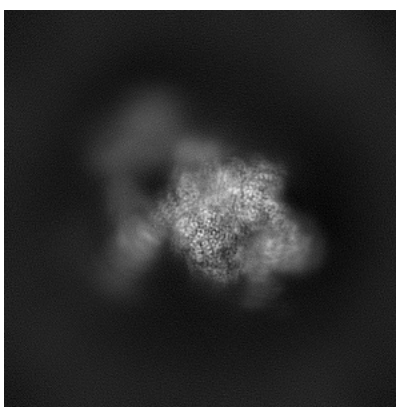


Z

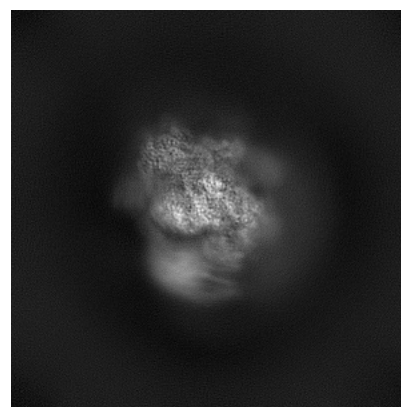
6.1.2 Raw map



X



Y

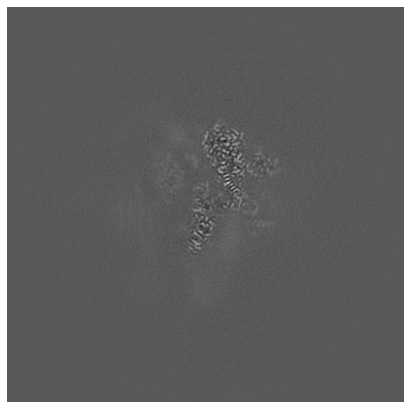


Z

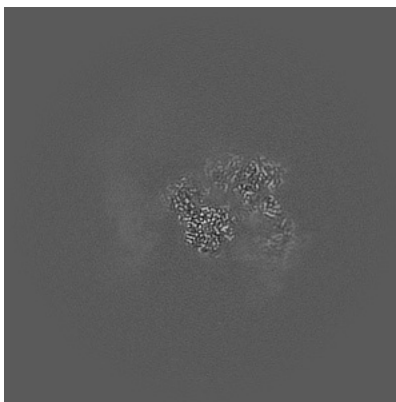
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

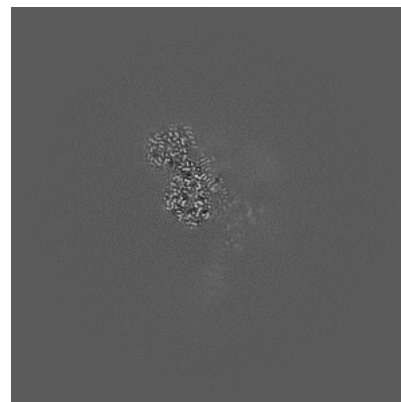
6.2.1 Primary map



X Index: 220

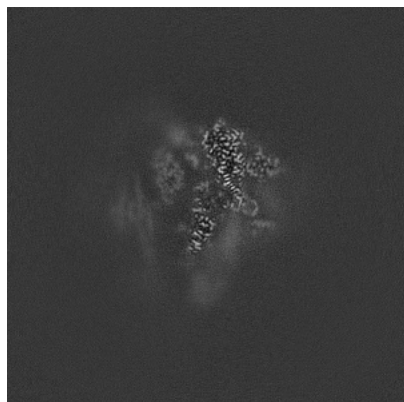


Y Index: 220

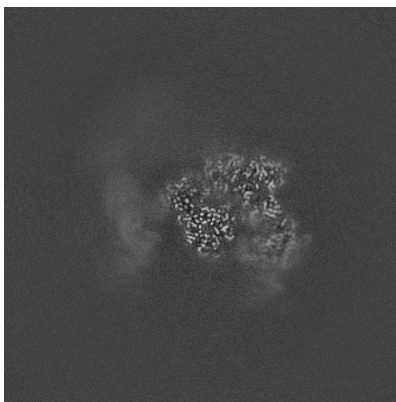


Z Index: 220

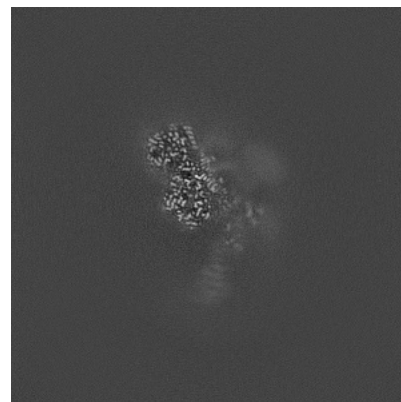
6.2.2 Raw map



X Index: 220



Y Index: 220

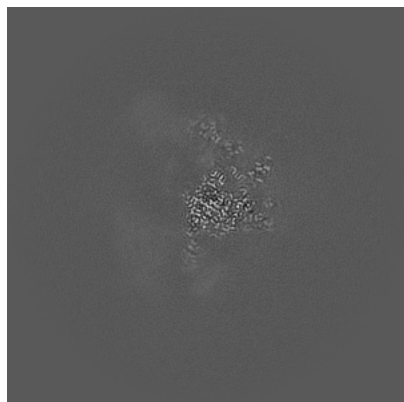


Z Index: 220

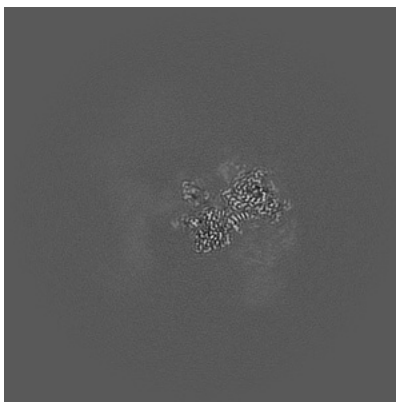
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

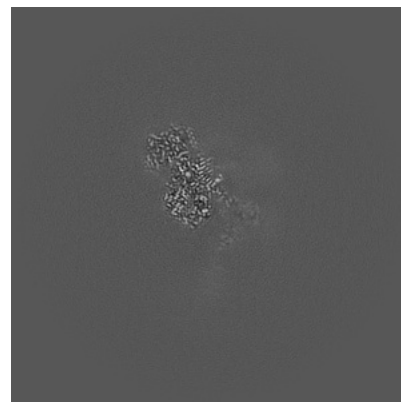
6.3.1 Primary map



X Index: 203

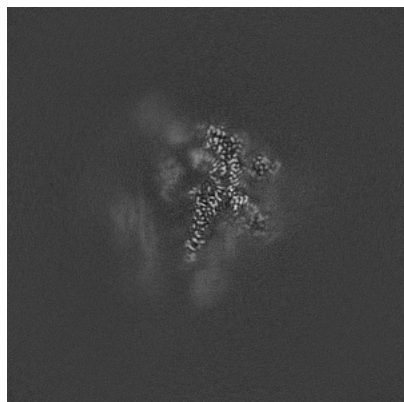


Y Index: 234

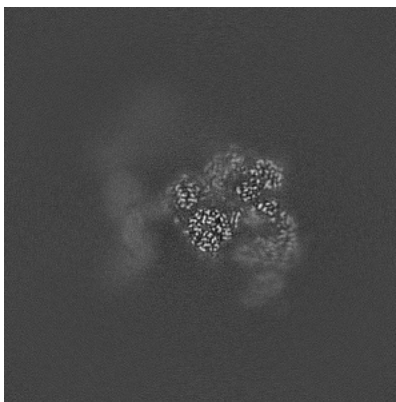


Z Index: 222

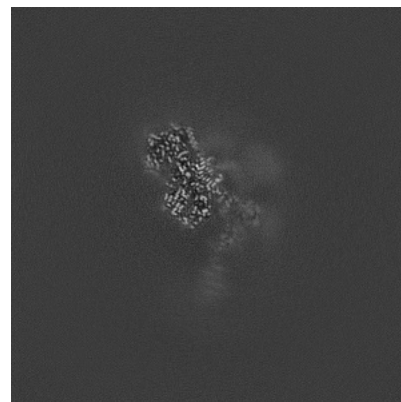
6.3.2 Raw map



X Index: 213



Y Index: 224

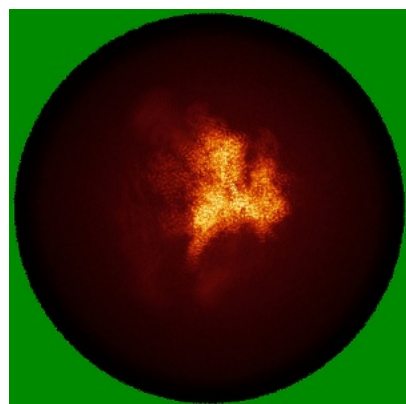


Z Index: 222

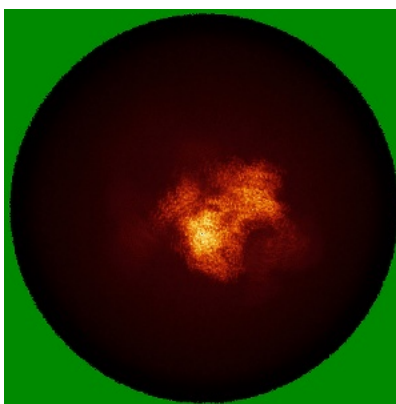
The images above show the largest variance slices of the map in three orthogonal directions.

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

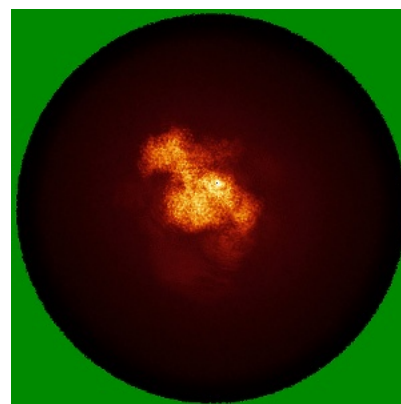
6.4.1 Primary map



X

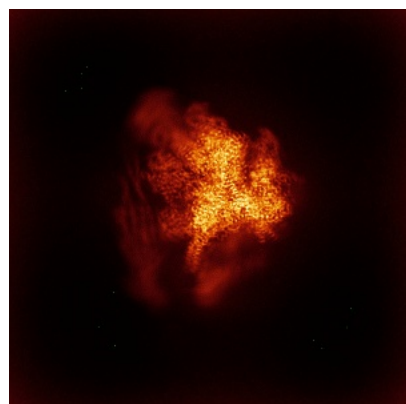


Y

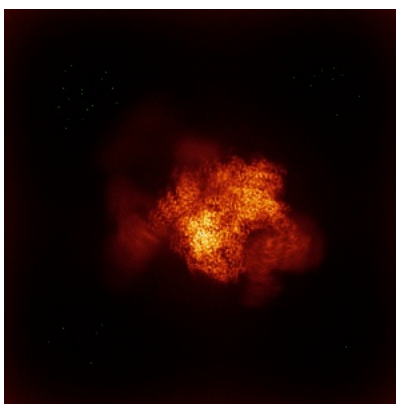


Z

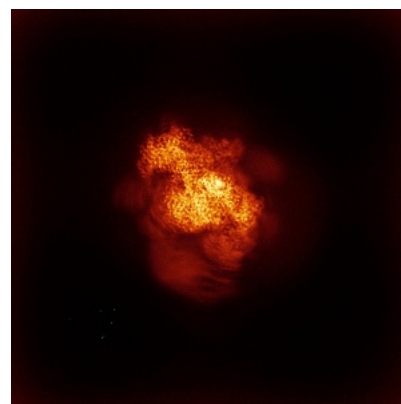
6.4.2 Raw map



X



Y

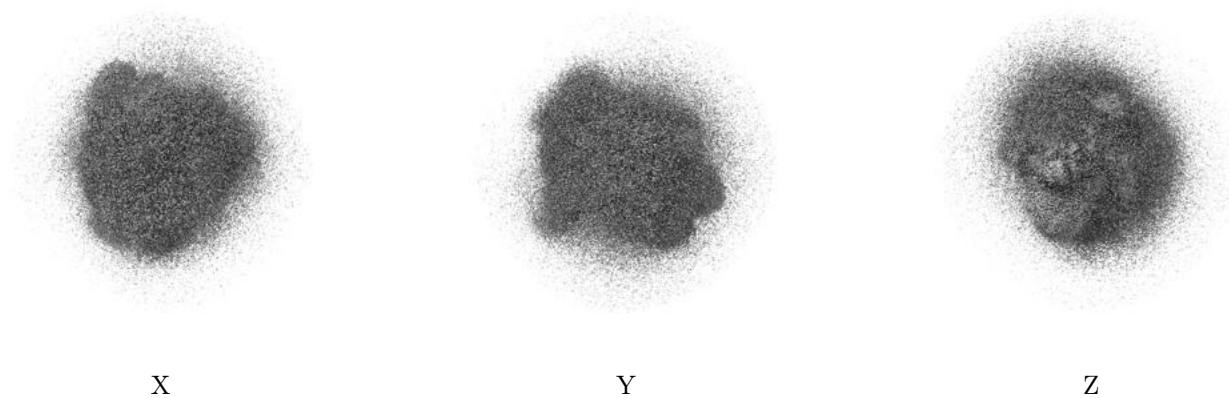


Z

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.

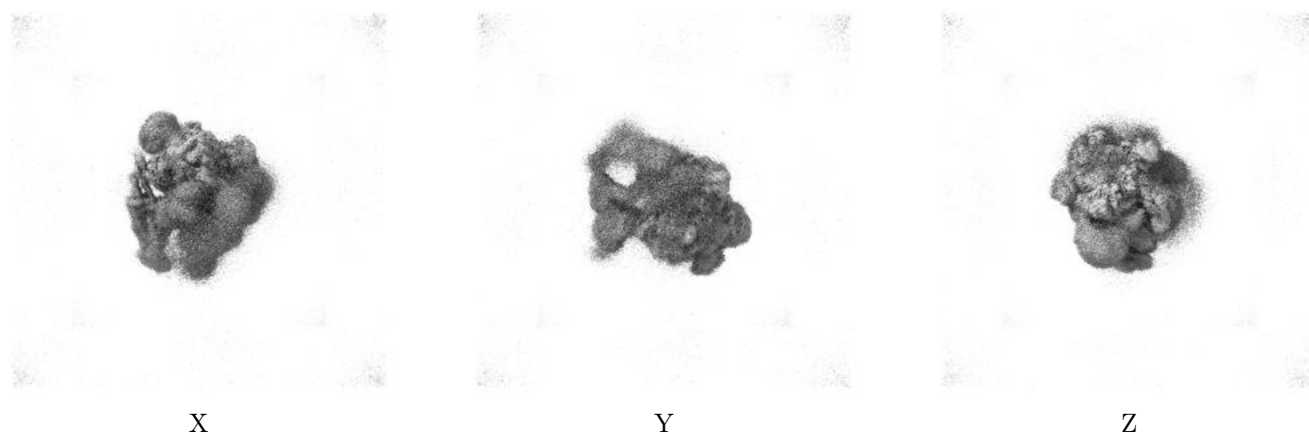
6.5 Orthogonal surface views [i](#)

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.

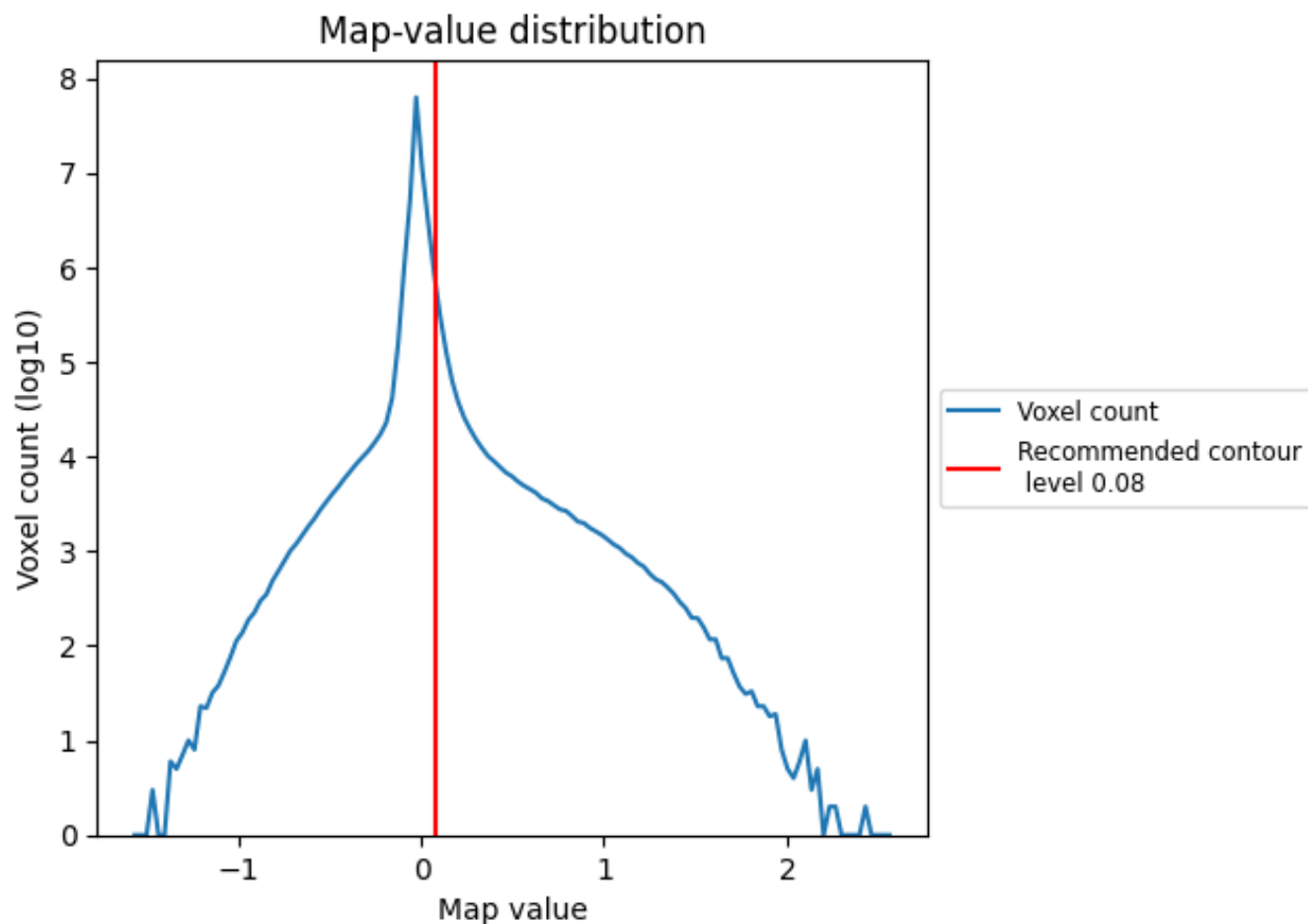
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

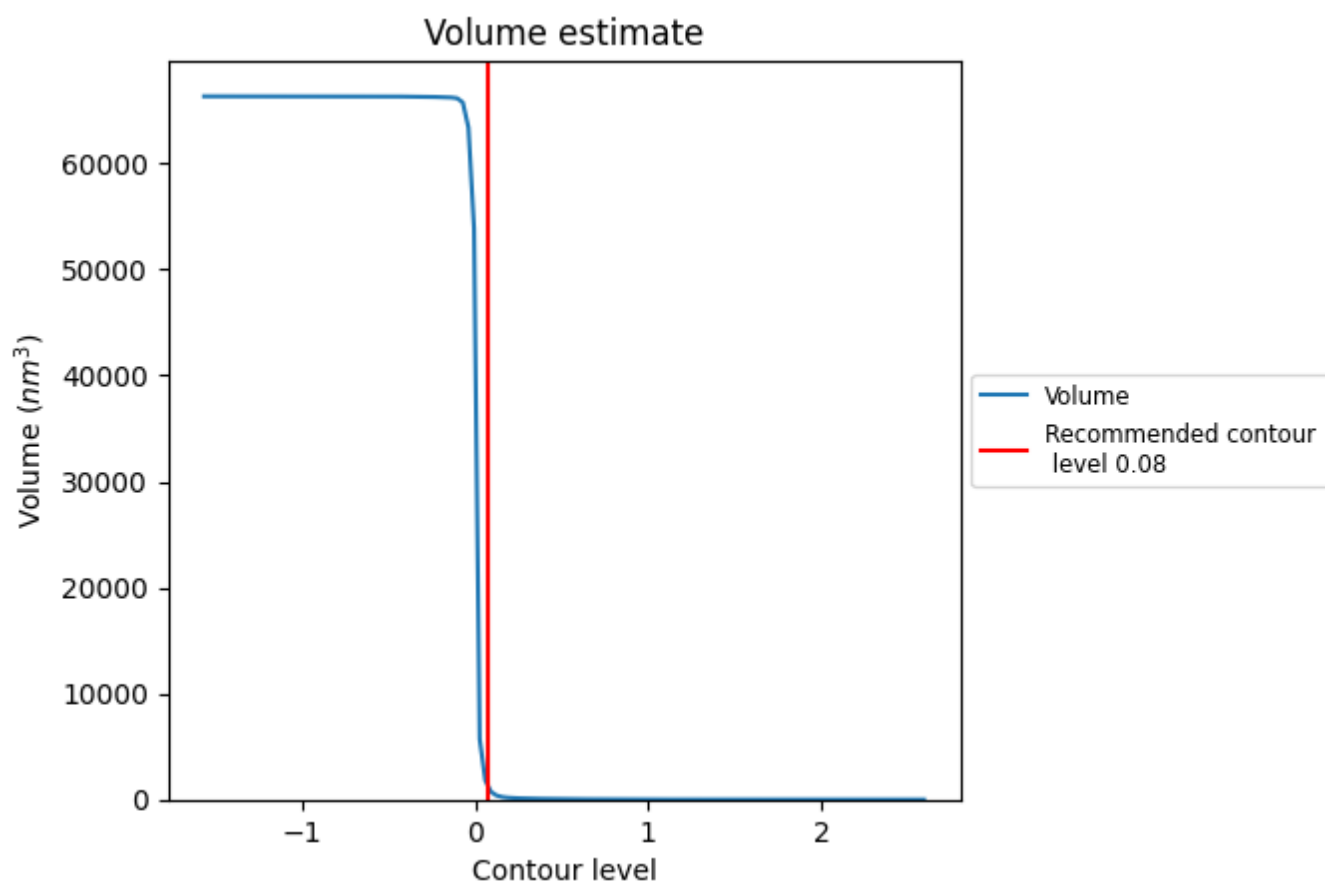
This section contains the results of statistical analysis of the map.

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.

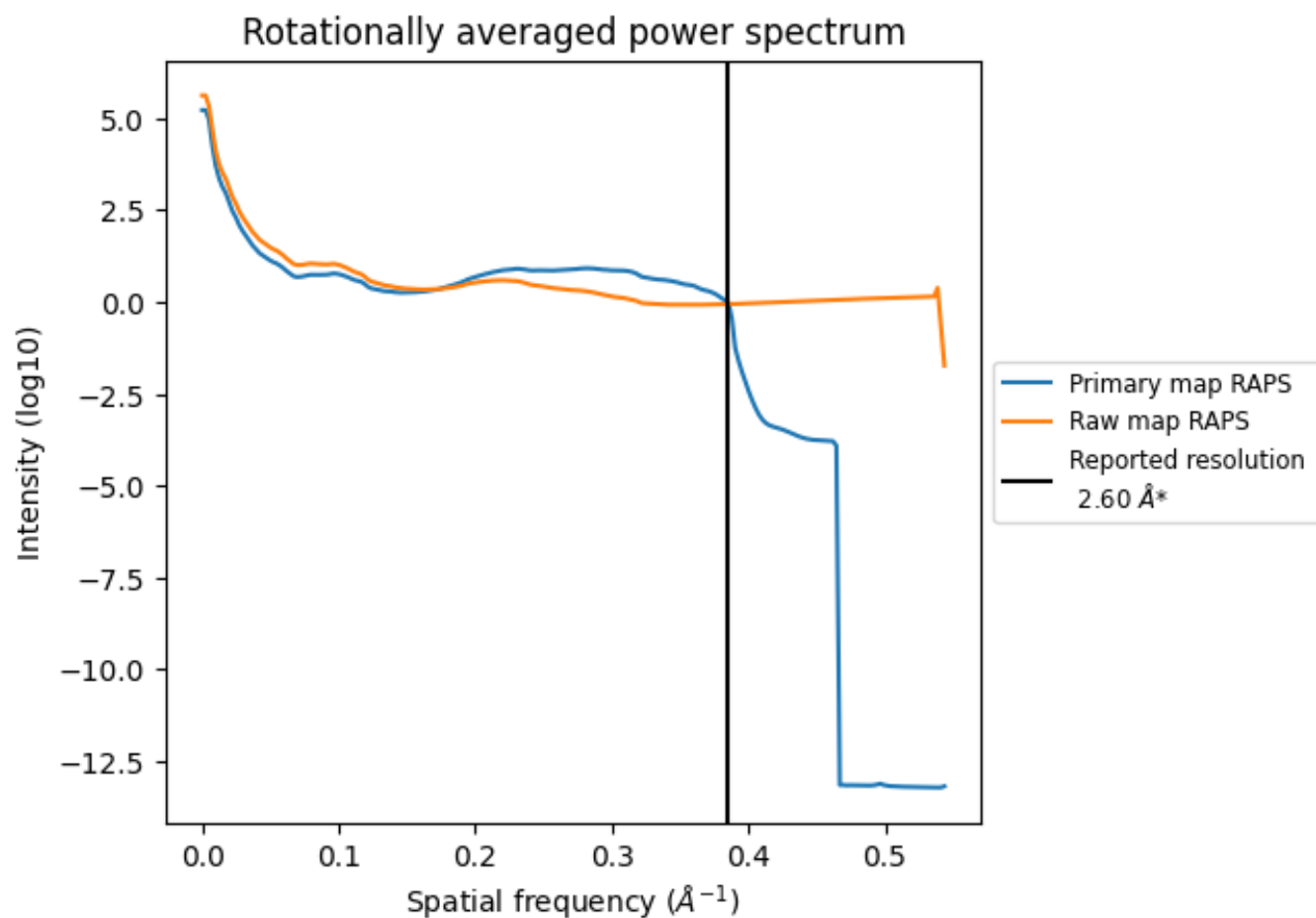
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1131 nm^3 ; this corresponds to an approximate mass of 1022 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 ⓘ

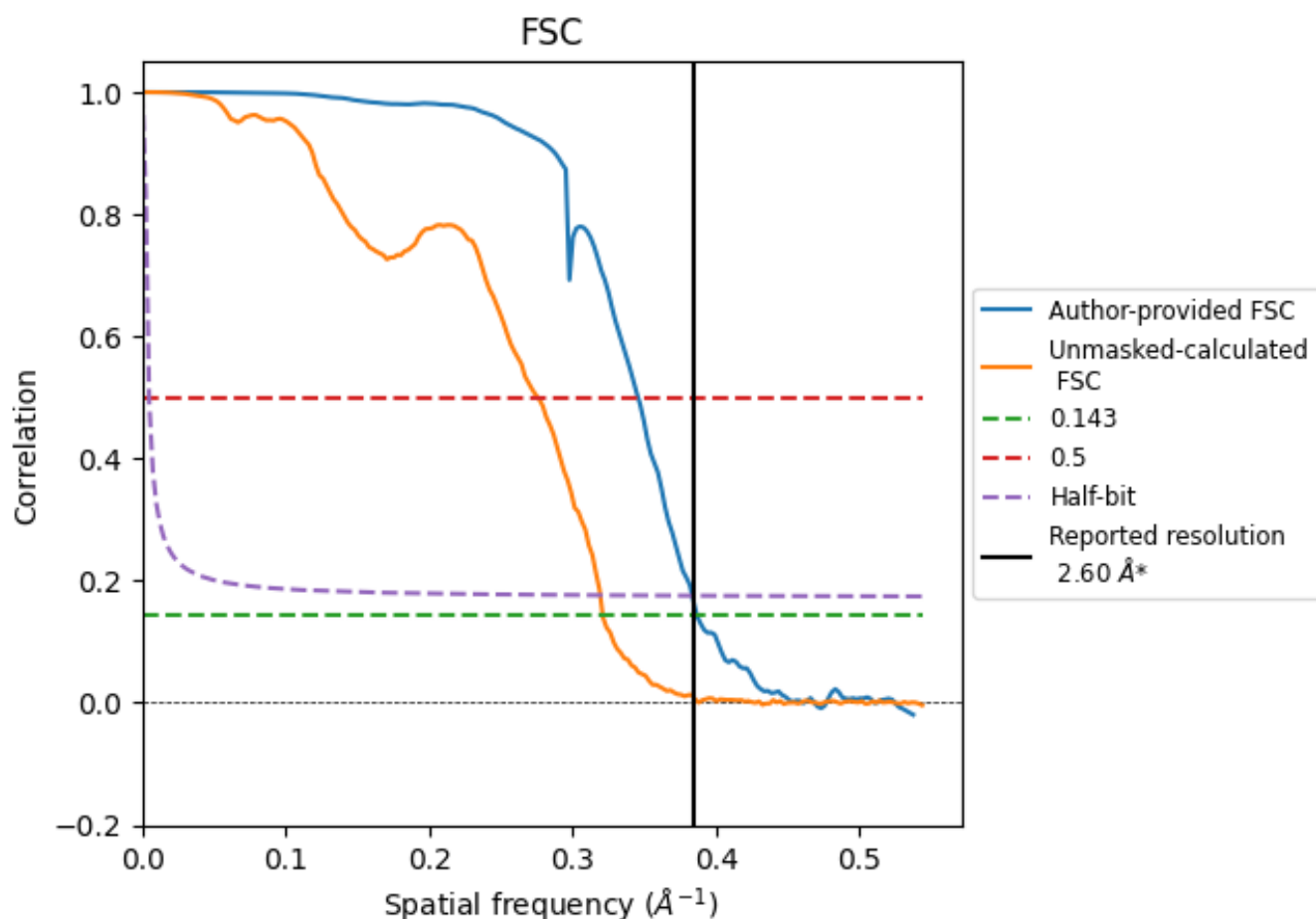


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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 0.385 Å⁻¹

8.2 Resolution estimates [i](#)

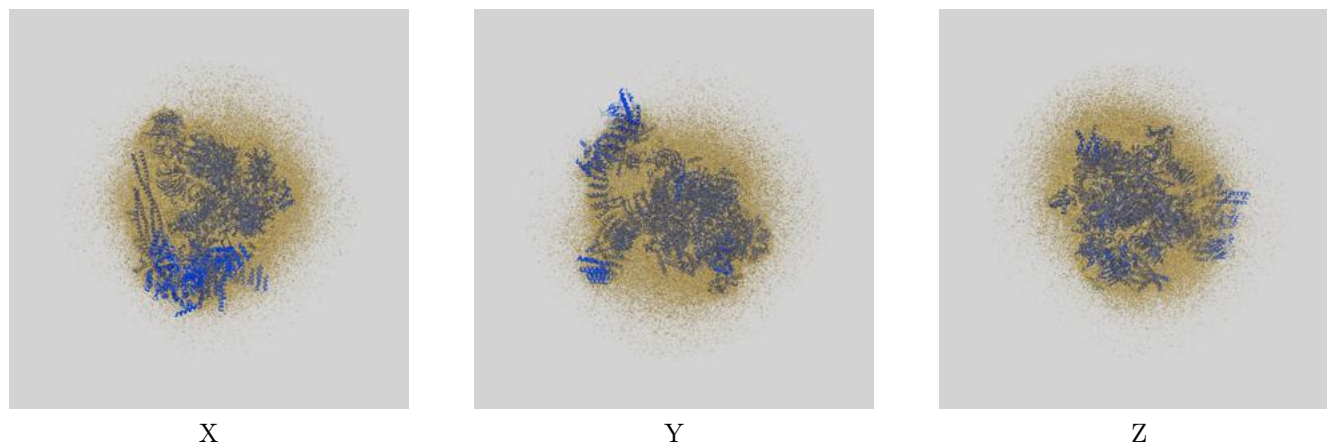
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.59	2.89	2.61
Unmasked-calculated*	3.12	3.63	3.13

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.12 differs from the reported value 2.6 by more than 10 %

9 Map-model fit [i](#)

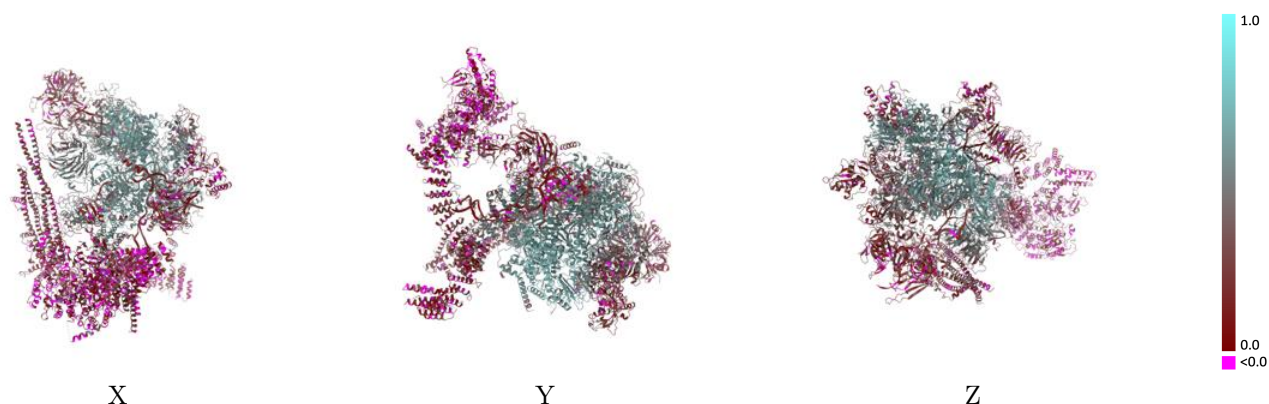
This section contains information regarding the fit between EMDB map EMD-38362 and PDB model 8XI2. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



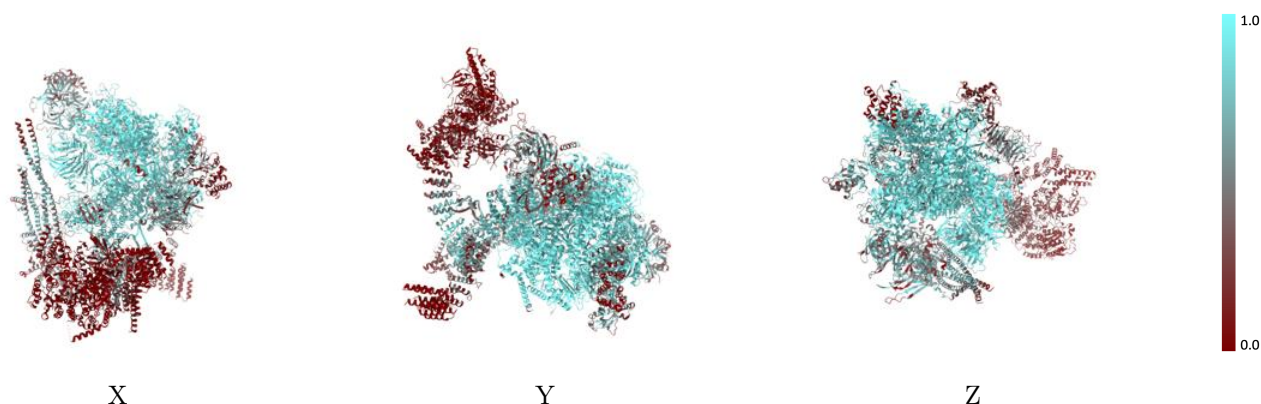
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



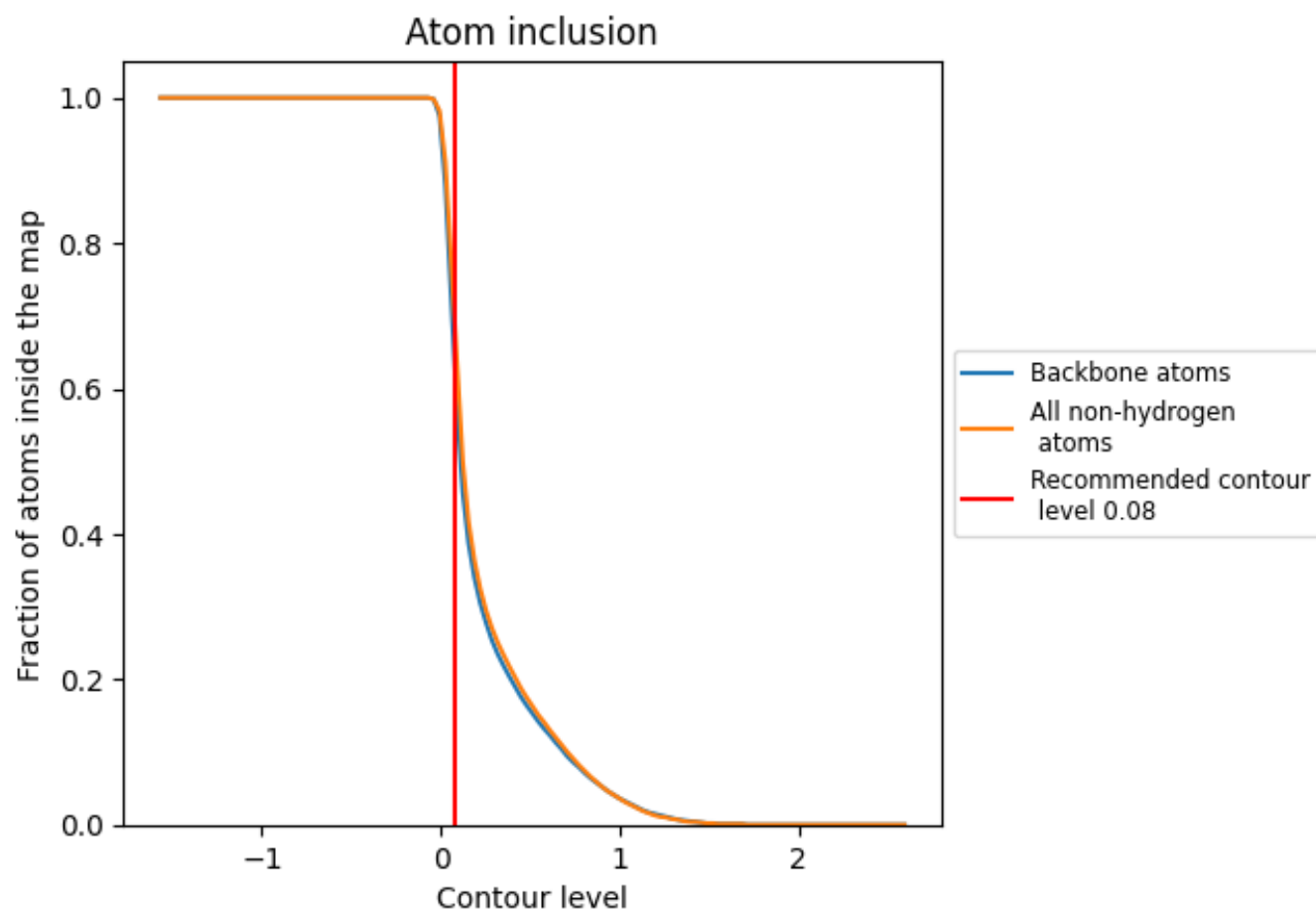
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 62% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6850	 0.3810
3	 0.7060	 0.2340
5	 0.9530	 0.6210
A	 0.8830	 0.5470
B	 0.8690	 0.3780
C	 0.7990	 0.3620
E	 0.9280	 0.4580
F	 0.9130	 0.4530
H	 0.6630	 0.2840
I	 0.4210	 0.1850
J	 0.6150	 0.3610
K	 0.4830	 0.2310
L	 0.6460	 0.3640
M	 0.7050	 0.3600
N	 0.9860	 0.6290
O	 0.7890	 0.4460
P	 0.9320	 0.5920
Q	 0.0410	 0.1050
R	 0.9330	 0.5620
S	 0.9540	 0.5290
T	 0.9960	 0.6770
U	 0.4390	 0.3290
V	 0.2680	 0.2470
W	 0.5890	 0.3040
a	 0.7190	 0.2760
b	 0.6710	 0.2880
c	 0.5790	 0.2130
d	 0.5490	 0.2310
e	 0.5280	 0.2160
f	 0.4730	 0.2010
g	 0.6610	 0.2630
q	 0.4630	 0.2050
r	 0.5790	 0.2140
s	 0.6220	 0.2370
t	 0.5040	 0.2050

