



wwPDB EM Validation Summary Report ⓘ

Nov 19, 2023 – 07:14 am GMT

PDB ID : 8Q6O
EMDB ID : EMD-18191
Title : X. laevis CMG dimer bound to dimeric DONSON - without ATPase
Authors : Butryn, A.; Cvetkovic, M.A.; Costa, A.
Deposited on : 2023-08-14
Resolution : 3.14 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:

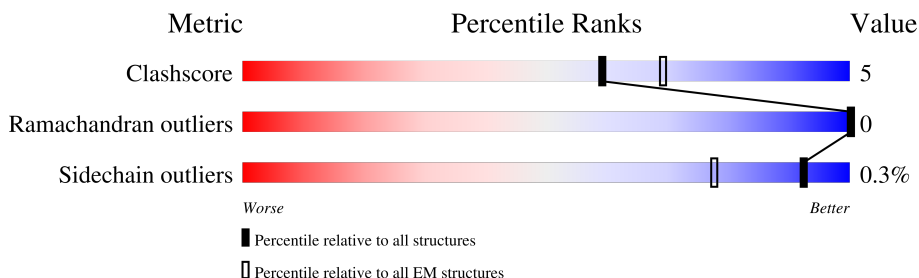
EMDB validation analysis : 0.0.1.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 3.14 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	2	886	
1	A	886	
2	3	807	
2	B	807	
3	4	863	
3	C	863	
4	5	735	
4	D	735	

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Mol	Chain	Length	Quality of chain
5	6	821	 26% 5% 70%
5	E	821	 26% 5% 70%
6	7	720	 31% 7% 62%
6	F	720	 30% 8% 62%
7	G	196	 82% 18%
7	M	196	 82% 18%
8	H	185	 84% 10% 5%
8	N	185	 84% 10% 5%
9	I	210	 89% 8% .
9	O	210	 89% 8% .
10	J	567	 81% 11% 8%
10	P	567	 80% 12% 8%
11	K	221	 81% 10% 8%
11	Q	221	 80% 12% 8%
12	L	579	 55% 7% 38%
12	R	579	 55% 7% 38%

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 51983 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 DNA replication licensing factor mcm2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	267	Total	C	N	O	S	0	0
			2141	1358	374	395	14		
1	2	267	Total	C	N	O	S	0	0
			2141	1358	374	395	14		

- Molecule 2 is a protein called Maternal DNA replication licensing factor mcm3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	262	Total	C	N	O	S	0	0
			2066	1292	361	403	10		
2	3	262	Total	C	N	O	S	0	0
			2066	1292	361	403	10		

- Molecule 3 is a protein called DNA replication licensing factor mcm4-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	258	Total	C	N	O	S	0	0
			2112	1331	378	387	16		
3	4	258	Total	C	N	O	S	0	0
			2112	1331	378	387	16		

- Molecule 4 is a protein called DNA replication licensing factor mcm5-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	256	Total	C	N	O	S	0	0
			2059	1297	369	379	14		
4	5	256	Total	C	N	O	S	0	0
			2059	1297	369	379	14		

- Molecule 5 is a protein called Maternal DNA replication licensing factor mcm6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	249	1997	1260	352	373	12	0	0
5	6	249	1997	1260	352	373	12	0	0

- Molecule 6 is a protein called DNA replication licensing factor mcm7-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	275	2227	1405	391	413	18	0	0
6	7	275	2227	1405	391	413	18	0	0

- Molecule 7 is a protein called DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	M	196	1622	1023	290	297	12	0	0
7	G	196	1623	1023	290	298	12	0	0

- Molecule 8 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	N	175	1418	907	237	267	7	0	0
8	H	175	1418	907	237	267	7	0	0

- Molecule 9 is a protein called DNA replication complex GINS protein PSF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	O	202	1621	1026	284	304	7	0	0
9	I	202	1621	1026	284	304	7	0	0

- Molecule 10 is a protein called Cell division control protein 45 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	P	523	4233	2700	701	799	33	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	523	4233	2700	701	799	33	0	0

- Molecule 11 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	Q	203	1655	1055	280	311	9	0	0
11	K	203	1655	1055	280	311	9	0	0

- Molecule 12 is a protein called Protein downstream neighbor of son homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	R	361	2835	1818	488	513	16	0	0
12	L	361	2835	1818	488	513	16	0	0

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
13	A	1	Total	Zn	0
			1	1	
13	C	1	Total	Zn	0
			1	1	
13	D	1	Total	Zn	0
			1	1	
13	E	1	Total	Zn	0
			1	1	
13	F	1	Total	Zn	0
			1	1	
13	2	1	Total	Zn	0
			1	1	
13	4	1	Total	Zn	0
			1	1	
13	5	1	Total	Zn	0
			1	1	
13	6	1	Total	Zn	0
			1	1	
13	7	1	Total	Zn	0
			1	1	

Chain 2:



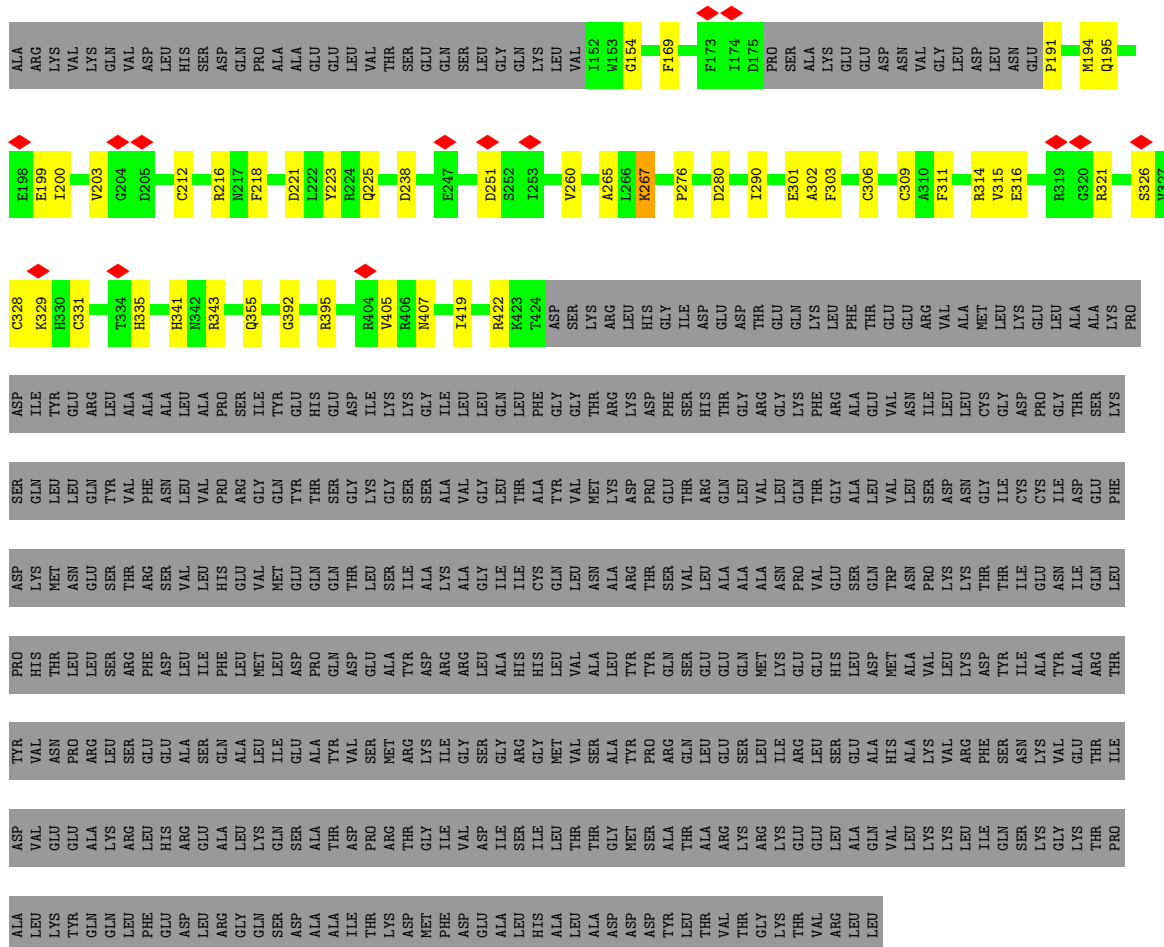
Table of amino acid residues for Chain 2, including labels like MET, ALA, ASP, SER, LEU, THR, and highlighted residues such as G196, L216, Y219, E226, A230, K242, R247, K311, N313, K316, R318, F319, L321, R333, P334, G335, S336, C337, P338, E339, C340, T353, A372, G373, R374, R377, K392, D408, and K432.

Molecule 2: Maternal DNA replication licensing factor mcm3

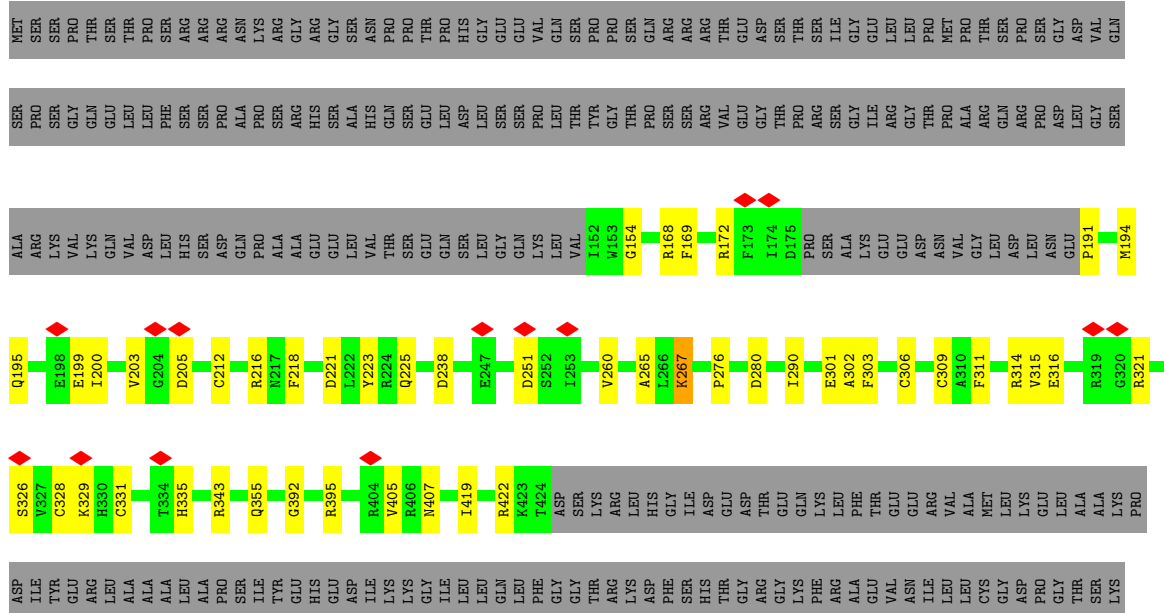
Chain B:

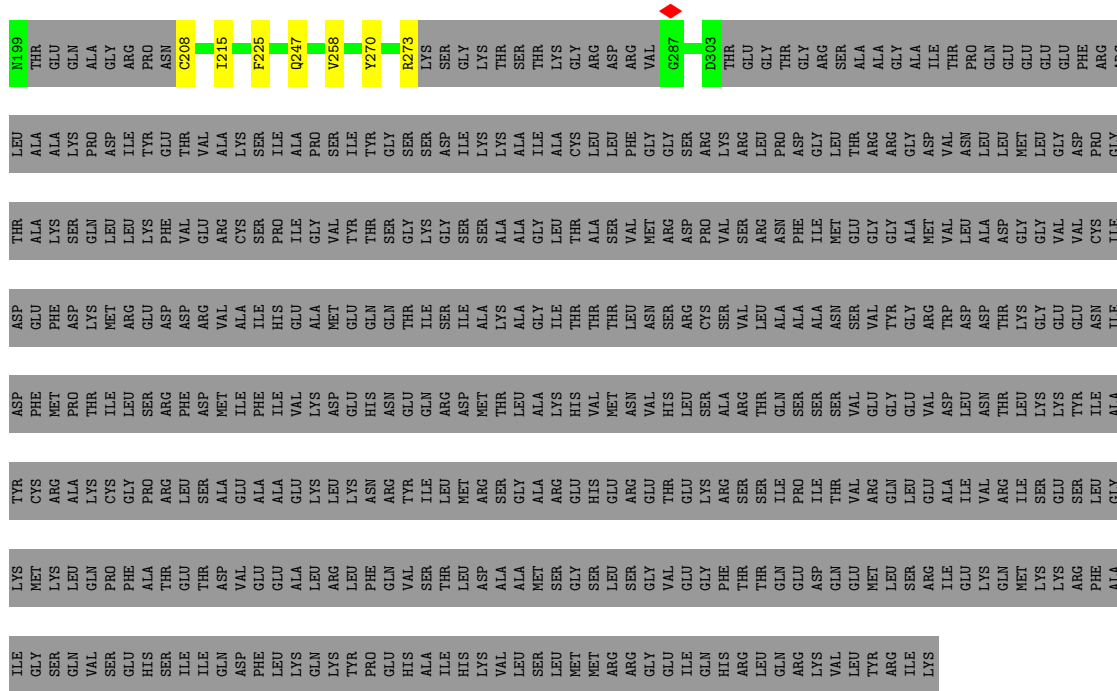


Table of amino acid residues for Chain B, including labels like MET, ASP, TYR, GLY, CYS, PHE, LEU, PHE, D9, E18, D25, G30, R61, F76, T90, Q94, V100, F106, H110, V111, L116, R138, M142, K194, E206, K207, D224, T252, K270, and LYS.

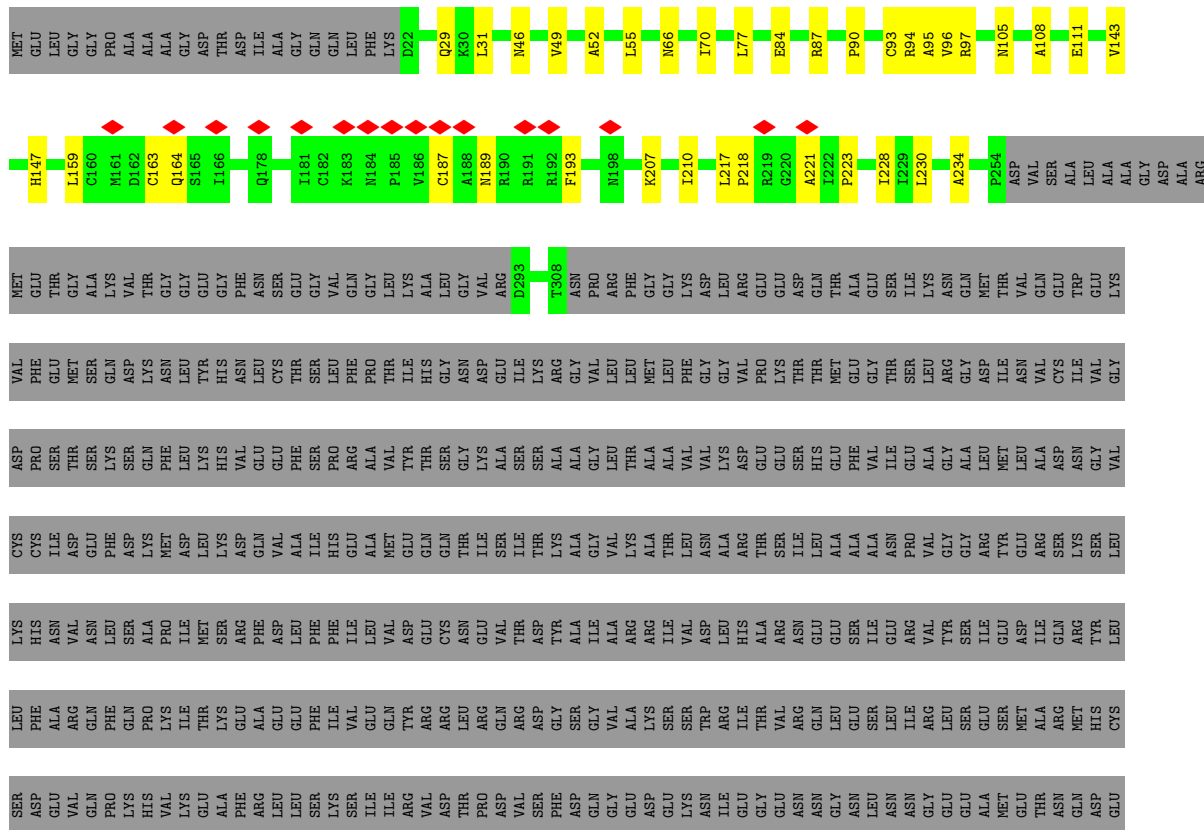


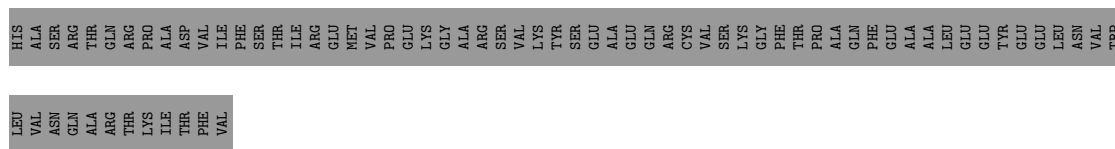
● Molecule 3: DNA replication licensing factor mcm4-B



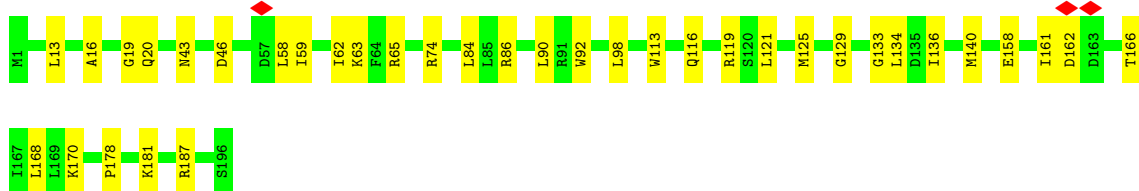
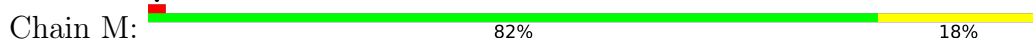


● Molecule 5: Maternal DNA replication licensing factor mcm6

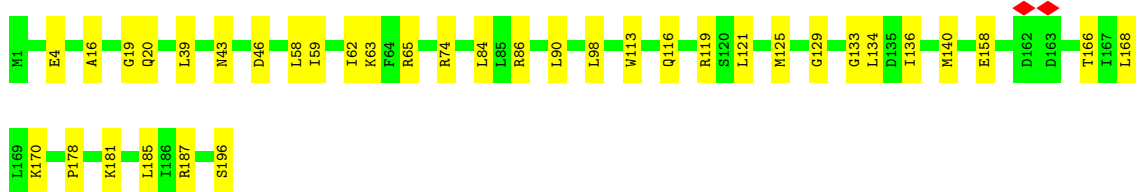
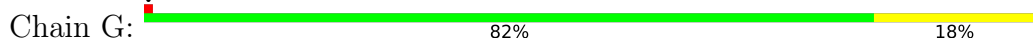




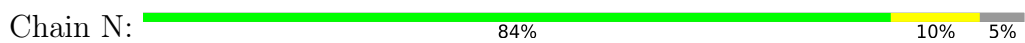
● Molecule 7: DNA replication complex GINS protein PSF1



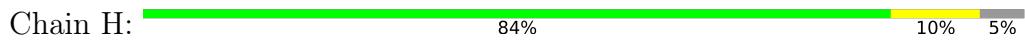
● Molecule 7: DNA replication complex GINS protein PSF1



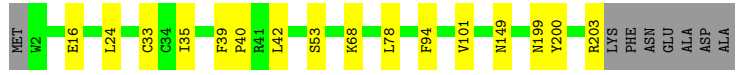
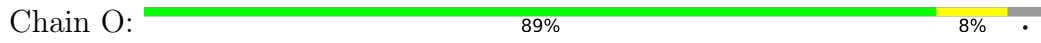
● Molecule 8: DNA replication complex GINS protein PSF2



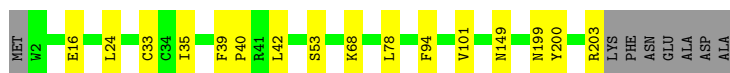
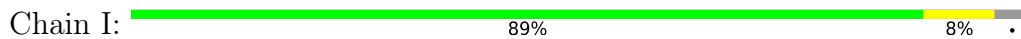
● Molecule 8: DNA replication complex GINS protein PSF2



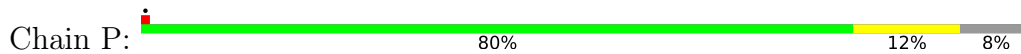
● Molecule 9: DNA replication complex GINS protein PSF3



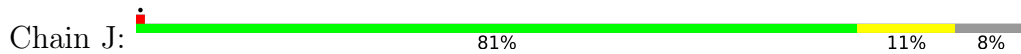
● Molecule 9: DNA replication complex GINS protein PSF3



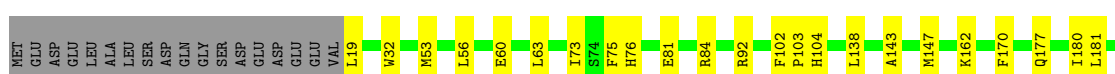
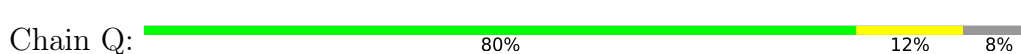
• Molecule 10: Cell division control protein 45 homolog



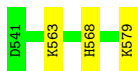
• Molecule 10: Cell division control protein 45 homolog



• Molecule 11: DNA replication complex GINS protein SLD5



• Molecule 11: DNA replication complex GINS protein SLD5



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	100667	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	33.0	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	3400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.750	Depositor
Minimum map value	-1.490	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	513.0, 513.0, 513.0	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
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	2	0.25	0/2188	0.48	0/2963
1	A	0.25	0/2188	0.48	0/2963
2	3	0.25	0/2101	0.49	0/2834
2	B	0.25	0/2101	0.49	0/2834
3	4	0.24	0/2157	0.48	0/2921
3	C	0.24	0/2157	0.48	0/2921
4	5	0.27	0/2096	0.51	0/2825
4	D	0.26	0/2096	0.51	0/2825
5	6	0.24	0/2033	0.50	0/2747
5	E	0.24	0/2033	0.50	0/2747
6	7	0.24	0/2266	0.48	0/3053
6	F	0.24	0/2266	0.49	0/3053
7	G	0.24	0/1653	0.48	0/2221
7	M	0.24	0/1652	0.48	0/2221
8	H	0.25	0/1448	0.45	0/1964
8	N	0.25	0/1448	0.45	0/1964
9	I	0.25	0/1658	0.47	0/2236
9	O	0.25	0/1658	0.47	0/2236
10	J	0.24	0/4314	0.44	0/5823
10	P	0.24	0/4314	0.44	0/5823
11	K	0.25	0/1690	0.44	0/2280
11	Q	0.25	0/1690	0.44	0/2280
12	L	0.24	0/2904	0.45	0/3938
12	R	0.24	0/2904	0.45	0/3938
All	All	0.25	0/53015	0.47	0/71610

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	2141	0	2124	22	0
1	A	2141	0	2124	22	0
2	3	2066	0	2059	18	0
2	B	2066	0	2059	13	0
3	4	2112	0	2090	31	0
3	C	2112	0	2090	30	0
4	5	2059	0	2074	15	0
4	D	2059	0	2074	15	0
5	6	1997	0	1987	22	0
5	E	1997	0	1987	21	0
6	7	2227	0	2232	33	0
6	F	2227	0	2232	38	0
7	G	1623	0	1623	27	0
7	M	1622	0	1623	25	0
8	H	1418	0	1433	15	0
8	N	1418	0	1433	14	0
9	I	1621	0	1589	10	0
9	O	1621	0	1589	11	0
10	J	4233	0	4211	37	0
10	P	4233	0	4211	38	0
11	K	1655	0	1669	19	0
11	Q	1655	0	1669	20	0
12	L	2835	0	2861	27	0
12	R	2835	0	2861	28	0
13	2	1	0	0	0	0
13	4	1	0	0	0	0
13	5	1	0	0	0	0
13	6	1	0	0	0	0
13	7	1	0	0	0	0
13	A	1	0	0	0	0
13	C	1	0	0	0	0
13	D	1	0	0	0	0
13	E	1	0	0	0	0
13	F	1	0	0	0	0
All	All	51983	0	51904	497	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 5.

The worst 5 of 497 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)
11:Q:63:LEU:HD11	11:Q:73:ILE:HA	1.65	0.79
11:K:63:LEU:HD11	11:K:73:ILE:HA	1.66	0.77
3:4:306:CYS:HB3	3:4:311:PHE:H	1.52	0.75
3:C:306:CYS:HB3	3:C:311:PHE:H	1.52	0.74
3:C:276:PRO:HB3	6:F:174:PRO:HB3	1.72	0.72

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	265/886 (30%)	256 (97%)	9 (3%)	0	100	100
1	A	265/886 (30%)	256 (97%)	9 (3%)	0	100	100
2	3	260/807 (32%)	252 (97%)	8 (3%)	0	100	100
2	B	260/807 (32%)	253 (97%)	7 (3%)	0	100	100
3	4	254/863 (29%)	253 (100%)	1 (0%)	0	100	100
3	C	254/863 (29%)	253 (100%)	1 (0%)	0	100	100
4	5	250/735 (34%)	244 (98%)	6 (2%)	0	100	100
4	D	250/735 (34%)	243 (97%)	7 (3%)	0	100	100
5	6	245/821 (30%)	240 (98%)	5 (2%)	0	100	100
5	E	245/821 (30%)	240 (98%)	5 (2%)	0	100	100
6	7	267/720 (37%)	260 (97%)	7 (3%)	0	100	100
6	F	267/720 (37%)	260 (97%)	7 (3%)	0	100	100
7	G	194/196 (99%)	192 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	M	194/196 (99%)	191 (98%)	3 (2%)	0	100	100
8	H	173/185 (94%)	170 (98%)	3 (2%)	0	100	100
8	N	173/185 (94%)	170 (98%)	3 (2%)	0	100	100
9	I	200/210 (95%)	197 (98%)	3 (2%)	0	100	100
9	O	200/210 (95%)	197 (98%)	3 (2%)	0	100	100
10	J	519/567 (92%)	502 (97%)	17 (3%)	0	100	100
10	P	519/567 (92%)	504 (97%)	15 (3%)	0	100	100
11	K	201/221 (91%)	197 (98%)	4 (2%)	0	100	100
11	Q	201/221 (91%)	198 (98%)	3 (2%)	0	100	100
12	L	351/579 (61%)	338 (96%)	13 (4%)	0	100	100
12	R	351/579 (61%)	337 (96%)	14 (4%)	0	100	100
All	All	6358/13580 (47%)	6203 (98%)	155 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	238/767 (31%)	238 (100%)	0	100	100
1	A	238/767 (31%)	238 (100%)	0	100	100
2	3	231/701 (33%)	231 (100%)	0	100	100
2	B	231/701 (33%)	231 (100%)	0	100	100
3	4	240/761 (32%)	239 (100%)	1 (0%)	91	96
3	C	240/761 (32%)	239 (100%)	1 (0%)	91	96
4	5	225/627 (36%)	222 (99%)	3 (1%)	69	86
4	D	225/627 (36%)	222 (99%)	3 (1%)	69	86
5	6	219/712 (31%)	219 (100%)	0	100	100
5	E	219/712 (31%)	219 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	7	248/629 (39%)	248 (100%)	0	100	100
6	F	248/629 (39%)	248 (100%)	0	100	100
7	G	176/176 (100%)	176 (100%)	0	100	100
7	M	176/176 (100%)	176 (100%)	0	100	100
8	H	159/168 (95%)	158 (99%)	1 (1%)	86	94
8	N	159/168 (95%)	158 (99%)	1 (1%)	86	94
9	I	174/180 (97%)	174 (100%)	0	100	100
9	O	174/180 (97%)	174 (100%)	0	100	100
10	J	478/515 (93%)	476 (100%)	2 (0%)	91	96
10	P	478/515 (93%)	476 (100%)	2 (0%)	91	96
11	K	187/203 (92%)	187 (100%)	0	100	100
11	Q	187/203 (92%)	187 (100%)	0	100	100
12	L	317/499 (64%)	315 (99%)	2 (1%)	86	94
12	R	317/499 (64%)	315 (99%)	2 (1%)	86	94
All	All	5784/11876 (49%)	5766 (100%)	18 (0%)	92	97

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	5	173	CYS
12	L	315	PRO
12	L	272	PHE
12	R	315	PRO
4	5	60	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
10	P	484	ASN
10	J	484	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

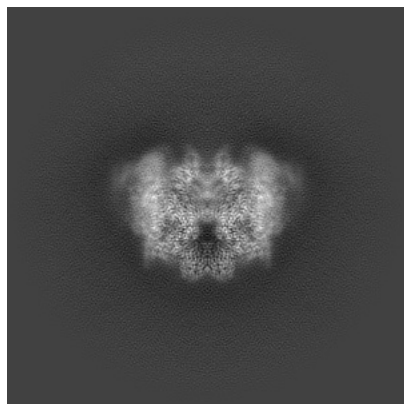
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18191. These allow visual inspection of the internal detail of the map and identification of artifacts.

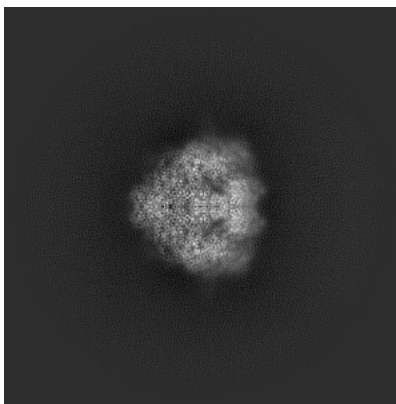
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

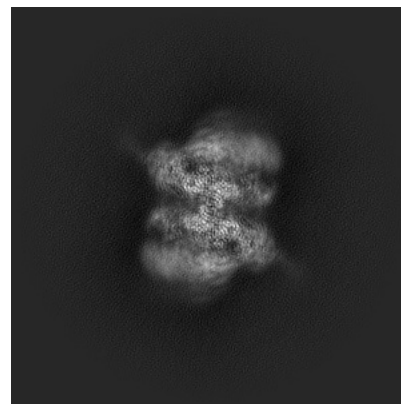
6.1.1 Primary map



X

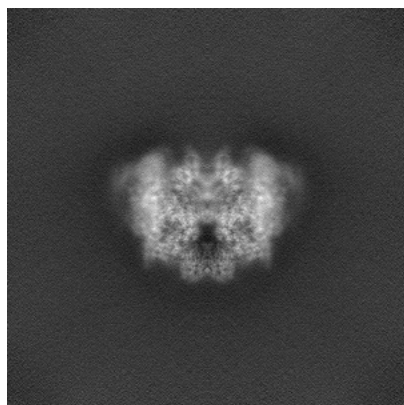


Y

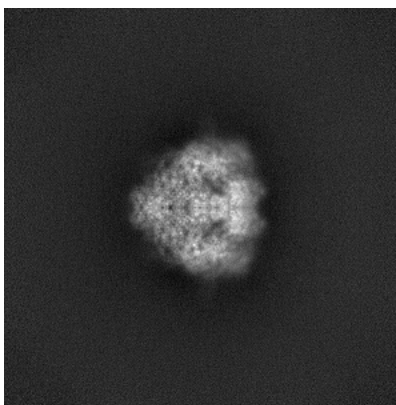


Z

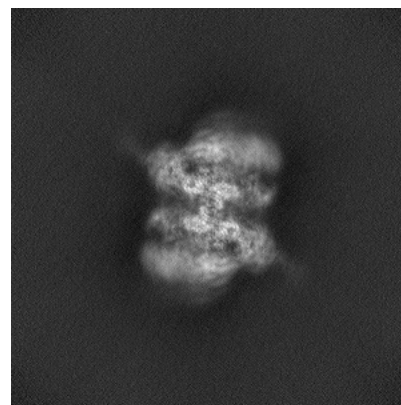
6.1.2 Raw map



X



Y

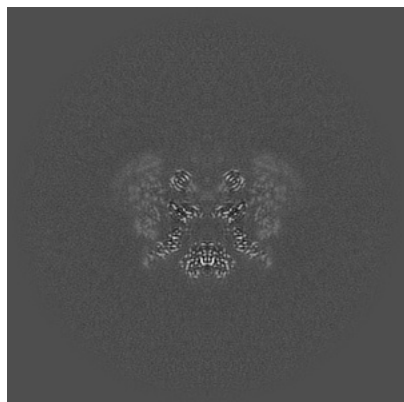


Z

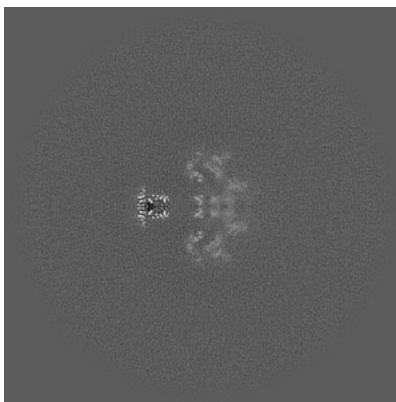
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

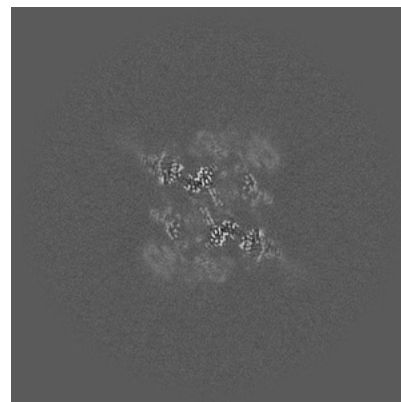
6.2.1 Primary map



X Index: 270

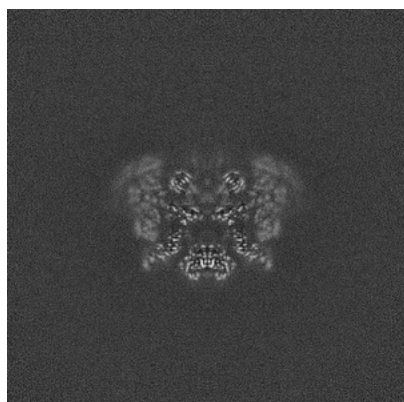


Y Index: 270

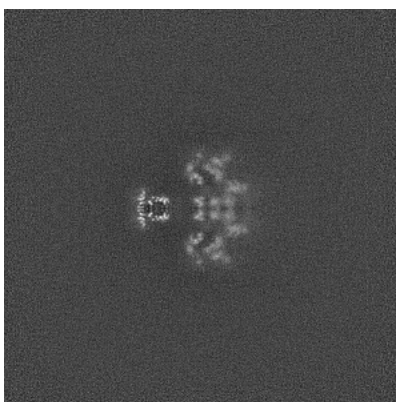


Z Index: 270

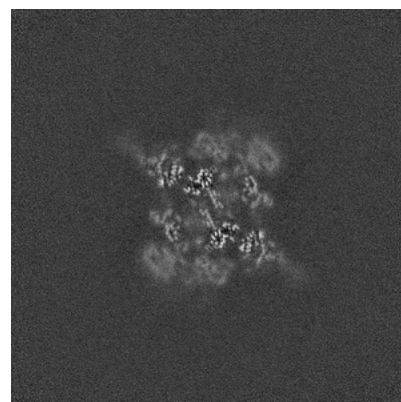
6.2.2 Raw map



X Index: 270



Y Index: 270

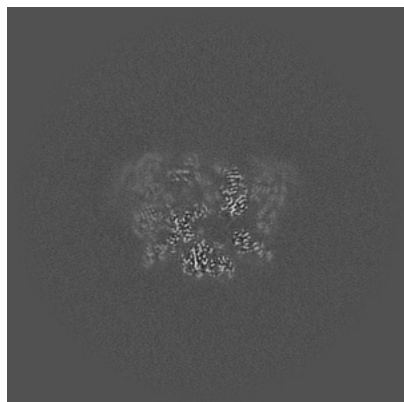


Z Index: 270

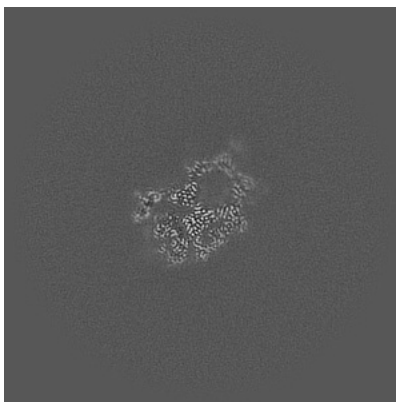
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

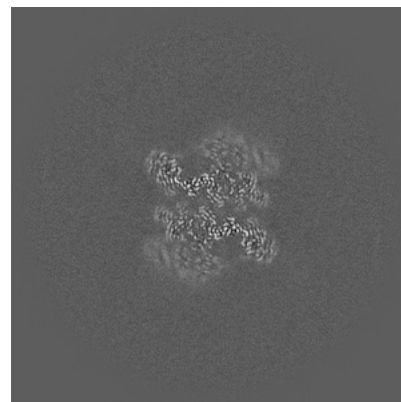
6.3.1 Primary map



X Index: 263

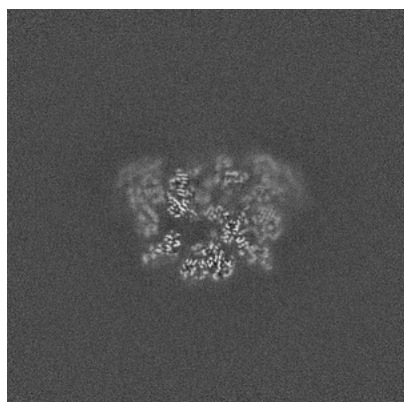


Y Index: 303

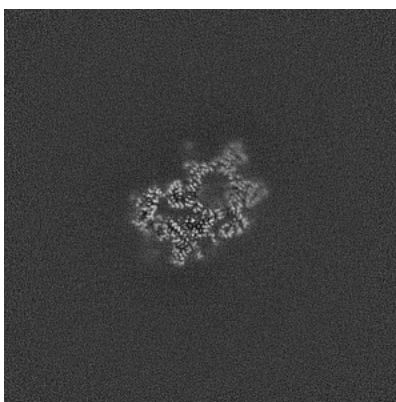


Z Index: 260

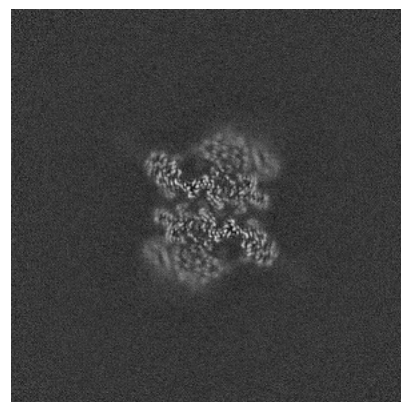
6.3.2 Raw map



X Index: 276



Y Index: 297

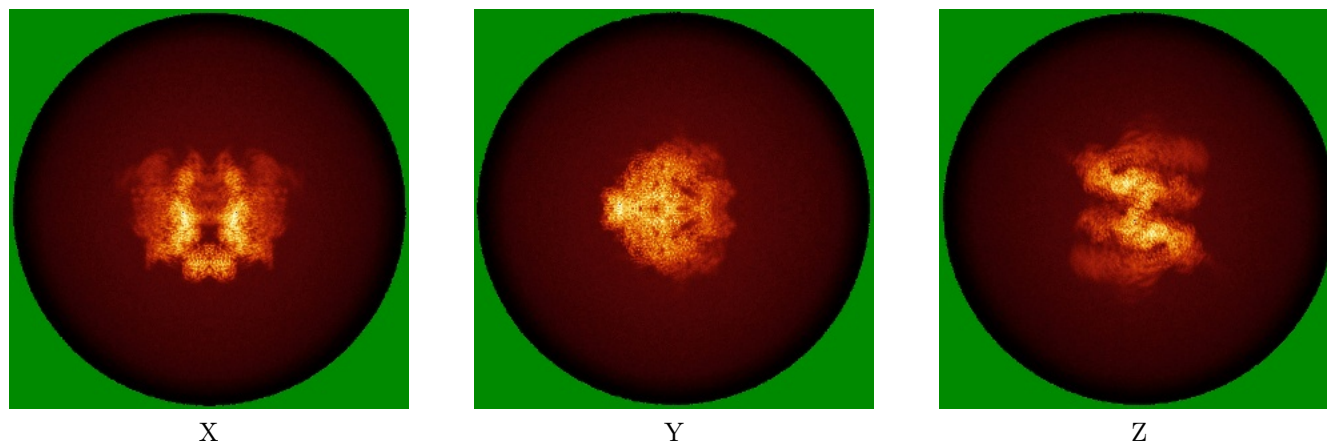


Z Index: 260

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

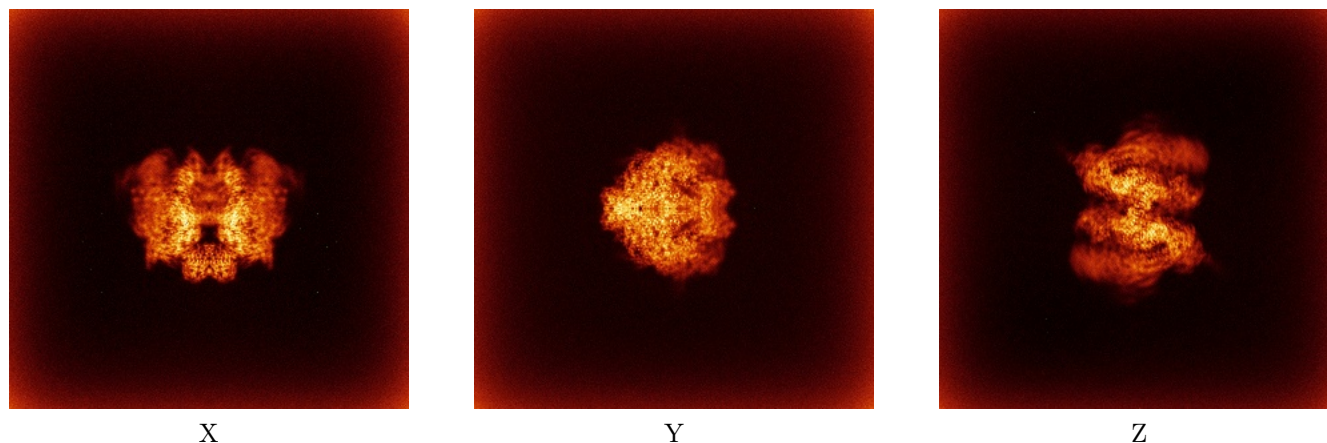


X

Y

Z

6.4.2 Raw map



X

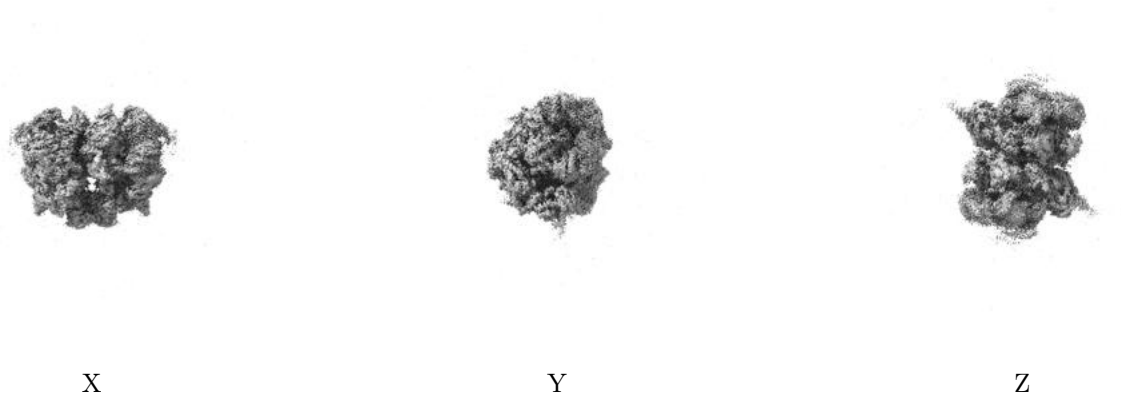
Y

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.

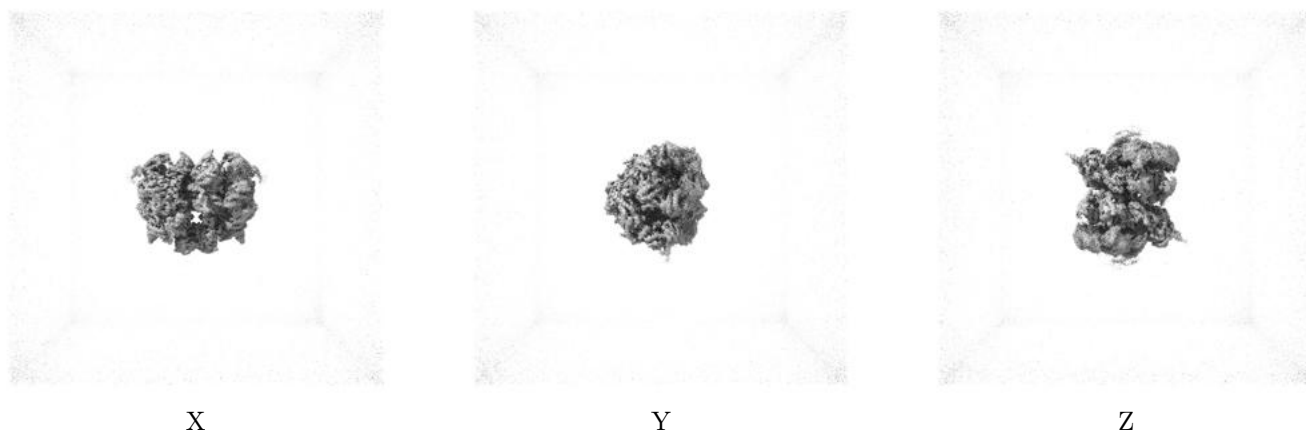
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. 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.

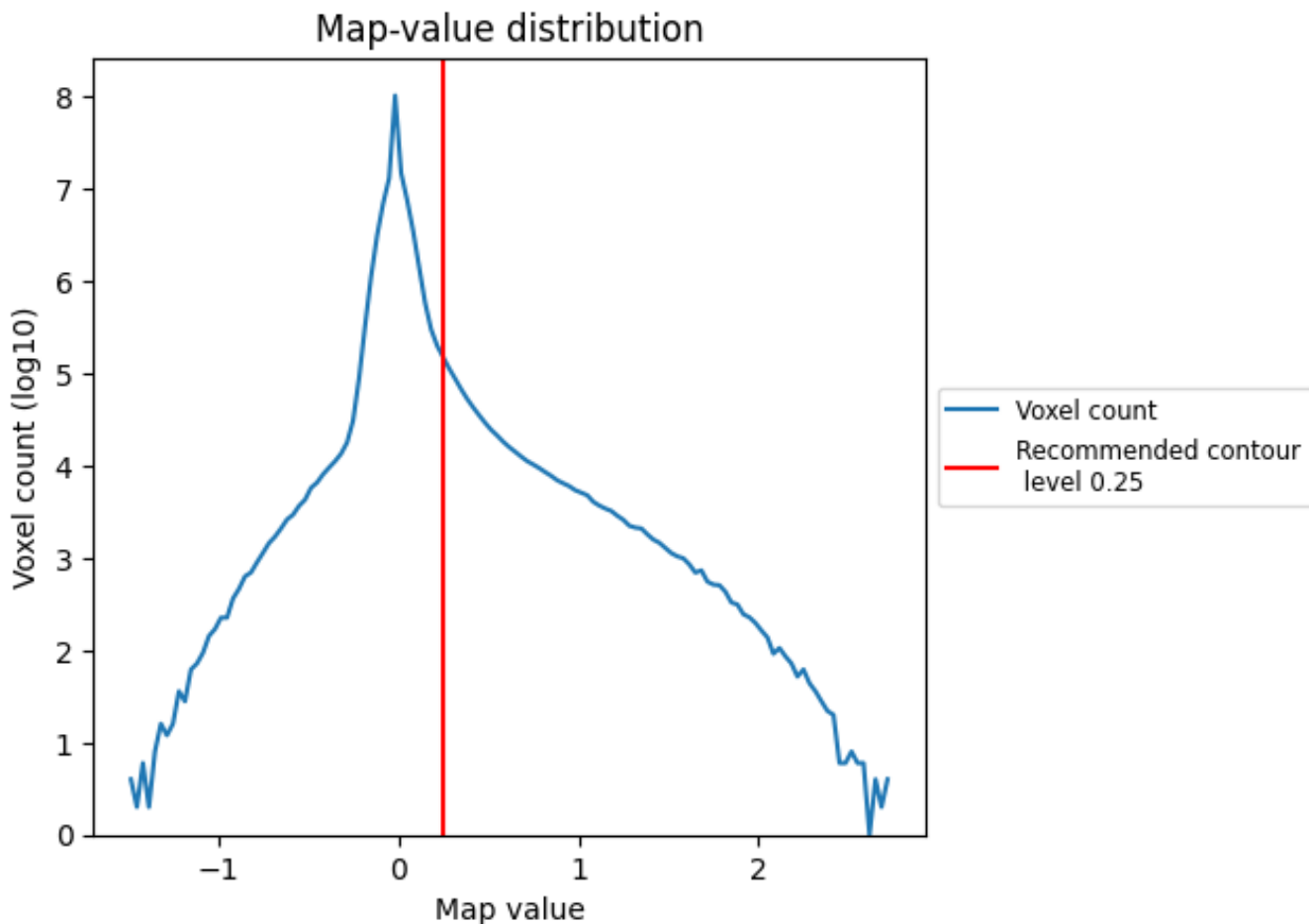
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

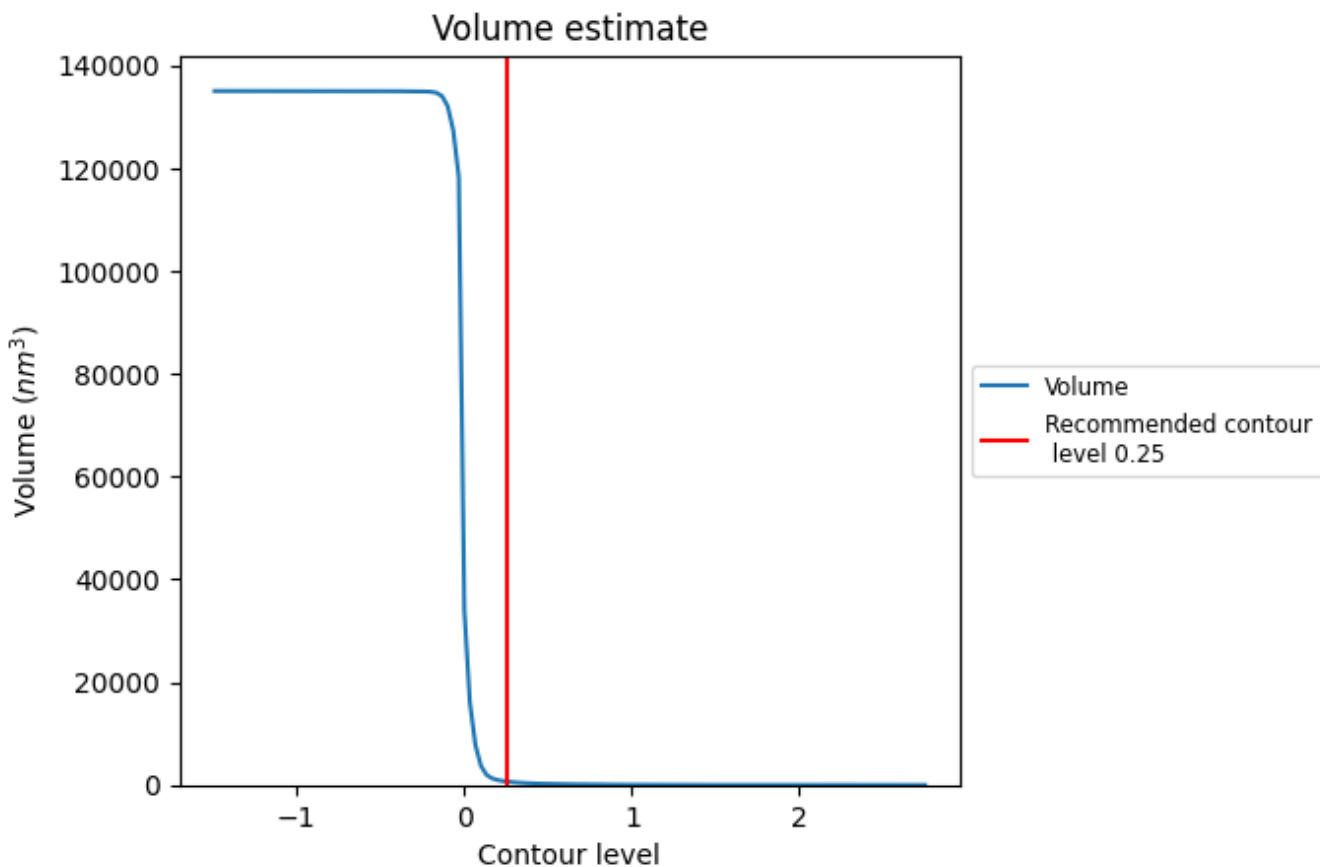
This section contains the results of statistical analysis of the map.

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.

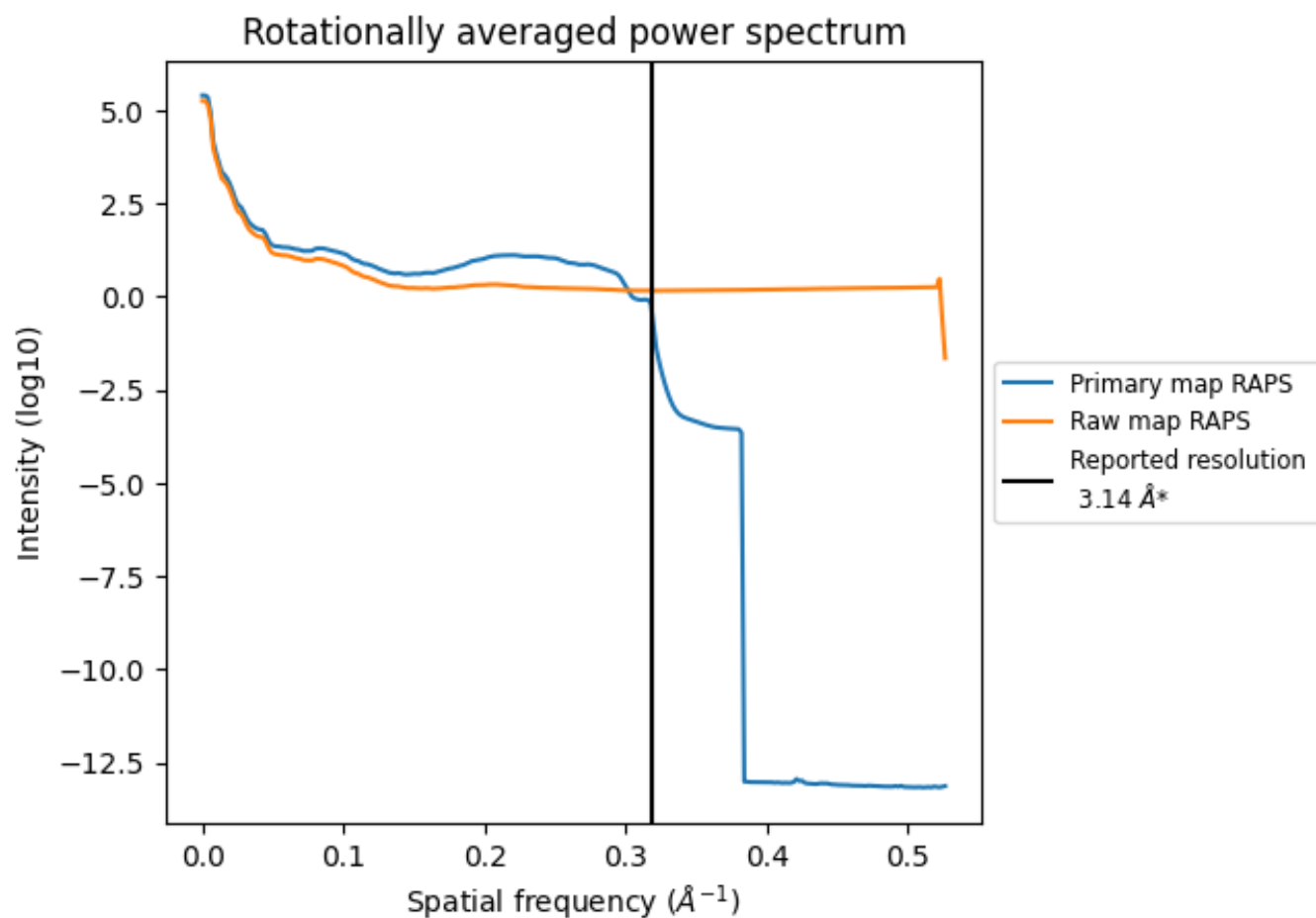
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 684 nm³; this corresponds to an approximate mass of 618 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

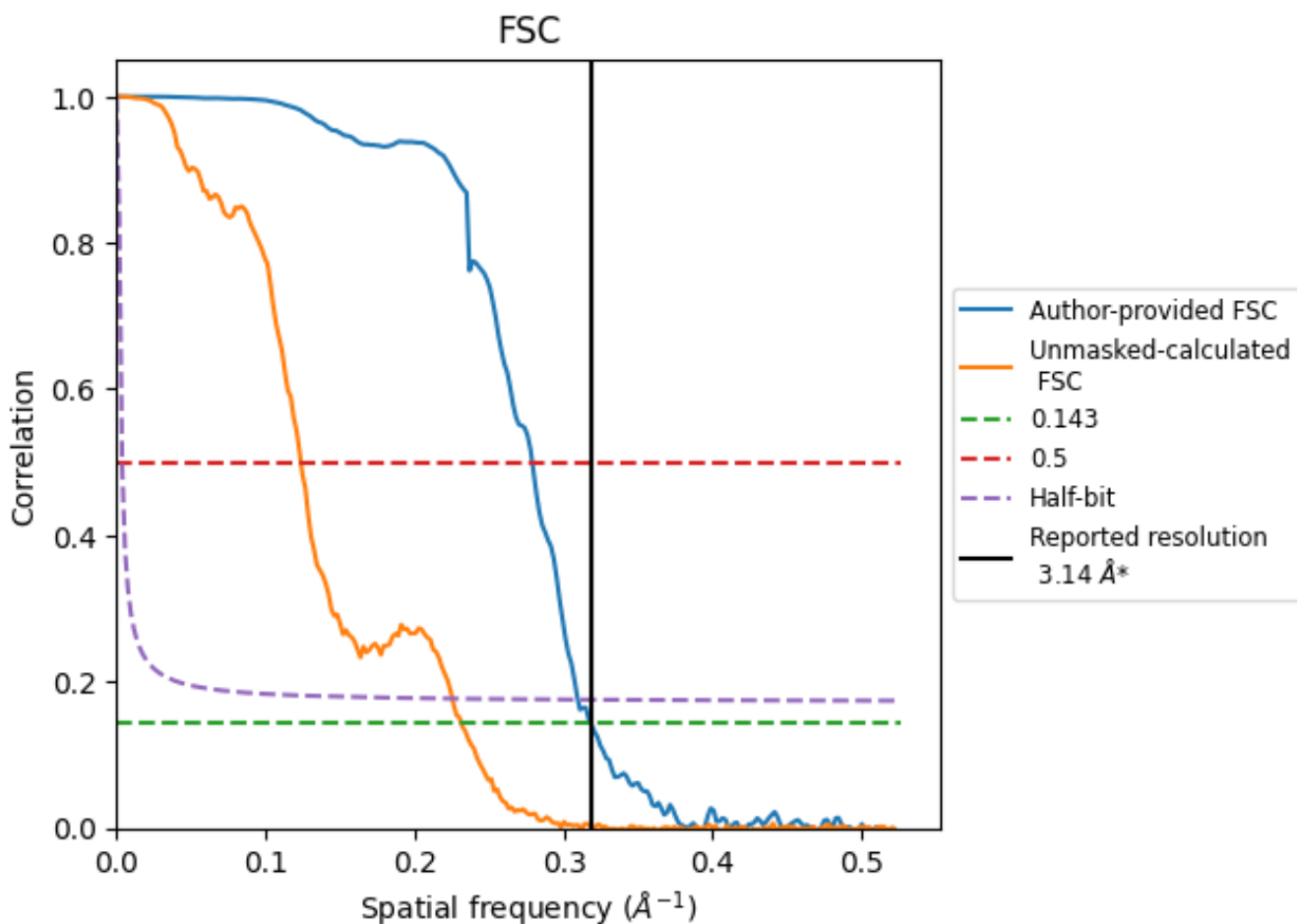


*Reported resolution corresponds to spatial frequency of 0.318 Å⁻¹

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 0.318 \AA^{-1}

8.2 Resolution estimates [i](#)

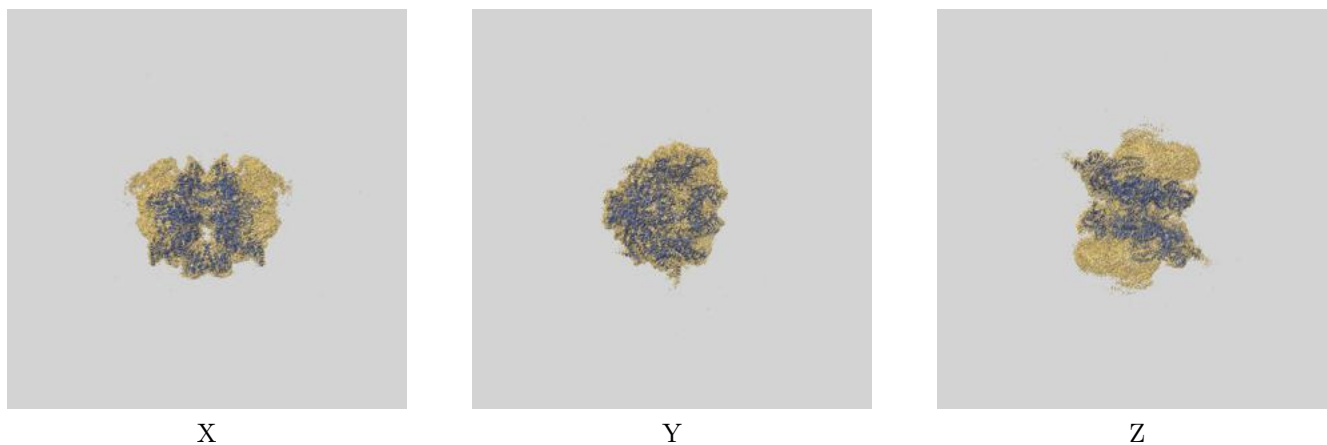
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.14	-	-
Author-provided FSC curve	3.14	3.59	3.23
Unmasked-calculated*	4.32	8.08	4.44

*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 4.32 differs from the reported value 3.14 by more than 10 %

9 Map-model fit [i](#)

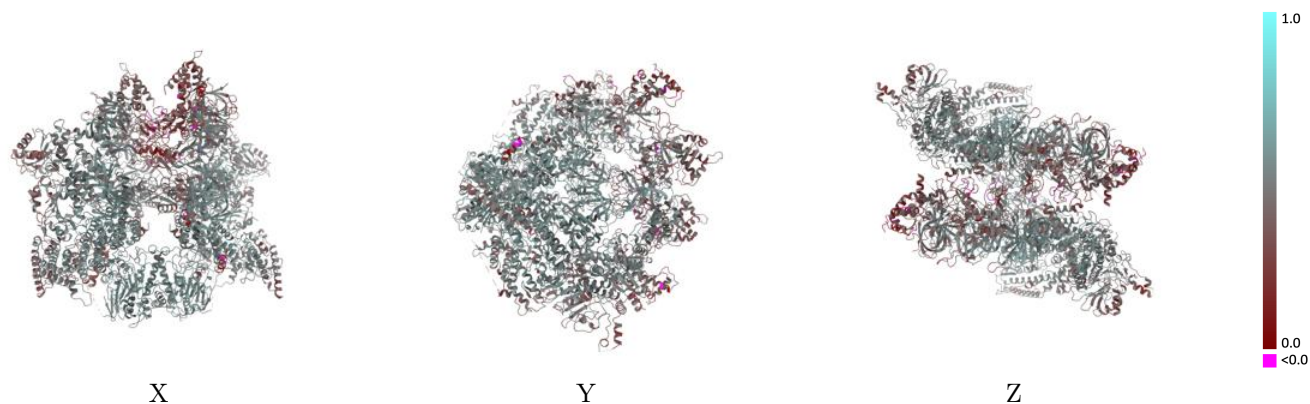
This section contains information regarding the fit between EMDB map EMD-18191 and PDB model 8Q6O. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



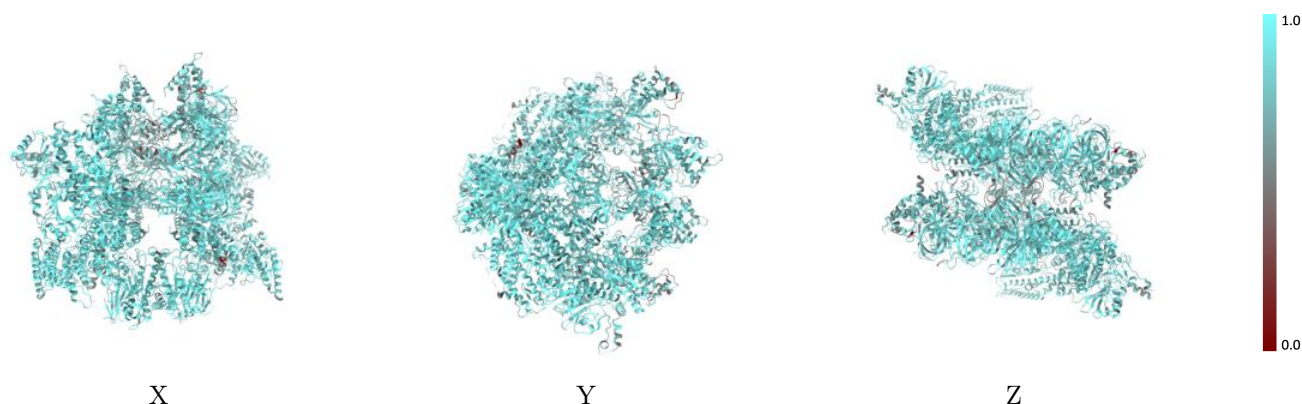
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



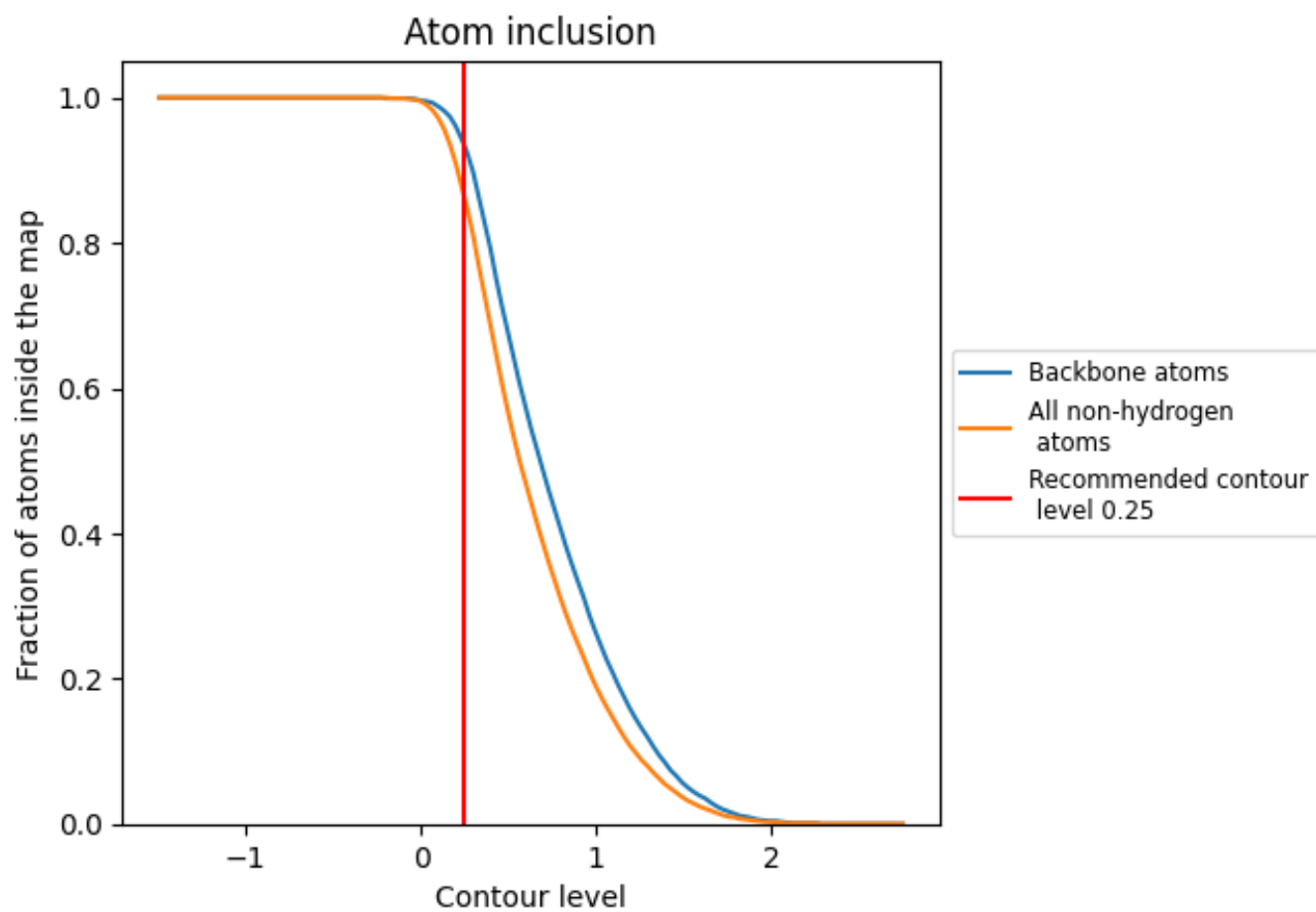
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 86% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8620	 0.4710
2	 0.8420	 0.4600
3	 0.9090	 0.5270
4	 0.7620	 0.3370
5	 0.9130	 0.5390
6	 0.7650	 0.3590
7	 0.8230	 0.4030
A	 0.8420	 0.4610
B	 0.9110	 0.5300
C	 0.7590	 0.3410
D	 0.9130	 0.5380
E	 0.7630	 0.3620
F	 0.8210	 0.4040
G	 0.8720	 0.4660
H	 0.9300	 0.5350
I	 0.9050	 0.5290
J	 0.8640	 0.4770
K	 0.8960	 0.5050
L	 0.8990	 0.5220
M	 0.8720	 0.4690
N	 0.9300	 0.5390
O	 0.9070	 0.5290
P	 0.8630	 0.4780
Q	 0.8960	 0.5040
R	 0.8980	 0.5200

