



wwPDB EM Validation Summary Report ⓘ

Nov 17, 2024 – 02:12 PM EST

PDB ID : 3JC6
EMDB ID : EMD-6534
Title : Structure of the eukaryotic replicative CMG helicase and pumpjack motion
Authors : Li, H.; Bai, L.; Yuan, Z.; Sun, J.; Georgescu, R.E.; Liu, J.; O'Donnell, M.E.
Deposited on : 2015-11-24
Resolution : 3.70 Å(reported)
Based on initial model : 2Q9Q

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

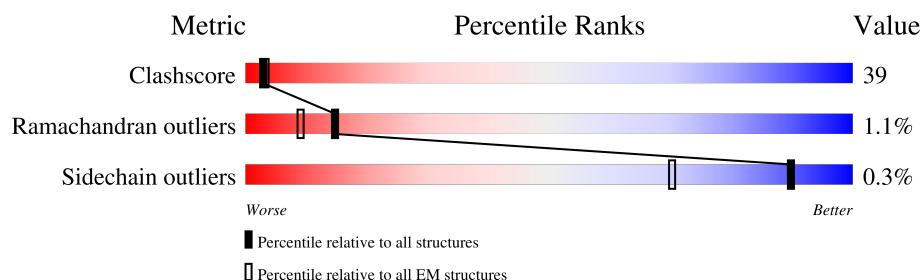
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 Å.

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



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

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	868	 16% 12% 72%
2	3	971	 14% 13% 72%
3	4	933	 14% 15% 71%
4	5	775	 16% 17% 67%
5	6	1017	 14% 12% 74%
6	7	845	 5% 20% 18% 62%
7	E	672	 8% 43% 38% 18%
8	D	294	 36% 37% 25%

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Mol	Chain	Length	Quality of chain
9	B	213	<div><div><div></div><div></div><div></div></div><div>39%45%15%</div></div>
10	A	208	<div><div><div></div><div></div><div></div></div><div>15%40%58%</div></div>
11	C	194	<div><div><div></div><div></div><div></div></div><div>39%42%18%</div></div>

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 23732 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
1	2	241	Total	C	N	O	S	0	0
			1911	1214	338	354	5		

- Molecule 2 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	269	Total	C	N	O	S	0	0
			2130	1354	368	404	4		

- Molecule 3 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	275	Total	C	N	O	S	0	0
			2203	1391	382	413	17		

- Molecule 4 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	254	Total	C	N	O	S	0	0
			2028	1284	347	388	9		

- Molecule 5 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	267	Total	C	N	O	S	0	0
			2049	1296	366	381	6		

- Molecule 6 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	325	Total	C	N	O	S	0	0
			2611	1653	455	491	12		

- Molecule 7 is a protein called Cell division control protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	553	Total	C	N	O	S	0	0
			4482	2862	763	844	13		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	651	ASP	-	expression tag	UNP Q08032
E	652	TYR	-	expression tag	UNP Q08032
E	653	LYS	-	expression tag	UNP Q08032
E	654	ASP	-	expression tag	UNP Q08032
E	655	HIS	-	expression tag	UNP Q08032
E	656	ASP	-	expression tag	UNP Q08032
E	657	GLY	-	expression tag	UNP Q08032
E	658	ASP	-	expression tag	UNP Q08032
E	659	TYR	-	expression tag	UNP Q08032
E	660	LYS	-	expression tag	UNP Q08032
E	661	ASP	-	expression tag	UNP Q08032
E	662	HIS	-	expression tag	UNP Q08032
E	663	ASP	-	expression tag	UNP Q08032
E	664	ILE	-	expression tag	UNP Q08032
E	665	ASP	-	expression tag	UNP Q08032
E	666	TYR	-	expression tag	UNP Q08032
E	667	LYS	-	expression tag	UNP Q08032
E	668	ASP	-	expression tag	UNP Q08032
E	669	ASP	-	expression tag	UNP Q08032
E	670	ASP	-	expression tag	UNP Q08032
E	671	ASP	-	expression tag	UNP Q08032
E	672	LYS	-	expression tag	UNP Q08032

- Molecule 8 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	221	Total	C	N	O	S	0	0
			1820	1159	300	348	13		

- Molecule 9 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	181	Total	C	N	O	S	0	0
			1513	978	261	270	4		

- Molecule 10 is a protein called DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	208	Total	C	N	O	S	0	0
			1696	1065	290	331	10		

- Molecule 11 is a protein called DNA replication complex GINS protein PSF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	159	Total	C	N	O	S	0	0
			1288	843	207	232	6		

- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
12	7	1	Total	Zn	0
			1	1	

- Molecule 2: DNA replication licensing factor MCM3



SER	THR	ARG	GLY	THR	ASN	LEU	ALA	THR	GLN	V294	A217	SER	GLU	MET
PRO	ARG	PRO	VAL	ALA	SER	LEU	HIS	ALA	SER	V295	T218	ARG	LYS	GLY
ARG	ARG	VAL	ILE	GLU	SER	LEU	LYS	SER	LEU	G296	T219	H151	GLU	GLY
ARG	ARG	ALA	VAL	VAL	ALA	VAL	ALA	LEU	ALA	V297	T220	P152	LYS	SER
GLJ	SER	ALA	GLN	MET	ILE	THR	GLY	PRO	SER	F298	L221	V153	ALA	GLY
HIS	THR	ASN	LEU	GLJ	ALA	ASP	ILE	SER	ILE	V299		K154	ALA	PHE
LEU	ALA	LEU	THR	GLN	THR	ASP	TYR	TYR	TYR	L301	T225	S156	SER	GLY
HIS	ALA	LEU	GLN	THR	THR	GLY	GLY	HIS	GLY	N307	T227	K158	THR	ASP
ALA	ASN	ILE	THR	VAL	ARG	ASP	ASP	ASP	HIS		A229	G159	SER	ALA
GLU	ALA	ARG	ILE	THR	GLY	SER	ILE	ILE	ILE	N310	T230	S160	ASN	THR
GLY	VAL	ASP	VAL	ALA	SER	SER	GLY	LYS	LYS	A163		H164	ASN	PHE
SER	PRO	GLY	ILE	GLY	GLY	ARG	GLY	LYS	LYS	H164	T233	H164	GLU	ALA
SER	THR	GLY	VAL	GLY	VAL	SER	ALA	ALA	ALA	T312	E234	A165	ALA	ALA
GLY	SER	ASP	VAL	GLY	GLY	ILE	GLY	ILE	ILE	T313	D235	L166		
PRO	ALA	ILE	ASN	THR	LEU	SER	THR	LEU	LEU	L314		S167		
LEU	ARG	GLY	THR	HIS	THR	GLU	THR	LEU	LEU	F317	G238	P168		D118
THR	ARG	ASN	THR	THR	ALA	GLU	ALA	MET	MET		N239			
THR	ILE	LEU	THR	VAL	VAL	VAL	VAL	LEU	LEU	L320	K240	L171		D23
GLY	THR	ARG	ASN	THR	THR	ARG	THR	GLY	GLY	T325	T243	A173		R24
GLY	THR	THR	THR	THR	THR	THR	THR	GLY	GLY	V326	E244	L176		R26
VAL	THR	THR	THR	THR	THR	THR	THR	VAL	VAL	Y327	T245	K177		D33
ASN	THR	THR	THR	THR	THR	THR	THR	GLY	GLY	H330	G246	K178		R39
ASN	THR	THR	THR	THR	THR	THR	THR	ASN	ASN	ALA	Y247	L179		D40
ASN	THR	THR	THR	THR	THR	THR	THR	LEU	LEU	ALA	S248	V180		S41
ASN	THR	THR	THR	THR	THR	THR	THR	GLY	GLY	ALA	T249	V186		V42
ASN	THR	THR	THR	THR	THR	THR	THR	ASN	ASN	ALA	F250	T187		R43
ASN	THR	THR	THR	THR	THR	THR	THR	GLY	GLY	ALA	L261	K188		N49
ASN	THR	THR	THR	THR	THR	THR	THR	VAL	SER	ALA	D252	T189		S50
ASN	THR	THR	THR	THR	THR	THR	THR	VAL	SER	ALA	H253	S190		A53
ASN	THR	THR	THR	THR	THR	THR	THR	VAL	SER	ALA	Q254	T189		N55
ASN	THR	THR	THR	THR	THR	THR	THR	VAL	SER	ALA	L256	S194		T56
ASN	THR	THR	THR	THR	THR	THR	THR	VAL	SER	ALA	T257	P194		ASN
ASN	THR	THR	THR	THR	THR	THR	THR	VAL	SER	ALA	V258	K195		ASP
ASN	THR	THR	THR	THR	THR	THR	THR	VAL	SER	ALA	Q259	L196		ASP
ASN	THR	THR	THR	THR	THR	THR	THR	VAL	SER	ALA	E260	T197		GLN
ASN	THR	THR	THR	THR	THR	THR	THR	VAL	SER	ALA	M261	S199		ASP
ASN	THR	THR	THR	THR	THR	THR	THR	VAL	SER	ALA	P262	H201		GLN
ASN	THR	THR	THR	THR	THR	THR	THR	VAL	SER	ALA	E263	V200		ASP
ASN	THR	THR	THR	THR	THR	THR	THR	VAL	SER	ALA	M264	H201		ALA
ASN	THR	THR	THR	THR	THR	THR	THR	VAL	SER	ALA	A265	T202		ALA
ASN	THR	THR	THR	THR	THR	THR	THR	VAL	SER	ALA	P266	A203		ASP
ASN	THR	THR	THR	THR	THR	THR	THR	VAL	SER	ALA	A267	A204		GLU
ASN	THR	THR	THR	THR	THR	THR	THR	VAL	SER	ALA	G268	A204		ARG
ASN	THR	THR	THR	THR	THR	THR	THR	VAL	SER	ALA	Q269	V205		ASP
ASN	THR	THR	THR	THR	THR	THR	THR	VAL	SER	ALA	L270	V205		LEU
ASN	THR	THR	THR	THR	THR	THR	THR	VAL	SER	ALA	P271	T206		LEU
ASN	THR	THR	THR	THR	THR	THR	THR	VAL	SER	ALA	R272	G207		LEU
ASN	THR	THR	THR	THR	THR	THR	THR	VAL	SER	ALA		P140		GLY
ASN	THR	THR	THR	THR	THR	THR	THR	VAL	SER	ALA		H136		ASP
ASN	THR	THR	THR	THR	THR	THR	THR	VAL	SER	ALA		D137		GLU
ASN	THR	THR	THR	THR	THR	THR	THR	VAL	SER	ALA		D138		ARG
ASN	THR	THR	THR	THR	THR	THR	THR	VAL	SER	ALA		V139		ASP
ASN	THR	THR	THR	THR	THR	THR	THR	VAL	SER	ALA		P140		LEU
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ASN	THR	THR	THR	THR	THR	THR	THR	VAL	SER	ALA		D138		ASP
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ASN	THR	THR	THR	THR	THR	THR	THR	VAL	SER	ALA		H136		GLY
ASN	THR	THR	THR	THR	THR	THR	THR	VAL	SER	ALA		D137		ASP
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ASN	THR	THR	THR	THR	THR	THR	THR	VAL	SER	ALA		V139		LEU
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ASN	THR	THR	THR	THR	THR	THR	THR	VAL	SER	ALA		H136		GLY
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ASN	THR	THR	THR	THR	THR	THR	THR	VAL	SER	ALA		H136		LEU
ASN	THR	THR	THR	THR	THR	THR	THR	VAL	SER	ALA		D137		GLY
ASN	THR	THR	THR	THR	THR	THR	THR	VAL	SER	ALA		D138		ASP
ASN	THR	THR	THR	THR	THR	THR	THR	VAL	SER	ALA		V139		LEU
ASN	THR	THR	THR	THR	THR	THR	THR	VAL	SER	ALA		P140		LEU
ASN	THR	THR	THR	THR	THR	THR	THR	VAL	SER	ALA		H136		GLY
ASN	THR	THR	THR	THR	THR	THR	THR	VAL	SER	ALA		D137		ASP
ASN	THR	THR	THR	THR	THR	THR								

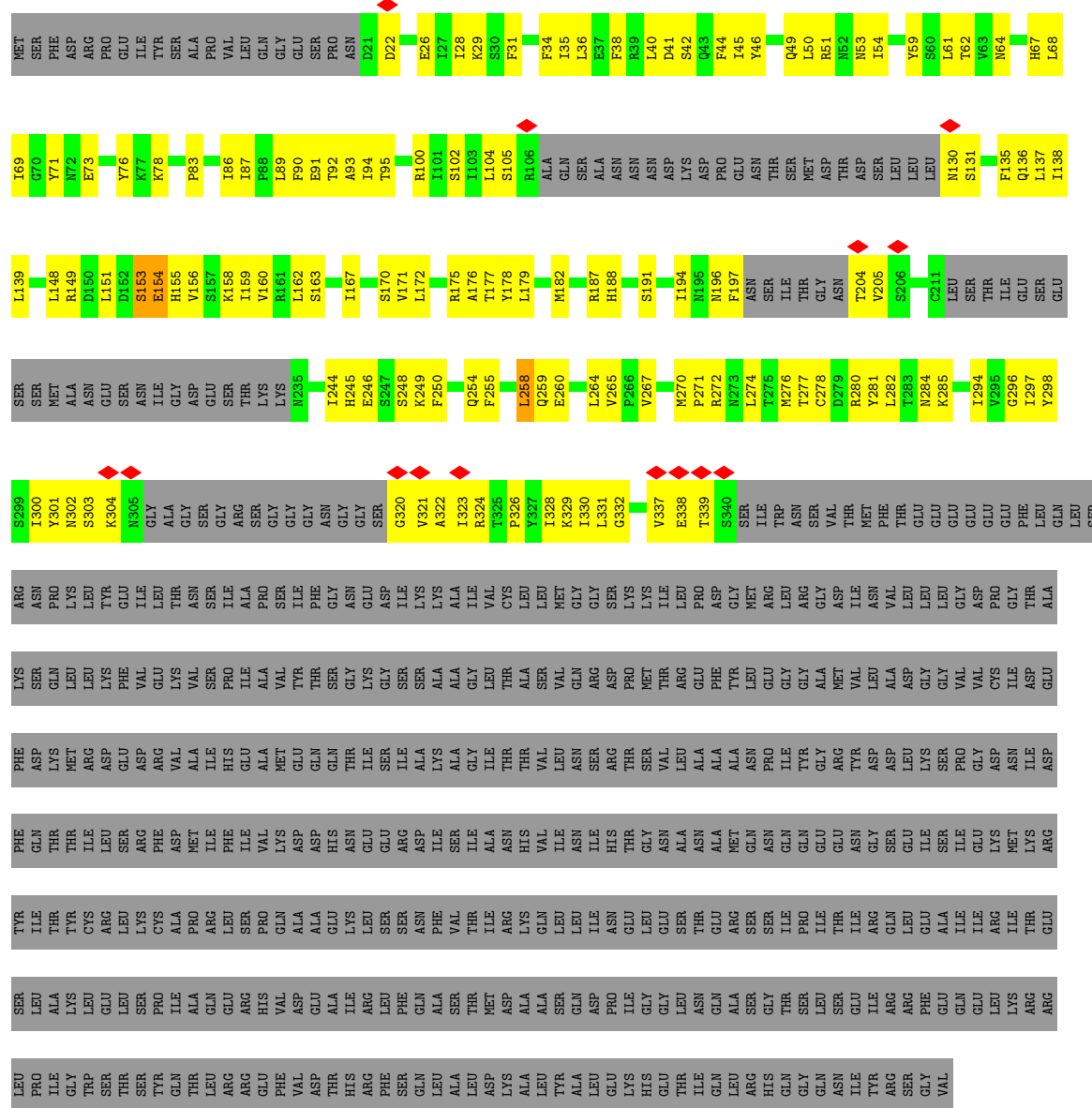
- Molecule 3: DNA replication licensing factor MCM4



GLU HIS SER GLN ASP ARG VAL GLU SER SER ASP ILE GLN GLU ALA LEU SER ARG LEU GLN GLN ASP LYS VAL ILE VAL VAL GLY GLU GLY GLY VAL ARG VAL ARG LEU ASN ASN ARG VAL

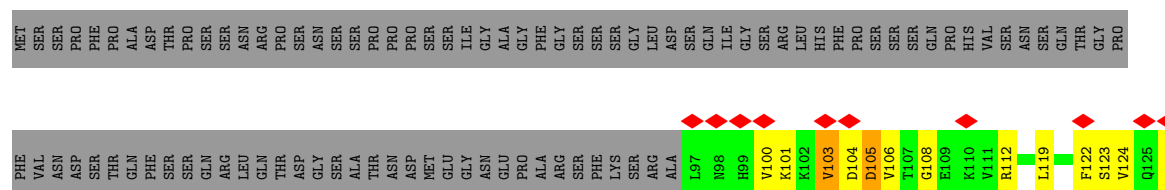
• Molecule 4: Minichromosome maintenance protein 5

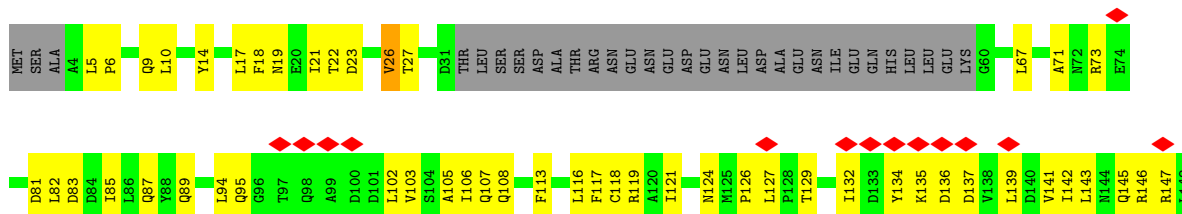
Chain 5:

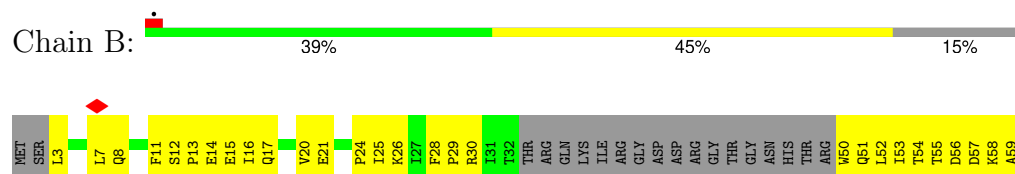


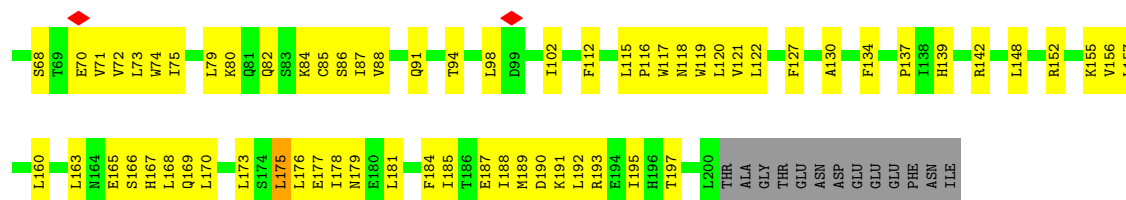
• Molecule 5: DNA replication licensing factor MCM6

Chain 6:

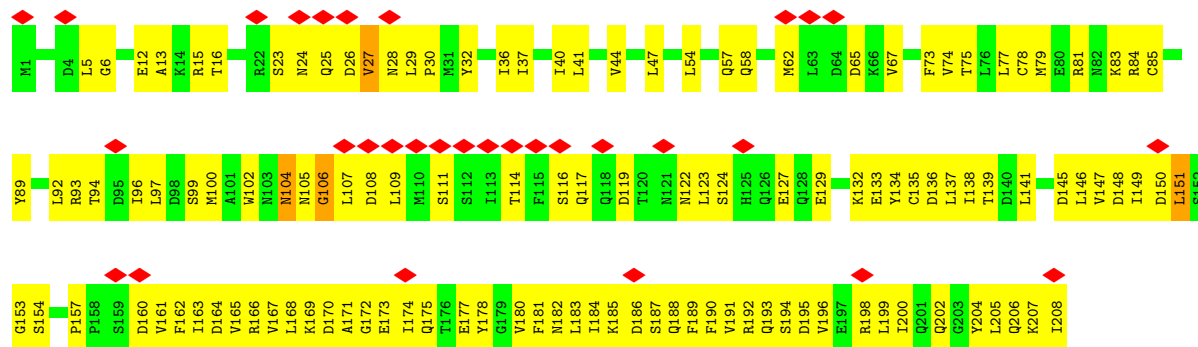




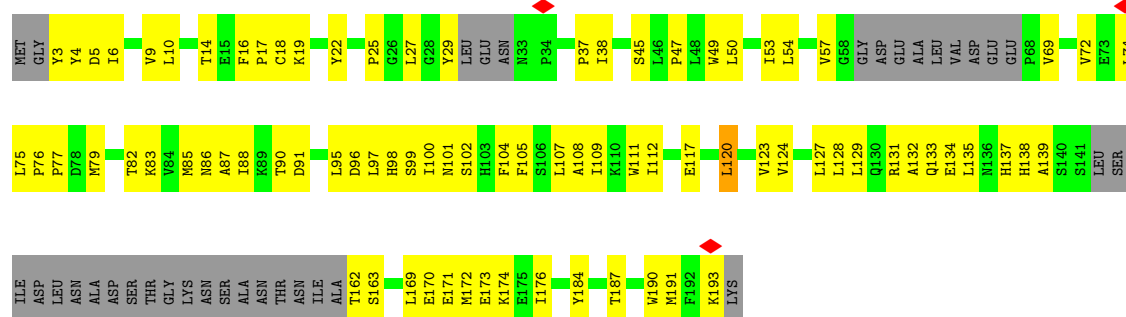




• Molecule 10: DNA replication complex GINS protein PSF1



• Molecule 11: DNA replication complex GINS protein PSF3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	469818	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	CTFFIND4	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	49505	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.155	Depositor
Minimum map value	-0.084	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (\AA)	258.56, 258.56, 258.56	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.01, 1.01, 1.01	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	0.41	0/1946	0.66	1/2633 (0.0%)
2	3	0.46	0/2179	0.70	1/2963 (0.0%)
3	4	0.38	0/2240	0.67	0/3029
4	5	0.50	0/2057	0.73	2/2781 (0.1%)
5	6	0.39	0/2081	0.66	1/2813 (0.0%)
6	7	0.41	0/2657	0.66	1/3592 (0.0%)
7	E	0.39	0/4563	0.63	2/6173 (0.0%)
8	D	0.43	0/1853	0.64	0/2500
9	B	0.44	0/1545	0.69	0/2092
10	A	0.39	0/1718	0.65	0/2314
11	C	0.46	0/1320	0.64	1/1784 (0.1%)
All	All	0.42	0/24159	0.66	9/32674 (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
2	3	0	2
3	4	0	5
5	6	0	3
6	7	0	4
7	E	0	1
8	D	0	2
10	A	0	4
All	All	0	21

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	27	LEU	CA-CB-CG	7.97	133.63	115.30
4	5	258	LEU	CA-CB-CG	7.60	132.78	115.30
2	3	171	LEU	CA-CB-CG	7.21	131.88	115.30
5	6	105	ASP	CB-CG-OD1	6.55	124.20	118.30
1	2	436	GLY	N-CA-C	5.96	128.01	113.10

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	3	163	ALA	Peptide
2	3	165	ALA	Peptide
3	4	202	LYS	Peptide
3	4	245	ALA	Peptide
3	4	372	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	1911	0	1908	126	0
2	3	2130	0	2105	172	0
3	4	2203	0	2188	198	0
4	5	2028	0	2055	177	0
5	6	2049	0	1959	132	0
6	7	2611	0	2623	165	0
7	E	4482	0	4497	322	0
8	D	1820	0	1823	214	0
9	B	1513	0	1558	150	0
10	A	1696	0	1698	310	0
11	C	1288	0	1298	104	0
12	7	1	0	0	0	0
All	All	23732	0	23712	1852	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 39.

The worst 5 of 1852 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)
4:5:197:PHE:CE2	4:5:329:LYS:HG2	1.19	1.65
6:7:17:LEU:HD11	6:7:102:LEU:CD2	1.37	1.55
5:6:290:ILE:HD13	5:6:454:PHE:CZ	1.40	1.51
3:4:342:MET:HB3	3:4:360:ILE:CD1	1.45	1.46
9:B:187:GLU:OE2	11:C:176:ILE:CG2	1.65	1.43

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	235/868 (27%)	205 (87%)	25 (11%)	5 (2%)	5	33
2	3	263/971 (27%)	236 (90%)	22 (8%)	5 (2%)	6	35
3	4	271/933 (29%)	230 (85%)	36 (13%)	5 (2%)	7	35
4	5	244/775 (32%)	222 (91%)	19 (8%)	3 (1%)	11	41
5	6	259/1017 (26%)	229 (88%)	27 (10%)	3 (1%)	11	41
6	7	319/845 (38%)	270 (85%)	45 (14%)	4 (1%)	10	40
7	E	543/672 (81%)	491 (90%)	47 (9%)	5 (1%)	14	47
8	D	215/294 (73%)	197 (92%)	16 (7%)	2 (1%)	14	47
9	B	177/213 (83%)	163 (92%)	14 (8%)	0	100	100
10	A	206/208 (99%)	180 (87%)	25 (12%)	1 (0%)	25	57
11	C	151/194 (78%)	144 (95%)	7 (5%)	0	100	100
All	All	2883/6990 (41%)	2567 (89%)	283 (10%)	33 (1%)	15	43

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	291	SER
3	4	450	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	7	26	VAL
7	E	601	ILE
3	4	419	VAL

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	2	206/770 (27%)	206 (100%)	0	100	100
2	3	236/835 (28%)	236 (100%)	0	100	100
3	4	249/848 (29%)	249 (100%)	0	100	100
4	5	241/688 (35%)	241 (100%)	0	100	100
5	6	207/886 (23%)	207 (100%)	0	100	100
6	7	295/753 (39%)	295 (100%)	0	100	100
7	E	499/607 (82%)	495 (99%)	4 (1%)	79	85
8	D	213/279 (76%)	212 (100%)	1 (0%)	86	92
9	B	171/198 (86%)	170 (99%)	1 (1%)	84	90
10	A	193/193 (100%)	192 (100%)	1 (0%)	86	92
11	C	144/173 (83%)	144 (100%)	0	100	100
All	All	2654/6230 (43%)	2647 (100%)	7 (0%)	90	94

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	E	152	LEU
8	D	168	LEU
10	A	151	LEU
9	B	175	LEU
7	E	27	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
6	7	145	GLN
10	A	104	ASN
7	E	26	GLN
10	A	202	GLN
9	B	146	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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.

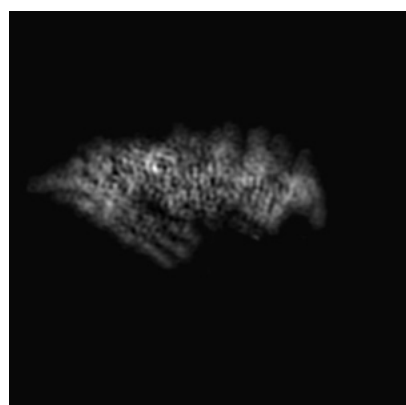
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6534. These allow visual inspection of the internal detail of the map and identification of artifacts.

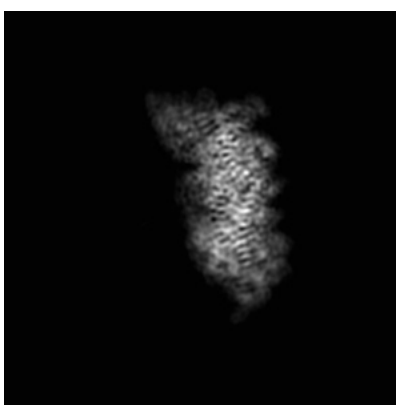
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

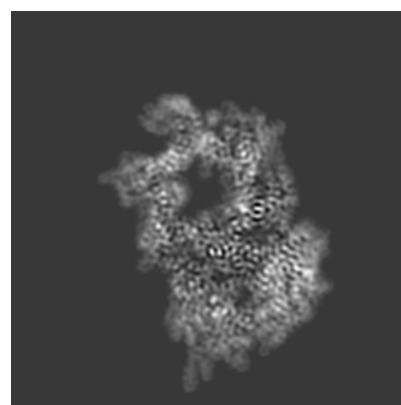
6.1.1 Primary map



X



Y

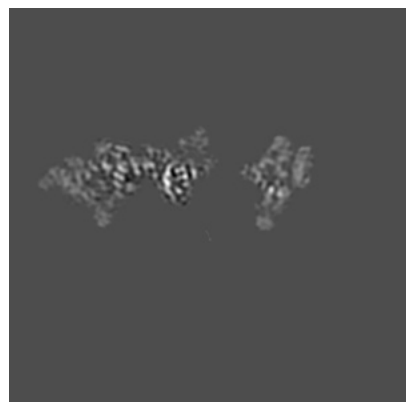


Z

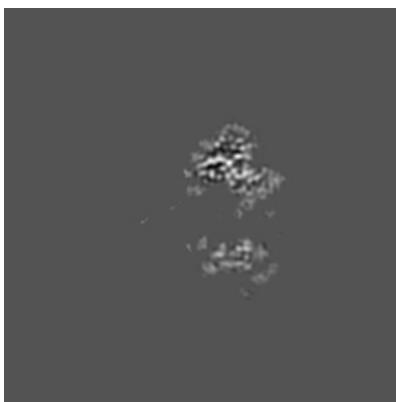
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

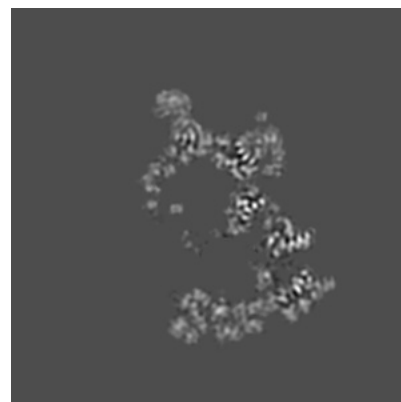
6.2.1 Primary map



X Index: 128



Y Index: 128

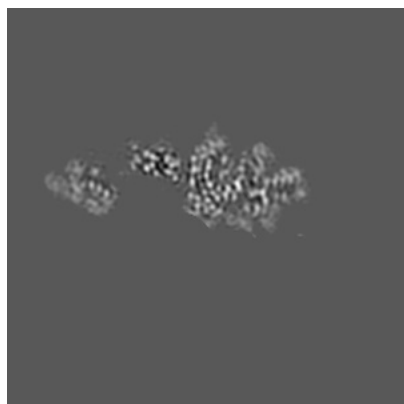


Z Index: 128

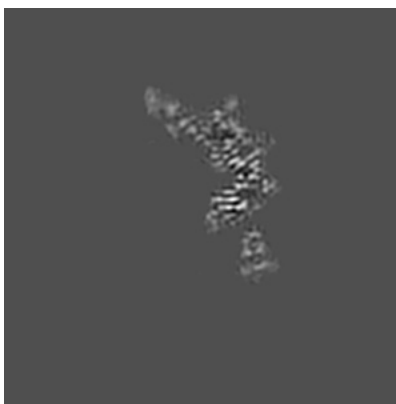
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

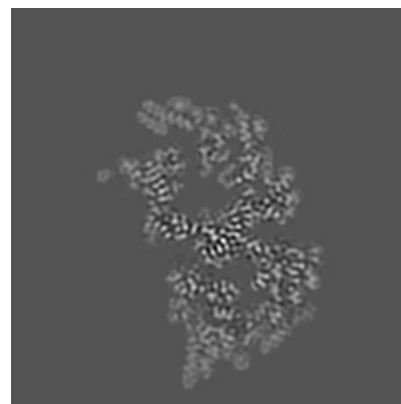
6.3.1 Primary map



X Index: 149



Y Index: 101

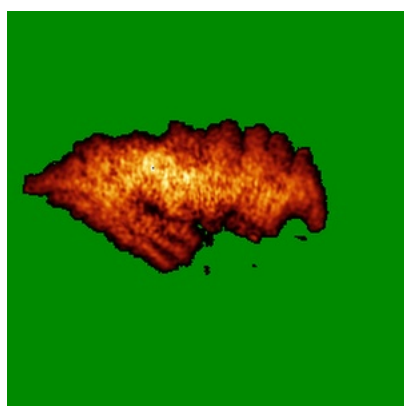


Z Index: 147

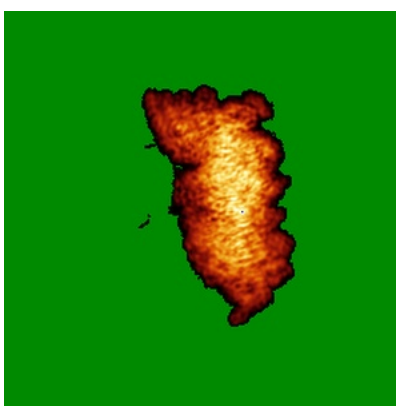
The images above show the largest variance slices of the map in three orthogonal directions.

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

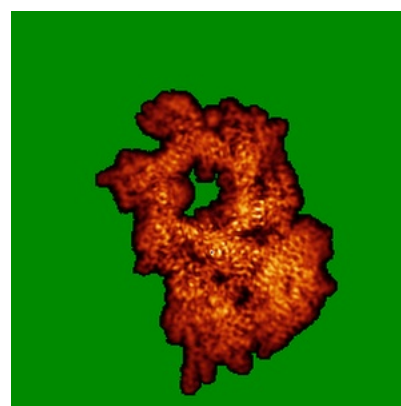
6.4.1 Primary map



X



Y

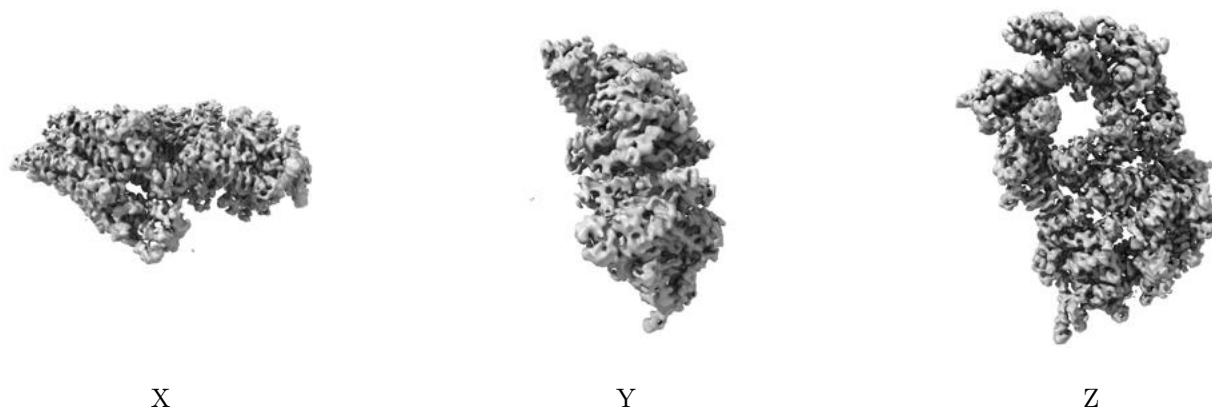


Z

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

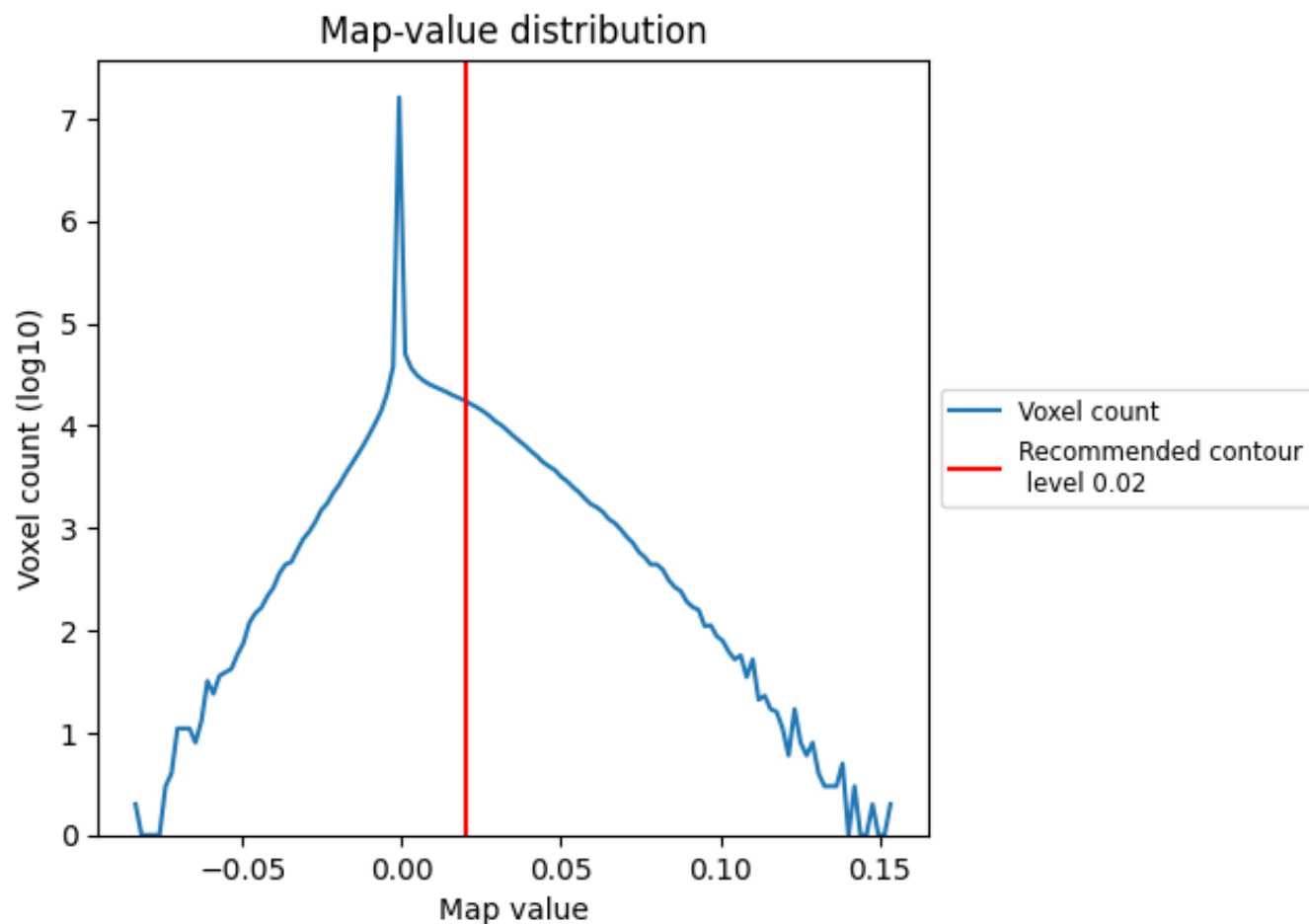
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

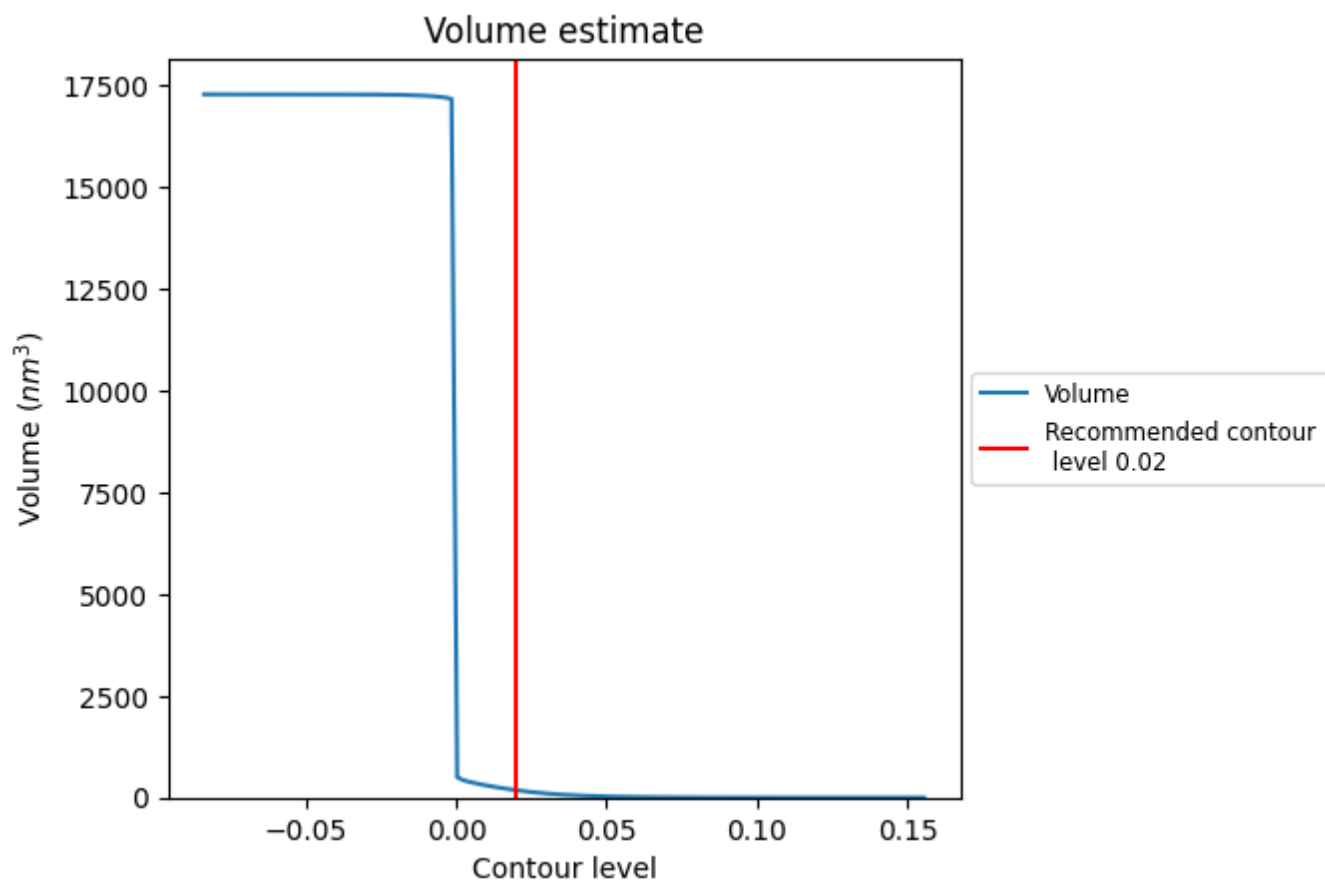
This section contains the results of statistical analysis of the map.

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.

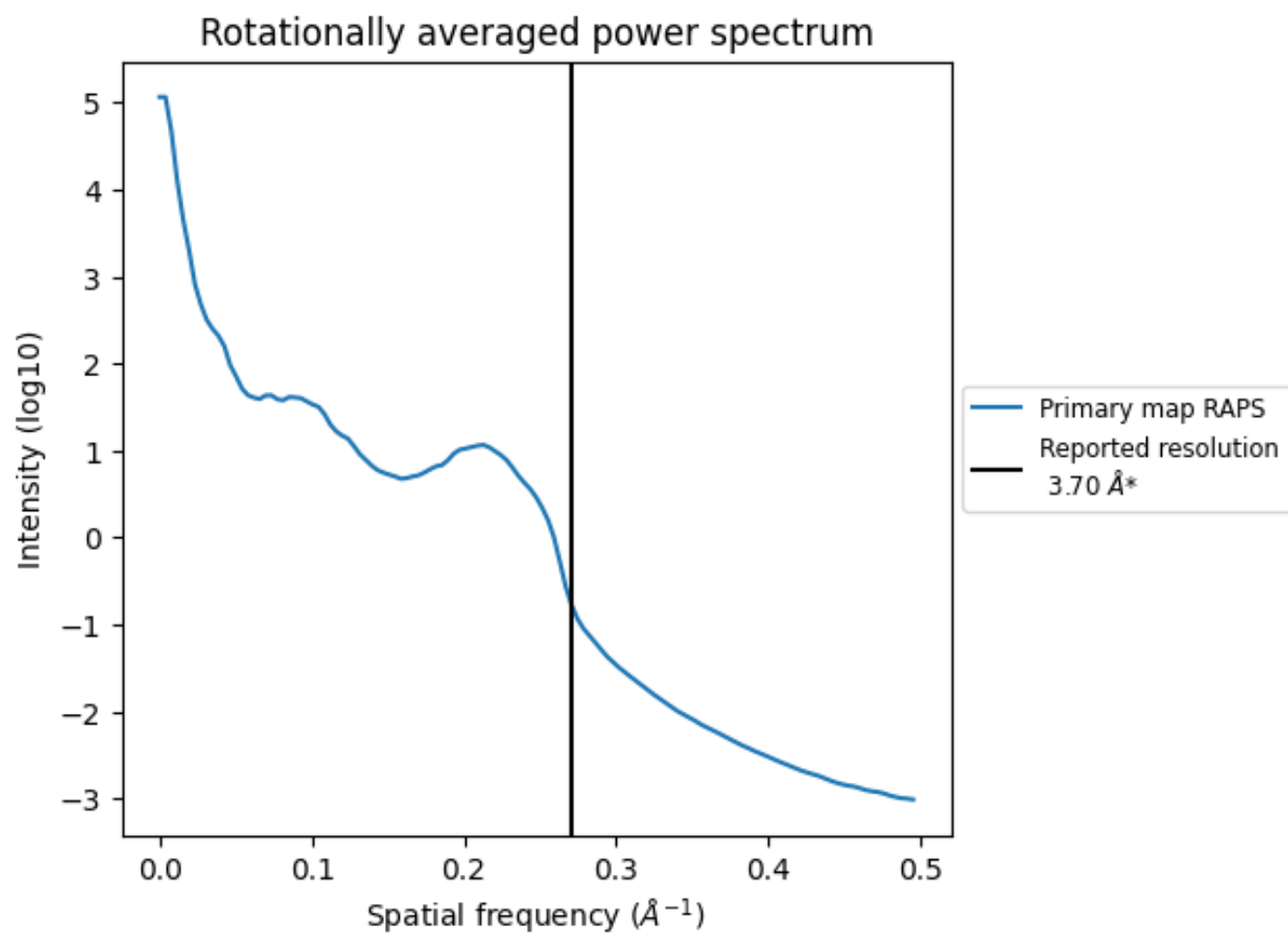
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 181 nm³; this corresponds to an approximate mass of 164 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 0.270 Å⁻¹

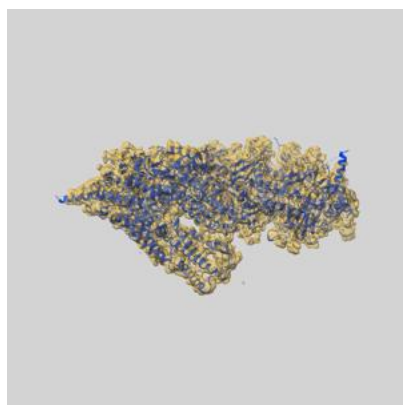
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

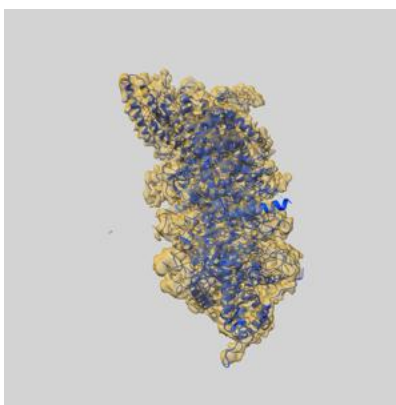
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6534 and PDB model 3JC6. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

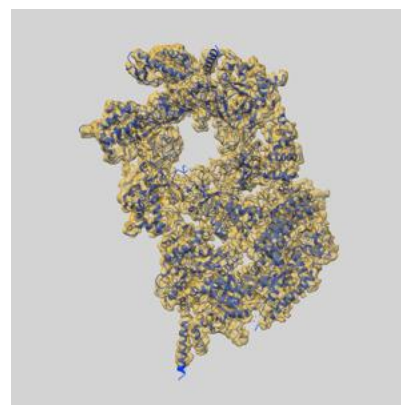
9.1 Map-model overlay [i](#)



X



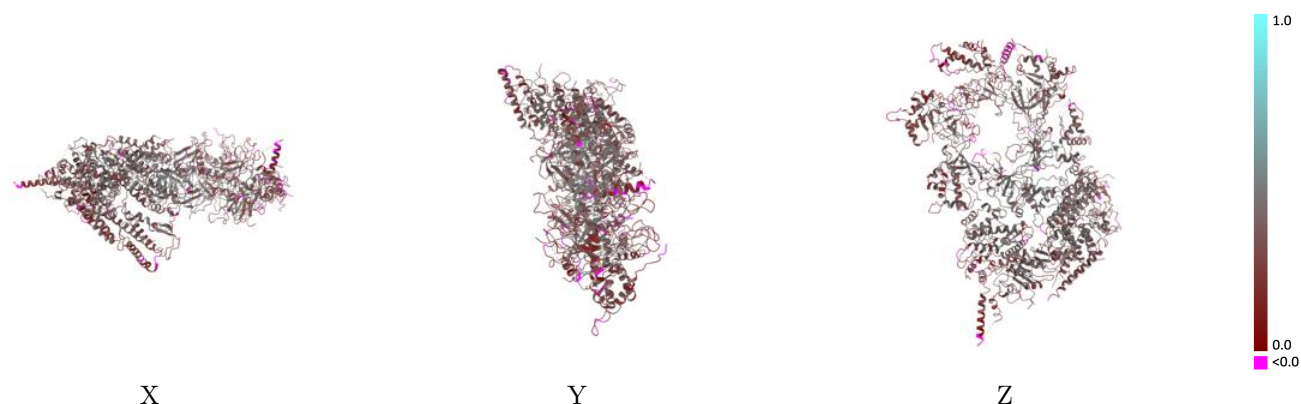
Y



Z

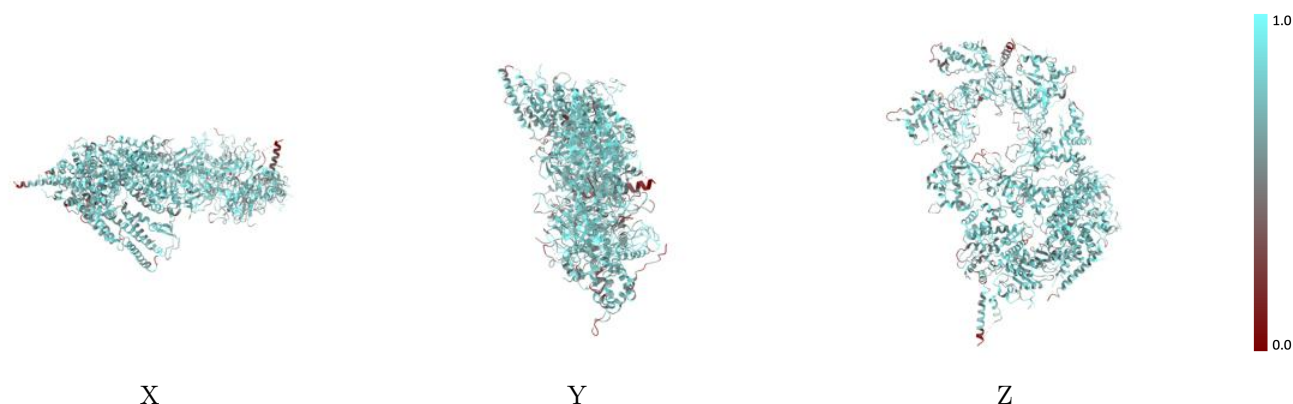
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



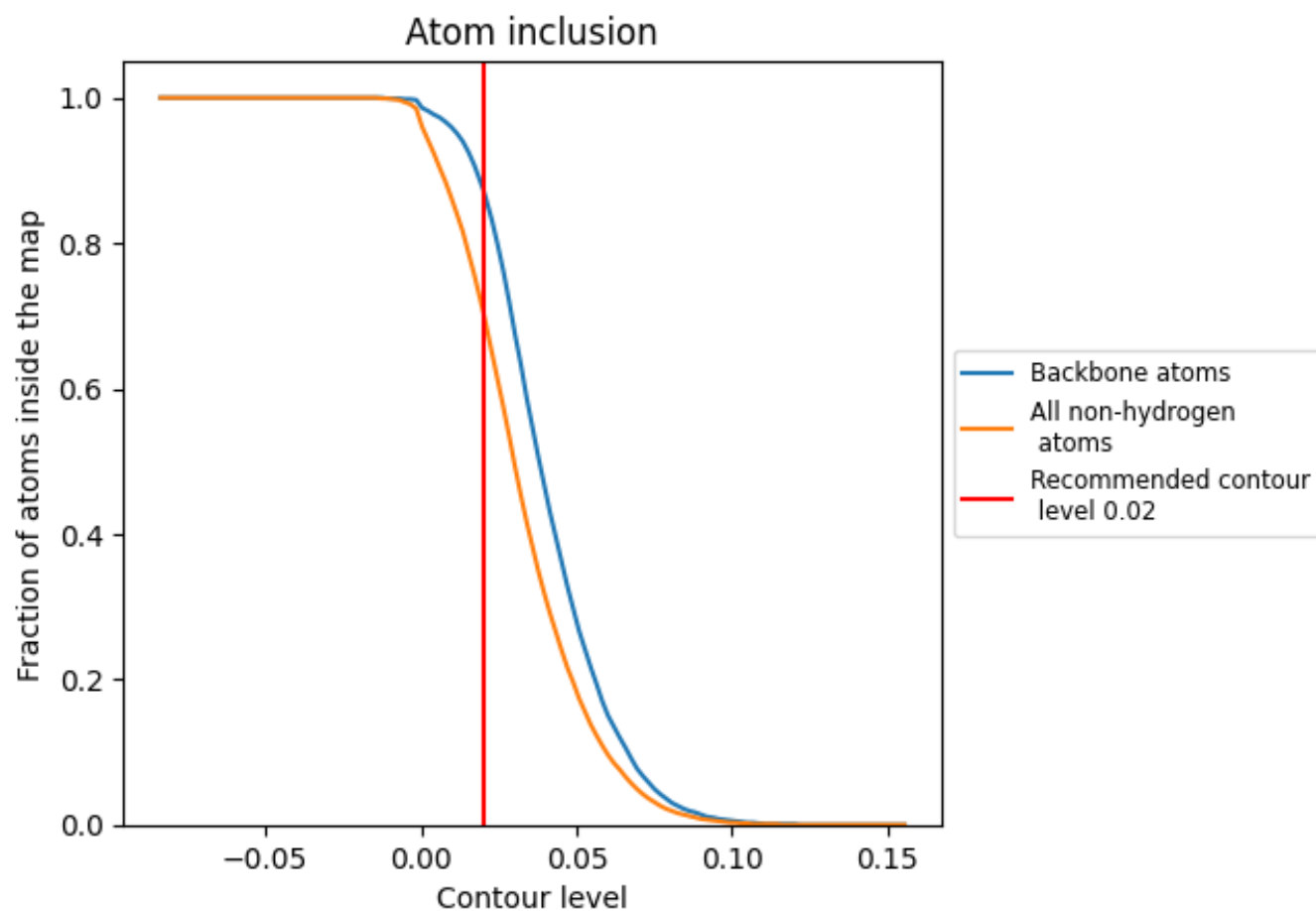
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion ⓘ



At the recommended contour level, 87% of all backbone atoms, 71% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.7060</div>	<div><div></div>0.3290</div>
2	<div><div></div>0.7000</div>	<div><div></div>0.3380</div>
3	<div><div></div>0.7450</div>	<div><div></div>0.3680</div>
4	<div><div></div>0.6760</div>	<div><div></div>0.2630</div>
5	<div><div></div>0.7680</div>	<div><div></div>0.4160</div>
6	<div><div></div>0.6790</div>	<div><div></div>0.2950</div>
7	<div><div></div>0.6520</div>	<div><div></div>0.2910</div>
A	<div><div></div>0.6490</div>	<div><div></div>0.2820</div>
B	<div><div></div>0.7470</div>	<div><div></div>0.3740</div>
C	<div><div></div>0.7680</div>	<div><div></div>0.3830</div>
D	<div><div></div>0.7240</div>	<div><div></div>0.3260</div>
E	<div><div></div>0.7000</div>	<div><div></div>0.3270</div>

1.0

0.0

<0.0