



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 11:27 AM UTC

PDB ID : 8Q6O / pdb_00008q6o
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 Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

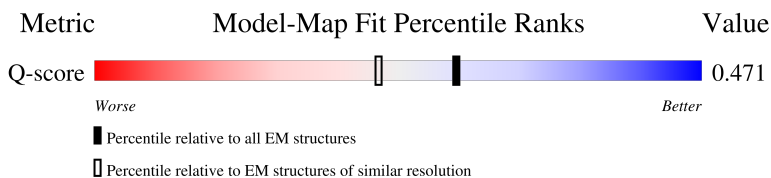
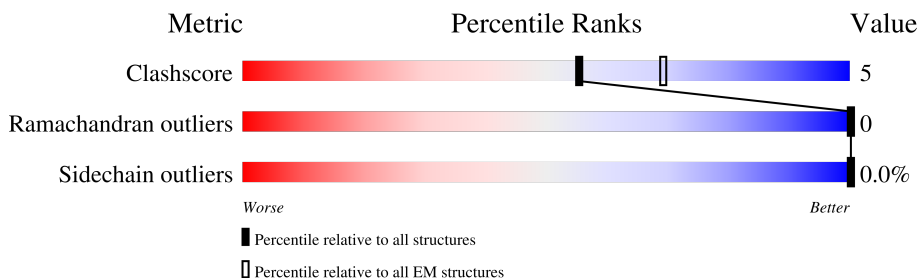
1 Overall quality at a glance

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.



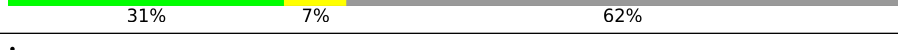
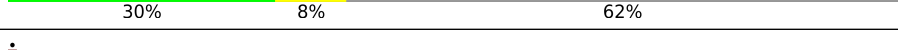
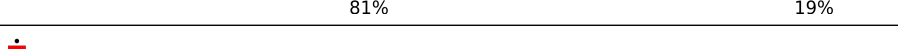
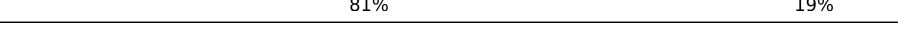
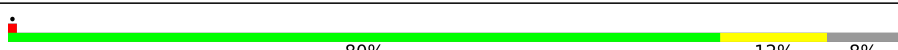
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14483 (2.64 - 3.64)

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	

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Mol	Chain	Length	Quality of chain
3	4	863	
3	C	863	
4	5	735	
4	D	735	
5	6	821	
5	E	821	
6	7	720	
6	F	720	
7	G	196	
7	M	196	
8	H	185	
8	N	185	
9	I	210	
9	O	210	
10	J	567	
10	P	567	
11	K	221	
11	Q	221	
12	L	579	
12	R	579	

2 Entry composition

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
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
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
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
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
5	E	249	Total	C	N	O	S	0	0
			1997	1260	352	373	12		
5	6	249	Total	C	N	O	S	0	0
			1997	1260	352	373	12		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn).

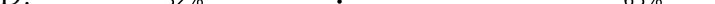
Mol	Chain	Residues	Atoms		AltConf
13	A	1	Total	Zn	0
			1	1	
13	C	1	Total	Zn	0
			1	1	
13	D	1	Total	Zn	0
			1	1	
13	E	1	Total	Zn	0
			1	1	
13	F	1	Total	Zn	0
			1	1	
13	2	1	Total	Zn	0
			1	1	
13	4	1	Total	Zn	0
			1	1	
13	5	1	Total	Zn	0
			1	1	
13	6	1	Total	Zn	0
			1	1	
13	7	1	Total	Zn	0
			1	1	





GLY	LYS	THR	VAL	TYR	ASN	ILE	GLY	ALA
THR	THR	THR	THR	ARG	GLN	ILE	THR	ALA
PRO	PRO	ILE	ILE	ARG	LEU	ASP	SER	LYS
ALA	ASP	VAL	VAL	TYR	PRO	PHE	LYS	PRO
LYS	GLU	VAL	GLU	ASN	THR	MET	GLN	ILE
TYR	TYR	GLU	GLU	PRO	LEU	ASN	LEU	GLU
GLN	GLN	ALA	ALA	ARG	SER	GLU	GLN	ARG
GLN	LYS	LYS	LYS	LEU	SER	SER	TYR	LEU
LEU	ARG	ARG	ARG	SER	THR	THR	VAL	ALA
PHE	LEU	LEU	LEU	GLU	PHE	THR	PHE	ALA
GLU	GLU	HIS	HIS	GLU	ASP	ARG	VAL	ALA
ASP	ASP	ARG	ARG	ALA	LEU	VAL	LEU	ALA
LEU	LEU	GLU	GLU	SER	ILE	LEU	VAL	ALA
ARG	ARG	ALA	ALA	GLN	PHE	HIS	PRO	SER
GLY	GLY	LEU	LEU	ALA	LEU	GLU	ARG	SER
GLN	GLN	LYS	LYS	ILE	MET	VAL	GLY	ILE
SER	SER	GLN	GLN	LEU	GLU	MET	GLN	TYR
ASP	ASP	SER	SER	GLU	ASP	GLU	THR	GLU
ALA	ALA	ALA	ALA	VAL	ASP	THR	GLY	ASP
LEU	LEU	ILE	ILE	SER	GLU	LEU	LYS	ILE
LYS	LYS	THR	THR	SER	ALA	SER	GLY	LYS
ASP	ASP	MET	THR	MET	ASP	ILE	SER	LYS
PHE	PHE	ILE	ILE	LYS	ASP	ALA	SER	GLY
GLU	GLU	VAL	VAL	GLY	ARG	ALA	VAL	LEU
ASP	ASP	ASP	ASP	SER	LEU	ILE	GLY	LEU
ALA	ALA	ILE	ILE	GLY	ALA	ILE	LEU	GLN
LEU	LEU	SER	SER	ARG	HIS	ILE	THR	LEU
HIS	HIS	ILE	ILE	GLY	HIS	CYS	ALA	PHE
ALA	ALA	LEU	LEU	MET	GLN	TYR	GLY	GLY
LEU	LEU	THR	THR	VAL	VAL	LEU	VAL	GLY
ALA	ALA	THR	THR	SER	ALA	ASN	MET	THR
ASP	ASP	GLY	GLY	ALA	LEU	ALA	LYS	ARG
ASP	ASP	MET	MET	TYR	THR	ARG	ASP	LYS
TYR	TYR	SER	SER	PRO	THR	THR	PRO	PHE
LEU	LEU	ALA	ALA	GLN	SER	VAL	GLU	THR
THR	THR	THR	THR	LEU	LEU	LEU	ARG	HIS
VAL	VAL	ARG	ARG	GLU	ALA	GLN	GLN	THR
THR	THR	LYS	LYS	SER	GLN	ALA	LEU	GLY
GLY	GLY	ARG	ARG	LEU	MET	ALA	VAL	ARG
LYS	LYS	ILE	ILE	ILE	LYS	ASN	LEU	GLY
GLU	GLU	GLU	GLU	GLU	PRO	VAL	GLN	LYS
VAL	VAL	GLU	GLU	GLU	VAL	GLY	THR	PHE
ARG	ARG	LEU	LEU	SER	GLU	ARG	ALA	ALA
LEU	LEU	ALA	ALA	GLU	LEU	SER	LEU	GLU
LEU	LEU	GLN	GLN	ALA	ASP	GLN	VAL	ASN
LEU	LEU	VAL	VAL	ALA	MET	THR	VAL	VAL
LYS	LYS	VAL	VAL	LYS	ASN	ASN	LEU	ASN
THR	THR	VAL	VAL	VAL	PRO	PRO	SER	ILE
VAL	VAL	ARG	ARG	VAL	LYS	LYS	ASP	LEU
GLN	GLN	PHE	PHE	ARG	LYS	THR	GLY	CYS
LEU	LEU	ILE	ILE	SER	THR	THR	ILE	GLY
GLN	GLN	GLN	GLN	SER	ILE	CYS	ASP	PRO
ASP	ASP	LYS	LYS	LYS	GLU	THR	CYS	PRO

- Molecule 4: DNA replication licensing factor mcm5-A

Chain D:  32% . 65%

[illegible]

- Molecule 4: DNA replication licensing factor mcm5-A

Chain 5: 32% . 65%

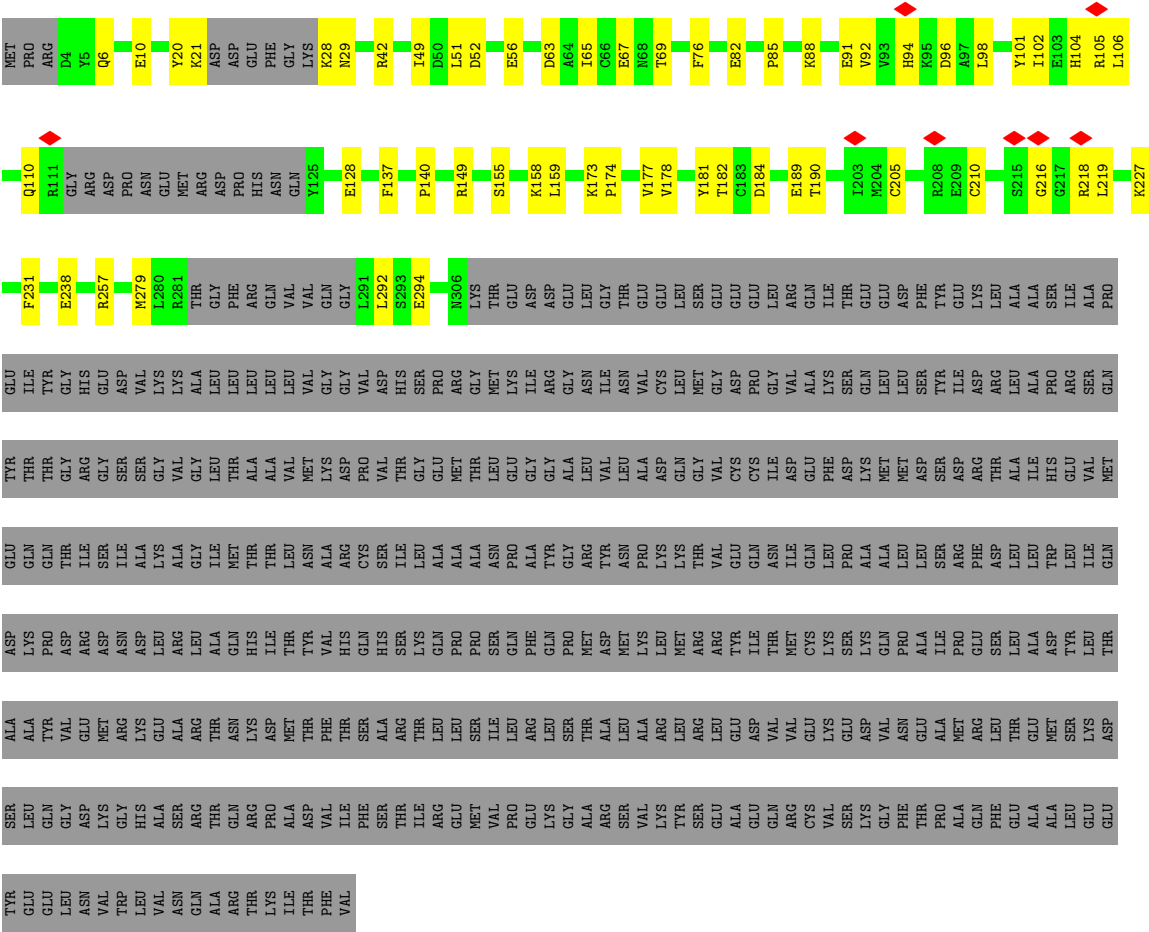
[illegible]

- Molecule 5: Maternal DNA replication licensing factor mcm6

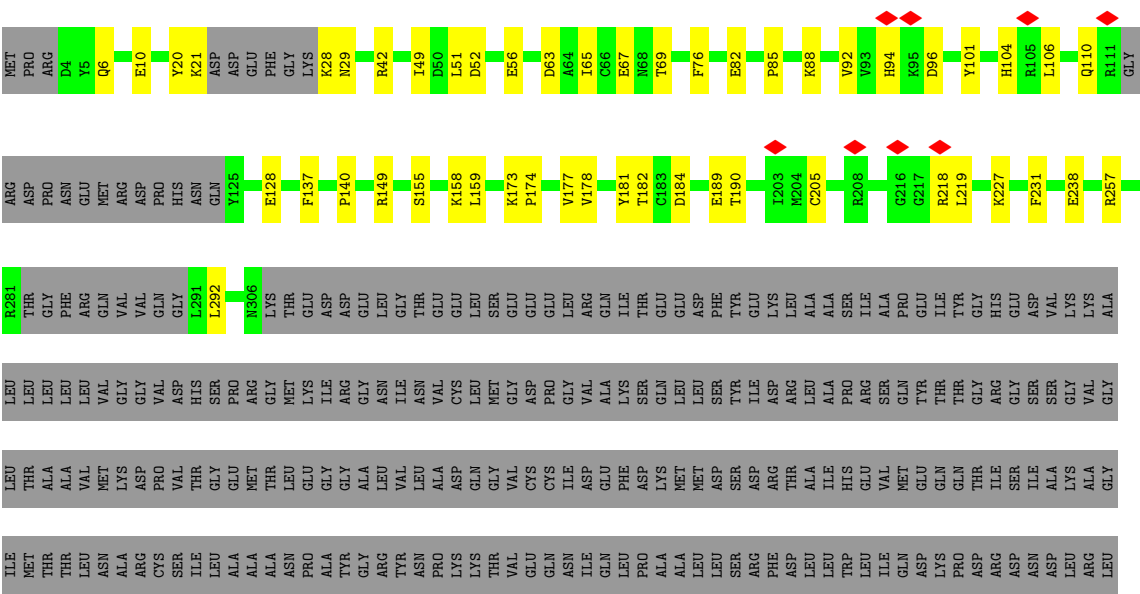
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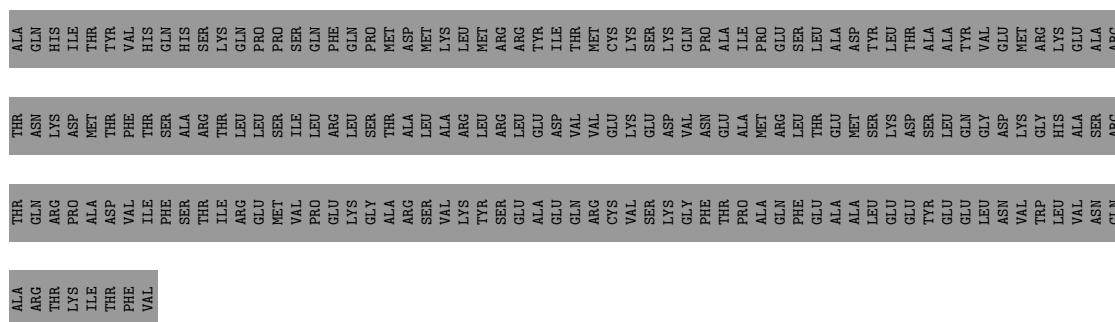
- Molecule 6: DNA replication licensing factor mcm7-B



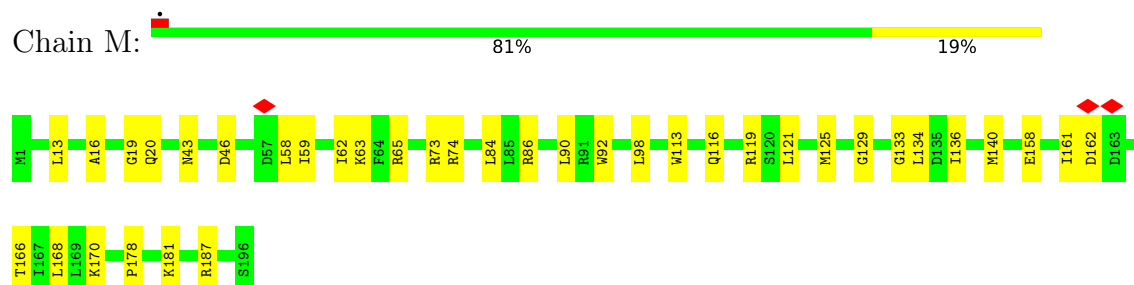


● Molecule 6: DNA replication licensing factor mcm7-B

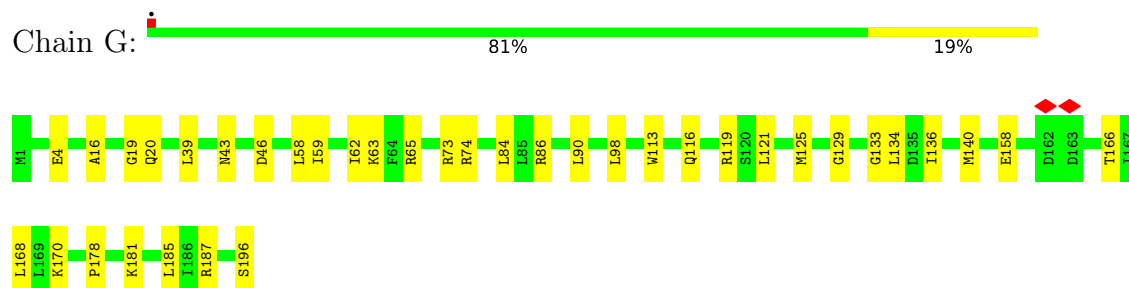




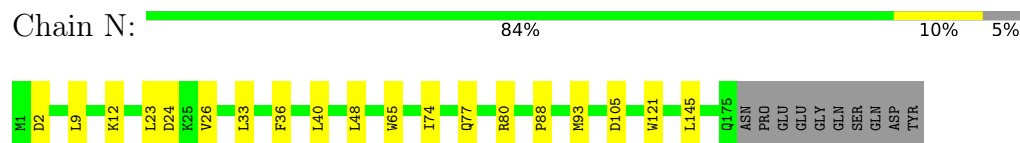
- Molecule 7: DNA replication complex GINS protein PSF1



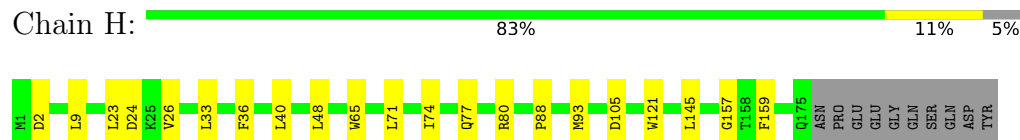
- Molecule 7: DNA replication complex GINS protein PSF1



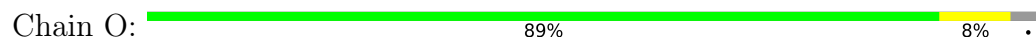
- Molecule 8: DNA replication complex GINS protein PSF2



- Molecule 8: DNA replication complex GINS protein PSF2



- Molecule 9: DNA replication complex GINS protein PSF3





- Molecule 9: DNA replication complex GINS protein PSF3

Chain I: 89% 8% .



- Molecule 10: Cell division control protein 45 homolog

Chain P: 80% 12% 8%



- Molecule 10: Cell division control protein 45 homolog

Chain J: 81% 11% 8%



- Molecule 11: DNA replication complex GINS protein SLD5

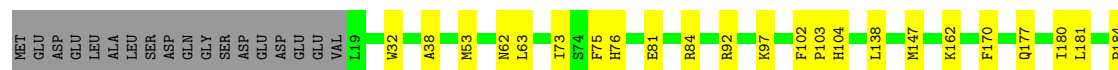
Chain Q: 79% 13% 8%





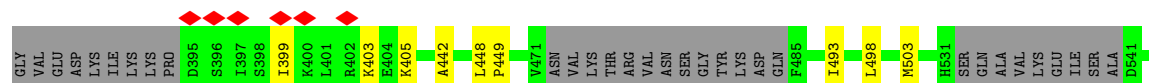
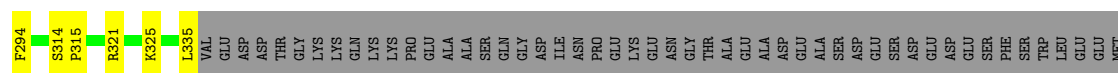
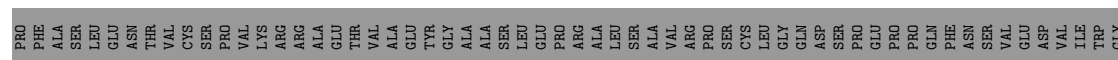
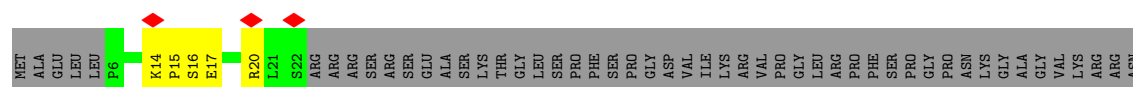
- Molecule 11: DNA replication complex GINS protein SLD5

Chain K: 80% 12% 8%



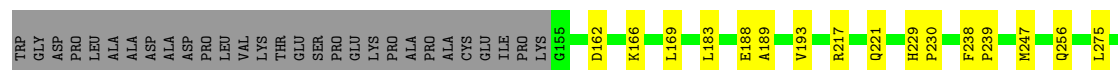
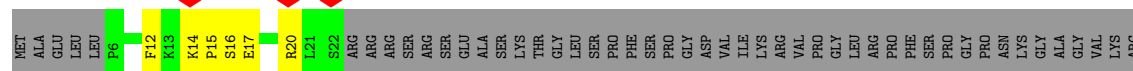
- Molecule 12: Protein downstream neighbor of son homolog

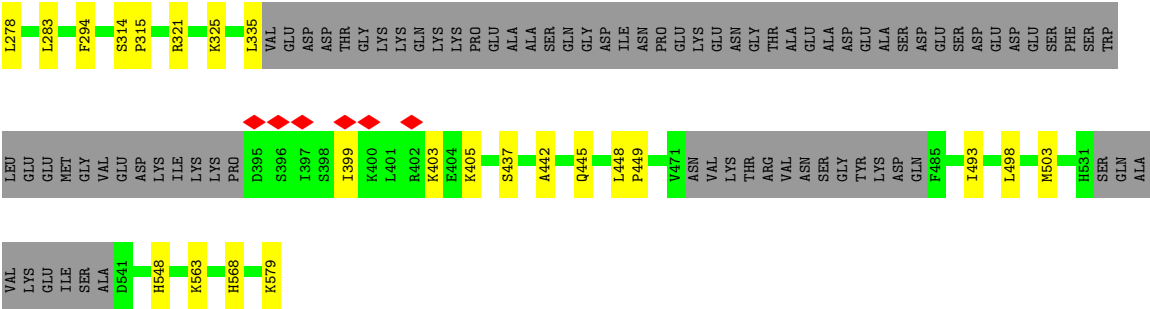
Chain R: 55% 7% 38%



- Molecule 12: Protein downstream neighbor of son homolog

Chain L: 55% 8% 38%





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	0.12	0/2188	0.28	0/2963
1	A	0.12	0/2188	0.29	0/2963
2	3	0.14	0/2101	0.30	0/2834
2	B	0.14	0/2101	0.31	0/2834
3	4	0.10	0/2157	0.27	0/2921
3	C	0.10	0/2157	0.27	0/2921
4	5	0.15	0/2096	0.30	0/2825
4	D	0.15	0/2096	0.30	0/2825
5	6	0.11	0/2033	0.26	0/2747
5	E	0.11	0/2033	0.26	0/2747
6	7	0.11	0/2266	0.28	0/3053
6	F	0.11	0/2266	0.27	0/3053
7	G	0.11	0/1653	0.27	0/2221
7	M	0.11	0/1652	0.27	0/2221
8	H	0.14	0/1448	0.30	0/1964
8	N	0.14	0/1448	0.31	0/1964
9	I	0.14	0/1658	0.31	0/2236
9	O	0.14	0/1658	0.31	0/2236
10	J	0.12	0/4314	0.29	0/5823
10	P	0.12	0/4314	0.30	0/5823
11	K	0.13	0/1690	0.30	0/2280
11	Q	0.13	0/1690	0.29	0/2280
12	L	0.15	0/2904	0.34	0/3938
12	R	0.15	0/2904	0.33	0/3938
All	All	0.13	0/53015	0.29	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	21	0
1	A	2141	0	2124	21	0
2	3	2066	0	2059	19	0
2	B	2066	0	2059	14	0
3	4	2112	0	2090	32	0
3	C	2112	0	2090	32	0
4	5	2059	0	2074	16	0
4	D	2059	0	2074	16	0
5	6	1997	0	1987	22	0
5	E	1997	0	1987	22	0
6	7	2227	0	2232	32	0
6	F	2227	0	2232	38	0
7	G	1623	0	1623	29	0
7	M	1622	0	1623	27	0
8	H	1418	0	1433	18	0
8	N	1418	0	1433	15	0
9	I	1621	0	1589	10	0
9	O	1621	0	1589	11	0
10	J	4233	0	4211	39	0
10	P	4233	0	4211	40	0
11	K	1655	0	1669	22	0
11	Q	1655	0	1669	23	0
12	L	2835	0	2861	30	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	521	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.

All (521) 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
3:4:276:PRO:HB3	6:7:174:PRO:HB3	1.72	0.72
6:F:205:CYS:HB2	6:F:219:LEU:HB3	1.77	0.67
6:F:21:LYS:HB3	6:F:29:ASN:HB3	1.77	0.66
6:7:21:LYS:HB3	6:7:29:ASN:HB3	1.77	0.66
6:7:205:CYS:HB2	6:7:219:LEU:HB3	1.77	0.66
5:6:56:ILE:HA	5:6:106:ILE:HD11	1.78	0.64
7:G:129:GLY:HA3	11:K:53:MET:HE2	1.80	0.64
7:M:129:GLY:HA3	11:Q:53:MET:HE2	1.81	0.63
10:P:288:TYR:HB2	10:P:326:VAL:HG12	1.80	0.62
2:B:18:GLU:HG2	12:R:442:ALA:HB1	1.81	0.62
10:J:475:LEU:HD13	10:J:492:LEU:HB2	1.81	0.62
1:2:310:VAL:HA	1:2:353:THR:HG23	1.82	0.62
2:3:18:GLU:HG2	12:L:442:ALA:HB1	1.83	0.61
4:5:144:GLU:OE1	4:5:144:GLU:N	2.33	0.61
6:7:51:LEU:HD12	6:7:140:PRO:HD3	1.84	0.60
12:L:314:SER:HB3	12:L:315:PRO:HD3	1.84	0.60
5:6:163:CYS:HB3	5:6:187:CYS:SG	2.42	0.60
6:F:51:LEU:HD12	6:F:140:PRO:HD3	1.83	0.59
5:E:163:CYS:HB3	5:E:187:CYS:SG	2.42	0.59
10:J:407:ARG:NH2	4:5:48:ASP:OD1	2.36	0.59
12:R:239:PRO:HB2	12:R:243:VAL:HG21	1.83	0.58
12:R:314:SER:HB3	12:R:315:PRO:HD3	1.84	0.58
4:D:48:ASP:OD1	10:P:407:ARG:NH2	2.36	0.58
7:G:19:GLY:O	7:G:86:ARG:NH1	2.37	0.58
7:G:196:SER:O	4:5:49:ARG:NH1	2.36	0.58
7:M:19:GLY:O	7:M:86:ARG:NH1	2.36	0.58
4:D:144:GLU:N	4:D:144:GLU:OE1	2.33	0.57
1:A:316:LYS:HG2	1:A:340:CYS:HB2	1.86	0.57
2:B:206:GLU:HG3	2:B:207:LYS:HG3	1.86	0.57
6:7:92:VAL:HB	6:7:94:HIS:HD2	1.70	0.56
10:J:300:THR:HG21	10:J:354:MET:HG3	1.88	0.56
5:6:210:ILE:HG12	5:6:228:ILE:HD11	1.87	0.56
12:R:283:LEU:HD13	12:L:193:VAL:HG21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:R:448:LEU:HD12	12:R:449:PRO:HD2	1.86	0.56
2:3:206:GLU:HG3	2:3:207:LYS:HG3	1.86	0.56
12:R:193:VAL:HG21	12:L:283:LEU:HD13	1.86	0.56
11:K:177:GLN:HB2	11:K:180:ILE:HD11	1.87	0.56
6:F:92:VAL:HB	6:F:94:HIS:HD2	1.70	0.56
10:P:300:THR:HG21	10:P:354:MET:HG3	1.88	0.56
1:A:310:VAL:HA	1:A:353:THR:HG23	1.88	0.55
1:2:316:LYS:HG2	1:2:340:CYS:HB2	1.87	0.55
6:7:42:ARG:NH1	6:7:96:ASP:OD2	2.39	0.55
1:A:241:LEU:HD21	1:A:270:ILE:HD11	1.89	0.55
9:I:16:GLU:OE2	9:I:68:LYS:NZ	2.40	0.55
1:2:241:LEU:HD21	1:2:270:ILE:HD11	1.88	0.55
5:E:210:ILE:HG12	5:E:228:ILE:HD11	1.88	0.55
11:Q:177:GLN:HB2	11:Q:180:ILE:HD11	1.88	0.55
6:7:69:THR:HG21	6:7:159:LEU:HB2	1.89	0.55
6:F:42:ARG:NH1	6:F:96:ASP:OD2	2.39	0.55
9:O:16:GLU:OE2	9:O:68:LYS:NZ	2.40	0.54
10:P:120:ARG:HG2	10:P:122:ASP:H	1.71	0.54
10:J:120:ARG:HG2	10:J:122:ASP:H	1.71	0.54
12:R:183:LEU:HA	12:R:217:ARG:HH21	1.73	0.54
1:2:166:THR:HB	1:2:169:GLU:HG3	1.90	0.54
12:L:294:PHE:HB2	12:L:315:PRO:HD2	1.90	0.54
12:L:183:LEU:HA	12:L:217:ARG:HH21	1.73	0.54
5:E:143:VAL:HA	5:E:210:ILE:HG22	1.90	0.53
3:4:216:ARG:HG2	3:4:223:TYR:CG	2.43	0.53
6:F:184:ASP:N	6:F:184:ASP:OD1	2.40	0.53
3:4:154:GLY:HA3	6:7:101:TYR:HD1	1.74	0.53
5:E:230:LEU:HB3	5:E:234:ALA:O	2.09	0.53
5:6:230:LEU:HB3	5:6:234:ALA:O	2.09	0.53
10:P:194:TYR:HB3	10:P:520:LYS:HG2	1.89	0.53
5:6:143:VAL:HA	5:6:210:ILE:HG22	1.90	0.53
6:F:69:THR:HG21	6:F:159:LEU:HB2	1.90	0.53
1:A:166:THR:HB	1:A:169:GLU:HG3	1.90	0.52
4:5:163:ARG:HB2	4:5:225:PHE:HD2	1.74	0.52
3:C:154:GLY:HA3	6:F:101:TYR:HD1	1.74	0.52
12:R:294:PHE:HB2	12:R:315:PRO:HD2	1.90	0.52
3:C:216:ARG:HG2	3:C:223:TYR:CG	2.43	0.52
6:F:181:TYR:HB2	6:F:190:THR:HB	1.90	0.52
10:P:427:ILE:HG22	10:P:461:PHE:HE1	1.74	0.52
3:C:392:GLY:HA2	3:C:419:ILE:HG12	1.92	0.52
10:J:550:LEU:HD21	10:J:555:ARG:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:63:LEU:HD13	11:Q:76:HIS:HB2	1.90	0.52
7:G:90:LEU:HB3	7:G:98:LEU:HD21	1.92	0.52
7:M:46:ASP:HB3	7:M:58:LEU:HD13	1.92	0.52
7:G:46:ASP:HB3	7:G:58:LEU:HD13	1.92	0.52
7:G:73:ARG:HG3	11:K:147:MET:HE2	1.92	0.52
4:D:163:ARG:HB2	4:D:225:PHE:HD2	1.74	0.52
5:E:97:ARG:NH2	5:E:111:GLU:OE2	2.42	0.52
3:4:191:PRO:HB2	3:4:194:MET:HB2	1.91	0.52
6:7:184:ASP:N	6:7:184:ASP:OD1	2.40	0.52
3:C:405:VAL:HG12	3:C:407:ASN:H	1.75	0.51
10:P:256:ARG:HA	10:P:261:GLU:HG3	1.91	0.51
10:P:550:LEU:HD21	10:P:555:ARG:HA	1.91	0.51
11:K:63:LEU:HD13	11:K:76:HIS:HB2	1.92	0.51
3:C:265:ALA:O	3:C:422:ARG:NH1	2.44	0.51
12:R:399:ILE:O	12:R:403:LYS:HG2	2.10	0.51
3:4:405:VAL:HG12	3:4:407:ASN:H	1.75	0.51
5:6:97:ARG:NH2	5:6:111:GLU:OE2	2.43	0.51
1:2:181:TYR:CZ	1:2:185:LYS:HD2	2.46	0.51
6:7:181:TYR:HB2	6:7:190:THR:HB	1.90	0.51
12:L:399:ILE:O	12:L:403:LYS:HG2	2.10	0.51
2:B:252:THR:HG21	4:D:215:ILE:HD11	1.93	0.51
8:H:105:ASP:OD1	8:H:105:ASP:N	2.44	0.51
10:J:427:ILE:HG22	10:J:461:PHE:HE1	1.74	0.51
7:M:73:ARG:HG3	11:Q:147:MET:HE2	1.92	0.51
9:I:149:ASN:HB3	4:5:62:ARG:HG3	1.93	0.51
10:J:194:TYR:HB3	10:J:520:LYS:HG2	1.91	0.51
1:A:179:GLU:O	1:A:183:ARG:HG3	2.11	0.51
6:F:182:THR:HG22	6:F:189:GLU:HG2	1.93	0.50
10:J:256:ARG:HA	10:J:261:GLU:HG3	1.91	0.50
3:4:392:GLY:HA2	3:4:419:ILE:HG12	1.93	0.50
7:M:74:ARG:HH11	9:O:24:LEU:HD13	1.76	0.50
7:M:90:LEU:HB3	7:M:98:LEU:HD21	1.93	0.50
9:O:33:CYS:HB3	9:O:78:LEU:HD11	1.93	0.50
4:D:62:ARG:HG3	9:O:149:ASN:HB3	1.93	0.50
2:3:252:THR:HG21	4:5:215:ILE:HD11	1.93	0.50
1:A:181:TYR:CZ	1:A:185:LYS:HD2	2.46	0.50
11:Q:185:GLU:HG2	11:Q:186:THR:HG23	1.94	0.50
11:K:185:GLU:HG2	11:K:186:THR:HG23	1.94	0.50
1:2:179:GLU:O	1:2:183:ARG:HG3	2.12	0.50
8:N:145:LEU:HD12	11:Q:170:PHE:HE1	1.76	0.50
6:F:20:TYR:HA	6:F:28:LYS:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:154:GLY:HA3	6:7:101:TYR:CD1	2.47	0.50
3:C:191:PRO:HB2	3:C:194:MET:HB2	1.92	0.50
9:O:35:ILE:HD12	9:O:39:PHE:HE2	1.77	0.50
7:G:74:ARG:HH11	9:I:24:LEU:HD13	1.77	0.50
10:J:390:ARG:HH12	10:J:397:ASN:HA	1.77	0.50
6:7:182:THR:HG22	6:7:189:GLU:HG2	1.92	0.50
9:I:33:CYS:HB3	9:I:78:LEU:HD11	1.93	0.49
10:J:219:TRP:HB2	10:J:269:MET:HE1	1.94	0.49
3:C:321:ARG:HH22	6:F:218:ARG:HD3	1.77	0.49
10:P:231:GLN:O	10:P:472:LYS:NZ	2.38	0.49
5:6:29:GLN:HG3	5:6:95:ALA:HB2	1.94	0.49
12:L:568:HIS:HB3	12:L:579:LYS:HB3	1.94	0.49
12:R:568:HIS:HB3	12:R:579:LYS:HB3	1.94	0.49
10:J:277:LEU:HD13	10:J:345:LEU:HD22	1.95	0.49
6:7:20:TYR:HA	6:7:28:LYS:HA	1.93	0.49
7:G:113:TRP:HB2	11:K:138:LEU:HD13	1.95	0.49
1:2:166:THR:HG22	1:2:168:ARG:H	1.77	0.49
3:4:321:ARG:HH22	6:7:218:ARG:HD3	1.77	0.49
9:I:39:PHE:HB3	9:I:42:LEU:HD12	1.94	0.49
1:A:313:ASN:HA	1:A:320:ILE:HA	1.94	0.49
5:E:46:ASN:O	5:E:49:VAL:HG12	2.13	0.49
5:E:218:PRO:HG2	5:E:221:ALA:HB3	1.95	0.49
9:I:35:ILE:HD12	9:I:39:PHE:HE2	1.77	0.49
3:4:265:ALA:O	3:4:422:ARG:NH1	2.45	0.49
3:4:169:PHE:HB2	3:4:218:PHE:CD2	2.48	0.49
5:6:46:ASN:O	5:6:49:VAL:HG12	2.13	0.49
12:L:188:GLU:HA	12:L:221:GLN:HG2	1.95	0.49
1:A:192:VAL:HB	1:A:196:GLY:HA2	1.95	0.49
3:C:169:PHE:HB2	3:C:218:PHE:CD2	2.48	0.49
3:C:301:GLU:HA	3:C:316:GLU:HA	1.95	0.49
11:K:170:PHE:HE1	8:H:145:LEU:HD12	1.77	0.49
1:2:313:ASN:HA	1:2:320:ILE:HA	1.95	0.49
12:L:448:LEU:HD12	12:L:449:PRO:HD2	1.95	0.49
3:C:154:GLY:HA3	6:F:101:TYR:CD1	2.47	0.48
3:C:212:CYS:O	3:C:216:ARG:HG3	2.13	0.48
10:P:390:ARG:HH12	10:P:397:ASN:HA	1.78	0.48
9:I:94:PHE:HE1	9:I:101:VAL:HG21	1.78	0.48
1:A:166:THR:HG22	1:A:168:ARG:H	1.77	0.48
9:O:39:PHE:HB3	9:O:42:LEU:HD12	1.93	0.48
3:4:212:CYS:O	3:4:216:ARG:HG3	2.13	0.48
5:E:29:GLN:HG3	5:E:95:ALA:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:113:TRP:HB2	11:Q:138:LEU:HD13	1.95	0.48
7:M:125:MET:O	7:M:133:GLY:HA3	2.13	0.48
10:P:219:TRP:HB2	10:P:269:MET:HE1	1.94	0.48
11:K:75:PHE:CE1	8:H:48:LEU:HD11	2.49	0.48
10:J:52:VAL:HG12	10:J:61:LEU:HD12	1.96	0.48
9:O:94:PHE:HE1	9:O:101:VAL:HG21	1.78	0.48
10:P:192:TYR:CG	10:P:520:LYS:HB3	2.48	0.48
3:4:303:PHE:HD2	3:4:314:ARG:HH11	1.61	0.48
12:L:17:GLU:HA	12:L:20:ARG:HD2	1.96	0.48
3:C:303:PHE:HD2	3:C:314:ARG:HH11	1.61	0.48
12:R:188:GLU:HA	12:R:221:GLN:HG2	1.95	0.48
2:3:111:VAL:HG21	2:3:116:LEU:HD13	1.95	0.48
5:6:218:PRO:HG2	5:6:221:ALA:HB3	1.95	0.48
7:G:125:MET:O	7:G:133:GLY:HA3	2.13	0.48
10:J:192:TYR:CG	10:J:520:LYS:HB3	2.48	0.48
3:4:301:GLU:HA	3:4:316:GLU:HA	1.95	0.48
4:D:113:ARG:HB3	4:D:114:PRO:HD3	1.96	0.48
10:P:277:LEU:HD13	10:P:345:LEU:HD22	1.95	0.48
11:Q:181:LEU:HD23	11:Q:184:PRO:HB3	1.96	0.48
4:D:156:ILE:HG13	4:D:258:VAL:HG11	1.95	0.48
10:P:52:VAL:HG12	10:P:61:LEU:HD12	1.96	0.47
1:2:192:VAL:HB	1:2:196:GLY:HA2	1.95	0.47
4:5:156:ILE:HG13	4:5:258:VAL:HG11	1.95	0.47
3:C:195:GLN:O	3:C:199:GLU:HG2	2.15	0.47
11:Q:102:PHE:CG	11:Q:103:PRO:HD3	2.49	0.47
11:K:102:PHE:CG	11:K:103:PRO:HD3	2.49	0.47
4:5:113:ARG:HB3	4:5:114:PRO:HD3	1.96	0.47
5:E:90:PRO:O	5:E:94:ARG:HG2	2.14	0.47
11:Q:38:ALA:O	11:Q:97:LYS:NZ	2.40	0.47
12:R:162:ASP:OD2	12:R:166:LYS:NZ	2.38	0.47
4:5:247:GLN:OE1	4:5:273:ARG:NH2	2.47	0.47
2:B:224:ASP:OD1	2:B:224:ASP:N	2.46	0.47
2:B:111:VAL:HG21	2:B:116:LEU:HD13	1.95	0.47
10:P:17:GLU:HG2	10:P:71:TYR:CE2	2.50	0.47
7:G:158:GLU:HB3	7:G:166:THR:HB	1.96	0.47
10:J:423:LEU:O	10:J:427:ILE:HG23	2.15	0.47
1:2:273:LEU:HD12	1:2:274:PRO:HD2	1.96	0.47
2:3:76:PHE:HD2	2:3:100:VAL:HG21	1.80	0.47
5:6:159:LEU:HD21	5:6:164:GLN:HG3	1.97	0.47
5:6:189:ASN:HB3	5:6:193:PHE:CE2	2.50	0.47
8:N:24:ASP:OD1	8:N:24:ASP:N	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:48:LEU:HD11	11:Q:75:PHE:CE1	2.49	0.47
10:P:423:LEU:O	10:P:427:ILE:HG23	2.15	0.47
12:R:17:GLU:HA	12:R:20:ARG:HD2	1.95	0.47
1:2:219:TYR:OH	1:2:230:ALA:O	2.23	0.47
1:2:312:TYR:O	1:2:321:LEU:N	2.44	0.47
10:P:342:ARG:HB3	10:P:358:ARG:HH21	1.79	0.47
12:L:16:SER:O	12:L:20:ARG:HG3	2.15	0.47
7:M:116:GLN:OE1	7:M:119:ARG:NH2	2.48	0.47
7:G:178:PRO:HD2	7:G:181:LYS:HD2	1.97	0.47
11:K:181:LEU:HD23	11:K:184:PRO:HB3	1.96	0.47
2:3:224:ASP:OD1	2:3:224:ASP:N	2.47	0.47
2:B:76:PHE:HD2	2:B:100:VAL:HG21	1.80	0.46
4:D:135:PRO:HB2	4:D:153:PRO:HD3	1.96	0.46
7:M:158:GLU:HB3	7:M:166:THR:HB	1.97	0.46
7:G:121:LEU:O	7:G:125:MET:HG2	2.15	0.46
10:J:342:ARG:HB3	10:J:358:ARG:HH21	1.79	0.46
4:D:247:GLN:OE1	4:D:273:ARG:NH2	2.48	0.46
5:E:52:ALA:HA	5:E:55:LEU:HB2	1.97	0.46
6:F:65:ILE:HD11	6:F:137:PHE:CZ	2.50	0.46
7:M:121:LEU:O	7:M:125:MET:HG2	2.15	0.46
7:G:116:GLN:OE1	7:G:119:ARG:NH2	2.48	0.46
3:4:195:GLN:O	3:4:199:GLU:HG2	2.14	0.46
6:7:6:GLN:O	6:7:10:GLU:HG2	2.15	0.46
5:E:189:ASN:HB3	5:E:193:PHE:CE2	2.49	0.46
8:N:77:GLN:HG3	8:N:80:ARG:HH21	1.80	0.46
10:P:269:MET:HG3	10:P:407:ARG:HH11	1.80	0.46
10:P:427:ILE:HG22	10:P:461:PHE:CE1	2.50	0.46
8:H:77:GLN:HG3	8:H:80:ARG:HH21	1.80	0.46
4:5:135:PRO:HB2	4:5:153:PRO:HD3	1.96	0.46
5:6:97:ARG:NH1	5:6:108:ALA:O	2.48	0.46
7:M:125:MET:HE1	7:M:136:ILE:HB	1.98	0.46
10:P:340:ASN:O	10:P:344:MET:HG2	2.16	0.46
3:4:326:SER:HB2	3:4:335:HIS:H	1.80	0.46
6:F:128:GLU:O	6:F:227:LYS:NZ	2.47	0.46
7:M:59:ILE:HG22	7:M:63:LYS:HE3	1.98	0.46
8:H:2:ASP:OD1	8:H:2:ASP:N	2.47	0.46
1:A:273:LEU:HD12	1:A:274:PRO:HD2	1.96	0.46
6:F:177:VAL:HG12	6:F:178:VAL:HG13	1.98	0.46
6:7:65:ILE:HD11	6:7:137:PHE:CZ	2.50	0.46
6:F:63:ASP:O	6:F:67:GLU:HG2	2.16	0.46
11:K:81:GLU:HG2	11:K:84:ARG:HH22	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:267:LYS:H	3:4:267:LYS:HD2	1.81	0.46
7:G:125:MET:HE1	7:G:136:ILE:HB	1.98	0.46
8:H:93:MET:HG3	8:H:121:TRP:CE3	2.51	0.46
3:4:221:ASP:O	3:4:225:GLN:HG3	2.16	0.46
6:F:6:GLN:O	6:F:10:GLU:HG2	2.15	0.45
8:N:93:MET:HG3	8:N:121:TRP:CE3	2.51	0.45
5:6:90:PRO:O	5:6:94:ARG:HG2	2.15	0.45
3:C:311:PHE:HE2	3:C:329:LYS:HD2	1.81	0.45
5:E:159:LEU:HD21	5:E:164:GLN:HG3	1.97	0.45
10:J:269:MET:HG3	10:J:407:ARG:HH11	1.81	0.45
10:J:427:ILE:HG22	10:J:461:PHE:CE1	2.51	0.45
3:4:311:PHE:HE2	3:4:329:LYS:HD2	1.81	0.45
6:7:63:ASP:O	6:7:67:GLU:HG2	2.17	0.45
1:A:312:TYR:O	1:A:321:LEU:N	2.43	0.45
1:A:317:CYS:SG	1:A:319:PHE:HB3	2.56	0.45
8:N:40:LEU:HD23	8:N:40:LEU:HA	1.84	0.45
10:P:507:MET:HE1	10:P:559:LEU:HD21	1.98	0.45
11:Q:81:GLU:HG2	11:Q:84:ARG:HH22	1.80	0.45
12:R:169:LEU:HD21	12:R:498:LEU:HD13	1.99	0.45
8:H:40:LEU:HD23	8:H:40:LEU:HA	1.84	0.45
6:F:155:SER:HA	6:F:158:LYS:HG3	1.99	0.45
8:N:105:ASP:OD1	8:N:105:ASP:N	2.43	0.45
8:H:23:LEU:HB3	8:H:36:PHE:HD2	1.82	0.45
5:6:31:LEU:HB3	5:6:77:LEU:HD22	1.98	0.45
5:E:166:ILE:HD13	5:E:199:LYS:HZ2	1.81	0.45
10:J:7:ARG:HD2	10:J:209:ILE:HG22	1.98	0.45
10:J:340:ASN:O	10:J:344:MET:HG2	2.16	0.45
1:2:226:GLU:HG3	1:2:229:LEU:HB2	1.99	0.45
1:2:317:CYS:SG	1:2:319:PHE:HB3	2.56	0.45
1:A:226:GLU:HG3	1:A:229:LEU:HB2	1.99	0.45
3:C:200:ILE:HA	3:C:203:VAL:HB	1.99	0.45
5:E:31:LEU:HB3	5:E:77:LEU:HD22	1.98	0.45
7:M:134:LEU:HD11	11:Q:84:ARG:HG3	1.98	0.45
12:R:16:SER:O	12:R:20:ARG:HG3	2.16	0.45
6:7:155:SER:HA	6:7:158:LYS:HG3	1.99	0.45
12:L:162:ASP:OD2	12:L:166:LYS:NZ	2.38	0.45
3:C:267:LYS:H	3:C:267:LYS:HD2	1.81	0.45
3:C:280:ASP:OD1	3:C:395:ARG:NH1	2.50	0.45
3:C:309:CYS:HB3	3:C:331:CYS:HB3	1.99	0.45
12:R:189:ALA:HB1	12:L:278:LEU:HD23	1.99	0.45
8:H:24:ASP:OD1	8:H:24:ASP:N	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:17:GLU:HG2	10:J:71:TYR:CE2	2.52	0.45
3:4:343:ARG:HD3	5:6:87:ARG:HD2	1.99	0.45
10:P:7:ARG:HD2	10:P:209:ILE:HG22	1.98	0.45
10:P:102:ARG:O	10:P:104:ILE:HG13	2.17	0.45
12:R:238:PHE:HB3	12:R:239:PRO:HD3	1.99	0.45
2:3:27:GLN:HG3	12:L:437:SER:HB3	1.99	0.45
3:4:309:CYS:HB3	3:4:331:CYS:HB3	1.99	0.45
12:R:503:MET:HE1	12:R:548:HIS:CE1	2.52	0.45
10:J:108:ASN:HB3	10:J:115:VAL:HG11	1.99	0.45
3:4:280:ASP:OD1	3:4:395:ARG:NH1	2.50	0.44
8:N:23:LEU:HB3	8:N:36:PHE:HD2	1.82	0.44
7:G:59:ILE:HG22	7:G:63:LYS:HE3	1.98	0.44
5:6:105:ASN:OD1	5:6:105:ASN:N	2.49	0.44
12:L:169:LEU:HD21	12:L:498:LEU:HD13	1.99	0.44
12:L:335:LEU:HD13	12:L:563:LYS:HE2	1.98	0.44
3:C:326:SER:HB2	3:C:335:HIS:H	1.82	0.44
7:M:178:PRO:HD2	7:M:181:LYS:HD2	1.98	0.44
10:J:507:MET:HE1	10:J:559:LEU:HD21	1.99	0.44
6:7:177:VAL:HG12	6:7:178:VAL:HG13	1.98	0.44
2:B:25:ASP:O	2:B:30:GLY:HA2	2.17	0.44
10:P:508:VAL:HG23	10:P:547:ILE:HG12	1.98	0.44
7:G:134:LEU:HD11	11:K:84:ARG:HG3	1.99	0.44
3:C:221:ASP:O	3:C:225:GLN:HG3	2.16	0.44
6:F:106:LEU:O	6:F:110:GLN:HG2	2.18	0.44
10:P:192:TYR:HE1	10:P:522:PHE:HD2	1.65	0.44
10:J:508:VAL:HG23	10:J:547:ILE:HG12	1.99	0.44
5:6:52:ALA:HA	5:6:55:LEU:HB2	1.97	0.44
12:L:405:LYS:HD3	12:L:405:LYS:HA	1.69	0.44
12:L:503:MET:HE1	12:L:548:HIS:CE1	2.52	0.44
12:R:278:LEU:HD23	12:L:189:ALA:HB1	1.99	0.44
10:J:102:ARG:O	10:J:104:ILE:HG13	2.17	0.44
7:G:16:ALA:O	7:G:86:ARG:NH2	2.51	0.44
2:3:61:ARG:HA	2:3:61:ARG:HD3	1.67	0.44
12:R:165:LEU:HD23	12:R:165:LEU:HA	1.87	0.44
10:J:306:LEU:HG	10:J:310:LYS:HE3	2.00	0.44
3:4:168:ARG:O	3:4:172:ARG:N	2.40	0.44
1:A:337:CYS:SG	1:A:338:PRO:HD2	2.58	0.44
6:F:82:GLU:O	6:F:85:PRO:HD2	2.18	0.44
10:P:108:ASN:HB3	10:P:115:VAL:HG11	1.99	0.44
12:R:335:LEU:HD13	12:R:563:LYS:HE2	1.98	0.43
7:G:168:LEU:HG	7:G:170:LYS:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:306:LEU:HG	10:P:310:LYS:HE3	2.00	0.43
10:P:475:LEU:HD13	10:P:492:LEU:HB2	1.99	0.43
2:B:106:PHE:HB2	2:B:110:HIS:CD2	2.53	0.43
3:C:238:ASP:OD1	3:C:260:VAL:HG12	2.19	0.43
10:J:559:LEU:O	10:J:563:ILE:HG13	2.19	0.43
2:3:106:PHE:HB2	2:3:110:HIS:CD2	2.53	0.43
7:M:13:LEU:HD23	7:M:13:LEU:HA	1.83	0.43
10:J:266:ILE:HG22	10:J:267:ASP:H	1.83	0.43
3:4:328:CYS:SG	3:4:329:LYS:N	2.91	0.43
3:C:343:ARG:HD3	5:E:87:ARG:HD2	1.99	0.43
6:F:88:LYS:HE3	6:F:92:VAL:HG13	2.00	0.43
3:C:232:GLU:C	3:C:235:PRO:HD2	2.44	0.43
4:D:66:LEU:HD23	4:D:66:LEU:HA	1.78	0.43
10:P:73:VAL:HG22	10:P:96:TYR:HB2	2.00	0.43
7:G:98:LEU:HD23	7:G:98:LEU:HA	1.84	0.43
1:2:337:CYS:SG	1:2:338:PRO:HD2	2.58	0.43
4:5:88:TYR:HB3	4:5:96:HIS:NE2	2.33	0.43
6:F:231:PHE:HD1	6:F:257:ARG:HG2	1.84	0.43
10:P:35:ILE:HG23	10:P:217:MET:HG2	2.00	0.43
10:J:73:VAL:HG22	10:J:96:TYR:HB2	2.00	0.43
3:4:238:ASP:OD1	3:4:260:VAL:HG12	2.18	0.43
6:7:82:GLU:O	6:7:85:PRO:HD2	2.18	0.43
6:7:106:LEU:O	6:7:110:GLN:HG2	2.18	0.43
7:M:16:ALA:O	7:M:86:ARG:NH2	2.51	0.43
3:4:200:ILE:HA	3:4:203:VAL:HB	2.00	0.43
3:4:232:GLU:C	3:4:235:PRO:HD2	2.44	0.43
6:F:49:ILE:HG21	6:F:76:PHE:CE2	2.54	0.43
7:M:46:ASP:OD2	7:M:65:ARG:NH1	2.52	0.43
6:7:49:ILE:HG21	6:7:76:PHE:CE2	2.53	0.43
2:B:65:MET:HE3	2:B:102:PHE:CZ	2.54	0.43
7:M:136:ILE:O	11:Q:92:ARG:NH1	2.52	0.43
10:P:133:ILE:HA	10:P:182:ARG:HD3	2.00	0.43
8:H:74:ILE:HD13	8:H:88:PRO:HD3	2.01	0.43
10:J:11:PHE:O	10:J:15:VAL:HG23	2.19	0.43
10:J:468:CYS:O	10:J:472:LYS:HG3	2.18	0.43
3:4:290:ILE:HG13	3:4:355:GLN:HG3	2.01	0.43
1:A:219:TYR:OH	1:A:230:ALA:O	2.23	0.42
3:C:290:ILE:HG13	3:C:355:GLN:HG3	2.01	0.42
10:P:559:LEU:O	10:P:563:ILE:HG13	2.19	0.42
7:G:84:LEU:HD21	11:K:138:LEU:HD22	2.01	0.42
4:5:83:GLU:CD	4:5:83:GLU:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:176:CYS:HB3	4:5:208:CYS:SG	2.59	0.42
3:C:251:ASP:N	3:C:251:ASP:OD1	2.52	0.42
1:2:374:ARG:HH11	1:2:377:ARG:HH21	1.68	0.42
3:C:328:CYS:SG	3:C:329:LYS:N	2.92	0.42
7:M:20:GLN:NE2	9:O:199:ASN:HB3	2.34	0.42
7:G:20:GLN:NE2	9:I:199:ASN:HB3	2.34	0.42
7:G:39:LEU:HD23	7:G:39:LEU:HA	1.85	0.42
7:G:46:ASP:OD2	7:G:65:ARG:NH1	2.52	0.42
1:2:180:ILE:HG23	1:2:229:LEU:HD21	2.01	0.42
2:3:65:MET:HE3	2:3:102:PHE:CZ	2.53	0.42
2:3:138:ARG:HD2	6:7:292:LEU:HD21	2.01	0.42
6:7:52:ASP:O	6:7:56:GLU:HG3	2.20	0.42
6:7:231:PHE:HD1	6:7:257:ARG:HG2	1.84	0.42
1:A:239:GLU:O	1:A:243:ILE:HG13	2.19	0.42
4:D:88:TYR:HB3	4:D:96:HIS:NE2	2.34	0.42
9:O:200:TYR:HA	9:O:203:ARG:HD3	2.01	0.42
10:P:266:ILE:HG22	10:P:267:ASP:H	1.83	0.42
10:P:468:CYS:O	10:P:472:LYS:HG3	2.19	0.42
11:K:38:ALA:O	11:K:97:LYS:NZ	2.38	0.42
10:J:35:ILE:HG23	10:J:217:MET:HG2	2.01	0.42
10:J:387:ASN:HD22	10:J:390:ARG:HE	1.66	0.42
6:7:128:GLU:O	6:7:227:LYS:NZ	2.47	0.42
4:D:83:GLU:CD	4:D:83:GLU:H	2.27	0.42
5:E:66:ASN:O	5:E:70:ILE:HG13	2.19	0.42
5:E:105:ASN:OD1	5:E:105:ASN:N	2.52	0.42
8:H:65:TRP:CD1	8:H:65:TRP:H	2.37	0.42
12:L:229:HIS:HB3	12:L:230:PRO:HD3	2.02	0.42
6:F:279:MET:HE2	6:F:294:GLU:HB2	2.01	0.42
7:M:84:LEU:HD21	11:Q:138:LEU:HD22	2.01	0.42
11:K:201:GLN:HB2	8:H:145:LEU:O	2.19	0.42
1:2:184:PHE:HD2	1:2:247:ALA:HB3	1.85	0.42
1:A:180:ILE:HG23	1:A:229:LEU:HD21	2.01	0.42
6:F:52:ASP:O	6:F:56:GLU:HG3	2.19	0.42
10:J:60:THR:O	10:J:64:GLU:HG3	2.20	0.42
6:7:149:ARG:HG3	6:7:238:GLU:OE2	2.20	0.42
6:7:205:CYS:HA	6:7:219:LEU:HD13	2.02	0.42
8:N:145:LEU:O	11:Q:201:GLN:HB2	2.19	0.42
10:P:60:THR:O	10:P:64:GLU:HG3	2.19	0.42
11:Q:53:MET:HE3	11:Q:53:MET:HB3	1.89	0.42
12:R:166:LYS:HB2	12:R:493:ILE:HB	2.02	0.42
10:J:192:TYR:HE1	10:J:522:PHE:HD2	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:14:LYS:HG3	12:L:15:PRO:HD2	2.01	0.42
6:F:98:LEU:HD23	6:F:98:LEU:HA	1.92	0.42
6:F:205:CYS:HA	6:F:219:LEU:HD13	2.02	0.42
8:N:65:TRP:H	8:N:65:TRP:CD1	2.37	0.42
1:A:184:PHE:HD2	1:A:247:ALA:HB3	1.85	0.41
1:A:374:ARG:HH11	1:A:377:ARG:HH21	1.68	0.41
3:C:154:GLY:HA2	6:F:104:HIS:HB2	2.01	0.41
5:E:217:LEU:HD21	5:E:223:PRO:HB3	2.01	0.41
8:N:74:ILE:HD13	8:N:88:PRO:HD3	2.01	0.41
12:R:229:HIS:HB3	12:R:230:PRO:HD3	2.01	0.41
11:K:32:TRP:HZ3	8:H:9:LEU:HD21	1.85	0.41
9:I:200:TYR:HA	9:I:203:ARG:HD3	2.01	0.41
3:4:251:ASP:OD1	3:4:251:ASP:N	2.52	0.41
4:5:107:VAL:O	4:5:111:VAL:HG23	2.20	0.41
5:6:66:ASN:O	5:6:70:ILE:HG13	2.19	0.41
4:D:176:CYS:HB3	4:D:208:CYS:SG	2.60	0.41
6:F:65:ILE:O	6:F:69:THR:HG22	2.20	0.41
7:M:168:LEU:HG	7:M:170:LYS:HG3	2.02	0.41
8:N:2:ASP:N	8:N:2:ASP:OD1	2.47	0.41
10:P:411:ASP:O	10:P:415:THR:HG23	2.19	0.41
1:2:239:GLU:O	1:2:243:ILE:HG13	2.19	0.41
2:3:10:HIS:NE2	12:L:256:GLN:OE1	2.49	0.41
10:P:11:PHE:O	10:P:15:VAL:HG23	2.20	0.41
7:G:136:ILE:O	11:K:92:ARG:NH1	2.52	0.41
8:H:71:LEU:HD23	8:H:71:LEU:HA	1.88	0.41
10:J:411:ASP:O	10:J:415:THR:HG23	2.19	0.41
2:B:90:THR:O	2:B:94:GLN:HG3	2.20	0.41
4:D:257:LYS:HE2	4:D:257:LYS:HB3	1.78	0.41
5:E:97:ARG:NH1	5:E:108:ALA:O	2.53	0.41
6:F:149:ARG:HG3	6:F:238:GLU:OE2	2.19	0.41
8:N:9:LEU:HD21	11:Q:32:TRP:HZ3	1.86	0.41
8:N:12:LYS:HB3	8:N:12:LYS:HE2	1.84	0.41
5:6:124:LYS:HE3	5:6:124:LYS:HB2	1.89	0.41
6:7:88:LYS:HE3	6:7:92:VAL:HG13	2.02	0.41
12:L:275:LEU:HD12	12:L:275:LEU:HA	1.92	0.41
7:G:140:MET:SD	7:G:187:ARG:NH1	2.93	0.41
2:3:162:LEU:HD11	2:3:169:PRO:HD3	2.03	0.41
4:5:61:LYS:HB2	4:5:111:VAL:HG11	2.02	0.41
5:6:217:LEU:HD21	5:6:223:PRO:HB3	2.01	0.41
12:R:14:LYS:HG3	12:R:15:PRO:HD2	2.02	0.41
12:R:321:ARG:O	12:R:325:LYS:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:104:HIS:NE2	11:K:162:LYS:HG2	2.36	0.41
8:H:26:VAL:HB	8:H:33:LEU:HB2	2.02	0.41
2:3:90:THR:O	2:3:94:GLN:HG3	2.20	0.41
2:3:162:LEU:HD21	2:3:169:PRO:HB3	2.03	0.41
4:D:61:LYS:HB2	4:D:111:VAL:HG11	2.02	0.41
7:G:43:ASN:OD1	7:G:62:ILE:HA	2.21	0.41
11:K:62:ASN:OD1	12:L:12:PHE:HA	2.20	0.41
2:3:25:ASP:O	2:3:30:GLY:HA2	2.20	0.41
6:7:65:ILE:O	6:7:69:THR:HG22	2.20	0.41
12:L:321:ARG:O	12:L:325:LYS:HG3	2.21	0.41
2:B:138:ARG:HB2	6:F:292:LEU:HD11	2.03	0.41
2:B:142:MET:HG2	2:B:194:LYS:HG2	2.02	0.41
9:O:35:ILE:HD12	9:O:39:PHE:CE2	2.56	0.41
9:O:40:PRO:HA	9:O:53:SER:HB3	2.03	0.41
7:G:84:LEU:HD11	11:K:138:LEU:HD22	2.03	0.41
8:H:93:MET:HE3	8:H:93:MET:HB3	1.92	0.41
8:H:157:GLY:C	8:H:159:PHE:H	2.28	0.41
1:2:392:LYS:HE2	1:2:392:LYS:HB3	1.84	0.41
2:3:146:HIS:CE1	2:3:186:THR:HG22	2.56	0.41
5:6:85:TYR:HD2	5:6:249:THR:HB	1.85	0.41
12:L:166:LYS:HB2	12:L:493:ILE:HB	2.03	0.41
2:B:61:ARG:HD3	2:B:61:ARG:HA	1.85	0.41
3:C:328:CYS:HA	3:C:337:MET:HE2	2.03	0.41
7:M:43:ASN:OD1	7:M:62:ILE:HA	2.21	0.41
7:M:92:TRP:O	7:M:187:ARG:NH2	2.54	0.41
7:M:98:LEU:HD23	7:M:98:LEU:HA	1.85	0.41
7:M:140:MET:SD	7:M:187:ARG:NH1	2.94	0.41
8:N:26:VAL:HB	8:N:33:LEU:HB2	2.03	0.41
2:3:199:LEU:HD13	2:3:219:ILE:HD11	2.02	0.41
3:4:154:GLY:HA2	6:7:104:HIS:HB2	2.01	0.41
12:L:247:MET:HE3	12:L:445:GLN:HG2	2.02	0.41
2:B:138:ARG:HD2	6:F:292:LEU:HD21	2.01	0.41
3:C:341:HIS:H	3:C:341:HIS:HD1	1.69	0.41
10:P:387:ASN:HD22	10:P:390:ARG:HE	1.67	0.41
11:Q:104:HIS:NE2	11:Q:162:LYS:HG2	2.36	0.41
8:H:48:LEU:HD12	8:H:48:LEU:HA	1.83	0.41
9:I:40:PRO:HA	9:I:53:SER:HB3	2.03	0.41
2:3:142:MET:HG2	2:3:194:LYS:HG2	2.03	0.41
5:E:93:CYS:O	5:E:96:VAL:HG12	2.21	0.40
5:E:147:HIS:ND1	5:E:207:LYS:O	2.54	0.40
10:P:71:TYR:CD1	10:P:94:ILE:HB	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:185:LEU:HD23	7:G:185:LEU:HA	1.91	0.40
10:J:393:LYS:HB3	10:J:396:ASP:HB2	2.04	0.40
3:C:302:ALA:N	3:C:315:VAL:O	2.54	0.40
6:F:102:ILE:HG12	6:F:105:ARG:HH22	1.86	0.40
11:Q:56:LEU:O	11:Q:60:GLU:HG3	2.22	0.40
11:Q:143:ALA:O	11:Q:147:MET:HG2	2.21	0.40
12:R:405:LYS:HD3	12:R:405:LYS:HA	1.69	0.40
1:2:215:LEU:HD12	1:2:216:PRO:HD2	2.03	0.40
4:5:173:CYS:SG	4:5:176:CYS:N	2.89	0.40
6:7:173:LYS:HB2	6:7:173:LYS:HE3	1.85	0.40
4:D:107:VAL:O	4:D:111:VAL:HG23	2.21	0.40
12:R:188:GLU:O	12:R:192:LEU:HG	2.22	0.40
11:K:53:MET:HE3	11:K:53:MET:HB3	1.89	0.40
10:J:71:TYR:CD1	10:J:94:ILE:HB	2.56	0.40
3:4:302:ALA:N	3:4:315:VAL:O	2.54	0.40
12:L:169:LEU:HD13	12:L:493:ILE:HG13	2.04	0.40
6:F:210:CYS:HB3	6:F:216:GLY:HA2	2.04	0.40
10:P:295:CYS:HB2	10:P:473:TYR:CE2	2.57	0.40
11:Q:19:LEU:HD23	11:Q:19:LEU:HA	1.92	0.40
7:G:4:GLU:H	7:G:4:GLU:HG2	1.71	0.40
10:J:277:LEU:HD21	10:J:342:ARG:HG2	2.03	0.40
1:A:215:LEU:HD12	1:A:216:PRO:HD2	2.03	0.40
1:A:241:LEU:HD23	1:A:241:LEU:HA	1.90	0.40
5:E:84:GLU:HB3	5:E:87:ARG:HB2	2.03	0.40
6:F:88:LYS:HE2	6:F:91:GLU:HA	2.03	0.40
6:F:173:LYS:HE3	6:F:173:LYS:HB2	1.85	0.40
7:M:161:ILE:HG22	7:M:162:ASP:H	1.85	0.40
12:R:169:LEU:HD13	12:R:493:ILE:HG13	2.03	0.40
10:J:205:GLU:O	10:J:209:ILE:HG12	2.20	0.40
3:4:203:VAL:HG12	3:4:205:ASP:H	1.87	0.40
5:6:147:HIS:ND1	5:6:207:LYS:O	2.54	0.40
12:L:238:PHE:HB3	12:L:239:PRO:HD3	2.02	0.40

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
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 ⓘ

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%)	230 (100%)	1 (0%)	84	84
2	B	231/701 (33%)	230 (100%)	1 (0%)	84	84
3	4	240/761 (32%)	240 (100%)	0	100	100
3	C	240/761 (32%)	240 (100%)	0	100	100
4	5	225/627 (36%)	225 (100%)	0	100	100
4	D	225/627 (36%)	225 (100%)	0	100	100
5	6	219/712 (31%)	219 (100%)	0	100	100
5	E	219/712 (31%)	219 (100%)	0	100	100
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%)	159 (100%)	0	100	100
8	N	159/168 (95%)	159 (100%)	0	100	100
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%)	478 (100%)	0	100	100
10	P	478/515 (93%)	478 (100%)	0	100	100
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%)	317 (100%)	0	100	100
12	R	317/499 (64%)	317 (100%)	0	100	100
All	All	5784/11876 (49%)	5782 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	217	VAL
2	3	217	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	341	GLN
1	A	364	GLN
3	C	209	ASN
3	C	259	GLN
3	C	383	GLN
4	D	98	GLN
4	D	172	GLN
4	D	178	ASN
4	D	301	GLN
5	E	75	GLN
5	E	82	GLN
6	F	110	GLN
6	F	192	GLN
6	F	195	GLN
6	F	211	GLN
7	M	20	GLN
7	M	115	ASN
8	N	14	GLN
9	O	198	GLN
10	P	68	GLN
10	P	284	HIS
10	P	293	ASN
10	P	484	ASN
11	Q	146	HIS
11	Q	189	GLN
7	G	115	ASN
11	K	146	HIS
11	K	189	GLN
8	H	14	GLN
9	I	198	GLN
10	J	121	GLN
10	J	284	HIS
10	J	293	ASN
10	J	428	GLN
10	J	484	ASN
1	2	341	GLN
1	2	364	GLN

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Mol	Chain	Res	Type
3	4	209	ASN
3	4	259	GLN
3	4	383	GLN
4	5	98	GLN
4	5	172	GLN
4	5	178	ASN
4	5	301	GLN
5	6	75	GLN
5	6	82	GLN
6	7	110	GLN
6	7	192	GLN
6	7	195	GLN
6	7	211	GLN
6	7	269	HIS

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 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.

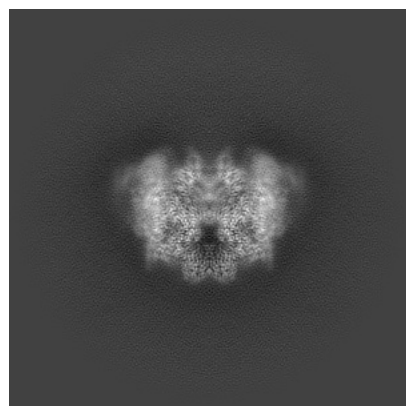
6 Map visualisation [i](#)

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.

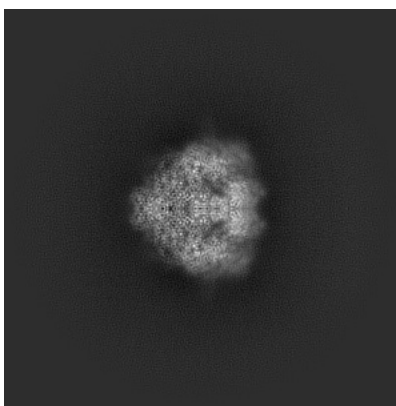
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

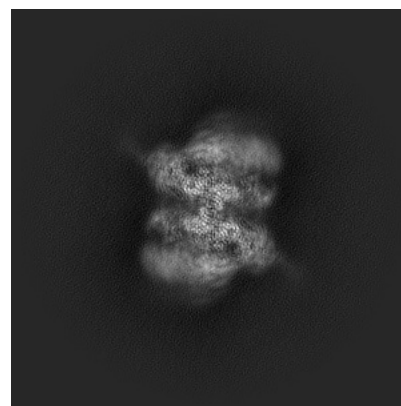
6.1.1 Primary map



X

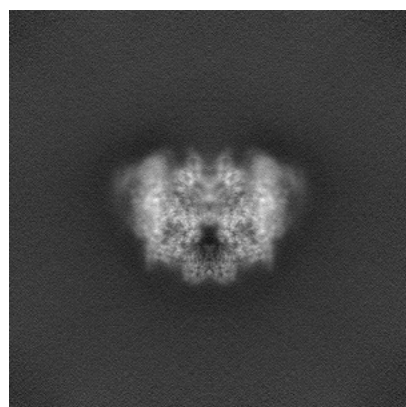


Y

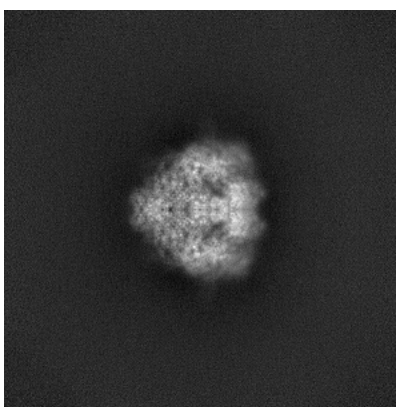


Z

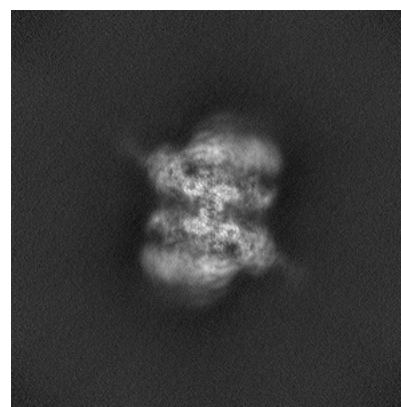
6.1.2 Raw map



X



Y

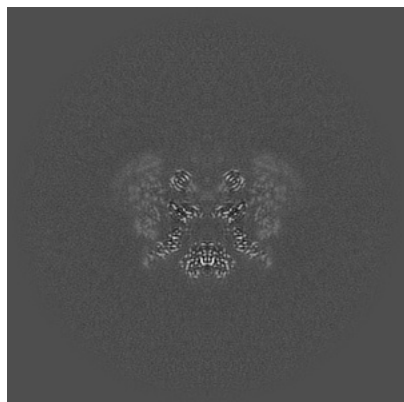


Z

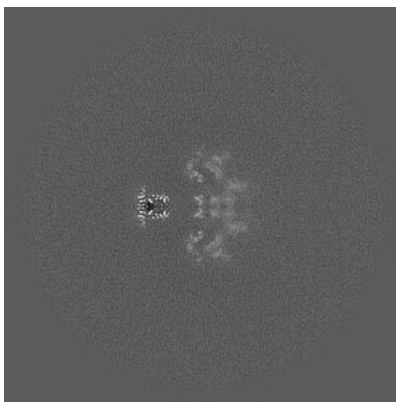
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

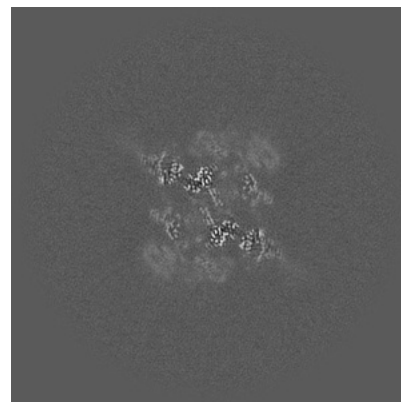
6.2.1 Primary map



X Index: 270

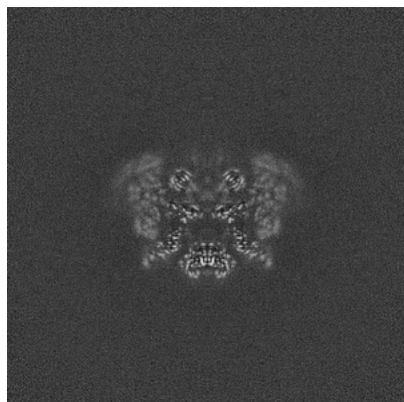


Y Index: 270

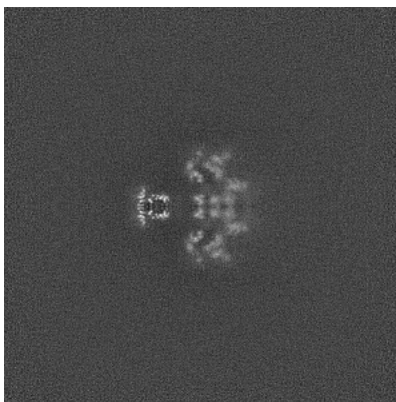


Z Index: 270

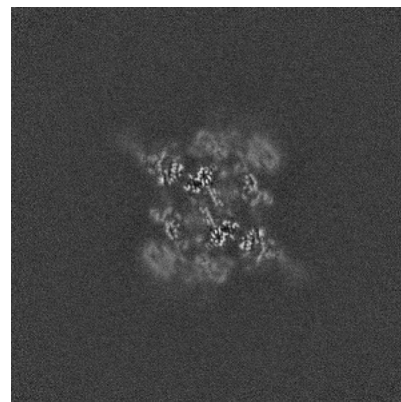
6.2.2 Raw map



X Index: 270



Y Index: 270

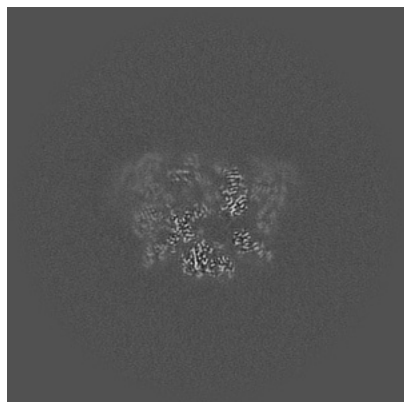


Z Index: 270

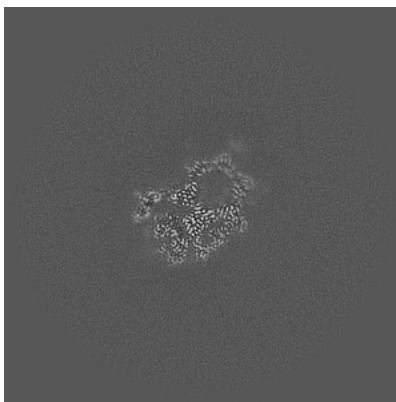
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

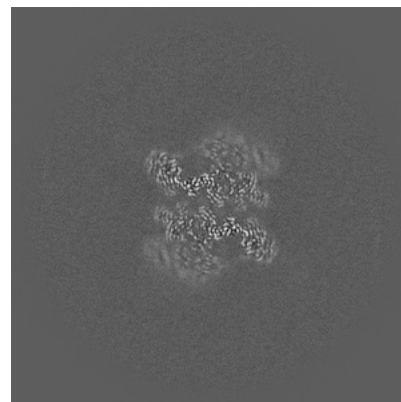
6.3.1 Primary map



X Index: 263

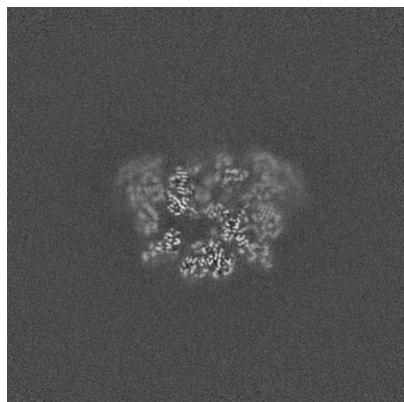


Y Index: 303

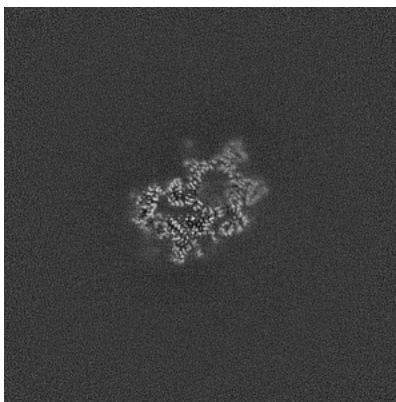


Z Index: 260

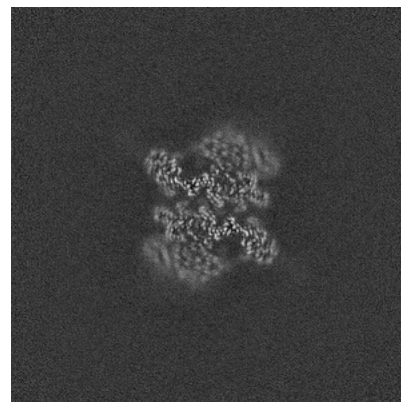
6.3.2 Raw map



X Index: 276



Y Index: 297

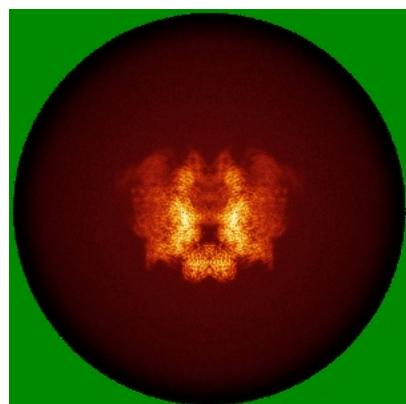


Z Index: 260

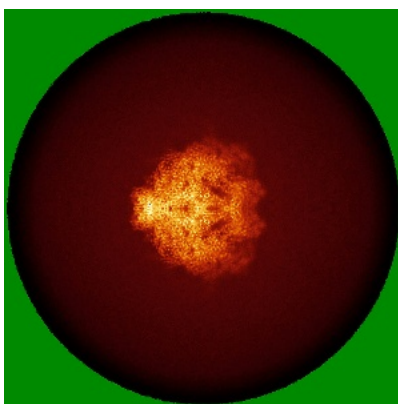
The images above show the largest variance slices of the map in three orthogonal directions.

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

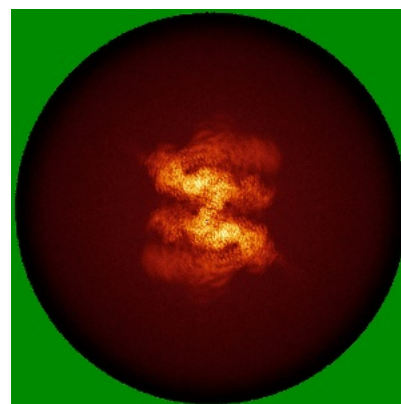
6.4.1 Primary map



X

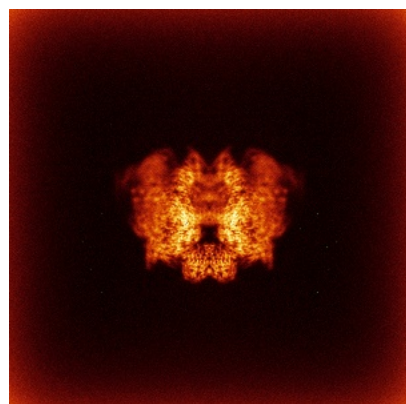


Y

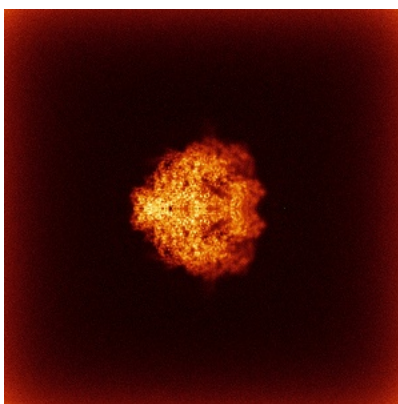


Z

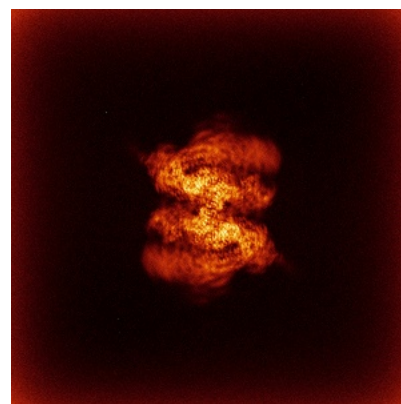
6.4.2 Raw map



X



Y

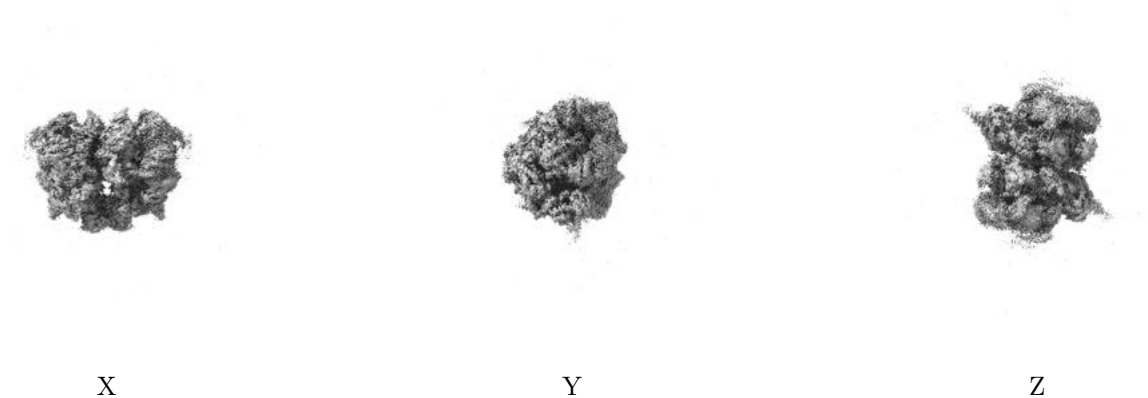


Z

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.

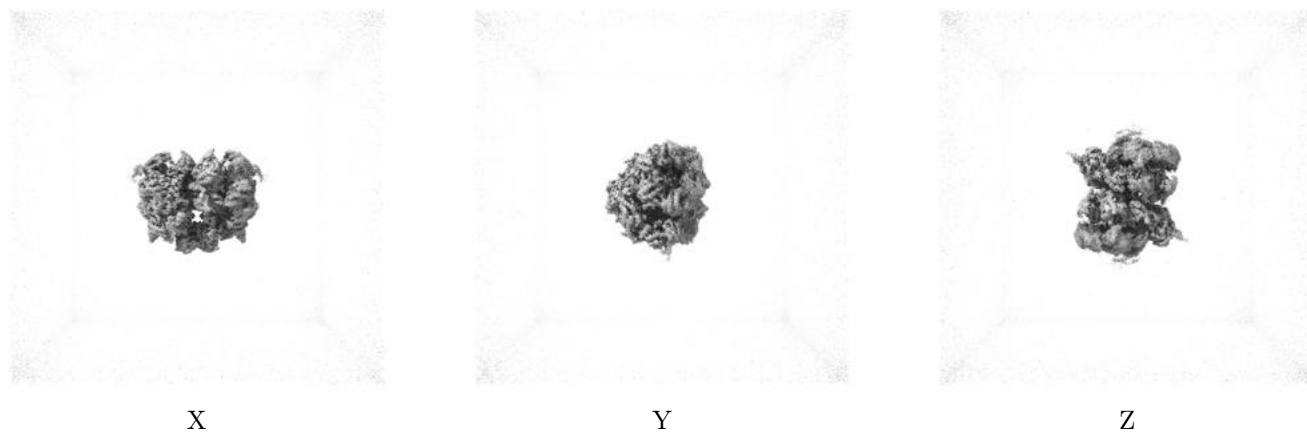
6.5 Orthogonal surface views [i](#)

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.

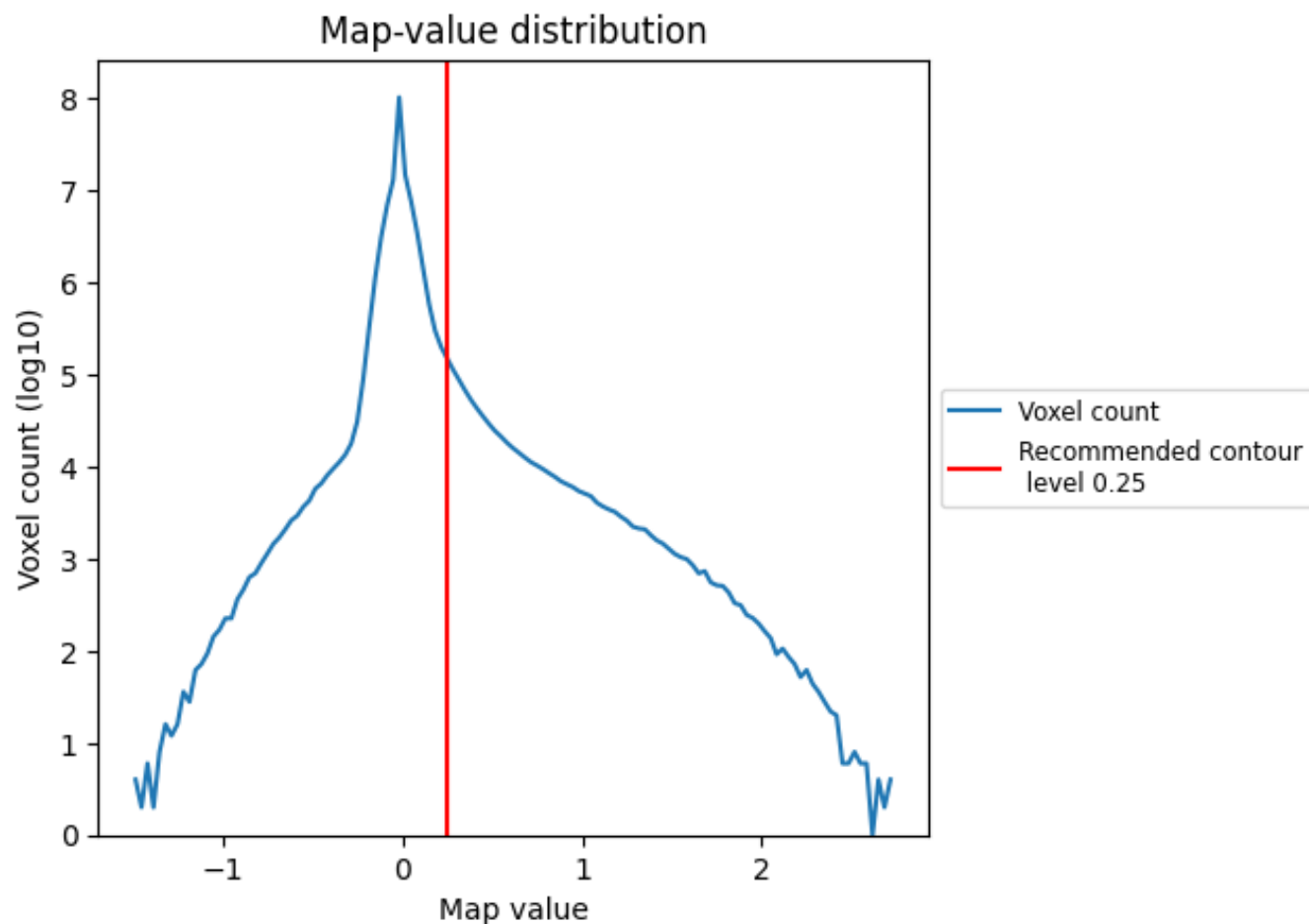
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

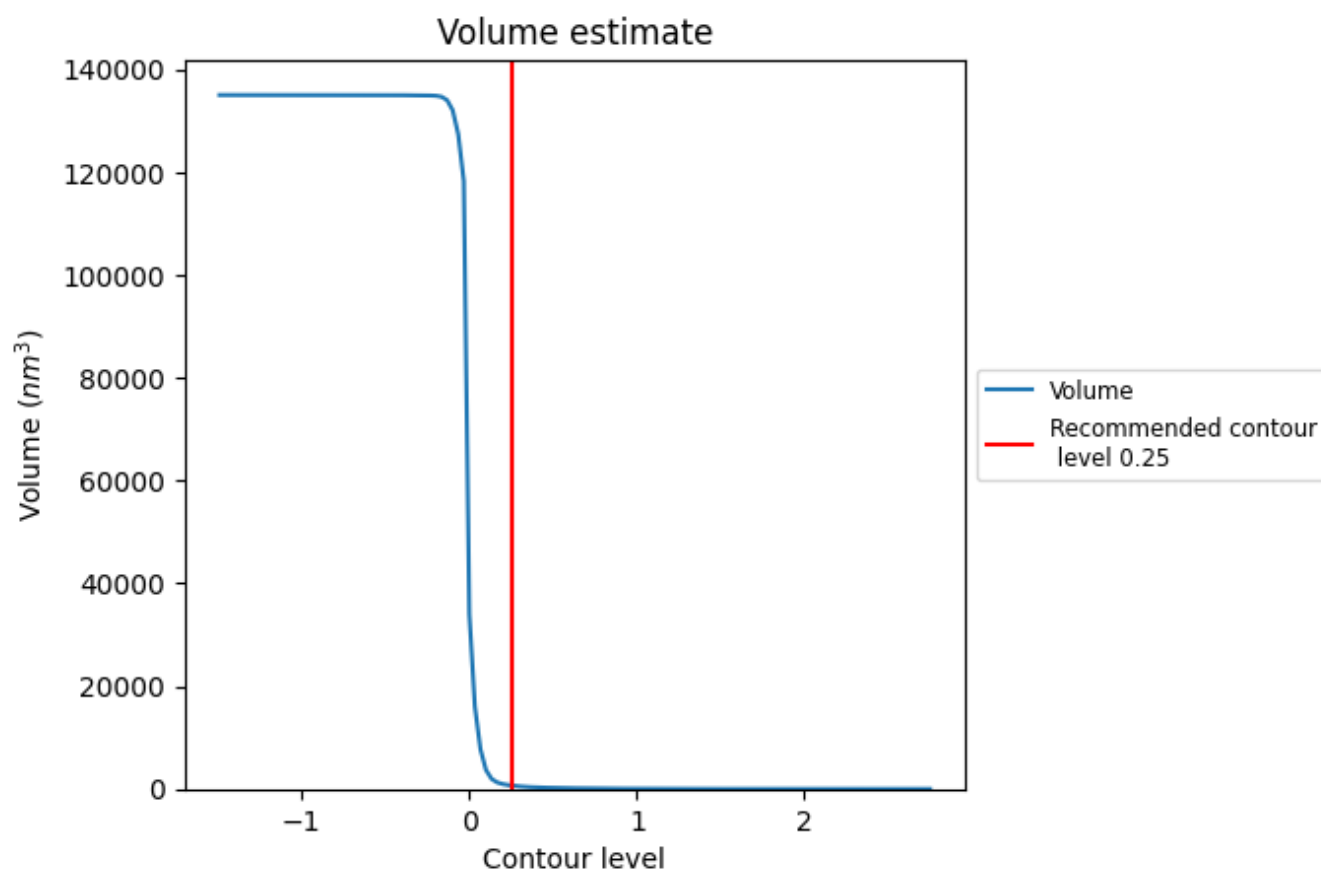
This section contains the results of statistical analysis of the map.

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.

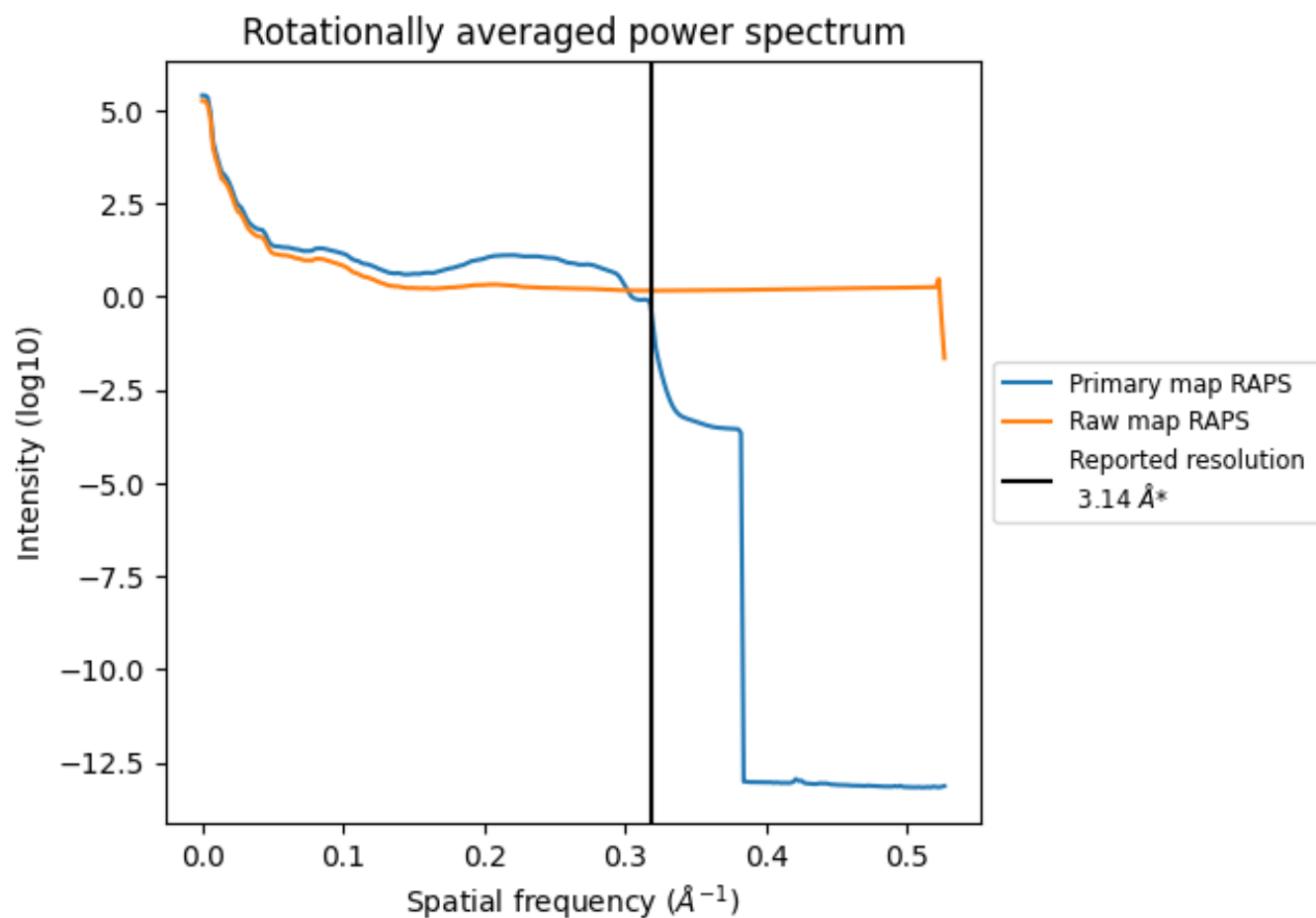
7.2 Volume estimate [i](#)



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 ⓘ

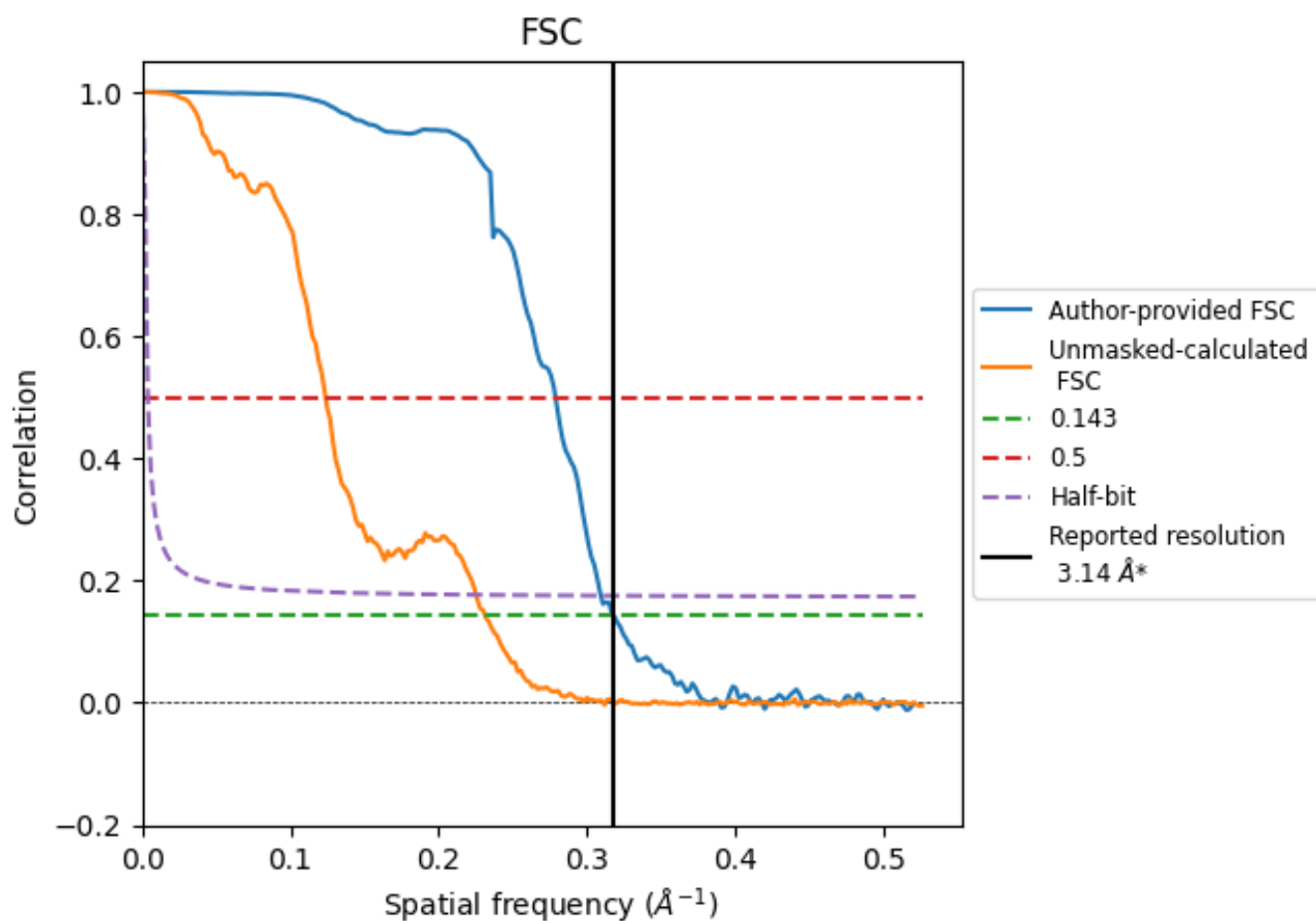


*Reported resolution corresponds to spatial frequency of 0.318 Å⁻¹

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 $\text{\AA}^{-1}$

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 %

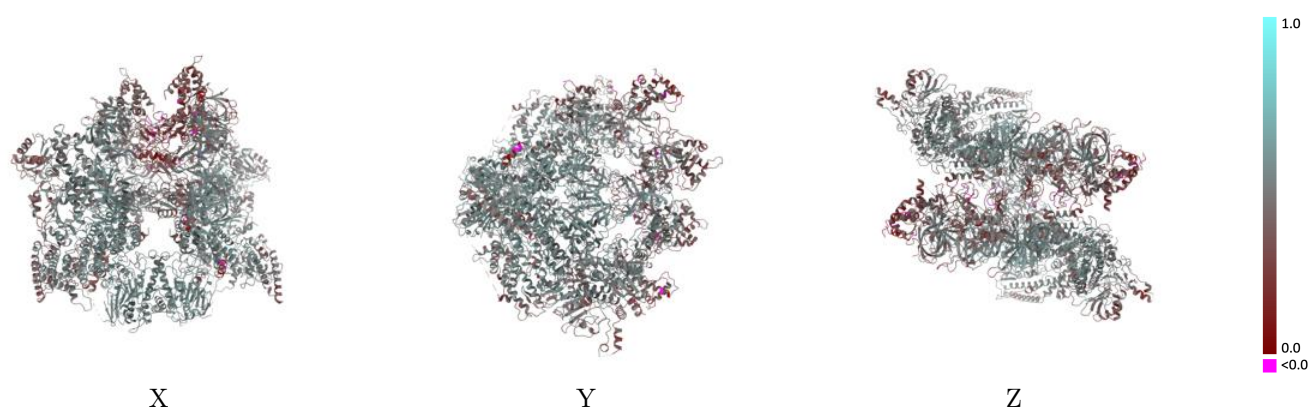
9 Map-model fit [i](#)

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](#)

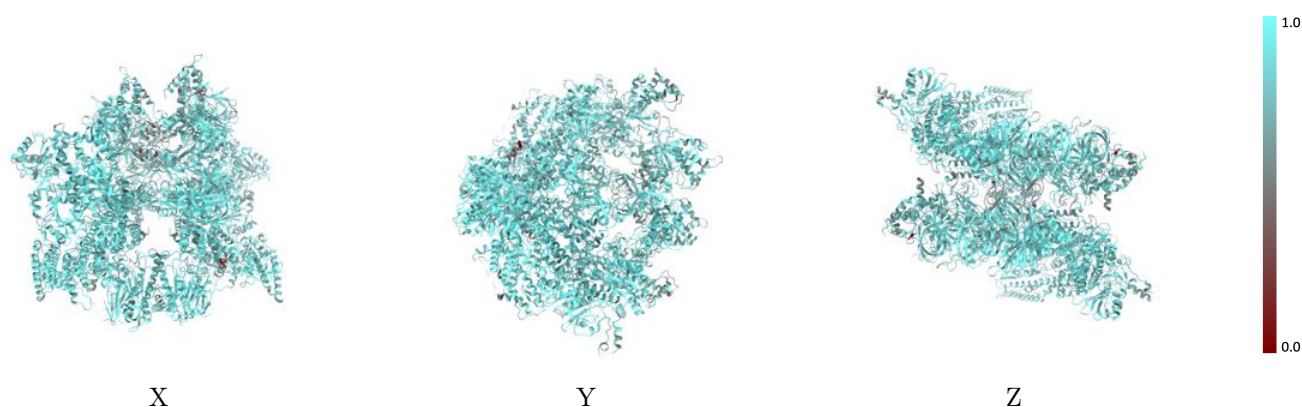
This section was not generated.

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



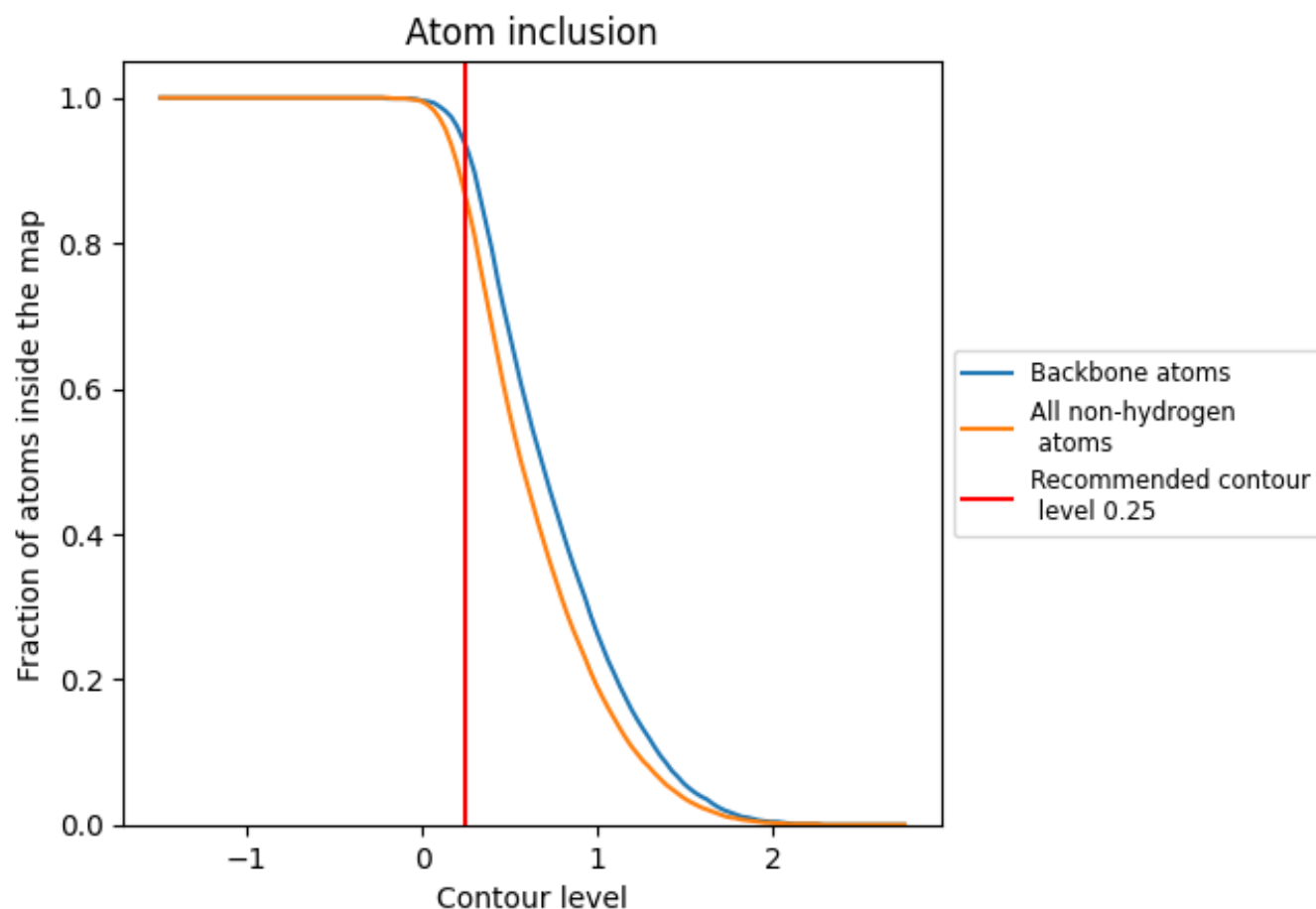
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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	 0.4670
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

