



Full wwPDB EM Validation Report ⓘ

May 29, 2025 – 05:06 pm BST

PDB ID : 9H2B / pdb_00009h2b
EMDB ID : EMD-51792
Title : AcMNPV basal cap - C14 anchor complex only
Authors : Effantin, G.; Kandiah, E.; Pelosse, M.
Deposited on : 2024-10-11
Resolution : 4.10 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.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.43.1

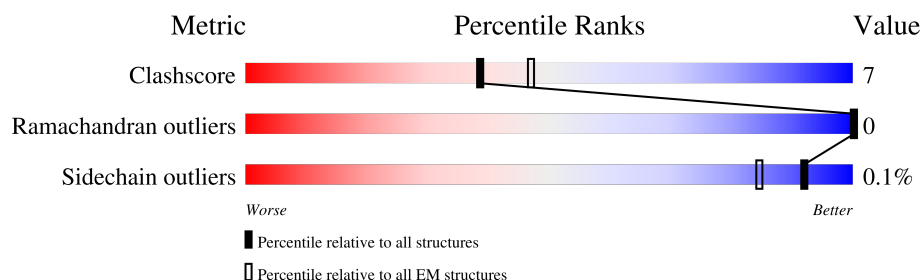
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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	A	290	
1	B	290	
2	C	361	
2	D	361	
3	E	320	
4	F	477	
5	G	347	
5	H	347	

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Mol	Chain	Length	Quality of chain
5	M	347	<div><div><div></div><div></div><div></div></div><div>6%58%13%29%</div></div>
5	N	347	<div><div><div></div><div></div><div></div></div><div>64%15%21%</div></div>
6	I	691	<div><div><div></div><div></div><div></div></div><div>27%69%</div></div>
6	J	691	<div><div><div></div><div></div><div></div></div><div>20%6%75%</div></div>
6	K	691	<div><div><div></div><div></div><div></div></div><div>22%75%</div></div>
7	L	390	<div><div><div></div><div></div><div></div></div><div>77%13%9%</div></div>

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 29762 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 Occlusion-derived virus envelope protein E27.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	246	Total	C	N	O	S	0	0
			1991	1276	324	382	9		
1	B	203	Total	C	N	O	S	0	0
			1649	1068	263	310	8		

- Molecule 2 is a protein called Protein C42.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	216	Total	C	N	O	S	0	0
			1790	1135	305	334	16		
2	D	201	Total	C	N	O	S	0	0
			1677	1065	286	312	14		

- Molecule 3 is a protein called Uncharacterized 38.0 kDa protein in P143-LEF5 intergenic region.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	299	Total	C	N	O	S	0	0
			2526	1648	413	451	14		

- Molecule 4 is a protein called Protein AC142.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	461	Total	C	N	O	S	0	0
			3792	2468	619	682	23		

- Molecule 5 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	275	Total	C	N	O	S	0	0
			2213	1397	388	413	15		
5	H	283	Total	C	N	O	S	0	0
			2274	1434	398	427	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	248	Total	C	N	O	S	0	0
			2008	1280	337	379	12		
5	N	275	Total	C	N	O	S	0	0
			2226	1413	384	417	12		

- Molecule 6 is a protein called Capsid-associated protein VP80.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	215	Total	C	N	O	S	0	0
			1802	1168	301	319	14		
6	J	176	Total	C	N	O	S	0	0
			1462	947	242	261	12		
6	K	176	Total	C	N	O	S	0	0
			1468	956	243	257	12		

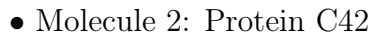
- Molecule 7 is a protein called Protein AC109.

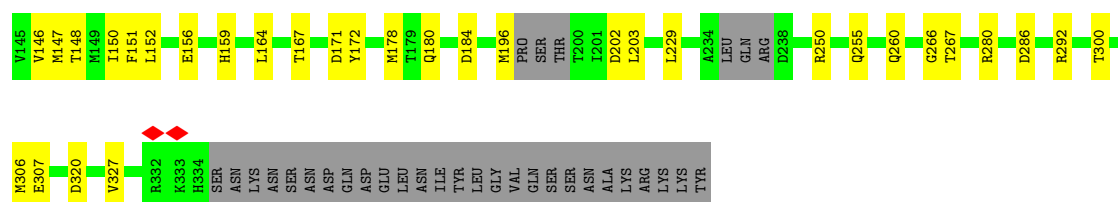
Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	353	Total	C	N	O	S	0	0
			2880	1861	480	523	16		

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
8	G	1	Total	Zn	0
			1	1	
8	H	1	Total	Zn	0
			1	1	
8	M	1	Total	Zn	0
			1	1	
8	N	1	Total	Zn	0
			1	1	

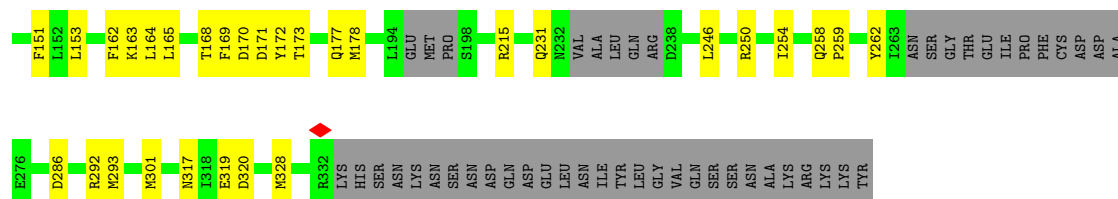
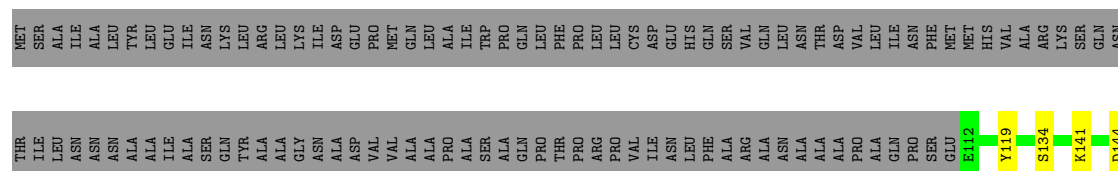
- Molecule 1: Occlusion-derived virus envelope protein E27





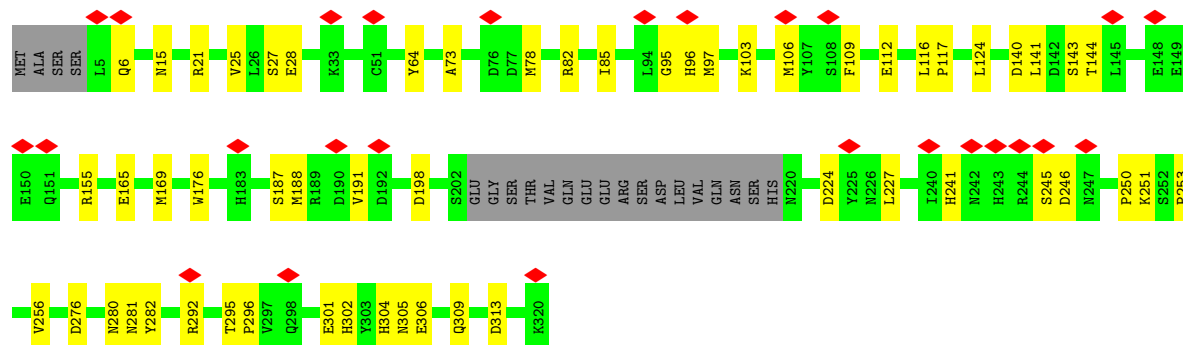
• Molecule 2: Protein C42

Chain D: 46% 9% 44%



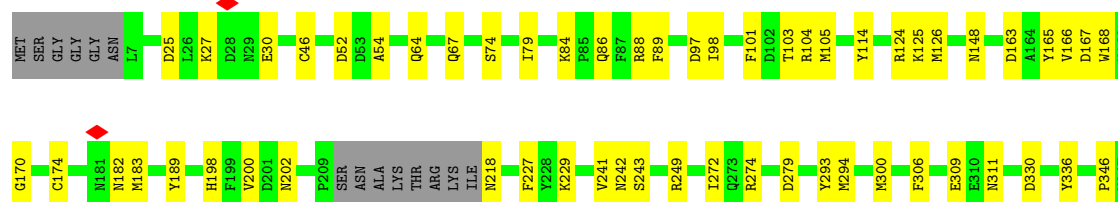
• Molecule 3: Uncharacterized 38.0 kDa protein in P143-LEF5 intergenic region

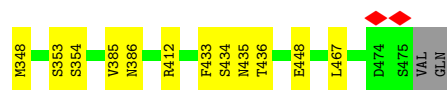
Chain E: 8% 76% 18% 7%



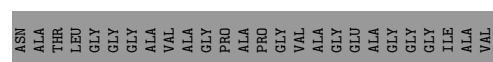
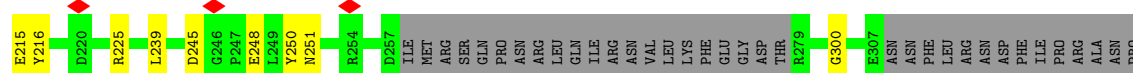
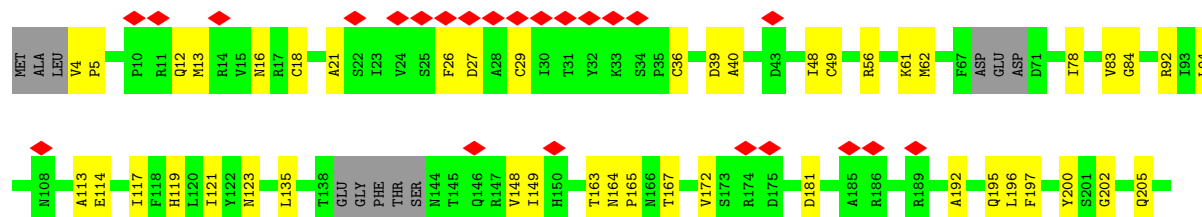
• Molecule 4: Protein AC142

Chain F: 82% 14%

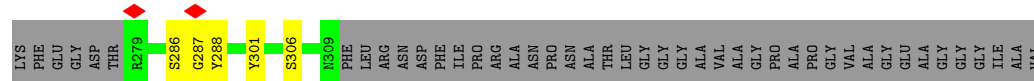
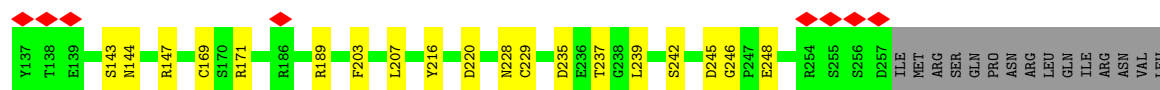
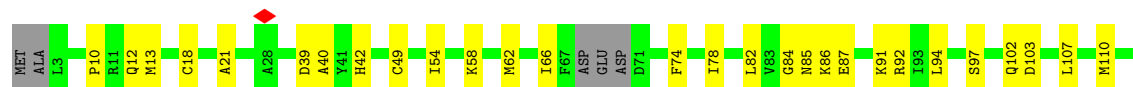




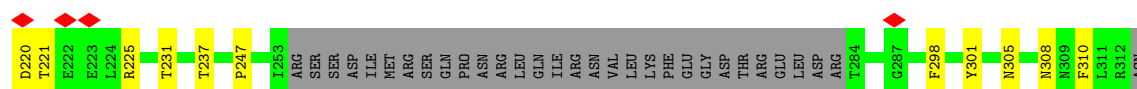
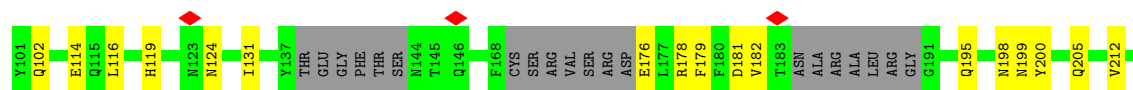
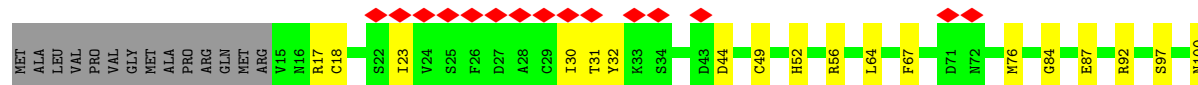
• Molecule 5: Major capsid protein



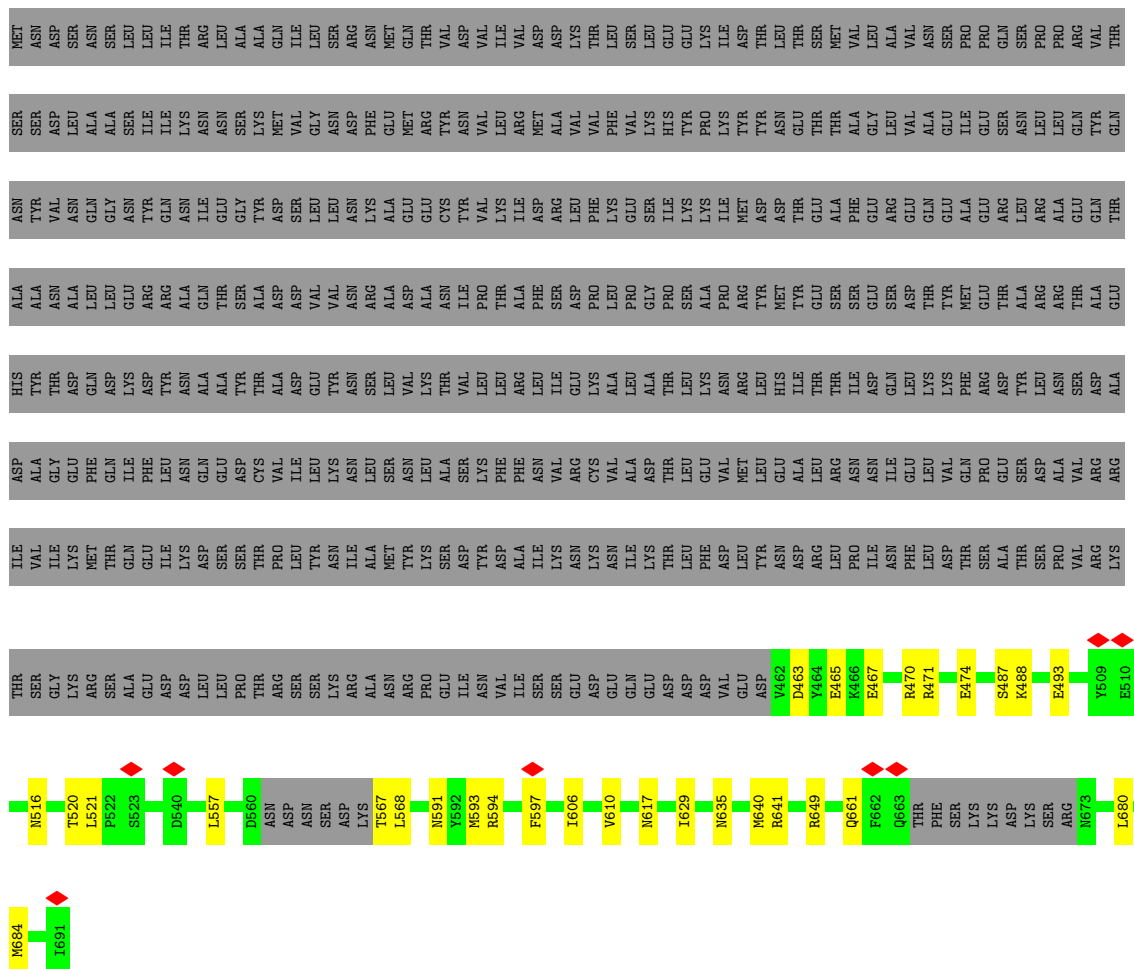
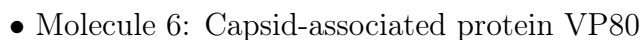
• Molecule 5: Major capsid protein



• Molecule 5: Major capsid protein



Chain N:



Chain J: 20% 6% 75%

LEU	LEU	THR	ILE	ASP	HIS	ALA	ASN	SER	MET
R594	LYS	SER	ILE	ALA	THR	ALA	TYR	SER	MET
E595	ALA	GLY	ILE	GLY	THR	ASN	VAL	ASP	
T596	LEU	LYS	LYS	LYS	ASP	ALA	ASN	LEU	
F597	GLU	ARG	MET	PHE	GLN	LEU	GLN	ALA	
F600	PHE	SER	THR	GLN	ASP	LEU	GLY	SER	
K604	S487	ALA	GLN	ILE	LYS	GLU	ASN	LEU	
	K488	GLU	GLU	PHE	ASP	ARG	TYR	ILE	
	V501	ASP	ILE	ASN	TYR	ARG	GLN	LYS	
	M505	LEU	ASP	GLN	ALA	THR	ILE	ASN	
	K506	PRO	SER	GLU	ALA	SER	GLY	ALA	
	B507	THR	THR	VAL	TYR	ALA	TYR	LYS	
	E510	ARG	PRO	CYS	ALA	ASP	ASP	MET	
	Y611	SER	LEU	ILE	ASP	ASP	SER	VAL	
	C512	LYS	ASN	LYS	GLU	VAL	LEU	GLY	
	N513	ARG	ILE	ASN	TYR	ASN	LEU	ASN	
	C514	ALA	THR	LYS	GLU	ALA	CYS	THR	
	E519	GLU	SER	ALA	THR	ASN	GLY	VAL	
	N526	ILE	ASP	SER	VAL	ILE	TYR	ASP	
	L530	VAL	TYR	LYS	VAL	PRO	VAL	VAL	
	L531	VAL	ASP	PHE	LEU	THR	LYS	ILE	
	K532	ILE	ALA	PHE	ARG	ALA	ILE	VAL	
	R533	SER	ILE	VAL	LEU	PHE	ASP	MET	
	F548	GLU	LYS	ARG	ILE	SER	ARG	ALA	
	Y549	ASP	ASN	GLY	GLU	ASP	LEU	VAL	
	E550	GLU	LYS	VAL	ALA	LEU	GLY	LYS	
	L551	GLU	ILE	ALA	LEU	PRO	LYS	SER	
	L552	ASP	THR	THR	ALA	GLY	ILE	HIS	
	L555	ASP	LEU	LEU	THR	PRO	LYS	GLU	
	D560	ASP	PHE	GLU	LEU	SER	LYS	GLU	
	N561	VAL	ASP	VAL	ASN	ALA	ILE	TYR	
	D562	GLU	ASP	VAL	THR	GLU	THR	SER	
	N563	GLU	LEU	ARG	THR	SER	ALA	THR	
	S564	LYS	PRO	ASN	ILE	SER	PHE	VAL	
	D565	GLU	ILE	ASN	ASP	GLU	GLY	LEU	
	K566	SER	ASN	ILE	GLN	SER	ARG	ALA	
	T567	LYS	PHE	GLU	LEU	ASP	GLU	VAL	
	L568	ARG	LEU	VAL	LYS	THR	GLN	VAL	
	Q571	LYS	THR	GLN	PHE	MET	ALA	ILE	
	F577	LEU	SER	PRO	ARG	THR	GLU	PRO	
	S580	GLU	ALA	GLU	ASP	ALA	LEU	SER	
	N581	GLU	THR	SER	TYR	ARG	ARG	LEU	
	N585	PHE	VAL	ALA	ASP	THR	GLU	GLN	
		LYS	ARG	ARG	ALA	THR	THR	VAL	

Chain K:

Amino Acid	Percentage
MET	22%
ASP	10%
THR	10%
GLY	10%
LEU	10%
PHE	10%
VAL	10%
ARG	10%
SER	10%
ASN	10%
GLN	10%

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	12164	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.031	Depositor
Minimum map value	-0.009	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	675.0, 675.0, 675.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.18	0/2024	0.29	0/2732
1	B	0.22	0/1681	0.32	0/2273
2	C	0.18	0/1821	0.30	0/2455
2	D	0.20	0/1704	0.36	0/2295
3	E	0.15	0/2598	0.31	0/3518
4	F	0.17	0/3890	0.31	0/5268
5	G	0.14	0/2257	0.29	0/3056
5	H	0.14	0/2320	0.28	0/3143
5	M	0.12	0/2050	0.28	0/2779
5	N	0.15	0/2271	0.30	0/3075
6	I	0.15	0/1836	0.28	0/2467
6	J	0.15	0/1493	0.33	0/2013
6	K	0.14	0/1499	0.32	0/2018
7	L	0.17	0/2952	0.27	0/4012
All	All	0.16	0/30396	0.30	0/41104

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1991	0	2012	37	0
1	B	1649	0	1652	25	0
2	C	1790	0	1789	28	0
2	D	1677	0	1685	32	0
3	E	2526	0	2476	37	0
4	F	3792	0	3777	50	0
5	G	2213	0	2169	36	0
5	H	2274	0	2222	44	0
5	M	2008	0	1944	33	0
5	N	2226	0	2170	38	0
6	I	1802	0	1821	20	0
6	J	1462	0	1462	32	0
6	K	1468	0	1481	19	0
7	L	2880	0	2878	39	0
8	G	1	0	0	0	0
8	H	1	0	0	0	0
8	M	1	0	0	0	0
8	N	1	0	0	0	0
All	All	29762	0	29538	423	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 7.

All (423) 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)
1:A:102:PHE:CE2	1:A:106:MET:HE2	2.02	0.95
5:H:144:ASN:OD1	5:H:147:ARG:NH2	2.13	0.81
6:J:571:GLN:O	5:N:189:ARG:NH2	2.12	0.81
3:E:176:TRP:O	3:E:251:LYS:NZ	2.14	0.81
2:D:134:SER:OG	2:D:215:ARG:NH2	2.15	0.80
6:J:519:GLU:OE1	6:J:519:GLU:N	2.16	0.78
4:F:433:PHE:O	4:F:436:THR:N	2.18	0.76
6:J:581:ASN:OD1	6:J:649:ARG:NH2	2.19	0.75
2:C:266:GLY:O	2:C:267:THR:OG1	2.05	0.75
6:I:493:GLU:N	6:I:493:GLU:OE1	2.19	0.75
5:M:18:CYS:SG	5:M:52:HIS:CE1	2.81	0.74
5:N:102:GLN:N	5:N:102:GLN:OE1	2.20	0.74
5:H:102:GLN:OE1	5:H:102:GLN:N	2.23	0.72
7:L:6:GLN:OE1	7:L:6:GLN:N	2.22	0.72
5:G:195:GLN:NE2	6:K:566:LYS:O	2.23	0.72
6:I:467:GLU:OE2	6:I:471:ARG:NE	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:591:ASN:OD1	6:J:594:ARG:NH1	2.22	0.72
5:M:102:GLN:OE1	5:M:102:GLN:N	2.22	0.72
5:M:87:GLU:N	5:M:87:GLU:OE1	2.24	0.71
2:D:141:LYS:N	2:D:144:ASP:OD2	2.23	0.71
5:N:248:GLU:OE1	5:N:248:GLU:N	2.24	0.70
5:N:37:SER:OG	5:N:49:CYS:SG	2.47	0.70
1:A:63:MET:SD	1:A:79:GLN:NE2	2.64	0.70
1:B:55:MET:HE1	1:B:209:TYR:CD2	2.26	0.70
5:M:220:ASP:O	5:M:221:THR:OG1	2.08	0.69
1:B:151:THR:O	2:D:292:ARG:NH1	2.24	0.69
5:H:301:TYR:OH	6:I:649:ARG:NH1	2.26	0.69
5:H:245:ASP:O	6:J:585:ASN:ND2	2.26	0.69
3:E:246:ASP:OD2	3:E:280:ASN:ND2	2.25	0.69
4:F:84:LYS:NZ	4:F:200:VAL:O	2.27	0.68
4:F:124:ARG:NH1	6:I:463:ASP:O	2.25	0.68
3:E:21:ARG:O	3:E:95:GLY:N	2.27	0.68
2:C:164:LEU:O	2:C:167:THR:OG1	2.12	0.67
6:K:629:ILE:HG22	6:K:629:ILE:O	1.93	0.67
5:M:176:GLU:OE2	5:M:305:ASN:ND2	2.28	0.67
6:I:467:GLU:OE1	6:I:470:ARG:NH2	2.28	0.67
5:M:200:TYR:O	5:M:205:GLN:NE2	2.26	0.67
5:N:125:GLU:N	5:N:125:GLU:OE1	2.25	0.67
1:B:236:LYS:NZ	3:E:124:LEU:O	2.27	0.67
3:E:28:GLU:N	3:E:28:GLU:OE1	2.28	0.67
4:F:126:MET:N	4:F:126:MET:HE2	2.09	0.67
1:A:107:GLU:N	1:A:107:GLU:OE1	2.28	0.66
1:A:65:GLN:N	1:A:65:GLN:OE1	2.28	0.66
1:A:175:ARG:NH1	1:A:176:LYS:O	2.28	0.66
5:N:36:CYS:SG	5:N:52:HIS:CE1	2.87	0.66
1:A:102:PHE:CZ	1:A:106:MET:CE	2.78	0.66
6:J:549:TYR:CE1	6:J:650:ASP:HB3	2.30	0.66
7:L:236:GLU:OE2	7:L:240:ARG:NE	2.29	0.66
6:I:470:ARG:NH1	6:I:474:GLU:OE2	2.29	0.66
5:H:235:ASP:OD1	5:H:237:THR:N	2.29	0.65
1:A:126:THR:OG1	2:C:255:GLN:NE2	2.29	0.65
5:G:27:ASP:OD1	5:G:29:CYS:N	2.30	0.65
6:J:565:ASP:OD1	6:J:568:LEU:N	2.29	0.65
1:B:115:ASP:O	2:D:250:ARG:NE	2.29	0.65
1:A:72:ARG:O	7:L:376:SER:OG	2.13	0.64
6:J:506:LYS:O	6:J:507:ARG:NH1	2.31	0.63
5:H:220:ASP:OD1	5:H:306:SER:N	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:353:SER:OG	4:F:385:VAL:O	2.13	0.63
5:M:97:SER:N	5:M:100:ASN:OD1	2.31	0.63
5:M:231:THR:OG1	5:M:298:PHE:N	2.31	0.63
2:D:317:ASN:OD1	2:D:320:ASP:N	2.25	0.63
6:J:630:ASP:OD1	6:J:631:GLU:N	2.31	0.62
5:G:197:PHE:O	5:G:205:GLN:NE2	2.33	0.62
2:C:171:ASP:OD1	2:C:172:TYR:N	2.32	0.62
5:G:181:ASP:OD2	5:G:192:ALA:N	2.33	0.62
4:F:249:ARG:NH1	7:L:349:ASN:O	2.33	0.62
6:I:591:ASN:OD1	6:I:594:ARG:NH2	2.32	0.62
5:G:216:TYR:CE1	5:G:225:ARG:HG3	2.34	0.62
2:C:113:LEU:O	2:D:163:LYS:NZ	2.32	0.61
5:H:66:ILE:N	5:H:74:PHE:O	2.32	0.61
1:A:102:PHE:CE2	1:A:106:MET:CE	2.80	0.61
5:N:56:ARG:NE	5:N:114:GLU:OE2	2.28	0.61
3:E:140:ASP:O	3:E:144:THR:OG1	2.17	0.61
2:C:280:ARG:NH1	5:H:12:GLN:O	2.34	0.60
5:G:84:GLY:O	5:G:92:ARG:NH2	2.34	0.60
5:G:92:ARG:NH1	5:G:248:GLU:OE1	2.34	0.60
5:M:84:GLY:N	5:M:87:GLU:OE2	2.34	0.60
4:F:166:VAL:O	7:L:341:ASN:ND2	2.35	0.60
2:D:293:MET:N	2:D:293:MET:HE2	2.17	0.60
5:N:215:GLU:N	5:N:300:GLY:O	2.34	0.59
7:L:224:GLU:OE1	7:L:224:GLU:N	2.33	0.59
2:C:202:ASP:OD1	2:C:203:LEU:N	2.35	0.59
2:C:148:THR:O	2:C:152:LEU:HD23	2.02	0.59
6:I:516:ASN:O	6:I:617:ASN:ND2	2.35	0.58
5:H:143:SER:O	5:H:147:ARG:NH2	2.36	0.58
4:F:242:ASN:OD1	4:F:243:SER:N	2.36	0.58
1:A:110:VAL:N	2:C:260:GLN:OE1	2.36	0.58
7:L:355:ASP:O	7:L:358:ASN:ND2	2.37	0.58
5:N:289:GLU:OE1	5:N:289:GLU:N	2.31	0.58
3:E:276:ASP:OD2	3:E:292:ARG:NH1	2.34	0.58
1:B:249:ARG:NH2	3:E:198:ASP:OD1	2.37	0.57
6:I:640:MET:HE3	6:I:640:MET:HA	1.84	0.57
6:K:503:ASP:OD1	6:K:623:ARG:NH1	2.36	0.57
7:L:169:GLU:OE1	7:L:169:GLU:N	2.36	0.57
1:A:151:THR:O	2:C:292:ARG:NH1	2.37	0.57
5:G:94:LEU:N	5:G:239:LEU:O	2.37	0.57
6:K:592:TYR:O	6:K:595:GLU:HG3	2.05	0.57
5:G:39:ASP:OD2	5:G:61:LYS:NZ	2.31	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:272:ASP:OD1	7:L:273:TYR:N	2.37	0.57
4:F:104:ARG:HG3	4:F:105:MET:N	2.19	0.56
5:G:164:ASN:O	5:G:167:THR:HG22	2.05	0.56
3:E:15:ASN:ND2	3:E:64:TYR:O	2.38	0.56
4:F:46:CYS:SG	4:F:218:ASN:ND2	2.78	0.56
5:H:58:LYS:NZ	5:H:91:LYS:O	2.35	0.56
6:J:549:TYR:N	6:J:650:ASP:OD2	2.37	0.56
2:D:170:ASP:CG	2:D:171:ASP:H	2.14	0.56
7:L:245:ASP:OD1	7:L:246:VAL:N	2.37	0.56
4:F:229:LYS:NZ	4:F:279:ASP:OD2	2.38	0.56
1:A:147:ARG:NH2	2:C:307:GLU:OE2	2.35	0.56
4:F:241:VAL:N	4:F:336:TYR:O	2.39	0.56
1:A:48:LYS:NZ	2:C:286:ASP:O	2.38	0.56
2:C:196:MET:HE3	2:C:196:MET:HA	1.87	0.55
4:F:64:GLN:O	4:F:67:GLN:NE2	2.39	0.55
7:L:106:SER:OG	7:L:108:LEU:O	2.15	0.55
2:D:172:TYR:HD1	2:D:173:THR:O	1.88	0.55
5:N:92:ARG:NH1	5:N:248:GLU:OE2	2.40	0.55
1:A:113:THR:OG1	1:A:115:ASP:OD1	2.20	0.55
5:H:66:ILE:O	5:H:74:PHE:N	2.38	0.55
6:K:629:ILE:HG23	6:K:632:LEU:HD12	1.87	0.55
7:L:328:ASP:OD1	7:L:329:SER:N	2.39	0.55
2:D:328:MET:HA	2:D:328:MET:HE3	1.87	0.55
3:E:143:SER:O	3:E:155:ARG:NH1	2.40	0.55
1:A:102:PHE:CG	1:A:102:PHE:O	2.61	0.54
2:D:165:LEU:O	2:D:168:THR:OG1	2.17	0.54
1:A:241:HIS:ND1	2:C:320:ASP:OD2	2.28	0.54
6:J:640:MET:HE2	6:J:640:MET:N	2.22	0.54
7:L:289:PHE:O	7:L:292:GLN:NE2	2.41	0.54
1:A:103:THR:HG22	1:A:104:ASN:N	2.24	0.53
3:E:169:MET:HE3	3:E:169:MET:O	2.08	0.53
7:L:342:MET:HA	7:L:342:MET:HE2	1.90	0.53
5:G:26:PHE:HD1	5:G:148:VAL:HG11	1.73	0.53
1:A:156:ASN:OD1	1:A:165:ARG:NH2	2.41	0.53
6:I:629:ILE:O	6:I:629:ILE:HG22	2.09	0.53
6:I:567:THR:OG1	6:I:568:LEU:N	2.41	0.53
5:G:12:GLN:NE2	5:G:13:MET:O	2.40	0.53
5:M:198:ASN:O	5:M:205:GLN:NE2	2.41	0.53
5:H:13:MET:SD	5:H:13:MET:N	2.81	0.53
1:A:147:ARG:NH1	2:C:300:THR:O	2.41	0.53
4:F:306:PHE:O	4:F:435:ASN:ND2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:98:ILE:O	4:F:98:ILE:HG22	2.09	0.52
5:G:18:CYS:SG	5:G:21:ALA:HB2	2.48	0.52
1:A:102:PHE:O	1:A:102:PHE:CD2	2.63	0.52
1:B:39:LEU:O	1:B:43:GLU:OE1	2.27	0.52
4:F:249:ARG:NE	4:F:330:ASP:OD2	2.32	0.52
4:F:354:SER:OG	4:F:386:ASN:OD1	2.28	0.52
5:H:171:ARG:O	6:I:641:ARG:NH2	2.37	0.52
6:K:631:GLU:OE1	6:K:631:GLU:N	2.33	0.51
4:F:104:ARG:HG3	4:F:105:MET:H	1.75	0.51
7:L:127:LYS:N	7:L:209:GLN:OE1	2.38	0.51
5:H:94:LEU:N	5:H:239:LEU:O	2.43	0.51
2:D:172:TYR:CD1	2:D:173:THR:O	2.64	0.51
2:D:258:GLN:NE2	2:D:259:PRO:O	2.40	0.51
3:E:309:GLN:NE2	3:E:313:ASP:OD1	2.42	0.51
5:H:10:PRO:O	5:H:12:GLN:NE2	2.43	0.51
6:J:591:ASN:O	6:J:595:GLU:OE1	2.28	0.51
1:B:78:ARG:NH1	2:D:262:TYR:O	2.41	0.51
1:B:121:GLU:OE2	1:B:241:HIS:NE2	2.43	0.51
3:E:106:MET:HA	3:E:106:MET:HE2	1.93	0.50
5:M:195:GLN:NE2	5:M:199:ASN:OD1	2.42	0.50
5:H:62:MET:N	5:H:78:ILE:O	2.44	0.50
5:H:92:ARG:NH1	5:H:248:GLU:OE1	2.45	0.50
5:H:107:LEU:HA	5:H:110:MET:HE3	1.92	0.50
6:K:544:MET:SD	6:K:611:MET:SD	3.09	0.50
3:E:253:PRO:HA	3:E:256:VAL:HG22	1.94	0.50
5:G:215:GLU:N	5:G:300:GLY:O	2.45	0.50
5:H:84:GLY:N	5:H:87:GLU:OE2	2.37	0.50
2:D:177:GLN:O	2:D:178:MET:HE2	2.12	0.50
6:J:618:PHE:O	6:J:622:MET:HG2	2.12	0.50
4:F:25:ASP:OD1	4:F:27:LYS:NZ	2.43	0.50
7:L:178:LEU:O	7:L:211:ARG:NH1	2.40	0.49
1:B:55:MET:HE1	1:B:209:TYR:HD2	1.75	0.49
5:M:308:ASN:O	5:M:310:PHE:N	2.45	0.49
5:G:196:LEU:O	5:G:200:TYR:CD1	2.65	0.49
1:B:152:GLU:OE1	1:B:152:GLU:N	2.35	0.49
5:H:84:GLY:O	5:H:92:ARG:NH2	2.45	0.49
3:E:165:GLU:OE1	3:E:304:HIS:NE2	2.45	0.49
7:L:43:THR:N	7:L:46:ASP:OD2	2.38	0.49
5:H:169:CYS:SG	7:L:220:ASN:ND2	2.81	0.48
3:E:144:THR:O	3:E:155:ARG:NH2	2.42	0.48
6:J:511:TYR:CD1	6:J:530:LEU:HD22	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:LYS:NZ	2:D:286:ASP:O	2.42	0.48
2:D:169:PHE:O	2:D:170:ASP:HB3	2.13	0.48
4:F:148:ASN:N	6:I:465:GLU:OE2	2.35	0.48
2:C:119:TYR:HB3	2:C:151:PHE:HB2	1.94	0.48
3:E:302:HIS:NE2	3:E:306:GLU:OE2	2.47	0.48
4:F:167:ASP:OD2	4:F:170:GLY:N	2.43	0.48
5:N:36:CYS:SG	5:N:52:HIS:CG	3.06	0.48
4:F:412:ARG:NH2	4:F:448:GLU:OE2	2.44	0.48
2:C:171:ASP:O	2:C:172:TYR:CG	2.67	0.48
5:H:189:ARG:NH1	6:J:589:ASN:OD1	2.47	0.48
6:K:518:LEU:HD21	6:K:521:LEU:C	2.39	0.48
5:M:100:ASN:ND2	5:M:237:THR:O	2.43	0.48
5:N:36:CYS:SG	5:N:51:ASN:HB2	2.54	0.48
5:G:163:THR:O	5:G:172:VAL:HG21	2.14	0.47
5:H:54:ILE:HG22	5:H:82:LEU:HD11	1.96	0.47
5:M:178:ARG:NH2	5:M:212:VAL:O	2.44	0.47
1:A:59:SER:O	1:A:62:GLU:N	2.47	0.47
3:E:301:GLU:OE1	3:E:305:ASN:ND2	2.46	0.47
4:F:101:PHE:CE1	4:F:103:THR:HA	2.50	0.47
6:J:513:ASN:ND2	6:J:526:ASN:O	2.47	0.47
1:A:121:GLU:OE2	1:A:241:HIS:NE2	2.47	0.47
4:F:300:MET:HE3	4:F:346:PRO:HD2	1.96	0.47
1:A:40:GLU:OE2	2:D:231:GLN:NE2	2.48	0.47
4:F:272:ILE:HG21	4:F:294:MET:HE2	1.97	0.47
6:K:635:ASN:OD1	6:K:636:LYS:N	2.45	0.47
1:A:202:THR:OG1	1:A:205:GLU:OE1	2.25	0.47
1:B:73:ASN:ND2	1:B:76:ASP:OD2	2.47	0.47
2:C:180:GLN:NE2	2:C:184:ASP:OD1	2.48	0.47
3:E:295:THR:HG23	3:E:296:PRO:HD2	1.97	0.47
4:F:104:ARG:CG	4:F:105:MET:H	2.28	0.47
7:L:183:ASP:OD1	7:L:216:ARG:NE	2.43	0.47
5:M:56:ARG:NE	5:M:114:GLU:OE2	2.40	0.47
2:C:156:GLU:OE1	2:C:159:HIS:NE2	2.47	0.47
3:E:82:ARG:HA	3:E:85:ILE:HG22	1.97	0.47
4:F:435:ASN:O	4:F:436:THR:OG1	2.29	0.47
5:G:48:ILE:O	5:G:61:LYS:NZ	2.39	0.47
5:G:245:ASP:OD1	5:M:225:ARG:NH1	2.45	0.47
4:F:198:HIS:ND1	4:F:202:ASN:OD1	2.48	0.47
6:J:549:TYR:CE1	6:J:650:ASP:CB	2.96	0.47
5:N:18:CYS:SG	5:N:21:ALA:HB2	2.55	0.47
5:N:195:GLN:NE2	5:N:199:ASN:OD1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:104:ARG:CG	4:F:105:MET:N	2.78	0.46
5:G:250:TYR:N	5:M:225:ARG:O	2.41	0.46
5:H:216:TYR:HB2	5:H:301:TYR:CD1	2.51	0.46
5:G:56:ARG:NE	5:G:114:GLU:OE2	2.45	0.46
6:K:629:ILE:CG2	6:K:632:LEU:HD12	2.45	0.46
7:L:182:ASN:OD1	7:L:211:ARG:NH2	2.48	0.46
1:B:113:THR:O	1:B:116:THR:OG1	2.29	0.46
4:F:97:ASP:HB3	7:L:251:ALA:HB2	1.96	0.46
4:F:274:ARG:HG2	4:F:294:MET:HE1	1.98	0.46
5:G:62:MET:N	5:G:78:ILE:O	2.48	0.46
1:A:244:PHE:HB3	2:C:327:VAL:HG11	1.95	0.46
1:B:78:ARG:NH2	2:D:262:TYR:O	2.47	0.46
5:M:64:LEU:O	5:M:76:MET:N	2.39	0.46
5:N:216:TYR:HB2	5:N:301:TYR:CD2	2.51	0.46
5:H:203:PHE:CE2	5:H:207:LEU:HD11	2.50	0.46
6:J:565:ASP:OD1	6:J:567:THR:OG1	2.21	0.46
2:D:293:MET:HE2	2:D:293:MET:CA	2.46	0.46
3:E:224:ASP:OD1	3:E:227:LEU:N	2.48	0.46
5:G:163:THR:O	5:G:164:ASN:C	2.59	0.46
5:H:245:ASP:OD1	5:H:246:GLY:N	2.49	0.46
6:K:594:ARG:HA	6:K:610:VAL:HG21	1.98	0.46
5:N:275:GLU:CD	5:N:275:GLU:O	2.59	0.46
1:B:118:ILE:HD11	2:D:250:ARG:HB2	1.99	0.46
5:H:18:CYS:SG	5:H:21:ALA:HB2	2.56	0.46
5:M:23:ILE:O	5:M:32:TYR:CZ	2.69	0.46
5:N:215:GLU:OE1	5:N:230:ALA:N	2.49	0.46
6:J:548:PHE:HB3	6:J:650:ASP:CG	2.41	0.45
5:M:49:CYS:SG	5:M:52:HIS:HD2	2.38	0.45
5:N:62:MET:N	5:N:78:ILE:O	2.48	0.45
2:C:119:TYR:CZ	2:C:147:MET:HE1	2.51	0.45
4:F:467:LEU:HD23	4:F:467:LEU:O	2.17	0.45
6:I:661:GLN:OE1	6:I:661:GLN:N	2.41	0.45
5:N:92:ARG:NH2	5:N:248:GLU:OE2	2.50	0.45
3:E:78:MET:HE2	3:E:109:PHE:HB3	1.97	0.45
2:D:319:GLU:OE1	2:D:319:GLU:N	2.34	0.45
3:E:78:MET:CE	3:E:109:PHE:HB3	2.47	0.45
6:K:629:ILE:O	6:K:629:ILE:CG2	2.63	0.45
6:J:531:LEU:HD21	6:J:597:PHE:CE1	2.52	0.45
2:D:170:ASP:CG	2:D:171:ASP:N	2.75	0.45
3:E:6:GLN:OE1	3:E:73:ALA:N	2.49	0.45
6:J:487:SER:OG	6:J:488:LYS:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:541:HIS:O	6:K:541:HIS:ND1	2.48	0.45
1:B:137:ASP:OD2	1:B:140:SER:OG	2.34	0.45
5:H:228:ASN:ND2	5:N:229:CYS:SG	2.90	0.45
1:A:57:MET:HE1	1:A:86:SER:HB3	1.98	0.45
4:F:182:ASN:OD1	4:F:183:MET:N	2.50	0.45
4:F:98:ILE:O	4:F:98:ILE:CG2	2.65	0.44
3:E:280:ASN:O	3:E:281:ASN:C	2.60	0.44
5:N:308:ASN:O	5:N:310:PHE:N	2.50	0.44
2:D:119:TYR:HB3	2:D:151:PHE:HB2	2.00	0.44
4:F:52:ASP:OD1	4:F:54:ALA:N	2.50	0.44
6:K:518:LEU:HD21	6:K:522:PRO:N	2.32	0.44
7:L:307:MET:N	7:L:307:MET:HE2	2.32	0.44
5:M:119:HIS:O	5:M:124:ASN:N	2.44	0.44
4:F:165:TYR:CZ	7:L:340:ILE:HB	2.52	0.44
7:L:9:VAL:HG23	7:L:116:CYS:SG	2.57	0.44
3:E:28:GLU:OE2	3:E:103:LYS:NZ	2.45	0.44
7:L:236:GLU:OE1	7:L:240:ARG:NH2	2.51	0.44
1:A:118:ILE:O	1:A:118:ILE:HG23	2.18	0.44
4:F:86:GLN:OE1	4:F:227:PHE:N	2.40	0.44
7:L:132:PHE:CG	7:L:132:PHE:O	2.69	0.44
7:L:213:GLN:NE2	7:L:214:PRO:O	2.44	0.44
3:E:116:LEU:HD12	3:E:117:PRO:HD2	2.00	0.44
5:N:37:SER:OG	5:N:39:ASP:OD1	2.35	0.44
5:N:200:TYR:O	5:N:205:GLN:NE2	2.49	0.44
1:A:137:ASP:OD2	1:A:140:SER:OG	2.33	0.44
5:N:265:ARG:O	5:N:267:GLN:NE2	2.40	0.44
2:C:172:TYR:CD1	2:C:172:TYR:C	2.95	0.44
3:E:96:HIS:CD2	3:E:116:LEU:HD22	2.52	0.44
4:F:348:MET:N	4:F:348:MET:SD	2.90	0.44
6:J:501:VAL:CG1	6:J:505:MET:HE1	2.48	0.44
7:L:43:THR:HG1	7:L:46:ASP:CG	2.25	0.44
5:M:84:GLY:O	5:M:92:ARG:NH2	2.47	0.44
1:A:63:MET:SD	1:A:79:GLN:CD	3.00	0.43
3:E:112:GLU:HB2	3:E:241:HIS:CD2	2.53	0.43
5:G:135:LEU:HB2	5:G:149:ILE:HD11	2.00	0.43
2:C:140:TYR:HA	2:C:144:ASP:OD2	2.17	0.43
6:I:606:ILE:O	6:I:610:VAL:HG23	2.18	0.43
5:M:67:PHE:CD1	5:M:67:PHE:C	2.96	0.43
5:N:144:ASN:OD1	5:N:147:ARG:NH1	2.45	0.43
1:B:55:MET:CE	1:B:209:TYR:HD2	2.30	0.43
4:F:309:GLU:OE2	4:F:311:ASN:N	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:225:ARG:NH1	5:M:247:PRO:O	2.32	0.43
5:H:286:SER:O	5:H:287:GLY:C	2.60	0.43
5:N:115:GLN:O	5:N:119:HIS:CD2	2.71	0.43
1:B:214:LEU:HB2	2:D:301:MET:HE1	2.01	0.43
3:E:27:SER:OG	3:E:28:GLU:OE1	2.22	0.43
4:F:274:ARG:NH1	4:F:293:TYR:O	2.44	0.43
6:J:577:PHE:CD2	5:N:182:VAL:HG12	2.53	0.43
6:J:580:SER:OG	6:J:649:ARG:NE	2.43	0.43
1:A:161:ASN:HB3	1:A:164:VAL:HG22	2.00	0.43
1:A:259:LEU:O	1:A:262:SER:OG	2.23	0.43
2:D:177:GLN:NE2	2:D:178:MET:O	2.51	0.43
5:H:102:GLN:NE2	5:H:103:ASP:OD2	2.52	0.43
6:I:487:SER:OG	6:I:488:LYS:N	2.52	0.43
7:L:321:ILE:HG22	7:L:322:ARG:N	2.33	0.43
5:N:219:ILE:O	5:N:220:ASP:OD1	2.36	0.43
1:A:113:THR:O	1:A:116:THR:OG1	2.36	0.43
3:E:245:SER:O	3:E:246:ASP:C	2.61	0.43
6:J:510:GLU:O	6:J:533:ARG:NH1	2.52	0.43
1:B:51:LEU:O	1:B:55:MET:HG2	2.19	0.42
2:D:141:LYS:O	2:D:144:ASP:N	2.51	0.42
5:H:85:ASN:O	5:H:92:ARG:NH2	2.52	0.42
5:N:219:ILE:O	5:N:220:ASP:C	2.62	0.42
2:C:141:LYS:N	2:C:144:ASP:OD2	2.51	0.42
2:D:164:LEU:O	2:D:168:THR:HG23	2.19	0.42
3:E:250:PRO:O	3:E:282:TYR:HB2	2.20	0.42
6:J:511:TYR:O	6:J:512:CYS:C	2.61	0.42
7:L:387:ASN:O	7:L:388:TYR:C	2.62	0.42
1:B:121:GLU:CD	1:B:218:HIS:HE2	2.26	0.42
3:E:141:LEU:HD22	3:E:188:MET:HE3	2.01	0.42
1:A:47:ILE:HD11	1:A:263:LYS:HB2	2.02	0.42
3:E:25:VAL:HG23	3:E:97:MET:HE2	2.02	0.42
5:H:245:ASP:OD1	5:N:225:ARG:NH1	2.46	0.42
5:N:77:THR:OG1	5:N:210:ARG:HD3	2.19	0.42
1:A:102:PHE:CZ	1:A:106:MET:HE1	2.53	0.42
5:H:40:ALA:HB2	5:H:49:CYS:HB3	2.00	0.42
6:K:593:MET:HE1	6:K:614:ILE:HG12	2.01	0.42
1:B:39:LEU:O	1:B:42:TYR:N	2.52	0.42
1:B:232:PHE:CZ	1:B:236:LYS:HD2	2.55	0.42
4:F:74:SER:H	4:F:79:ILE:HD11	1.85	0.42
6:I:557:LEU:O	6:I:635:ASN:N	2.44	0.42
5:M:179:PHE:O	5:M:301:TYR:N	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:83:VAL:O	5:G:251:ASN:ND2	2.49	0.42
5:M:116:LEU:HD21	5:M:131:ILE:HB	2.02	0.42
4:F:89:PHE:CE1	4:F:168:TRP:CD1	3.08	0.41
4:F:125:LYS:C	4:F:126:MET:HE2	2.45	0.41
6:I:593:MET:O	6:I:597:PHE:CD2	2.73	0.41
6:J:591:ASN:O	6:J:594:ARG:HB3	2.20	0.41
2:C:178:MET:SD	2:C:178:MET:N	2.93	0.41
2:D:153:LEU:HB2	2:D:162:PHE:CE1	2.55	0.41
4:F:174:CYS:HB2	7:L:325:CYS:SG	2.60	0.41
5:G:26:PHE:CE2	5:G:135:LEU:HD21	2.56	0.41
5:G:40:ALA:HB2	5:G:49:CYS:HB3	2.02	0.41
5:G:117:ILE:O	5:G:121:ILE:HG12	2.19	0.41
6:J:548:PHE:HB3	6:J:650:ASP:OD2	2.20	0.41
1:A:107:GLU:OE2	1:A:131:VAL:HG11	2.21	0.41
3:E:140:ASP:O	3:E:141:LEU:C	2.62	0.41
6:J:549:TYR:HE2	6:K:658:SER:HA	1.85	0.41
7:L:285:GLN:HA	7:L:288:ILE:HD12	2.02	0.41
1:B:223:TYR:CD1	1:B:223:TYR:C	2.97	0.41
5:H:286:SER:O	5:H:288:TYR:HB2	2.20	0.41
6:I:520:THR:OG1	6:I:521:LEU:N	2.52	0.41
6:J:644:SER:O	6:J:648:MET:HG2	2.20	0.41
7:L:47:ARG:HG2	7:L:63:VAL:HG12	2.02	0.41
5:M:17:ARG:NH2	5:M:44:ASP:O	2.53	0.41
1:B:67:LEU:HD12	1:B:209:TYR:CE1	2.55	0.41
5:G:250:TYR:HH	5:M:67:PHE:CB	2.32	0.41
5:H:97:SER:N	5:H:237:THR:O	2.51	0.41
5:H:229:CYS:SG	5:N:228:ASN:HB3	2.61	0.41
6:I:680:LEU:O	6:I:684:MET:HG2	2.20	0.41
5:N:87:GLU:OE1	5:N:87:GLU:N	2.41	0.41
4:F:30:GLU:OE1	4:F:30:GLU:N	2.43	0.41
4:F:300:MET:HB3	4:F:348:MET:HE2	2.02	0.41
5:H:39:ASP:HA	5:H:42:HIS:CD2	2.56	0.41
5:H:86:LYS:N	5:H:86:LYS:HD2	2.36	0.41
6:K:601:GLY:O	6:K:602:PRO:C	2.64	0.41
5:M:87:GLU:O	5:M:92:ARG:NE	2.53	0.41
2:D:293:MET:HE2	2:D:293:MET:HA	2.03	0.41
5:G:26:PHE:CD1	5:G:148:VAL:HG11	2.55	0.41
5:H:216:TYR:HB2	5:H:301:TYR:CE1	2.55	0.41
6:J:548:PHE:CZ	6:J:552:LEU:HD12	2.56	0.41
7:L:127:LYS:HB3	7:L:209:GLN:O	2.21	0.41
7:L:168:CYS:SG	7:L:186:LEU:HB3	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:181:ASP:OD1	5:M:182:VAL:N	2.50	0.41
1:B:221:LEU:HD21	1:B:244:PHE:CG	2.56	0.41
4:F:88:ARG:NE	4:F:114:TYR:OH	2.47	0.41
4:F:434:SER:C	4:F:436:THR:H	2.29	0.41
5:G:4:VAL:N	5:G:5:PRO:HD2	2.36	0.41
5:M:30:ILE:O	5:M:31:THR:HB	2.21	0.41
5:N:192:ALA:O	5:N:195:GLN:HB3	2.21	0.41
2:C:146:VAL:HG12	2:C:150:ILE:HD12	2.02	0.41
5:H:62:MET:SD	5:N:291:TYR:N	2.94	0.41
5:H:235:ASP:OD1	5:H:235:ASP:C	2.64	0.41
6:J:555:LEU:HD11	6:J:622:MET:CE	2.51	0.41
6:K:610:VAL:O	6:K:613:VAL:HG12	2.21	0.41
7:L:322:ARG:NH1	7:L:342:MET:O	2.45	0.41
5:G:16:ASN:ND2	5:G:36:CYS:SG	2.87	0.40
5:G:26:PHE:CE1	5:G:113:ALA:HB2	2.56	0.40
5:G:119:HIS:O	5:G:123:ASN:O	2.40	0.40
5:H:245:ASP:OD1	5:H:245:ASP:C	2.65	0.40
7:L:287:ILE:O	7:L:288:ILE:C	2.64	0.40
5:N:67:PHE:O	5:N:73:GLN:HA	2.21	0.40
5:N:200:TYR:OH	5:N:238:GLY:HA2	2.22	0.40
1:A:244:PHE:O	1:A:245:THR:C	2.63	0.40
5:H:189:ARG:NH2	5:H:242:SER:OG	2.53	0.40
6:K:572:LEU:O	6:K:576:ILE:HG12	2.21	0.40
7:L:340:ILE:O	7:L:341:ASN:HB2	2.21	0.40
1:A:117:SER:O	2:C:250:ARG:NE	2.55	0.40
2:D:246:LEU:O	2:D:250:ARG:HG2	2.22	0.40
5:G:245:ASP:OD2	5:M:225:ARG:NH2	2.46	0.40
2:C:229:LEU:HD22	2:C:306:MET:HE1	2.03	0.40
4:F:166:VAL:HG12	4:F:167:ASP:N	2.35	0.40
5:G:165:PRO:HD2	5:G:202:GLY:HA2	2.03	0.40
5:H:39:ASP:HA	5:H:42:HIS:HD2	1.87	0.40
7:L:290:PRO:O	7:L:292:GLN:NE2	2.54	0.40
5:M:52:HIS:H	5:M:52:HIS:CD2	2.40	0.40
2:D:250:ARG:O	2:D:254:ILE:HG12	2.22	0.40
3:E:187:SER:O	3:E:191:VAL:HG22	2.22	0.40
3:E:276:ASP:OD1	3:E:276:ASP:N	2.50	0.40
4:F:163:ASP:O	4:F:189:TYR:OH	2.33	0.40
5:N:141:PHE:HA	5:N:145:THR:HB	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	240/290 (83%)	230 (96%)	10 (4%)	0	100	100
1	B	197/290 (68%)	187 (95%)	10 (5%)	0	100	100
2	C	210/361 (58%)	204 (97%)	6 (3%)	0	100	100
2	D	193/361 (54%)	183 (95%)	10 (5%)	0	100	100
3	E	295/320 (92%)	258 (88%)	37 (12%)	0	100	100
4	F	457/477 (96%)	433 (95%)	24 (5%)	0	100	100
5	G	267/347 (77%)	244 (91%)	23 (9%)	0	100	100
5	H	277/347 (80%)	254 (92%)	23 (8%)	0	100	100
5	M	238/347 (69%)	215 (90%)	23 (10%)	0	100	100
5	N	267/347 (77%)	230 (86%)	37 (14%)	0	100	100
6	I	209/691 (30%)	196 (94%)	13 (6%)	0	100	100
6	J	174/691 (25%)	163 (94%)	11 (6%)	0	100	100
6	K	172/691 (25%)	160 (93%)	12 (7%)	0	100	100
7	L	347/390 (89%)	335 (96%)	12 (4%)	0	100	100
All	All	3543/5950 (60%)	3292 (93%)	251 (7%)	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	A	230/273 (84%)	230 (100%)	0	100	100
1	B	188/273 (69%)	186 (99%)	2 (1%)	70	80
2	C	204/326 (63%)	204 (100%)	0	100	100
2	D	192/326 (59%)	192 (100%)	0	100	100
3	E	285/304 (94%)	285 (100%)	0	100	100
4	F	428/440 (97%)	428 (100%)	0	100	100
5	G	247/299 (83%)	247 (100%)	0	100	100
5	H	254/299 (85%)	254 (100%)	0	100	100
5	M	225/299 (75%)	225 (100%)	0	100	100
5	N	247/299 (83%)	247 (100%)	0	100	100
6	I	204/634 (32%)	204 (100%)	0	100	100
6	J	167/634 (26%)	167 (100%)	0	100	100
6	K	167/634 (26%)	167 (100%)	0	100	100
7	L	334/366 (91%)	334 (100%)	0	100	100
All	All	3372/5406 (62%)	3370 (100%)	2 (0%)	92	95

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

Mol	Chain	Res	Type
1	B	158	GLU
1	B	159	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	B	65	GLN
1	B	79	GLN
1	B	163	ASN
2	C	255	GLN
2	C	322	ASN
2	D	299	ASN
2	D	313	ASN
3	E	15	ASN
3	E	52	ASN
3	E	96	HIS
3	E	102	ASN

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Mol	Chain	Res	Type
3	E	241	HIS
3	E	243	HIS
3	E	298	GLN
4	F	78	ASN
5	G	42	HIS
5	G	115	GLN
5	H	42	HIS
6	I	570	HIS
6	I	574	ASN
6	I	581	ASN
6	J	496	GLN
6	K	581	ASN
7	L	223	HIS
7	L	249	ASN
5	M	42	HIS
5	N	119	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 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.

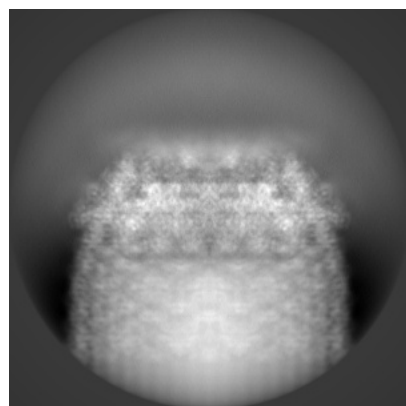
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51792. These allow visual inspection of the internal detail of the map and identification of artifacts.

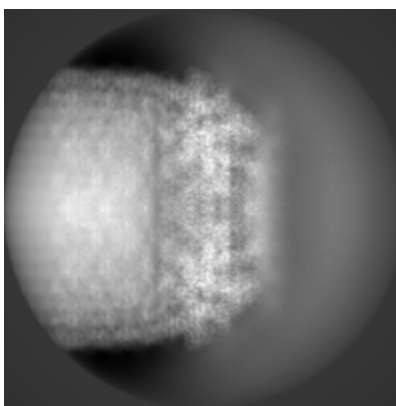
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

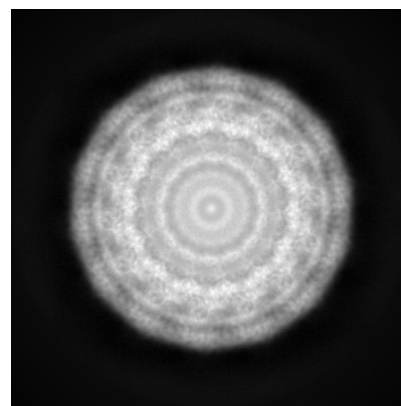
6.1.1 Primary map



X

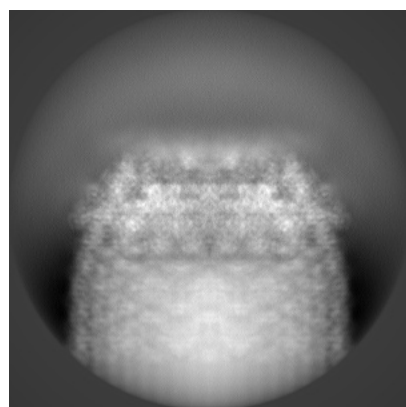


Y

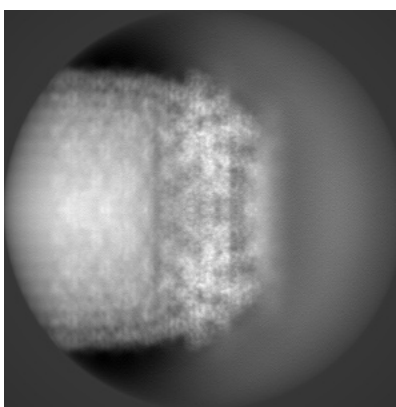


Z

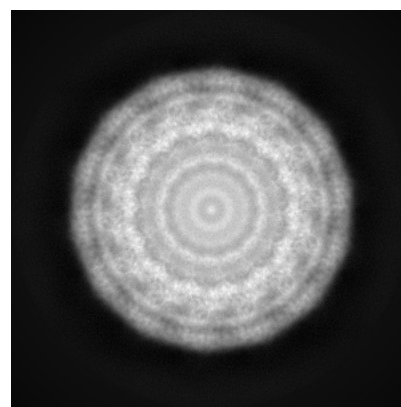
6.1.2 Raw map



X



Y

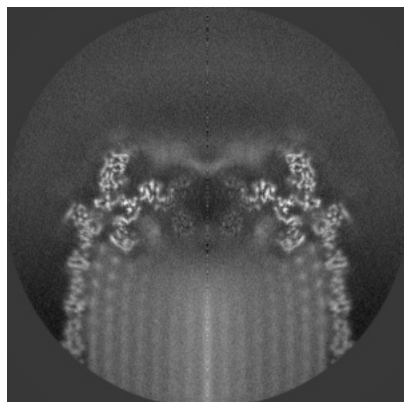


Z

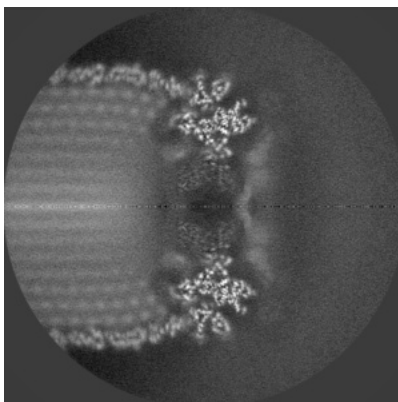
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

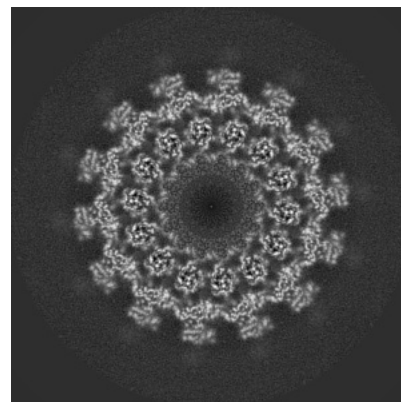
6.2.1 Primary map



X Index: 250

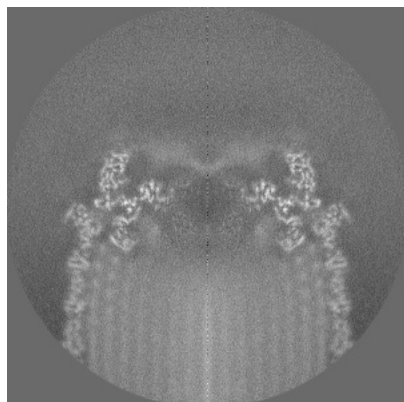


Y Index: 250

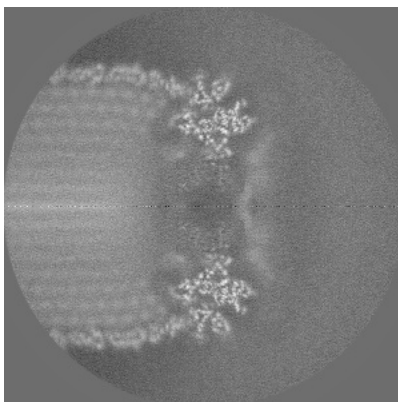


Z Index: 250

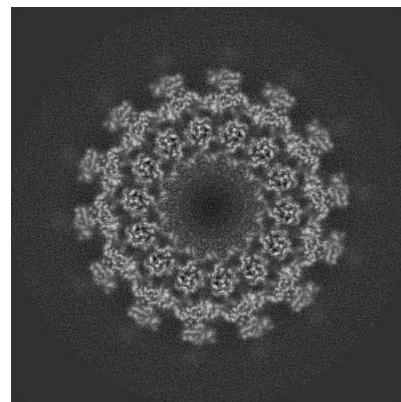
6.2.2 Raw map



X Index: 250



Y Index: 250

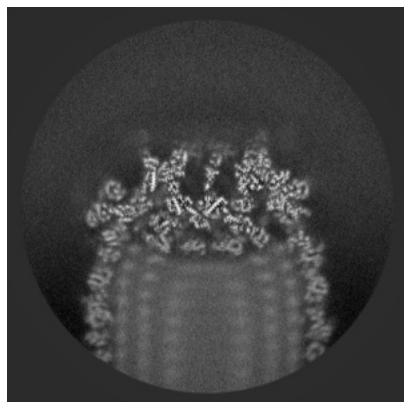


Z Index: 250

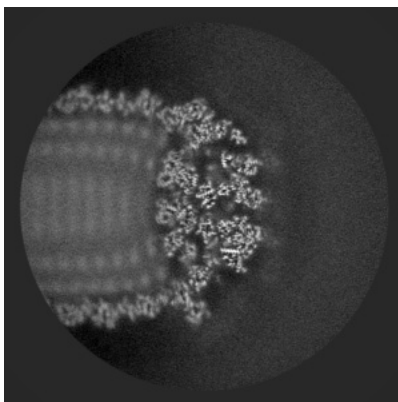
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

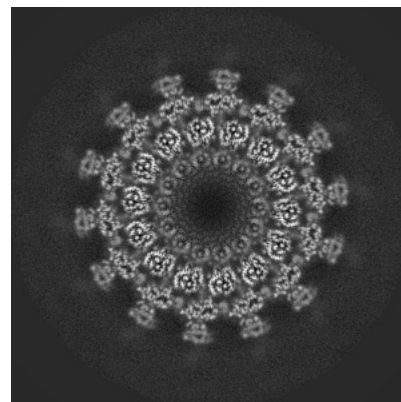
6.3.1 Primary map



X Index: 156

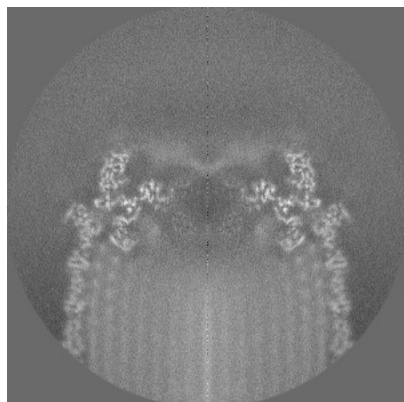


Y Index: 149

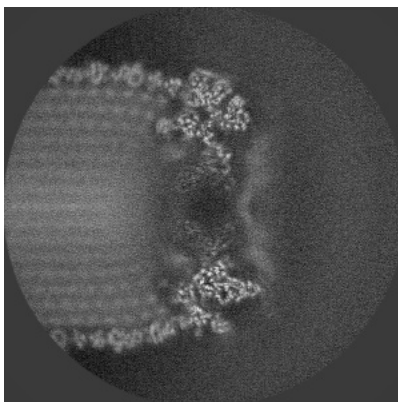


Z Index: 254

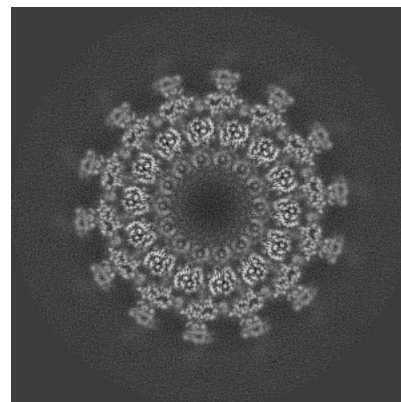
6.3.2 Raw map



X Index: 250



Y Index: 255

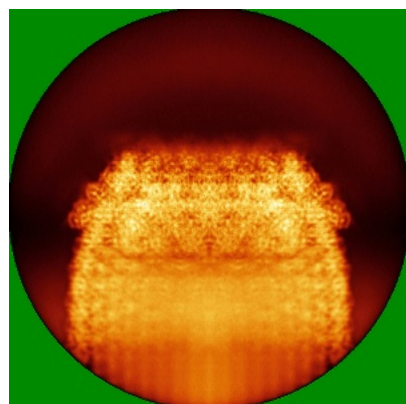


Z Index: 254

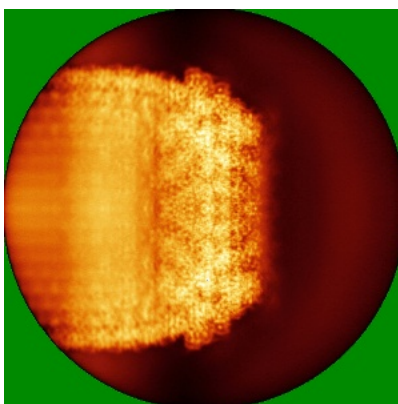
The images above show the largest variance slices of the map in three orthogonal directions.

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

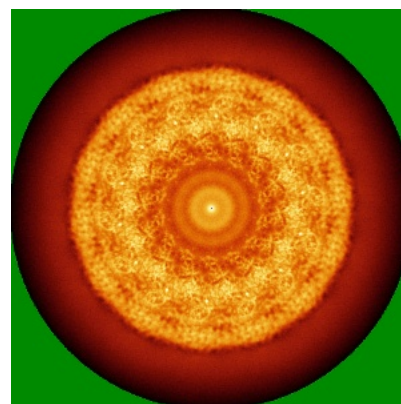
6.4.1 Primary map



X

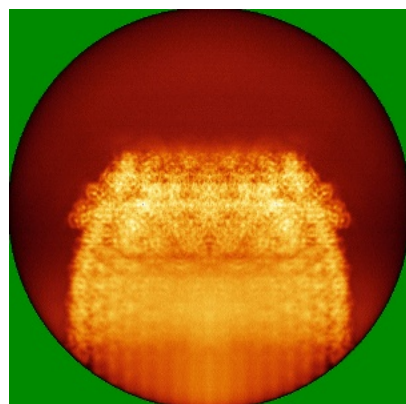


Y

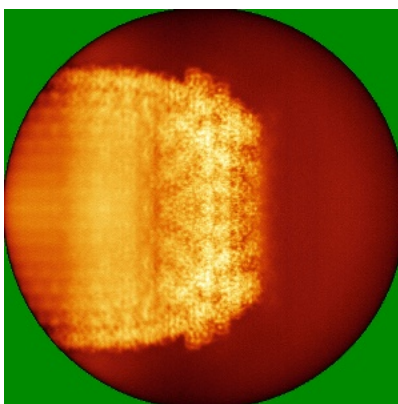


Z

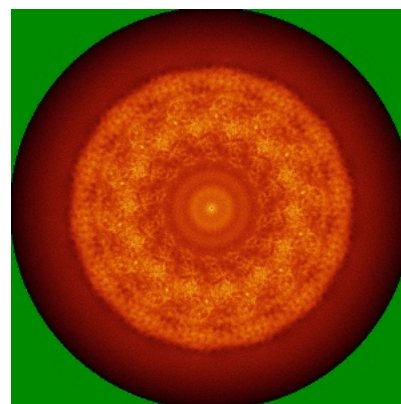
6.4.2 Raw map



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](#)

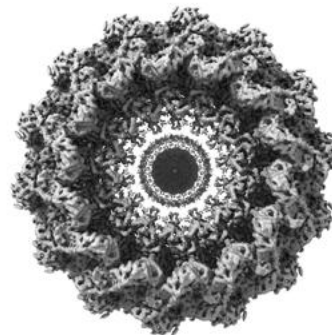
6.5.1 Primary map



X



Y



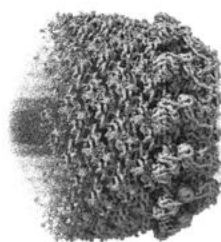
Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. 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



X



Y



Z

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.

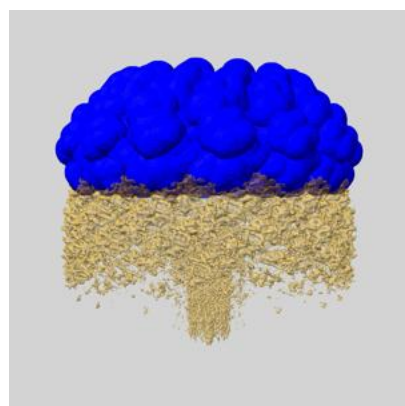
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

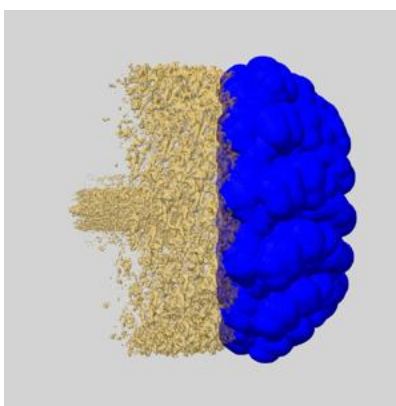
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

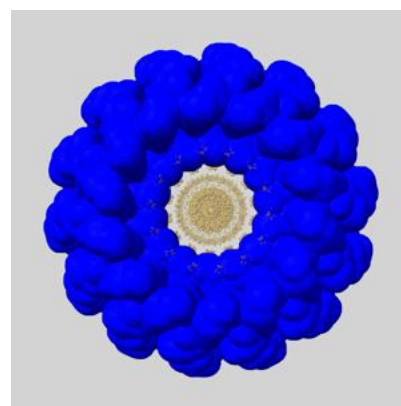
6.6.1 emd_51792_msk_1.map [i](#)



X



Y

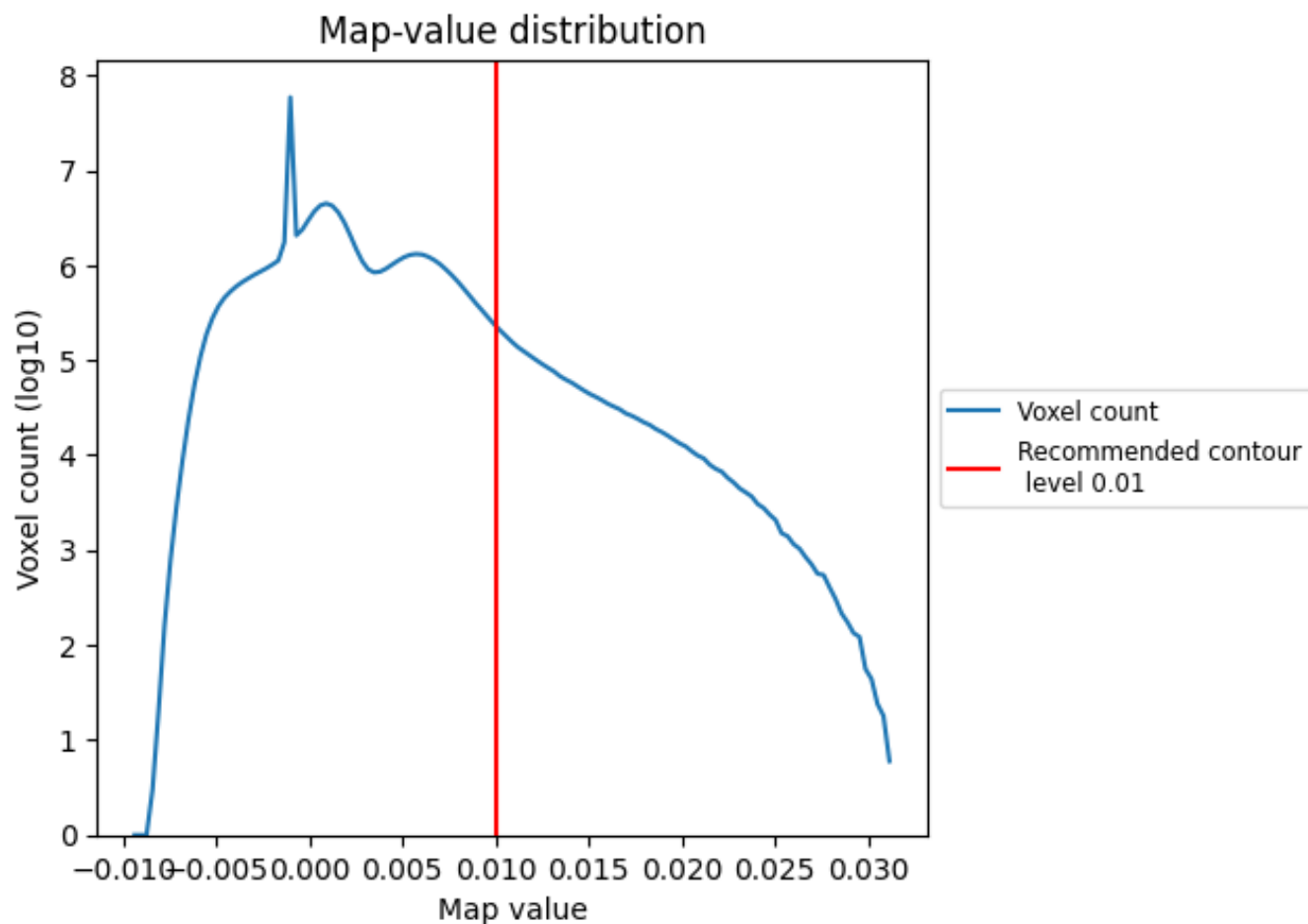


Z

7 Map analysis [i](#)

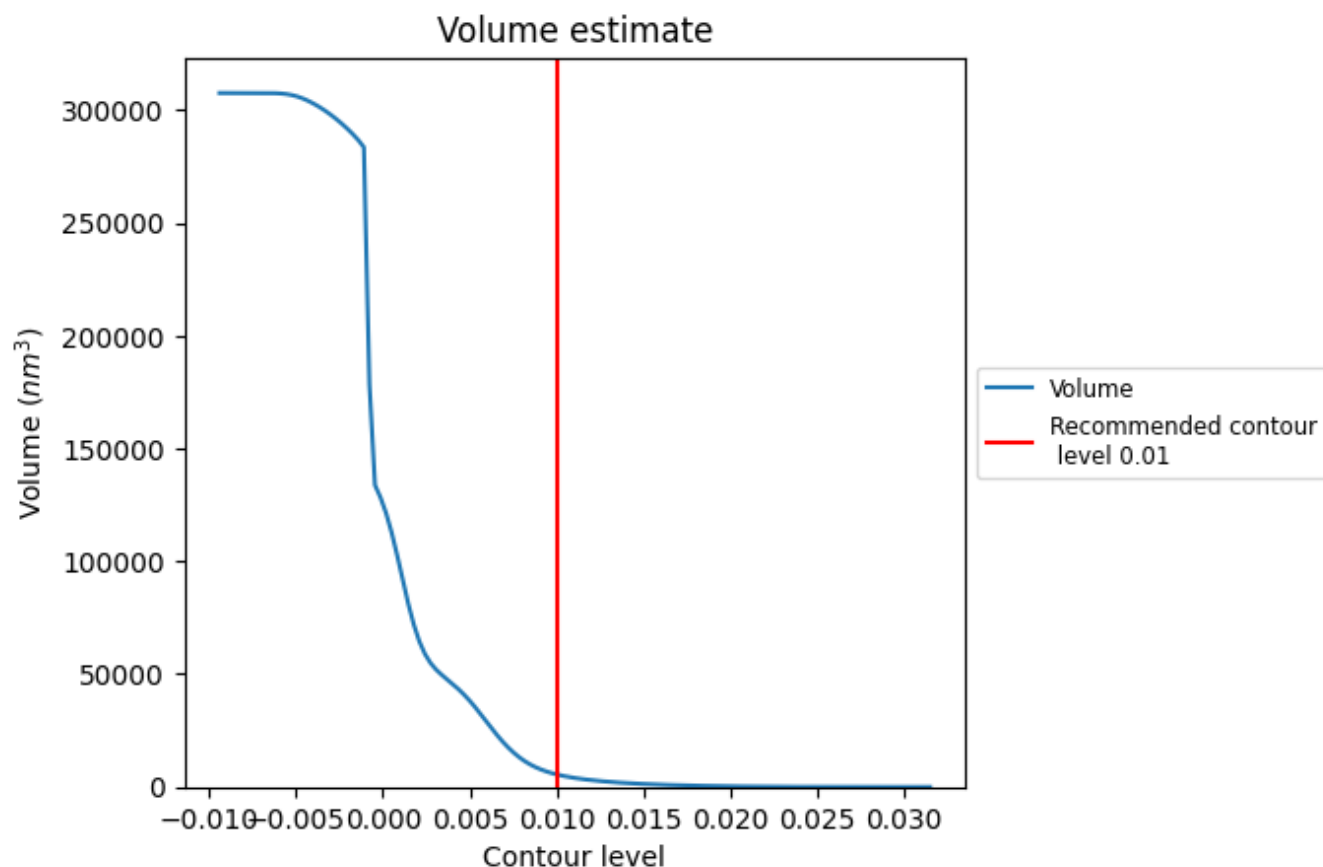
This section contains the results of statistical analysis of the map.

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.

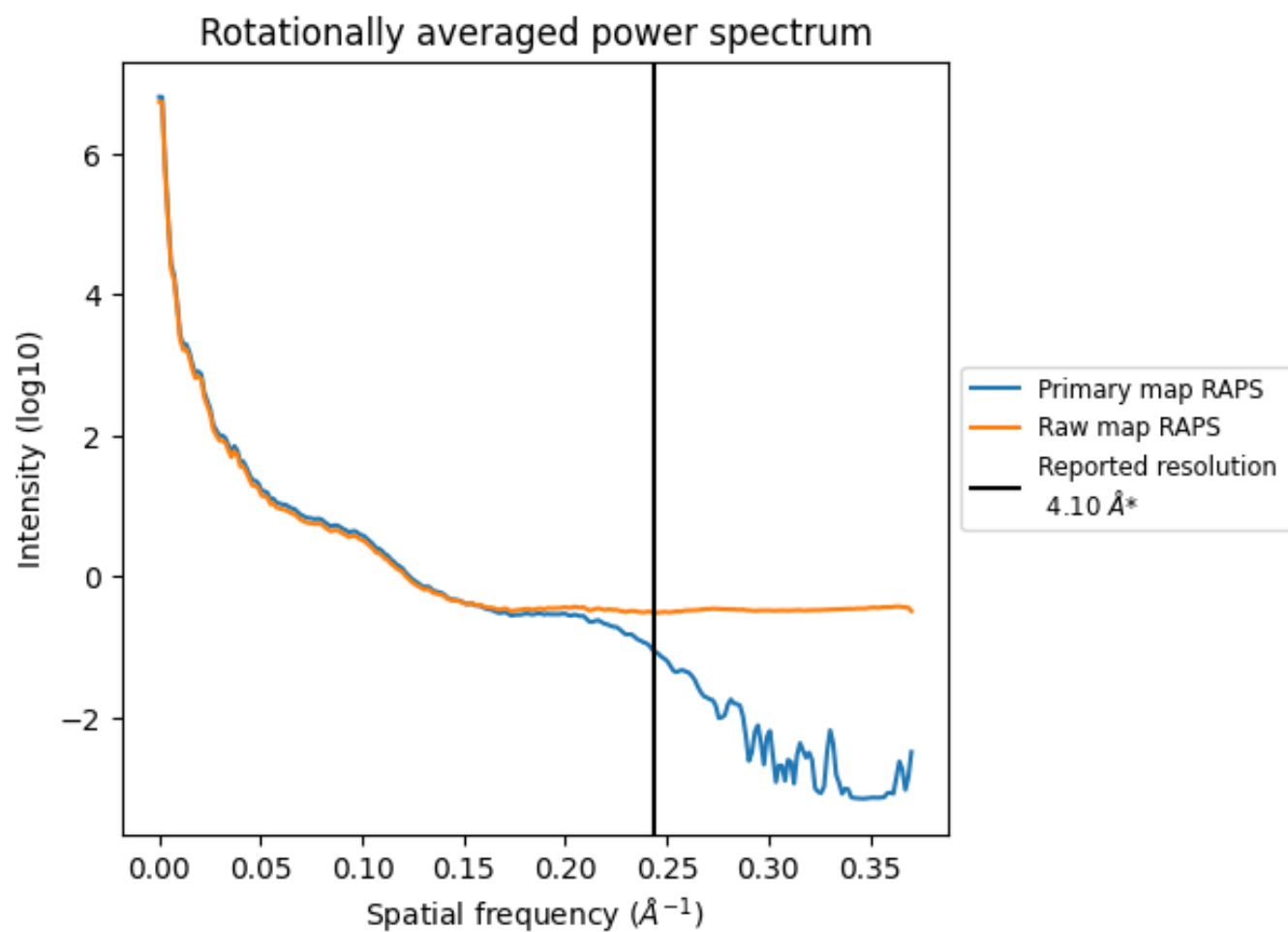
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5555 nm^3 ; this corresponds to an approximate mass of 5018 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 ⓘ

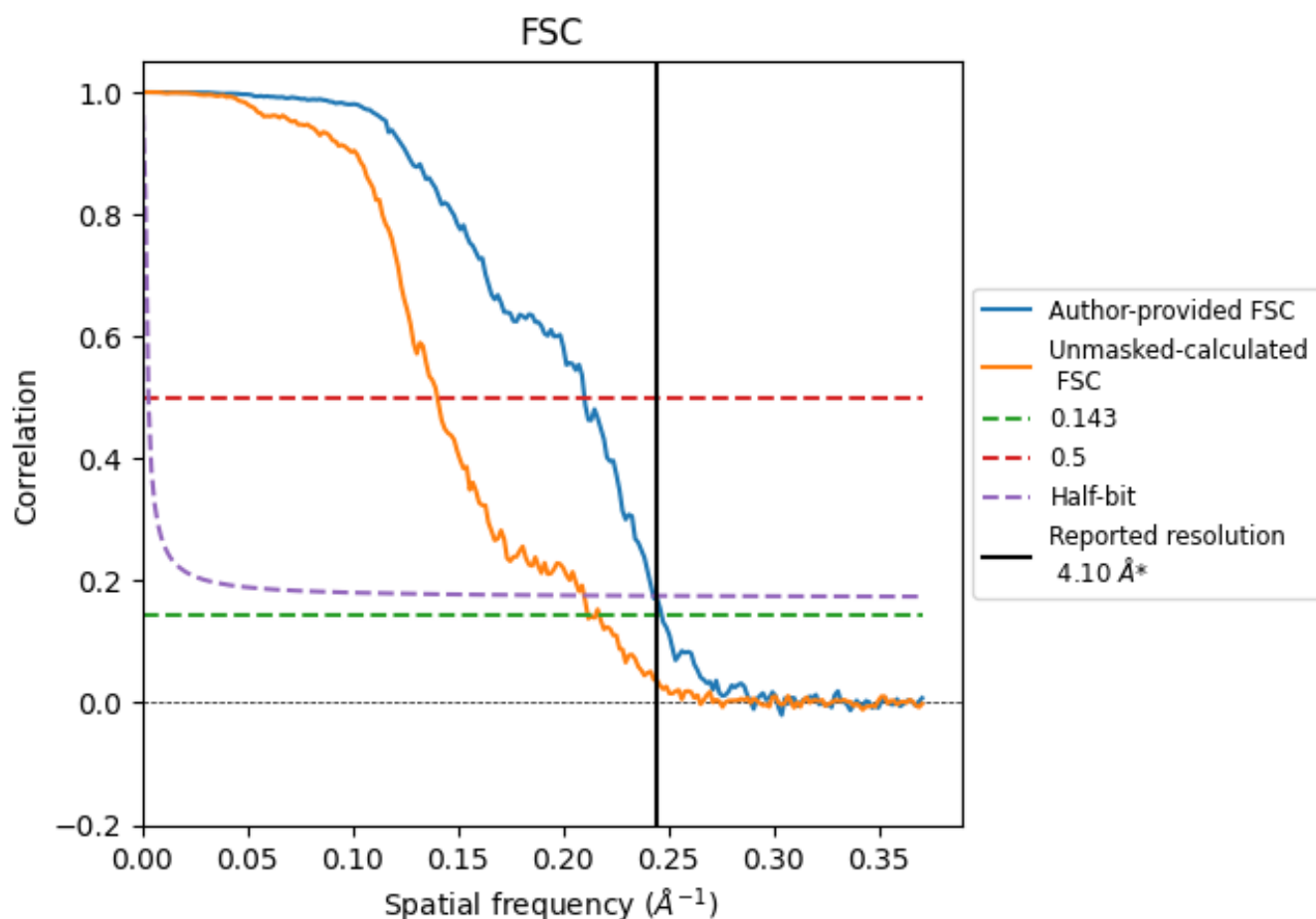


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

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 0.244 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.05	4.76	4.12
Unmasked-calculated*	4.73	7.13	4.77

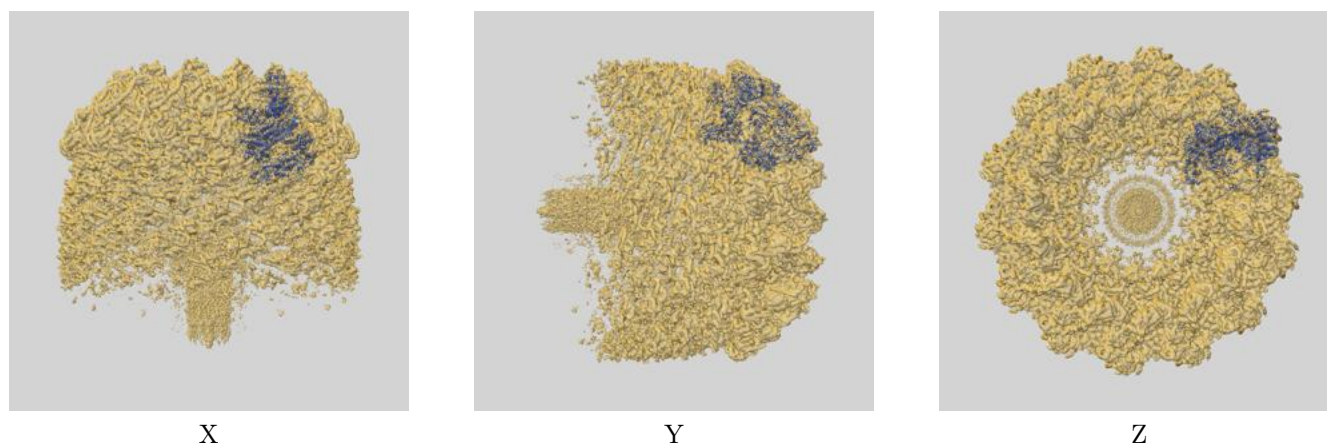
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.73 differs from the reported value 4.1 by more than 10 %

9 Map-model fit [i](#)

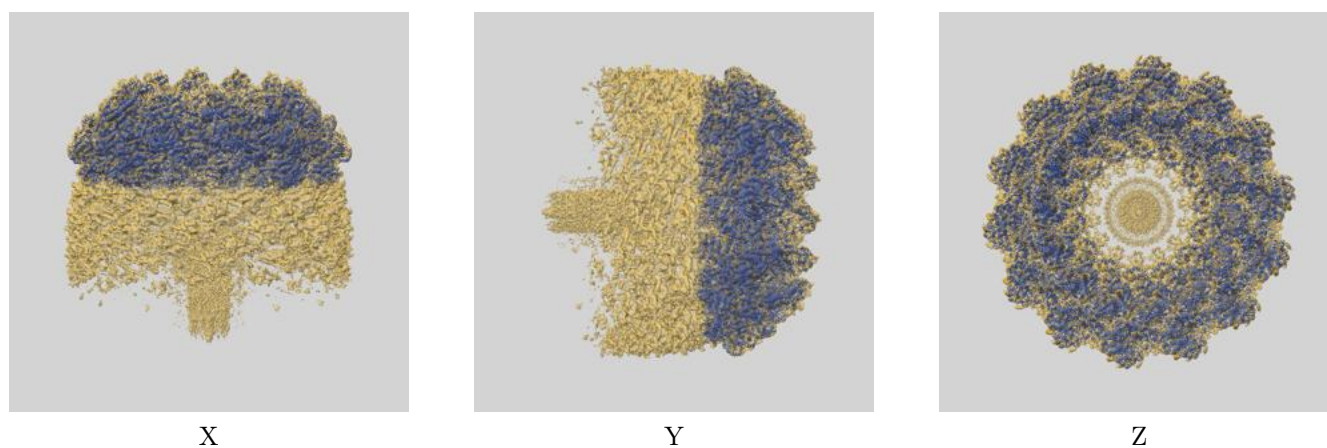
This section contains information regarding the fit between EMDB map EMD-51792 and PDB model 9H2B. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

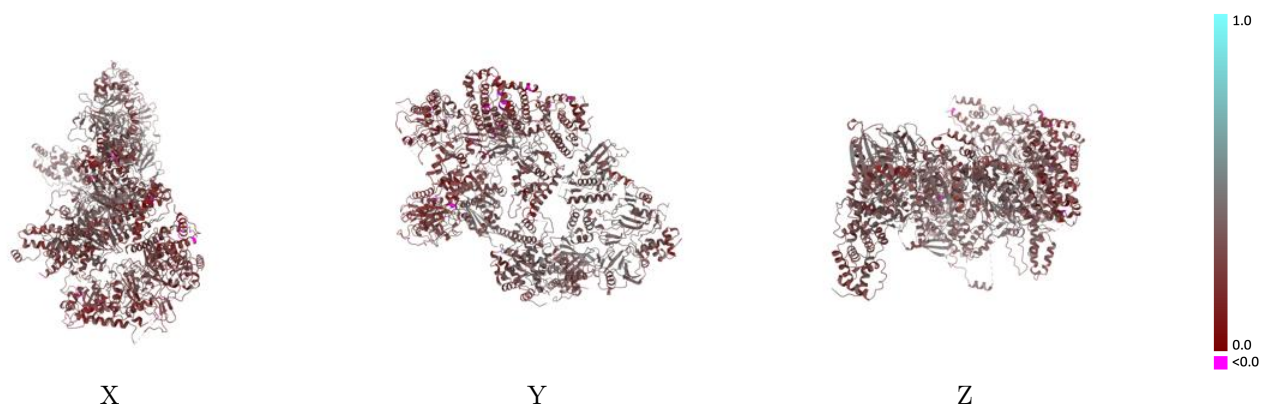


9.1.2 Map-model assembly overlay [i](#)



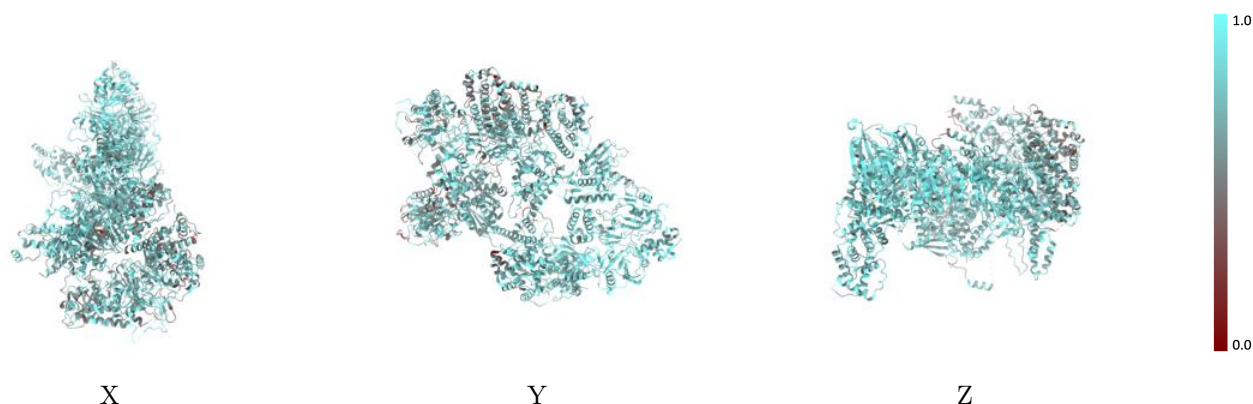
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



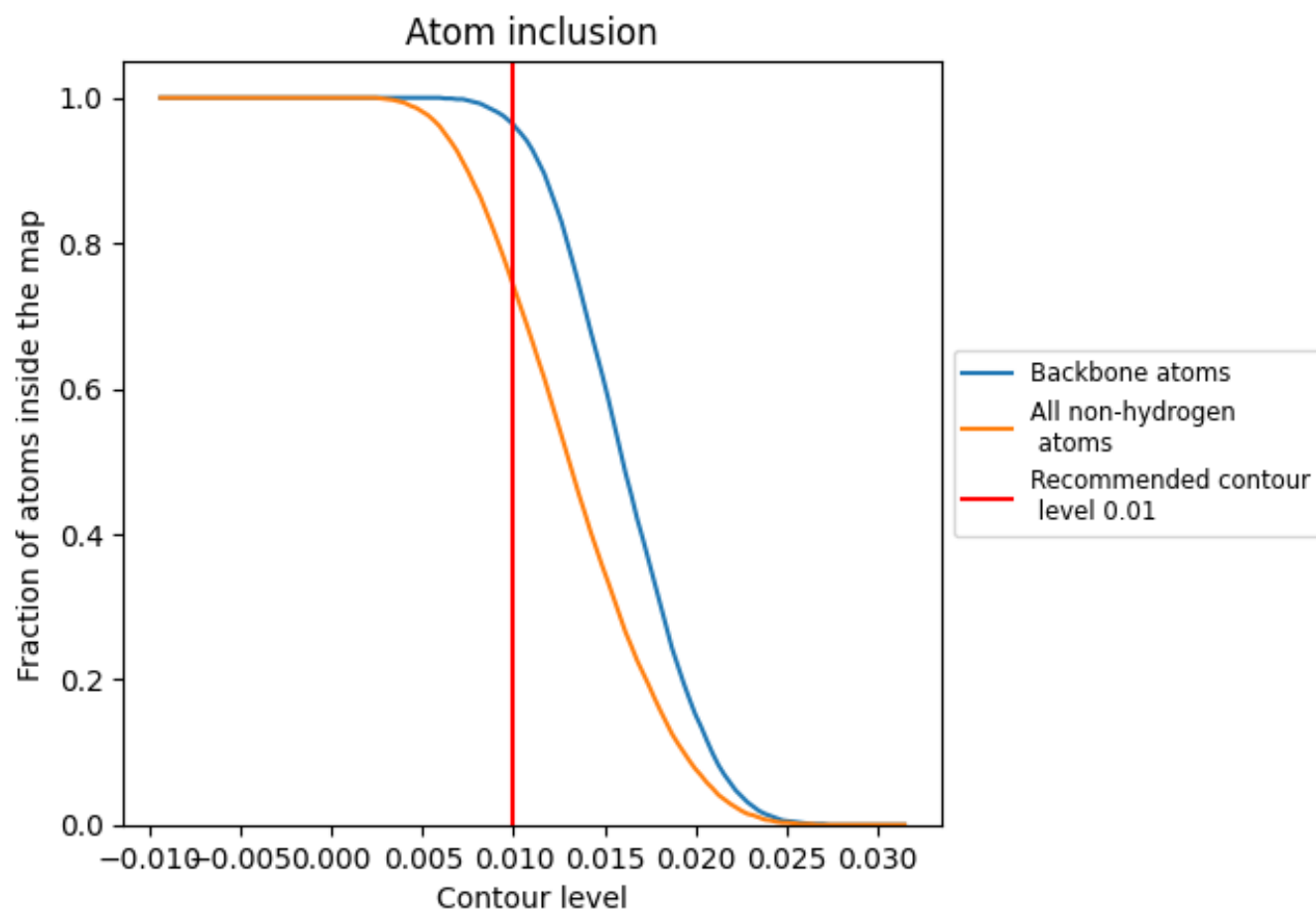
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 74% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7410	<div></div> 0.3080
A	<div></div> 0.7590	<div></div> 0.3490
B	<div></div> 0.7200	<div></div> 0.3070
C	<div></div> 0.7970	<div></div> 0.3270
D	<div></div> 0.7700	<div></div> 0.3090
E	<div></div> 0.6560	<div></div> 0.2520
F	<div></div> 0.8190	<div></div> 0.3610
G	<div></div> 0.6770	<div></div> 0.2650
H	<div></div> 0.7690	<div></div> 0.3250
I	<div></div> 0.7110	<div></div> 0.2640
J	<div></div> 0.6420	<div></div> 0.2560
K	<div></div> 0.5880	<div></div> 0.2370
L	<div></div> 0.8390	<div></div> 0.3820
M	<div></div> 0.6960	<div></div> 0.2460
N	<div></div> 0.7770	<div></div> 0.3290

1.0

0.0

<0.0