



Full wwPDB EM Validation Report ⓘ

Dec 2, 2025 – 04:30 PM EST

PDB ID : 9N8A / pdb_00009n8a
EMDB ID : EMD-49125
Title : In situ structure of the sheathed FlaD flagellar filament in *Vibrio cholerae*
Authors : Wangbiao, G.; Jun, L.
Deposited on : 2025-02-08
Resolution : 2.92 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.dev129
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

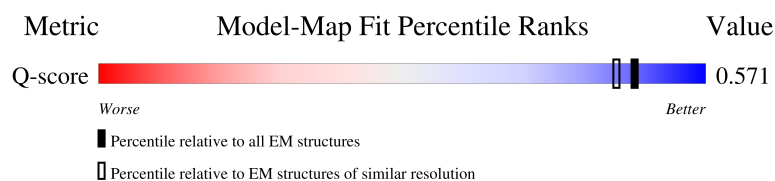
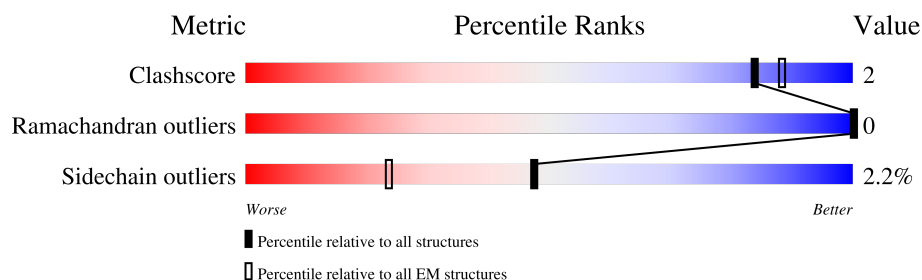
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.92 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.



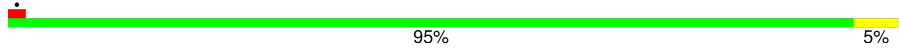
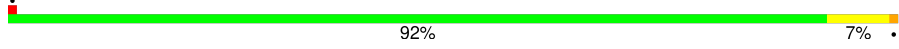
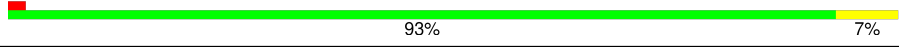
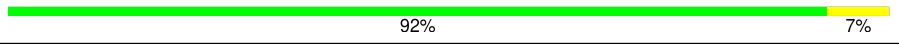
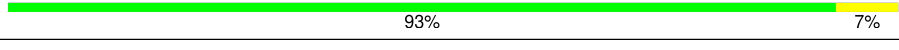
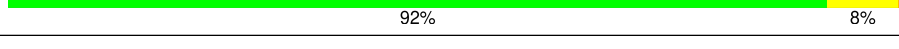
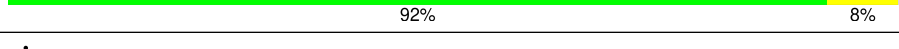
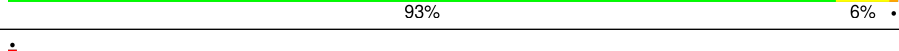
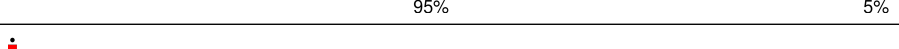
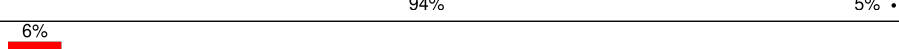
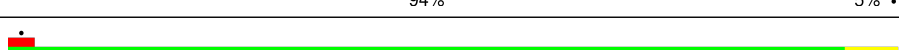
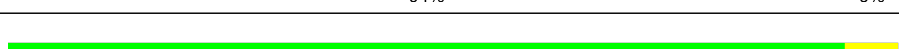
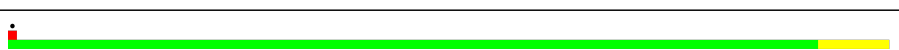
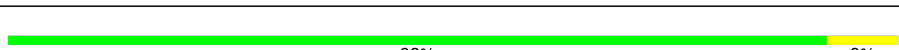
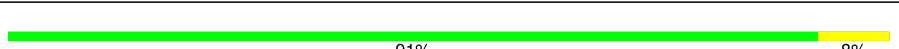

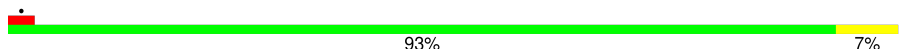
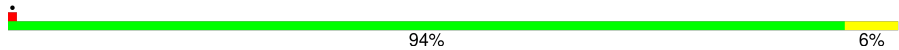
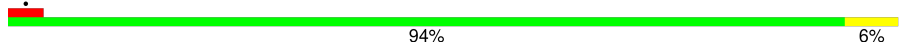
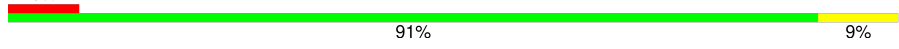
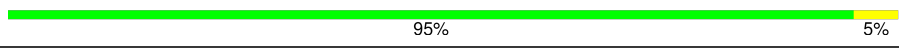
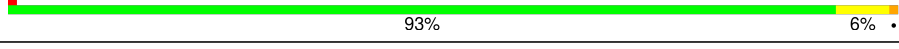
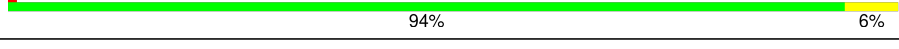


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	13007 (2.42 - 3.42)

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	A1	377	
1	A2	377	
1	A3	377	
1	B1	377	

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Mol	Chain	Length	Quality of chain
1	B2	377	
1	B3	377	
1	C1	377	
1	C2	377	
1	C3	377	
1	D1	377	
1	E1	377	
1	F1	377	
1	G1	377	
1	H1	377	
1	I1	377	
1	J1	377	
1	K1	377	
1	L1	377	
1	M1	377	
1	N1	377	
1	O1	377	
1	P1	377	
1	Q1	377	
1	R1	377	
1	S1	377	
1	T1	377	
1	U1	377	
1	V1	377	
1	W1	377	

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Mol	Chain	Length	Quality of chain
1	X1	377	<div><div></div><div>92%</div><div>8%</div></div>
1	Y1	377	<div><div></div><div>92%</div><div>8%</div></div>
1	Z1	377	<div><div>8%</div><div>92%</div><div>7%</div></div>
1	a1	377	<div><div></div><div>95%</div><div>5%</div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 182292 atoms, of which 90387 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 Flagellin D.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A1	376	Total 5524	C 1685	H 2739	N 501	O 589	S 10	0	0
1	B1	376	Total 5524	C 1685	H 2739	N 501	O 589	S 10	0	0
1	C1	376	Total 5524	C 1685	H 2739	N 501	O 589	S 10	0	0
1	D1	376	Total 5524	C 1685	H 2739	N 501	O 589	S 10	0	0
1	E1	376	Total 5524	C 1685	H 2739	N 501	O 589	S 10	0	0
1	F1	376	Total 5524	C 1685	H 2739	N 501	O 589	S 10	0	0
1	G1	376	Total 5524	C 1685	H 2739	N 501	O 589	S 10	0	0
1	H1	376	Total 5524	C 1685	H 2739	N 501	O 589	S 10	0	0
1	I1	376	Total 5524	C 1685	H 2739	N 501	O 589	S 10	0	0
1	J1	376	Total 5524	C 1685	H 2739	N 501	O 589	S 10	0	0
1	K1	376	Total 5524	C 1685	H 2739	N 501	O 589	S 10	0	0
1	L1	376	Total 5524	C 1685	H 2739	N 501	O 589	S 10	0	0
1	M1	376	Total 5524	C 1685	H 2739	N 501	O 589	S 10	0	0
1	N1	376	Total 5524	C 1685	H 2739	N 501	O 589	S 10	0	0
1	O1	376	Total 5524	C 1685	H 2739	N 501	O 589	S 10	0	0
1	P1	376	Total 5524	C 1685	H 2739	N 501	O 589	S 10	0	0
1	Q1	376	Total 5524	C 1685	H 2739	N 501	O 589	S 10	0	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
1	R1	376	Total	C	H	N	O	S	0	0
			5524	1685	2739	501	589	10		
1	S1	376	Total	C	H	N	O	S	0	0
			5524	1685	2739	501	589	10		
1	T1	376	Total	C	H	N	O	S	0	0
			5524	1685	2739	501	589	10		
1	U1	376	Total	C	H	N	O	S	0	0
			5524	1685	2739	501	589	10		
1	V1	376	Total	C	H	N	O	S	0	0
			5524	1685	2739	501	589	10		
1	W1	376	Total	C	H	N	O	S	0	0
			5524	1685	2739	501	589	10		
1	X1	376	Total	C	H	N	O	S	0	0
			5524	1685	2739	501	589	10		
1	Y1	376	Total	C	H	N	O	S	0	0
			5524	1685	2739	501	589	10		
1	Z1	376	Total	C	H	N	O	S	0	0
			5524	1685	2739	501	589	10		
1	a1	376	Total	C	H	N	O	S	0	0
			5524	1685	2739	501	589	10		
1	A2	376	Total	C	H	N	O	S	0	0
			5524	1685	2739	501	589	10		
1	B2	376	Total	C	H	N	O	S	0	0
			5524	1685	2739	501	589	10		
1	C2	376	Total	C	H	N	O	S	0	0
			5524	1685	2739	501	589	10		
1	A3	376	Total	C	H	N	O	S	0	0
			5524	1685	2739	501	589	10		
1	B3	376	Total	C	H	N	O	S	0	0
			5524	1685	2739	501	589	10		
1	C3	376	Total	C	H	N	O	S	0	0
			5524	1685	2739	501	589	10		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

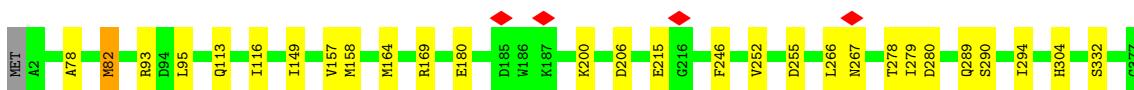
- Molecule 1: Flagellin D

Chain A1: 



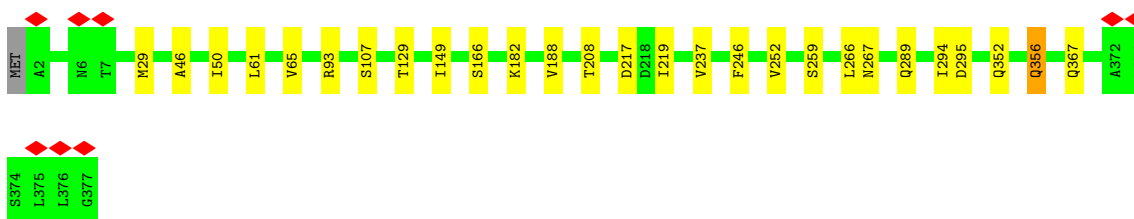
- Molecule 1: Flagellin D

Chain B1: 



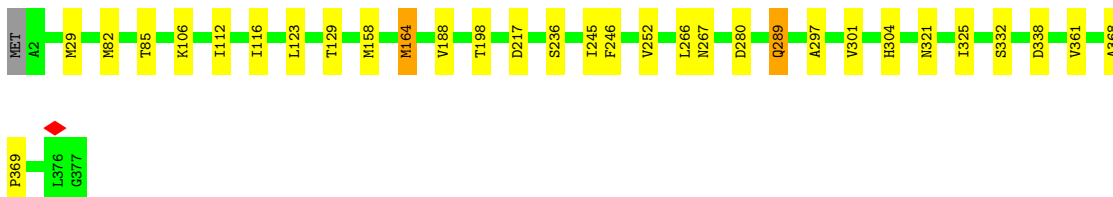
- Molecule 1: Flagellin D

Chain C1: 



- Molecule 1: Flagellin D

Chain D1: 



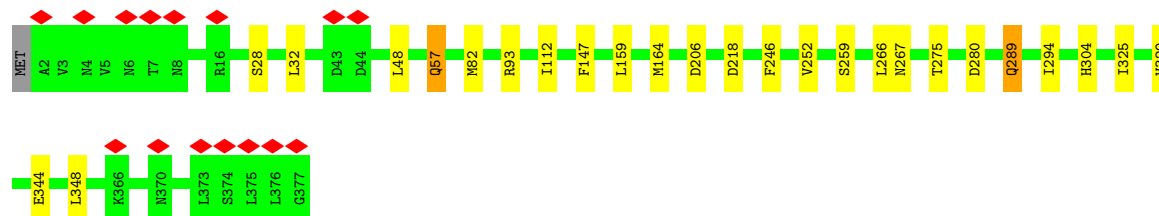
- Molecule 1: Flagellin D

Chain E1:  92% 8%



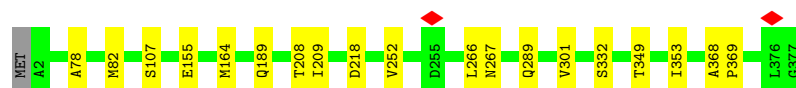
• Molecule 1: Flagellin D

Chain F1:  93% 6%



• Molecule 1: Flagellin D

Chain G1:  95% 5%



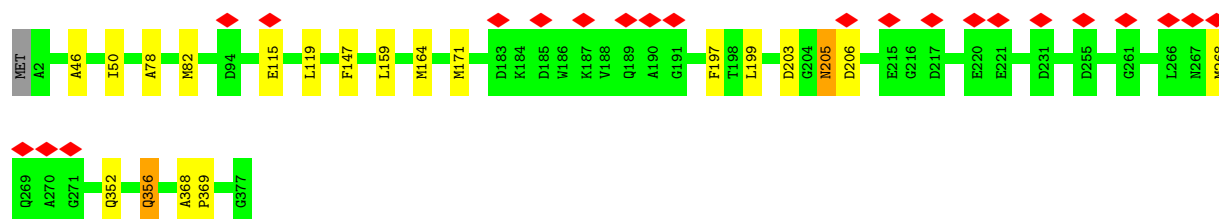
• Molecule 1: Flagellin D

Chain H1:  94% 5%



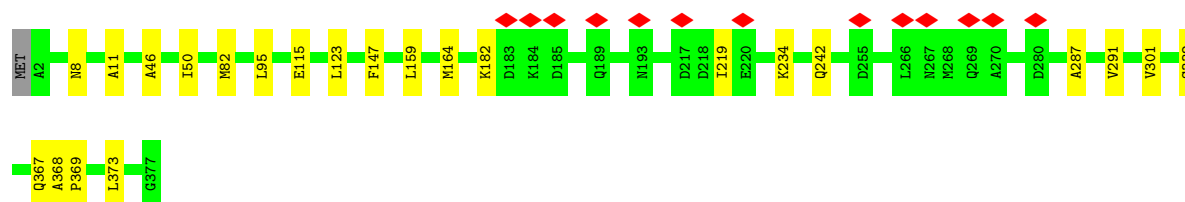
• Molecule 1: Flagellin D

Chain I1:  94% 5% 6%



• Molecule 1: Flagellin D

Chain J1:  94% 6%



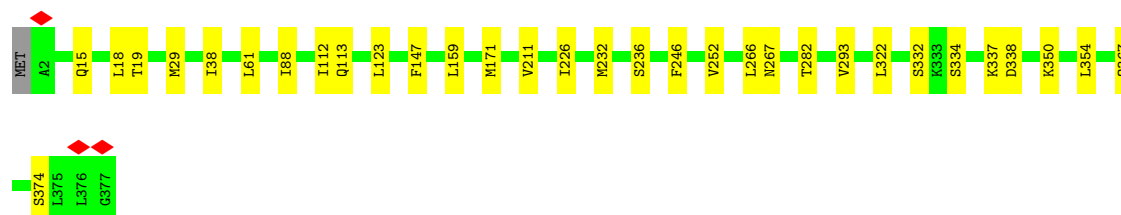
- Molecule 1: Flagellin D

Chain K1: 94% 6%



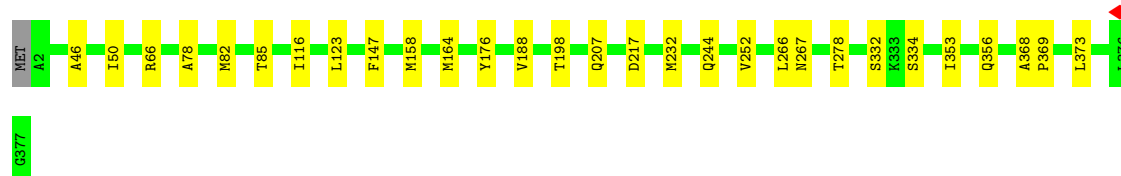
- Molecule 1: Flagellin D

Chain L1: 91% 8%



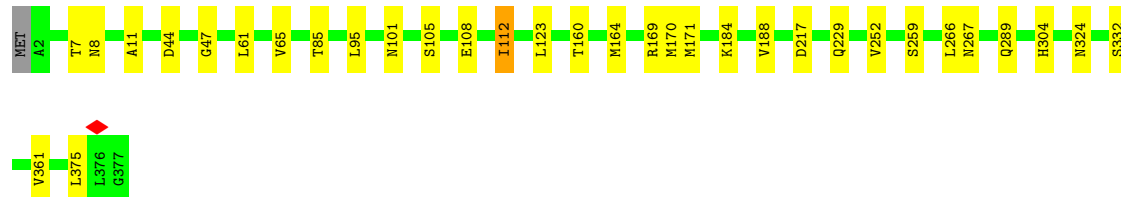
- Molecule 1: Flagellin D

Chain M1: 92% 8%



- Molecule 1: Flagellin D

Chain N1: 91% 8%

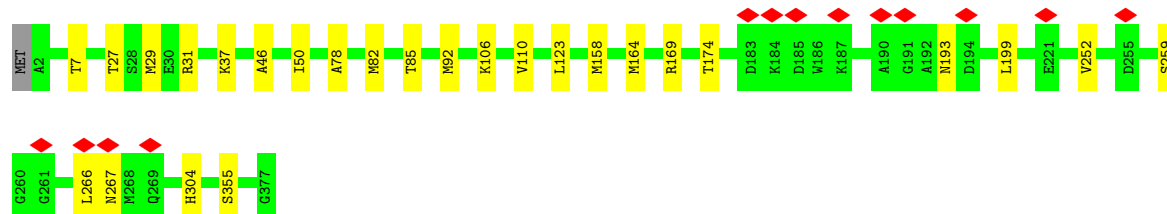


- Molecule 1: Flagellin D

Chain O1: 94% 6%



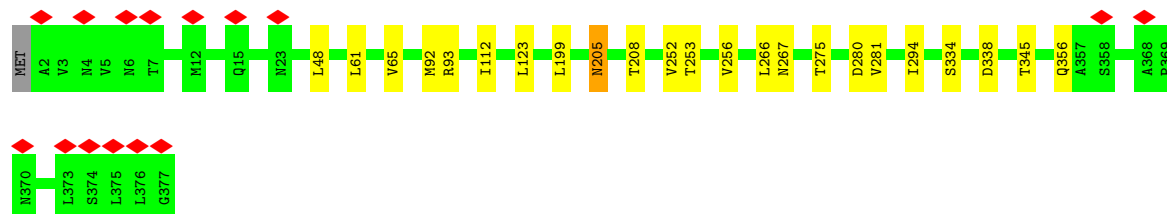
- Molecule 1: Flagellin D



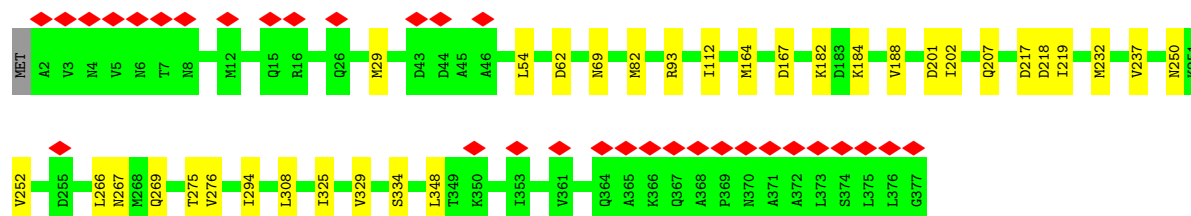
- Molecule 1: Flagellin D



- Molecule 1: Flagellin D



- Molecule 1: Flagellin D



- Molecule 1: Flagellin D





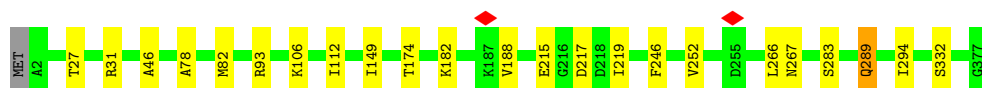
- Molecule 1: Flagellin D

Chain U1: 93% 6%



- Molecule 1: Flagellin D

Chain V1: 94% 6%



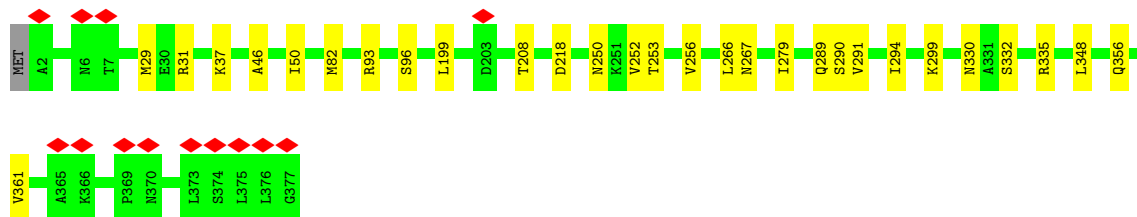
- Molecule 1: Flagellin D

Chain W1: 92% 7%



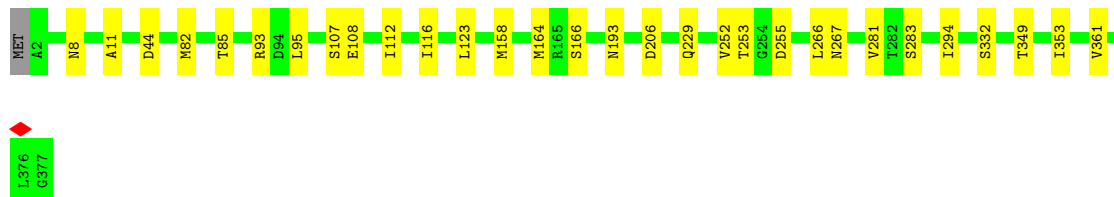
- Molecule 1: Flagellin D

Chain X1: 92% 8%

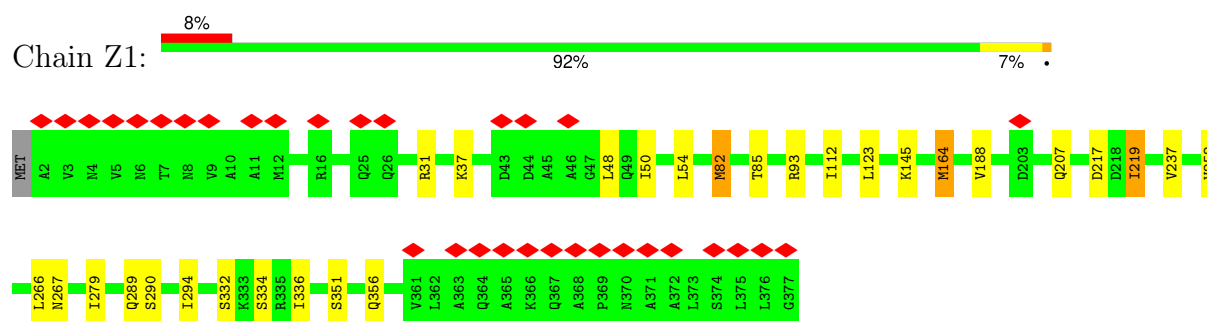


- Molecule 1: Flagellin D

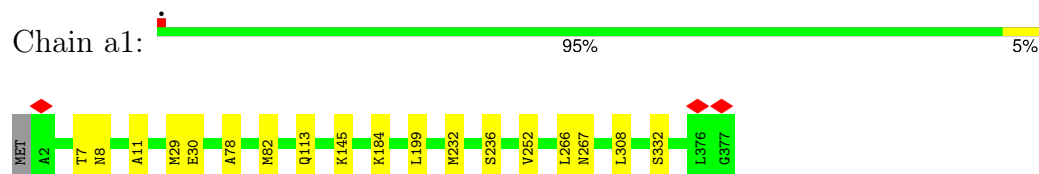
Chain Y1: 92% 8%



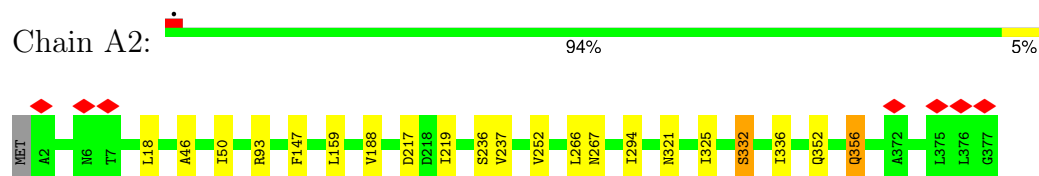
- Molecule 1: Flagellin D



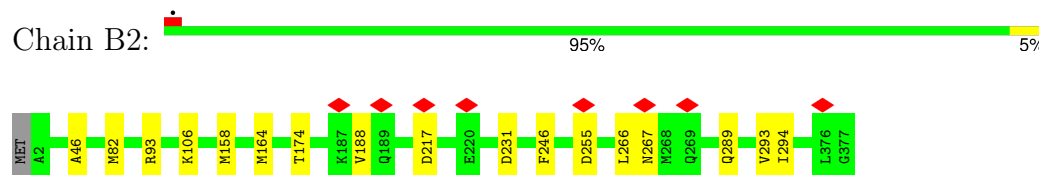
- Molecule 1: Flagellin D



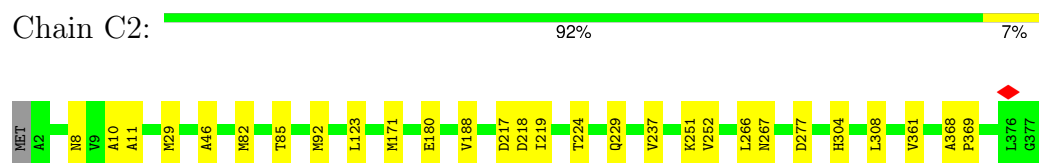
- Molecule 1: Flagellin D



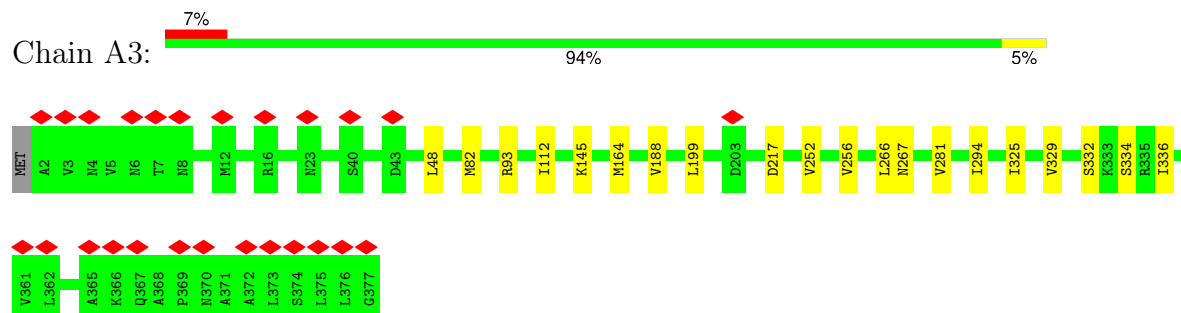
- Molecule 1: Flagellin D



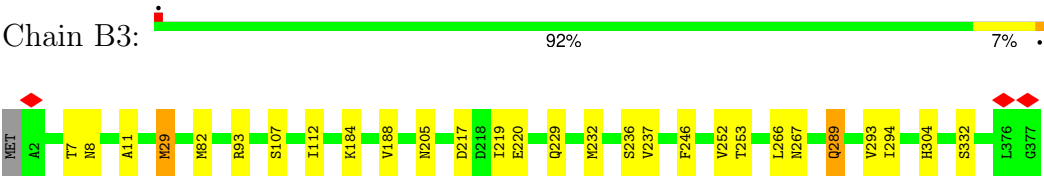
- Molecule 1: Flagellin D



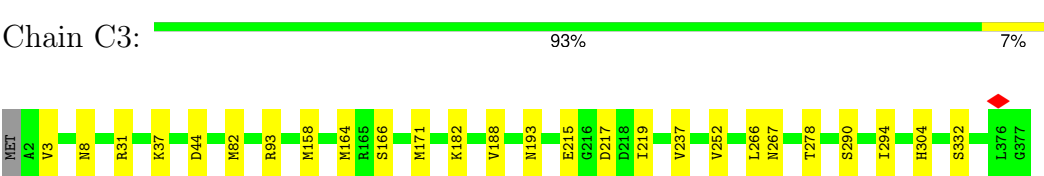
- Molecule 1: Flagellin D



● Molecule 1: Flagellin D



● Molecule 1: Flagellin D



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	2331318	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	70	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.152	Depositor
Minimum map value	-0.695	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	478.464, 478.464, 478.464	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.068, 1.068, 1.068	Depositor

5 Model quality

5.1 Standard geometry

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	A1	0.17	0/2803	0.27	0/3783
1	A2	0.16	0/2803	0.25	0/3783
1	A3	0.15	0/2803	0.27	0/3783
1	B1	0.15	0/2803	0.28	0/3783
1	B2	0.15	0/2803	0.26	0/3783
1	B3	0.17	0/2803	0.27	0/3783
1	C1	0.16	0/2803	0.26	0/3783
1	C2	0.17	0/2803	0.27	0/3783
1	C3	0.17	0/2803	0.27	0/3783
1	D1	0.17	0/2803	0.27	0/3783
1	E1	0.16	0/2803	0.26	0/3783
1	F1	0.15	0/2803	0.26	0/3783
1	G1	0.17	0/2803	0.26	0/3783
1	H1	0.16	0/2803	0.26	0/3783
1	I1	0.13	0/2803	0.25	0/3783
1	J1	0.14	0/2803	0.25	0/3783
1	K1	0.17	0/2803	0.26	0/3783
1	L1	0.16	0/2803	0.26	0/3783
1	M1	0.16	0/2803	0.25	0/3783
1	N1	0.17	0/2803	0.27	0/3783
1	O1	0.16	0/2803	0.26	0/3783
1	P1	0.14	0/2803	0.24	0/3783
1	Q1	0.17	0/2803	0.26	0/3783
1	R1	0.15	0/2803	0.24	0/3783
1	S1	0.15	0/2803	0.26	0/3783
1	T1	0.16	0/2803	0.26	0/3783
1	U1	0.17	0/2803	0.25	0/3783
1	V1	0.16	0/2803	0.27	0/3783
1	W1	0.17	0/2803	0.28	0/3783
1	X1	0.16	0/2803	0.26	0/3783
1	Y1	0.16	0/2803	0.26	0/3783
1	Z1	0.15	0/2803	0.25	0/3783
1	a1	0.17	0/2803	0.26	0/3783
All	All	0.16	0/92499	0.26	0/124839

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	A1	2785	2739	2738	11	0
1	A2	2785	2739	2738	9	0
1	A3	2785	2739	2738	12	0
1	B1	2785	2739	2738	15	0
1	B2	2785	2739	2738	11	0
1	B3	2785	2739	2738	17	0
1	C1	2785	2739	2738	14	0
1	C2	2785	2739	2738	15	0
1	C3	2785	2739	2738	19	0
1	D1	2785	2739	2738	16	0
1	E1	2785	2739	2738	14	0
1	F1	2785	2739	2738	13	0
1	G1	2785	2739	2738	10	0
1	H1	2785	2739	2738	11	0
1	I1	2785	2739	2738	12	0
1	J1	2785	2739	2738	12	0
1	K1	2785	2739	2738	12	0
1	L1	2785	2739	2738	17	0
1	M1	2785	2739	2738	14	0
1	N1	2785	2739	2738	18	0
1	O1	2785	2739	2738	10	0
1	P1	2785	2739	2738	18	0
1	Q1	2785	2739	2738	11	0
1	R1	2785	2739	2738	14	0
1	S1	2785	2739	2738	21	0
1	T1	2785	2739	2738	9	0
1	U1	2785	2739	2738	15	0
1	V1	2785	2739	2738	11	0
1	W1	2785	2739	2738	13	0
1	X1	2785	2739	2738	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Y1	2785	2739	2738	13	0
1	Z1	2785	2739	2738	16	0
1	a1	2785	2739	2738	11	0
All	All	91905	90387	90354	397	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 2.

All (397) 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:D1:321:ASN:O	1:D1:325:ILE:HD12	1.85	0.75
1:W1:170:MET:HE2	1:W1:170:MET:HA	1.69	0.75
1:S1:325:ILE:O	1:S1:329:VAL:HG23	1.87	0.74
1:K1:7:THR:HG21	1:L1:334:SER:HB2	1.70	0.73
1:R1:205:ASN:O	1:R1:205:ASN:ND2	2.20	0.72
1:B2:82:MET:HE2	1:B2:164:MET:HE3	1.71	0.72
1:A3:82:MET:SD	1:A3:164:MET:HE3	2.30	0.71
1:D1:158:MET:HE2	1:F1:218:ASP:OD2	1.91	0.70
1:W1:232:MET:HA	1:W1:232:MET:HE2	1.72	0.70
1:A1:170:MET:HE2	1:A1:170:MET:HA	1.74	0.69
1:B1:82:MET:SD	1:B1:164:MET:HE3	2.35	0.67
1:B3:82:MET:HE1	1:B3:304:HIS:ND1	2.10	0.66
1:I1:268:MET:HE3	1:I1:268:MET:HA	1.78	0.66
1:I1:352:GLN:O	1:I1:356:GLN:NE2	2.30	0.64
1:V1:106:LYS:HE2	1:V1:106:LYS:H	1.63	0.63
1:W1:61:LEU:O	1:W1:65:VAL:HG23	1.98	0.63
1:A3:334:SER:HB2	1:B3:7:THR:HG21	1.80	0.63
1:J1:182:LYS:HG3	1:J1:219:ILE:HD11	1.79	0.63
1:K1:7:THR:HG22	1:L1:338:ASP:OD2	1.98	0.63
1:N1:170:MET:HE2	1:N1:170:MET:HA	1.80	0.63
1:Y1:95:LEU:HD22	1:Y1:112:ILE:HG23	1.82	0.62
1:A3:332:SER:O	1:A3:336:ILE:HD12	2.00	0.62
1:A2:352:GLN:O	1:A2:356:GLN:NE2	2.32	0.62
1:H1:349:THR:O	1:H1:353:ILE:HD12	2.00	0.62
1:E1:164:MET:HE3	1:E1:301:VAL:HG22	1.81	0.61
1:Z1:334:SER:HB2	1:a1:7:THR:HG21	1.81	0.61
1:C1:352:GLN:O	1:C1:356:GLN:NE2	2.35	0.60
1:L1:350:LYS:O	1:L1:354:LEU:HD12	2.02	0.59
1:R1:205:ASN:HD22	1:R1:205:ASN:C	2.05	0.59
1:Q1:46:ALA:HB2	1:R1:112:ILE:HG13	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N1:61:LEU:O	1:N1:65:VAL:HG23	2.02	0.58
1:S1:334:SER:HB2	1:U1:7:THR:HG21	1.86	0.57
1:F1:348:LEU:C	1:F1:348:LEU:HD23	2.29	0.57
1:Y1:108:GLU:O	1:Y1:112:ILE:HD12	2.04	0.57
1:R1:199:LEU:HB3	1:R1:256:VAL:HG22	1.87	0.57
1:M1:188:VAL:HG23	1:M1:217:ASP:O	2.05	0.57
1:Z1:188:VAL:HG23	1:Z1:217:ASP:O	2.04	0.57
1:W1:321:ASN:O	1:W1:325:ILE:HD12	2.05	0.57
1:B3:232:MET:HA	1:B3:232:MET:HE2	1.87	0.56
1:A3:48:LEU:HD13	1:A3:48:LEU:C	2.29	0.56
1:B3:188:VAL:HG23	1:B3:217:ASP:O	2.05	0.56
1:Z1:336:ILE:HD12	1:Z1:336:ILE:H	1.70	0.56
1:I1:46:ALA:HB2	1:W1:112:ILE:HG13	1.87	0.56
1:Y1:85:THR:HG23	1:Y1:123:LEU:HD22	1.87	0.56
1:A2:332:SER:O	1:A2:336:ILE:HD12	2.07	0.55
1:a1:199:LEU:HD11	1:a1:232:MET:CE	2.36	0.55
1:D1:112:ILE:HG13	1:J1:46:ALA:HB2	1.87	0.55
1:G1:82:MET:HE1	1:G1:164:MET:HE3	1.88	0.55
1:X1:348:LEU:C	1:X1:348:LEU:HD23	2.32	0.55
1:J1:82:MET:HE2	1:J1:164:MET:HE3	1.89	0.54
1:B3:82:MET:HE1	1:B3:304:HIS:CE1	2.42	0.54
1:Z1:50:ILE:O	1:Z1:54:LEU:HD22	2.08	0.53
1:C3:31:ARG:HD3	1:C3:37:LYS:HA	1.90	0.53
1:O1:188:VAL:HG23	1:O1:217:ASP:O	2.08	0.53
1:Y1:158:MET:HE1	1:a1:184:LYS:HA	1.89	0.53
1:B3:289:GLN:HE21	1:B3:289:GLN:HA	1.73	0.53
1:F1:48:LEU:HD23	1:F1:48:LEU:O	2.09	0.53
1:Y1:116:ILE:HD12	1:Y1:281:VAL:HG21	1.91	0.53
1:A3:188:VAL:HG23	1:A3:217:ASP:O	2.09	0.53
1:V1:78:ALA:O	1:V1:82:MET:HE3	2.09	0.53
1:B1:246:PHE:HB2	1:B1:289:GLN:NE2	2.24	0.52
1:U1:232:MET:HE2	1:U1:251:LYS:HD3	1.91	0.52
1:P1:199:LEU:N	1:P1:199:LEU:HD23	2.25	0.52
1:C3:219:ILE:HG22	1:C3:237:VAL:CG2	2.39	0.52
1:B2:231:ASP:OD2	1:B2:231:ASP:C	2.52	0.52
1:R1:61:LEU:O	1:R1:65:VAL:HG23	2.09	0.52
1:U1:246:PHE:HB2	1:U1:289:GLN:NE2	2.25	0.52
1:A1:361:VAL:HG13	1:a1:29:MET:HG2	1.91	0.52
1:R1:48:LEU:HD23	1:R1:48:LEU:C	2.34	0.51
1:Q1:218:ASP:C	1:Q1:218:ASP:OD1	2.53	0.51
1:C3:82:MET:CE	1:C3:164:MET:HE3	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F1:28:SER:O	1:F1:32:LEU:HD12	2.10	0.51
1:F1:57:GLN:OE1	1:F1:329:VAL:HG21	2.09	0.51
1:Z1:48:LEU:HD23	1:Z1:48:LEU:C	2.35	0.51
1:K1:218:ASP:OD2	1:K1:218:ASP:C	2.54	0.51
1:S1:82:MET:HE3	1:S1:308:LEU:CD1	2.41	0.51
1:V1:27:THR:HG22	1:V1:31:ARG:HE	1.76	0.51
1:Q1:246:PHE:CE1	1:Q1:293:VAL:HG22	2.46	0.51
1:Z1:332:SER:O	1:Z1:336:ILE:HD12	2.11	0.51
1:S1:275:THR:HG22	1:S1:276:VAL:N	2.26	0.51
1:G1:208:THR:HG23	1:G1:208:THR:O	2.10	0.50
1:L1:112:ILE:HG13	1:M1:46:ALA:HB2	1.93	0.50
1:S1:184:LYS:HA	1:U1:158:MET:HE1	1.92	0.50
1:K1:82:MET:CE	1:K1:164:MET:HE3	2.41	0.50
1:M1:82:MET:SD	1:M1:164:MET:HE3	2.50	0.50
1:D1:246:PHE:HB2	1:D1:289:GLN:NE2	2.26	0.50
1:Y1:361:VAL:HG13	1:C2:29:MET:HG2	1.94	0.50
1:M1:158:MET:HE1	1:N1:184:LYS:HA	1.93	0.50
1:Z1:93:ARG:HB2	1:Z1:294:ILE:HG21	1.93	0.50
1:B2:188:VAL:HG23	1:B2:217:ASP:O	2.11	0.50
1:B1:280:ASP:C	1:B1:280:ASP:OD2	2.55	0.50
1:T1:219:ILE:HG22	1:T1:237:VAL:HG21	1.93	0.50
1:H1:361:VAL:HG13	1:X1:29:MET:HG2	1.94	0.50
1:I1:115:GLU:O	1:I1:119:LEU:HD22	2.12	0.50
1:C3:44:ASP:OD1	1:C3:44:ASP:C	2.55	0.50
1:C1:266:LEU:O	1:C1:267:ASN:C	2.53	0.49
1:E1:188:VAL:HG23	1:E1:217:ASP:O	2.12	0.49
1:P1:82:MET:SD	1:P1:164:MET:HE2	2.52	0.49
1:S1:348:LEU:C	1:S1:348:LEU:HD23	2.36	0.49
1:C3:215:GLU:OE2	1:C3:215:GLU:N	2.45	0.49
1:A1:114:GLU:OE1	1:A1:114:GLU:O	2.30	0.49
1:O1:15:GLN:O	1:O1:19:THR:HG23	2.12	0.49
1:S1:188:VAL:HG23	1:S1:217:ASP:O	2.12	0.49
1:D1:338:ASP:OD2	1:E1:7:THR:HG22	2.12	0.49
1:T1:188:VAL:HG23	1:T1:217:ASP:O	2.13	0.49
1:Q1:46:ALA:O	1:Q1:50:ILE:HG22	2.13	0.49
1:O1:266:LEU:O	1:O1:267:ASN:C	2.55	0.49
1:R1:280:ASP:C	1:R1:280:ASP:OD1	2.55	0.49
1:C3:290:SER:O	1:C3:294:ILE:HD12	2.13	0.49
1:I1:206:ASP:C	1:I1:206:ASP:OD1	2.55	0.49
1:S1:269:GLN:OE1	1:S1:269:GLN:HA	2.13	0.49
1:H1:18:LEU:O	1:H1:18:LEU:HD12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D1:112:ILE:HG22	1:D1:116:ILE:HD12	1.94	0.49
1:J1:46:ALA:O	1:J1:50:ILE:HG22	2.13	0.49
1:K1:202:ILE:HG23	1:K1:203:ASP:OD1	2.12	0.49
1:L1:15:GLN:O	1:L1:19:THR:HG23	2.12	0.49
1:B3:184:LYS:HA	1:C3:158:MET:HE1	1.95	0.48
1:I1:46:ALA:O	1:I1:50:ILE:HG22	2.13	0.48
1:D1:164:MET:HE2	1:D1:301:VAL:HG22	1.95	0.48
1:I1:199:LEU:C	1:I1:199:LEU:HD12	2.38	0.48
1:N1:266:LEU:O	1:N1:267:ASN:C	2.56	0.48
1:W1:85:THR:HG23	1:W1:123:LEU:HD22	1.94	0.48
1:A2:266:LEU:O	1:A2:267:ASN:C	2.55	0.48
1:C1:219:ILE:HG22	1:C1:237:VAL:HG21	1.95	0.48
1:G1:78:ALA:O	1:G1:82:MET:HG3	2.14	0.48
1:F1:246:PHE:HB2	1:F1:289:GLN:NE2	2.29	0.48
1:P1:92:MET:HE1	1:P1:123:LEU:CD1	2.43	0.48
1:C3:82:MET:HE2	1:C3:164:MET:HE3	1.95	0.48
1:P1:46:ALA:O	1:P1:50:ILE:HG22	2.14	0.48
1:a1:266:LEU:O	1:a1:267:ASN:C	2.55	0.48
1:C1:246:PHE:HB2	1:C1:289:GLN:NE2	2.28	0.48
1:N1:169:ARG:NH2	1:N1:170:MET:HE3	2.29	0.48
1:C2:361:VAL:HG13	1:B3:29:MET:HG2	1.96	0.48
1:K1:266:LEU:O	1:K1:267:ASN:C	2.56	0.47
1:V1:149:ILE:O	1:V1:149:ILE:CG1	2.62	0.47
1:C3:219:ILE:HG22	1:C3:237:VAL:HG21	1.96	0.47
1:D1:266:LEU:O	1:D1:267:ASN:C	2.57	0.47
1:E1:85:THR:HG23	1:E1:123:LEU:HD22	1.96	0.47
1:N1:188:VAL:HG23	1:N1:217:ASP:O	2.14	0.47
1:E1:297:ALA:O	1:E1:301:VAL:HG23	2.13	0.47
1:O1:61:LEU:HD22	1:O1:322:LEU:HD22	1.96	0.47
1:P1:27:THR:HG22	1:P1:31:ARG:HD2	1.96	0.47
1:C1:367:GLN:N	1:C1:367:GLN:OE1	2.47	0.47
1:S1:207:GLN:OE1	1:S1:232:MET:HE3	2.14	0.47
1:T1:8:ASN:OD1	1:T1:8:ASN:O	2.33	0.47
1:U1:188:VAL:HG23	1:U1:217:ASP:O	2.14	0.47
1:U1:266:LEU:O	1:U1:267:ASN:C	2.57	0.47
1:L1:266:LEU:O	1:L1:267:ASN:C	2.56	0.47
1:P1:92:MET:HE1	1:P1:123:LEU:HD11	1.97	0.47
1:O1:364:GLN:OE1	1:O1:364:GLN:C	2.58	0.47
1:N1:85:THR:HG23	1:N1:123:LEU:HD22	1.97	0.47
1:T1:266:LEU:O	1:T1:267:ASN:C	2.58	0.47
1:Z1:48:LEU:HD23	1:Z1:48:LEU:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I1:82:MET:SD	1:I1:164:MET:HE3	2.55	0.47
1:V1:188:VAL:HG23	1:V1:217:ASP:O	2.15	0.47
1:O1:164:MET:HE3	1:O1:301:VAL:HG22	1.98	0.46
1:V1:246:PHE:HB2	1:V1:289:GLN:NE2	2.29	0.46
1:X1:266:LEU:O	1:X1:267:ASN:C	2.56	0.46
1:N1:8:ASN:OD1	1:N1:11:ALA:HB2	2.14	0.46
1:a1:82:MET:HE1	1:a1:308:LEU:HD11	1.96	0.46
1:C2:266:LEU:O	1:C2:267:ASN:C	2.57	0.46
1:H1:266:LEU:O	1:H1:267:ASN:C	2.58	0.46
1:L1:113:GLN:HG3	1:L1:282:THR:HG23	1.98	0.46
1:P1:7:THR:HG21	1:Q1:334:SER:HB2	1.98	0.46
1:R1:93:ARG:HB2	1:R1:294:ILE:HG21	1.98	0.46
1:a1:78:ALA:O	1:a1:82:MET:HE3	2.16	0.46
1:C3:188:VAL:HG23	1:C3:217:ASP:O	2.15	0.46
1:R1:266:LEU:O	1:R1:267:ASN:C	2.58	0.46
1:S1:218:ASP:OD2	1:U1:158:MET:HE2	2.16	0.46
1:T1:85:THR:HG23	1:T1:123:LEU:HD22	1.98	0.46
1:A3:325:ILE:O	1:A3:329:VAL:HG22	2.15	0.46
1:U1:29:MET:HG2	1:W1:361:VAL:HG13	1.96	0.46
1:Q1:266:LEU:O	1:Q1:267:ASN:C	2.59	0.46
1:S1:266:LEU:O	1:S1:267:ASN:C	2.59	0.46
1:X1:199:LEU:HB3	1:X1:256:VAL:HG22	1.97	0.46
1:Y1:93:ARG:HB2	1:Y1:294:ILE:HG21	1.98	0.46
1:E1:180:GLU:OE2	1:E1:180:GLU:HA	2.14	0.46
1:G1:266:LEU:O	1:G1:267:ASN:C	2.59	0.46
1:Y1:193:ASN:OD1	1:Y1:193:ASN:C	2.58	0.46
1:C3:267:ASN:OD1	1:C3:267:ASN:C	2.58	0.46
1:H1:246:PHE:HB2	1:H1:289:GLN:NE2	2.30	0.46
1:Z1:266:LEU:O	1:Z1:267:ASN:C	2.58	0.46
1:A3:266:LEU:O	1:A3:267:ASN:C	2.58	0.46
1:F1:266:LEU:O	1:F1:267:ASN:C	2.58	0.46
1:M1:85:THR:HG23	1:M1:123:LEU:HD22	1.98	0.46
1:a1:113:GLN:HA	1:a1:113:GLN:OE1	2.15	0.46
1:C3:266:LEU:O	1:C3:267:ASN:C	2.59	0.46
1:Y1:266:LEU:O	1:Y1:267:ASN:C	2.58	0.45
1:M1:207:GLN:OE1	1:M1:232:MET:HE2	2.17	0.45
1:C2:188:VAL:HG23	1:C2:217:ASP:O	2.17	0.45
1:A1:30:GLU:HG3	1:T1:13:THR:HG21	1.97	0.45
1:G1:208:THR:C	1:G1:209:ILE:HD13	2.41	0.45
1:H1:82:MET:HE1	1:H1:304:HIS:CD2	2.51	0.45
1:H1:108:GLU:O	1:H1:112:ILE:HD12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N1:164:MET:HE3	1:N1:304:HIS:HD2	1.80	0.45
1:W1:266:LEU:O	1:W1:267:ASN:C	2.57	0.45
1:X1:208:THR:O	1:X1:208:THR:HG23	2.16	0.45
1:A1:266:LEU:O	1:A1:267:ASN:C	2.58	0.45
1:J1:95:LEU:HD13	1:J1:115:GLU:HG2	1.98	0.45
1:M1:266:LEU:O	1:M1:267:ASN:C	2.60	0.45
1:A3:334:SER:CB	1:B3:7:THR:HG21	2.46	0.45
1:B1:280:ASP:OD2	1:B1:280:ASP:O	2.34	0.45
1:I1:78:ALA:O	1:I1:82:MET:HG3	2.17	0.45
1:A3:199:LEU:HB3	1:A3:256:VAL:HG22	1.98	0.45
1:B3:266:LEU:O	1:B3:267:ASN:C	2.59	0.45
1:D1:82:MET:HE1	1:D1:304:HIS:CD2	2.51	0.45
1:G1:218:ASP:C	1:G1:218:ASP:OD2	2.60	0.45
1:S1:112:ILE:HG13	1:W1:46:ALA:HB2	1.98	0.45
1:B1:164:MET:HE2	1:B1:304:HIS:HD2	1.82	0.45
1:D1:297:ALA:O	1:D1:301:VAL:HG23	2.17	0.45
1:Q1:82:MET:HE2	1:Q1:164:MET:HE3	1.98	0.45
1:J1:287:ALA:O	1:J1:291:VAL:HG23	2.17	0.45
1:N1:112:ILE:HG13	1:P1:46:ALA:HB2	1.98	0.45
1:T1:82:MET:HE2	1:T1:164:MET:SD	2.57	0.45
1:a1:82:MET:HE1	1:a1:308:LEU:CD1	2.47	0.45
1:R1:205:ASN:ND2	1:R1:205:ASN:C	2.73	0.45
1:S1:202:ILE:HG21	1:S1:250:ASN:O	2.17	0.45
1:T1:149:ILE:O	1:T1:149:ILE:CG1	2.65	0.45
1:D1:188:VAL:HG23	1:D1:217:ASP:O	2.16	0.45
1:P1:82:MET:HE1	1:P1:304:HIS:CD2	2.52	0.45
1:S1:167:ASP:HA	1:S1:275:THR:HG21	1.99	0.45
1:C3:8:ASN:OD1	1:C3:8:ASN:O	2.35	0.45
1:E1:182:LYS:HG3	1:E1:219:ILE:HD11	1.99	0.44
1:U1:112:ILE:HG13	1:V1:46:ALA:HB2	1.98	0.44
1:B2:93:ARG:HB2	1:B2:294:ILE:HG21	1.98	0.44
1:J1:373:LEU:HD13	1:M1:353:ILE:HG23	1.99	0.44
1:M1:78:ALA:O	1:M1:82:MET:HE3	2.17	0.44
1:S1:93:ARG:HB2	1:S1:294:ILE:HG21	1.98	0.44
1:Y1:8:ASN:HD21	1:Y1:11:ALA:HB2	1.83	0.44
1:C3:182:LYS:HB2	1:C3:219:ILE:HG13	1.99	0.44
1:B1:149:ILE:HD11	1:B1:157:VAL:HG21	1.99	0.44
1:C2:85:THR:HG23	1:C2:123:LEU:HD22	1.98	0.44
1:E1:93:ARG:HB2	1:E1:294:ILE:HG21	1.99	0.44
1:F1:93:ARG:HB2	1:F1:294:ILE:HG21	1.98	0.44
1:G1:209:ILE:HD13	1:G1:209:ILE:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H1:164:MET:HE2	1:H1:301:VAL:HG22	1.99	0.44
1:C2:8:ASN:OD1	1:C2:11:ALA:HB2	2.18	0.44
1:E1:82:MET:CE	1:E1:308:LEU:HD12	2.47	0.44
1:E1:164:MET:CE	1:E1:301:VAL:HG22	2.47	0.44
1:F1:164:MET:HE2	1:F1:304:HIS:HD2	1.83	0.44
1:U1:246:PHE:HB2	1:U1:289:GLN:HE22	1.82	0.44
1:Z1:219:ILE:HG22	1:Z1:237:VAL:HG21	2.00	0.44
1:C1:289:GLN:HA	1:C1:289:GLN:HE21	1.82	0.44
1:K1:85:THR:HG23	1:K1:123:LEU:HD22	2.00	0.44
1:S1:29:MET:HB3	1:X1:361:VAL:HG13	1.99	0.44
1:V1:93:ARG:HB2	1:V1:294:ILE:HG21	1.99	0.44
1:A2:219:ILE:HG22	1:A2:237:VAL:HG21	2.00	0.44
1:S1:182:LYS:HB2	1:S1:219:ILE:HG13	2.00	0.43
1:E1:266:LEU:O	1:E1:267:ASN:C	2.61	0.43
1:F1:48:LEU:HD23	1:F1:48:LEU:C	2.43	0.43
1:G1:349:THR:O	1:G1:353:ILE:HD12	2.18	0.43
1:O1:246:PHE:HB2	1:O1:289:GLN:NE2	2.33	0.43
1:U1:8:ASN:OD1	1:U1:11:ALA:HB2	2.18	0.43
1:Z1:82:MET:HE2	1:Z1:164:MET:SD	2.58	0.43
1:B1:149:ILE:HD11	1:B1:157:VAL:CG2	2.48	0.43
1:D1:361:VAL:HG13	1:H1:29:MET:HG2	1.99	0.43
1:S1:201:ASP:OD2	1:S1:232:MET:HE1	2.17	0.43
1:B2:246:PHE:CE1	1:B2:293:VAL:HG22	2.53	0.43
1:P1:169:ARG:NH1	1:P1:169:ARG:HB3	2.33	0.43
1:X1:250:ASN:HD22	1:X1:299:LYS:HD2	1.84	0.43
1:J1:164:MET:HE1	1:J1:301:VAL:HA	2.01	0.43
1:V1:266:LEU:O	1:V1:267:ASN:C	2.61	0.43
1:X1:46:ALA:O	1:X1:50:ILE:HG22	2.18	0.43
1:C1:46:ALA:O	1:C1:50:ILE:HG22	2.19	0.43
1:J1:147:PHE:CE1	1:J1:159:LEU:HD23	2.53	0.43
1:P1:85:THR:HG23	1:P1:123:LEU:HD22	2.01	0.43
1:T1:27:THR:HG22	1:T1:31:ARG:HE	1.82	0.43
1:C3:3:VAL:O	1:C3:3:VAL:HG13	2.19	0.43
1:A1:46:ALA:HB2	1:Z1:112:ILE:HG13	2.01	0.43
1:L1:38:ILE:HD12	1:L1:337:LYS:HA	2.00	0.43
1:N1:375:LEU:O	1:R1:345:THR:HG21	2.19	0.43
1:X1:93:ARG:HB2	1:X1:294:ILE:HG21	2.01	0.43
1:L1:29:MET:HG2	1:N1:361:VAL:HG13	1.99	0.43
1:P1:78:ALA:O	1:P1:82:MET:HG2	2.18	0.43
1:C2:82:MET:HE1	1:C2:304:HIS:CD2	2.54	0.43
1:C3:93:ARG:HB2	1:C3:294:ILE:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D1:29:MET:HE3	1:K1:10:ALA:HB1	2.01	0.43
1:B1:266:LEU:O	1:B1:267:ASN:C	2.62	0.42
1:N1:7:THR:HG23	1:R1:338:ASP:OD2	2.19	0.42
1:N1:95:LEU:HB3	1:N1:112:ILE:HG23	2.01	0.42
1:V1:182:LYS:HG3	1:V1:219:ILE:HD11	2.02	0.42
1:W1:188:VAL:HG23	1:W1:217:ASP:O	2.19	0.42
1:A3:336:ILE:HD12	1:A3:336:ILE:H	1.84	0.42
1:D1:129:THR:HG22	1:K1:155:GLU:HG2	2.00	0.42
1:S1:82:MET:SD	1:S1:164:MET:SD	3.17	0.42
1:Z1:31:ARG:HG2	1:Z1:37:LYS:HA	2.01	0.42
1:B2:46:ALA:HB2	1:B3:112:ILE:HG13	2.00	0.42
1:C2:219:ILE:HG22	1:C2:237:VAL:HG21	2.01	0.42
1:A3:93:ARG:HB2	1:A3:294:ILE:HG21	2.00	0.42
1:A1:219:ILE:CG2	1:A1:237:VAL:HG11	2.50	0.42
1:L1:232:MET:HE3	1:L1:232:MET:HB3	1.97	0.42
1:B2:82:MET:HE2	1:B2:164:MET:CE	2.46	0.42
1:F1:325:ILE:O	1:F1:329:VAL:HG23	2.19	0.42
1:Q1:321:ASN:O	1:Q1:325:ILE:HD12	2.19	0.42
1:A2:93:ARG:HB2	1:A2:294:ILE:HG21	2.00	0.42
1:L1:367:GLN:N	1:L1:367:GLN:CD	2.78	0.42
1:M1:66:ARG:HH11	1:M1:66:ARG:HB2	1.84	0.42
1:U1:373:LEU:HD11	1:X1:356:GLN:HB2	2.01	0.42
1:Y1:44:ASP:OD2	1:Y1:44:ASP:C	2.61	0.42
1:C1:29:MET:HG2	1:U1:361:VAL:HG13	2.01	0.42
1:F1:147:PHE:CE1	1:F1:159:LEU:HD23	2.55	0.42
1:L1:18:LEU:HD12	1:L1:18:LEU:O	2.20	0.42
1:N1:105:SER:N	1:N1:108:GLU:OE2	2.52	0.42
1:R1:356:GLN:N	1:R1:356:GLN:OE1	2.52	0.42
1:a1:8:ASN:OD1	1:a1:11:ALA:HB2	2.20	0.42
1:O1:367:GLN:N	1:O1:367:GLN:CD	2.77	0.42
1:B2:158:MET:HE2	1:C2:218:ASP:OD1	2.20	0.42
1:C1:129:THR:HG22	1:U1:155:GLU:HG2	2.01	0.42
1:P1:31:ARG:HG2	1:P1:37:LYS:HA	2.02	0.42
1:X1:31:ARG:HG2	1:X1:37:LYS:HA	2.02	0.42
1:B2:106:LYS:HE3	1:B2:106:LYS:HA	2.02	0.42
1:B2:289:GLN:O	1:B2:293:VAL:HG23	2.20	0.42
1:A1:13:THR:HG21	1:a1:30:GLU:HG3	2.02	0.42
1:Z1:279:ILE:HG23	1:Z1:290:SER:HB2	2.02	0.42
1:B3:220:GLU:HG3	1:C3:158:MET:HG2	2.00	0.42
1:C1:188:VAL:HG23	1:C1:217:ASP:O	2.20	0.42
1:O1:164:MET:CE	1:O1:301:VAL:HG22	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W1:12:MET:HE1	1:X1:330:ASN:CB	2.49	0.42
1:X1:279:ILE:HG23	1:X1:290:SER:HB2	2.01	0.42
1:B1:95:LEU:HB2	1:B1:116:ILE:HD11	2.01	0.41
1:W1:158:MET:HE2	1:X1:218:ASP:OD2	2.20	0.41
1:C2:10:ALA:HB1	1:B3:29:MET:CE	2.50	0.41
1:P1:193:ASN:OD1	1:P1:193:ASN:C	2.63	0.41
1:V1:182:LYS:HB2	1:V1:219:ILE:HG13	2.02	0.41
1:B1:93:ARG:HB2	1:B1:294:ILE:HG21	2.02	0.41
1:J1:373:LEU:HD21	1:M1:356:GLN:OE1	2.20	0.41
1:N1:44:ASP:OD2	1:N1:47:GLY:HA3	2.20	0.41
1:R1:92:MET:HE1	1:R1:123:LEU:HD11	2.03	0.41
1:A2:147:PHE:CE1	1:A2:159:LEU:HD23	2.56	0.41
1:B2:266:LEU:O	1:B2:267:ASN:C	2.63	0.41
1:C2:46:ALA:HB2	1:A3:112:ILE:HG13	2.00	0.41
1:G1:368:ALA:N	1:G1:369:PRO:HD2	2.35	0.41
1:O1:169:ARG:HB3	1:O1:169:ARG:NH1	2.35	0.41
1:B3:219:ILE:HG22	1:B3:237:VAL:HG21	2.01	0.41
1:E1:82:MET:HE1	1:E1:308:LEU:HD12	2.02	0.41
1:I1:147:PHE:CE1	1:I1:159:LEU:HD23	2.56	0.41
1:A2:188:VAL:HG23	1:A2:217:ASP:O	2.21	0.41
1:B3:93:ARG:HB2	1:B3:294:ILE:HG21	2.03	0.41
1:B1:169:ARG:NH1	1:B1:169:ARG:HB3	2.35	0.41
1:L1:61:LEU:HD22	1:L1:322:LEU:HD22	2.02	0.41
1:N1:184:LYS:HB3	1:N1:184:LYS:HE2	1.89	0.41
1:W1:246:PHE:CE1	1:W1:293:VAL:HG22	2.56	0.41
1:C1:61:LEU:O	1:C1:65:VAL:HG23	2.20	0.41
1:E1:246:PHE:CE1	1:E1:293:VAL:HG22	2.55	0.41
1:H1:297:ALA:O	1:H1:301:VAL:HG23	2.20	0.41
1:I1:368:ALA:N	1:I1:369:PRO:HD2	2.36	0.41
1:P1:266:LEU:O	1:P1:267:ASN:C	2.64	0.41
1:S1:219:ILE:HG22	1:S1:237:VAL:HG21	2.01	0.41
1:Z1:356:GLN:N	1:Z1:356:GLN:OE1	2.53	0.41
1:B3:8:ASN:OD1	1:B3:11:ALA:HB2	2.21	0.41
1:B1:113:GLN:NE2	1:B1:280:ASP:HA	2.36	0.41
1:D1:368:ALA:N	1:D1:369:PRO:HD2	2.36	0.41
1:J1:8:ASN:HB3	1:J1:11:ALA:HB3	2.02	0.41
1:M1:46:ALA:O	1:M1:50:ILE:HG22	2.20	0.41
1:M1:368:ALA:N	1:M1:369:PRO:HD2	2.36	0.41
1:P1:106:LYS:O	1:P1:110:VAL:HG23	2.21	0.41
1:Q1:368:ALA:N	1:Q1:369:PRO:HD2	2.36	0.41
1:Y1:82:MET:HG2	1:Y1:164:MET:HE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B3:246:PHE:CE1	1:B3:293:VAL:HG22	2.56	0.41
1:D1:85:THR:HG23	1:D1:123:LEU:HD22	2.02	0.41
1:F1:112:ILE:HG13	1:K1:46:ALA:HB2	2.02	0.41
1:G1:82:MET:HE2	1:G1:301:VAL:HG13	2.01	0.41
1:X1:96:SER:HB2	1:X1:291:VAL:HG22	2.03	0.41
1:Y1:349:THR:O	1:Y1:353:ILE:HG12	2.21	0.41
1:Z1:85:THR:HG23	1:Z1:123:LEU:HD22	2.02	0.41
1:C3:193:ASN:OD1	1:C3:193:ASN:C	2.64	0.41
1:C1:93:ARG:HB2	1:C1:294:ILE:HG21	2.03	0.40
1:L1:211:VAL:HG11	1:L1:226:ILE:HG12	2.02	0.40
1:L1:246:PHE:CE1	1:L1:293:VAL:HG22	2.56	0.40
1:M1:147:PHE:CD2	1:N1:101:ASN:OD1	2.74	0.40
1:A2:321:ASN:O	1:A2:325:ILE:HG13	2.21	0.40
1:C2:92:MET:HE1	1:C2:123:LEU:HD12	2.03	0.40
1:L1:147:PHE:CE1	1:L1:159:LEU:HD23	2.56	0.40
1:Q1:231:ASP:N	1:Q1:231:ASP:OD1	2.55	0.40
1:E1:32:LEU:HD21	1:E1:344:GLU:HB3	2.03	0.40
1:K1:177:VAL:HG23	1:K1:244:GLN:HG2	2.03	0.40
1:P1:158:MET:HE2	1:Q1:218:ASP:OD2	2.20	0.40
1:C2:82:MET:HE3	1:C2:308:LEU:HD12	2.03	0.40
1:A1:82:MET:HE1	1:A1:308:LEU:HD12	2.04	0.40
1:C1:182:LYS:HB2	1:C1:219:ILE:HG13	2.04	0.40
1:H1:95:LEU:HB3	1:H1:112:ILE:HG23	2.02	0.40
1:J1:368:ALA:N	1:J1:369:PRO:HD2	2.37	0.40
1:K1:368:ALA:N	1:K1:369:PRO:HD2	2.37	0.40
1:S1:69:ASN:HB3	1:X1:335:ARG:HD2	2.03	0.40
1:U1:219:ILE:HG22	1:U1:237:VAL:HG21	2.03	0.40
1:A2:46:ALA:O	1:A2:50:ILE:HG22	2.22	0.40
1:C2:218:ASP:OD2	1:C2:218:ASP:N	2.55	0.40
1:C2:368:ALA:N	1:C2:369:PRO:HD2	2.37	0.40
1:A1:184:LYS:HA	1:B1:158:MET:HE1	2.03	0.40
1:A1:246:PHE:CE1	1:A1:293:VAL:HG22	2.57	0.40
1:B1:78:ALA:O	1:B1:82:MET:HG3	2.21	0.40
1:B1:200:LYS:HE3	1:B1:200:LYS:HB3	1.94	0.40
1:C1:149:ILE:O	1:C1:149:ILE:HG13	2.22	0.40
1:I1:205:ASN:HD22	1:I1:205:ASN:C	2.27	0.40
1:L1:88:ILE:HG21	1:L1:123:LEU:HG	2.04	0.40
1:P1:199:LEU:HD23	1:P1:199:LEU:H	1.85	0.40
1:C3:82:MET:HE1	1:C3:304:HIS:CD2	2.56	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	A1	374/377 (99%)	367 (98%)	7 (2%)	0	100	100
1	A2	374/377 (99%)	367 (98%)	7 (2%)	0	100	100
1	A3	374/377 (99%)	367 (98%)	7 (2%)	0	100	100
1	B1	374/377 (99%)	367 (98%)	7 (2%)	0	100	100
1	B2	374/377 (99%)	364 (97%)	10 (3%)	0	100	100
1	B3	374/377 (99%)	365 (98%)	9 (2%)	0	100	100
1	C1	374/377 (99%)	367 (98%)	7 (2%)	0	100	100
1	C2	374/377 (99%)	367 (98%)	7 (2%)	0	100	100
1	C3	374/377 (99%)	366 (98%)	8 (2%)	0	100	100
1	D1	374/377 (99%)	366 (98%)	8 (2%)	0	100	100
1	E1	374/377 (99%)	367 (98%)	7 (2%)	0	100	100
1	F1	374/377 (99%)	365 (98%)	9 (2%)	0	100	100
1	G1	374/377 (99%)	364 (97%)	10 (3%)	0	100	100
1	H1	374/377 (99%)	366 (98%)	8 (2%)	0	100	100
1	I1	374/377 (99%)	366 (98%)	8 (2%)	0	100	100
1	J1	374/377 (99%)	364 (97%)	10 (3%)	0	100	100
1	K1	374/377 (99%)	364 (97%)	10 (3%)	0	100	100
1	L1	374/377 (99%)	369 (99%)	5 (1%)	0	100	100
1	M1	374/377 (99%)	363 (97%)	11 (3%)	0	100	100
1	N1	374/377 (99%)	364 (97%)	10 (3%)	0	100	100
1	O1	374/377 (99%)	367 (98%)	7 (2%)	0	100	100
1	P1	374/377 (99%)	367 (98%)	7 (2%)	0	100	100
1	Q1	374/377 (99%)	366 (98%)	8 (2%)	0	100	100
1	R1	374/377 (99%)	367 (98%)	7 (2%)	0	100	100
1	S1	374/377 (99%)	369 (99%)	5 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	T1	374/377 (99%)	364 (97%)	10 (3%)	0	100	100
1	U1	374/377 (99%)	367 (98%)	7 (2%)	0	100	100
1	V1	374/377 (99%)	366 (98%)	8 (2%)	0	100	100
1	W1	374/377 (99%)	366 (98%)	8 (2%)	0	100	100
1	X1	374/377 (99%)	367 (98%)	7 (2%)	0	100	100
1	Y1	374/377 (99%)	367 (98%)	7 (2%)	0	100	100
1	Z1	374/377 (99%)	368 (98%)	6 (2%)	0	100	100
1	a1	374/377 (99%)	365 (98%)	9 (2%)	0	100	100
All	All	12342/12441 (99%)	12081 (98%)	261 (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	A1	298/299 (100%)	294 (99%)	4 (1%)	65	86
1	A2	298/299 (100%)	293 (98%)	5 (2%)	56	82
1	A3	298/299 (100%)	295 (99%)	3 (1%)	73	90
1	B1	298/299 (100%)	288 (97%)	10 (3%)	32	65
1	B2	298/299 (100%)	296 (99%)	2 (1%)	81	93
1	B3	298/299 (100%)	289 (97%)	9 (3%)	36	69
1	C1	298/299 (100%)	291 (98%)	7 (2%)	45	75
1	C2	298/299 (100%)	291 (98%)	7 (2%)	45	75
1	C3	298/299 (100%)	293 (98%)	5 (2%)	56	82
1	D1	298/299 (100%)	289 (97%)	9 (3%)	36	69
1	E1	298/299 (100%)	290 (97%)	8 (3%)	40	72
1	F1	298/299 (100%)	289 (97%)	9 (3%)	36	69
1	G1	298/299 (100%)	292 (98%)	6 (2%)	50	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H1	298/299 (100%)	292 (98%)	6 (2%)	50	78
1	I1	298/299 (100%)	293 (98%)	5 (2%)	56	82
1	J1	298/299 (100%)	293 (98%)	5 (2%)	56	82
1	K1	298/299 (100%)	292 (98%)	6 (2%)	50	78
1	L1	298/299 (100%)	293 (98%)	5 (2%)	56	82
1	M1	298/299 (100%)	289 (97%)	9 (3%)	36	69
1	N1	298/299 (100%)	289 (97%)	9 (3%)	36	69
1	O1	298/299 (100%)	290 (97%)	8 (3%)	40	72
1	P1	298/299 (100%)	293 (98%)	5 (2%)	56	82
1	Q1	298/299 (100%)	291 (98%)	7 (2%)	45	75
1	R1	298/299 (100%)	291 (98%)	7 (2%)	45	75
1	S1	298/299 (100%)	295 (99%)	3 (1%)	73	90
1	T1	298/299 (100%)	294 (99%)	4 (1%)	65	86
1	U1	298/299 (100%)	291 (98%)	7 (2%)	45	75
1	V1	298/299 (100%)	291 (98%)	7 (2%)	45	75
1	W1	298/299 (100%)	289 (97%)	9 (3%)	36	69
1	X1	298/299 (100%)	293 (98%)	5 (2%)	56	82
1	Y1	298/299 (100%)	289 (97%)	9 (3%)	36	69
1	Z1	298/299 (100%)	290 (97%)	8 (3%)	40	72
1	a1	298/299 (100%)	294 (99%)	4 (1%)	65	86
All	All	9834/9867 (100%)	9622 (98%)	212 (2%)	47	76

All (212) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A1	174	THR
1	A1	198	THR
1	A1	229	GLN
1	A1	252	VAL
1	B1	82	MET
1	B1	180	GLU
1	B1	206	ASP
1	B1	215	GLU
1	B1	252	VAL
1	B1	255	ASP

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Mol	Chain	Res	Type
1	B1	278	THR
1	B1	279	ILE
1	B1	290	SER
1	B1	332	SER
1	C1	107	SER
1	C1	166	SER
1	C1	208	THR
1	C1	252	VAL
1	C1	259	SER
1	C1	295	ASP
1	C1	356	GLN
1	D1	106	LYS
1	D1	164	MET
1	D1	198	THR
1	D1	236	SER
1	D1	245	ILE
1	D1	252	VAL
1	D1	280	ASP
1	D1	289	GLN
1	D1	332	SER
1	E1	174	THR
1	E1	229	GLN
1	E1	252	VAL
1	E1	255	ASP
1	E1	259	SER
1	E1	279	ILE
1	E1	332	SER
1	E1	373	LEU
1	F1	57	GLN
1	F1	82	MET
1	F1	206	ASP
1	F1	252	VAL
1	F1	259	SER
1	F1	275	THR
1	F1	280	ASP
1	F1	289	GLN
1	F1	344	GLU
1	G1	107	SER
1	G1	155	GLU
1	G1	189	GLN
1	G1	252	VAL
1	G1	289	GLN

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Mol	Chain	Res	Type
1	G1	332	SER
1	H1	107	SER
1	H1	164	MET
1	H1	252	VAL
1	H1	283	SER
1	H1	289	GLN
1	H1	332	SER
1	I1	171	MET
1	I1	197	PHE
1	I1	203	ASP
1	I1	205	ASN
1	I1	356	GLN
1	J1	123	LEU
1	J1	234	LYS
1	J1	242	GLN
1	J1	332	SER
1	J1	367	GLN
1	K1	5	VAL
1	K1	145	LYS
1	K1	236	SER
1	K1	252	VAL
1	K1	259	SER
1	K1	295	ASP
1	L1	171	MET
1	L1	236	SER
1	L1	252	VAL
1	L1	332	SER
1	L1	374	SER
1	M1	116	ILE
1	M1	176	TYR
1	M1	198	THR
1	M1	244	GLN
1	M1	252	VAL
1	M1	278	THR
1	M1	332	SER
1	M1	334	SER
1	M1	373	LEU
1	N1	112	ILE
1	N1	160	THR
1	N1	171	MET
1	N1	229	GLN
1	N1	252	VAL

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Mol	Chain	Res	Type
1	N1	259	SER
1	N1	289	GLN
1	N1	324	ASN
1	N1	332	SER
1	O1	107	SER
1	O1	116	ILE
1	O1	171	MET
1	O1	215	GLU
1	O1	252	VAL
1	O1	259	SER
1	O1	289	GLN
1	O1	332	SER
1	P1	29	MET
1	P1	174	THR
1	P1	252	VAL
1	P1	259	SER
1	P1	355	SER
1	Q1	5	VAL
1	Q1	107	SER
1	Q1	198	THR
1	Q1	229	GLN
1	Q1	236	SER
1	Q1	289	GLN
1	Q1	332	SER
1	R1	205	ASN
1	R1	208	THR
1	R1	252	VAL
1	R1	253	THR
1	R1	275	THR
1	R1	281	VAL
1	R1	334	SER
1	S1	54	LEU
1	S1	62	ASP
1	S1	252	VAL
1	T1	267	ASN
1	T1	289	GLN
1	T1	332	SER
1	T1	373	LEU
1	U1	112	ILE
1	U1	171	MET
1	U1	198	THR
1	U1	252	VAL

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Mol	Chain	Res	Type
1	U1	259	SER
1	U1	289	GLN
1	U1	332	SER
1	V1	112	ILE
1	V1	174	THR
1	V1	215	GLU
1	V1	252	VAL
1	V1	283	SER
1	V1	289	GLN
1	V1	332	SER
1	W1	107	SER
1	W1	160	THR
1	W1	198	THR
1	W1	206	ASP
1	W1	252	VAL
1	W1	253	THR
1	W1	332	SER
1	W1	334	SER
1	W1	356	GLN
1	X1	82	MET
1	X1	252	VAL
1	X1	253	THR
1	X1	289	GLN
1	X1	332	SER
1	Y1	107	SER
1	Y1	166	SER
1	Y1	206	ASP
1	Y1	229	GLN
1	Y1	252	VAL
1	Y1	253	THR
1	Y1	255	ASP
1	Y1	283	SER
1	Y1	332	SER
1	Z1	82	MET
1	Z1	145	LYS
1	Z1	164	MET
1	Z1	207	GLN
1	Z1	219	ILE
1	Z1	252	VAL
1	Z1	289	GLN
1	Z1	351	SER
1	a1	145	LYS

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Mol	Chain	Res	Type
1	a1	236	SER
1	a1	252	VAL
1	a1	332	SER
1	A2	18	LEU
1	A2	236	SER
1	A2	252	VAL
1	A2	332	SER
1	A2	356	GLN
1	B2	174	THR
1	B2	255	ASP
1	C2	171	MET
1	C2	180	GLU
1	C2	224	THR
1	C2	229	GLN
1	C2	251	LYS
1	C2	252	VAL
1	C2	277	ASP
1	A3	145	LYS
1	A3	252	VAL
1	A3	281	VAL
1	B3	29	MET
1	B3	107	SER
1	B3	205	ASN
1	B3	229	GLN
1	B3	236	SER
1	B3	252	VAL
1	B3	253	THR
1	B3	289	GLN
1	B3	332	SER
1	C3	166	SER
1	C3	171	MET
1	C3	252	VAL
1	C3	278	THR
1	C3	332	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (151) such sidechains are listed below:

Mol	Chain	Res	Type
1	A1	120	ASN
1	A1	212	ASN
1	A1	244	GLN
1	A1	269	GLN

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Mol	Chain	Res	Type
1	B1	120	ASN
1	B1	269	GLN
1	C1	212	ASN
1	C1	242	GLN
1	C1	244	GLN
1	C1	289	GLN
1	D1	101	ASN
1	D1	120	ASN
1	D1	207	GLN
1	D1	250	ASN
1	D1	267	ASN
1	D1	330	ASN
1	E1	168	ASN
1	E1	250	ASN
1	E1	269	GLN
1	F1	49	GLN
1	F1	101	ASN
1	F1	104	ASN
1	F1	120	ASN
1	F1	242	GLN
1	F1	244	GLN
1	F1	321	ASN
1	G1	212	ASN
1	G1	229	GLN
1	G1	250	ASN
1	G1	269	GLN
1	H1	39	ASN
1	H1	76	GLN
1	H1	101	ASN
1	H1	120	ASN
1	H1	189	GLN
1	H1	212	ASN
1	H1	244	GLN
1	H1	249	ASN
1	H1	289	GLN
1	H1	326	ASN
1	I1	244	GLN
1	I1	289	GLN
1	I1	312	GLN
1	J1	39	ASN
1	J1	244	GLN
1	K1	55	ASN

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Mol	Chain	Res	Type
1	K1	120	ASN
1	K1	212	ASN
1	K1	250	ASN
1	K1	326	ASN
1	L1	39	ASN
1	L1	212	ASN
1	L1	269	GLN
1	L1	288	GLN
1	L1	364	GLN
1	M1	120	ASN
1	M1	244	GLN
1	M1	250	ASN
1	M1	267	ASN
1	M1	269	GLN
1	N1	87	ASN
1	N1	120	ASN
1	N1	244	GLN
1	N1	328	ASN
1	N1	330	ASN
1	N1	367	GLN
1	O1	4	ASN
1	O1	244	GLN
1	O1	250	ASN
1	P1	212	ASN
1	P1	267	ASN
1	P1	367	GLN
1	Q1	120	ASN
1	Q1	212	ASN
1	Q1	250	ASN
1	Q1	269	GLN
1	Q1	289	GLN
1	R1	4	ASN
1	R1	55	ASN
1	R1	205	ASN
1	R1	324	ASN
1	S1	212	ASN
1	S1	242	GLN
1	S1	250	ASN
1	S1	316	ASN
1	S1	321	ASN
1	S1	324	ASN
1	T1	39	ASN

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Mol	Chain	Res	Type
1	T1	87	ASN
1	T1	212	ASN
1	T1	229	GLN
1	T1	269	GLN
1	U1	8	ASN
1	U1	15	GLN
1	U1	39	ASN
1	U1	101	ASN
1	U1	120	ASN
1	U1	269	GLN
1	V1	244	GLN
1	V1	269	GLN
1	W1	76	GLN
1	W1	120	ASN
1	W1	250	ASN
1	W1	269	GLN
1	X1	120	ASN
1	X1	242	GLN
1	X1	267	ASN
1	X1	324	ASN
1	X1	328	ASN
1	Y1	212	ASN
1	Y1	250	ASN
1	Y1	267	ASN
1	Y1	269	GLN
1	Z1	23	ASN
1	Z1	120	ASN
1	Z1	212	ASN
1	Z1	244	GLN
1	Z1	321	ASN
1	Z1	324	ASN
1	a1	120	ASN
1	a1	244	GLN
1	a1	250	ASN
1	A2	120	ASN
1	A2	212	ASN
1	A2	244	GLN
1	A2	321	ASN
1	B2	39	ASN
1	B2	104	ASN
1	B2	120	ASN
1	B2	168	ASN

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Mol	Chain	Res	Type
1	B2	250	ASN
1	B2	269	GLN
1	C2	25	GLN
1	C2	269	GLN
1	C2	364	GLN
1	A3	23	ASN
1	A3	25	GLN
1	A3	205	ASN
1	A3	242	GLN
1	A3	244	GLN
1	A3	269	GLN
1	B3	87	ASN
1	B3	120	ASN
1	B3	250	ASN
1	B3	269	GLN
1	B3	289	GLN
1	B3	328	ASN
1	C3	55	ASN
1	C3	212	ASN
1	C3	330	ASN
1	C3	370	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

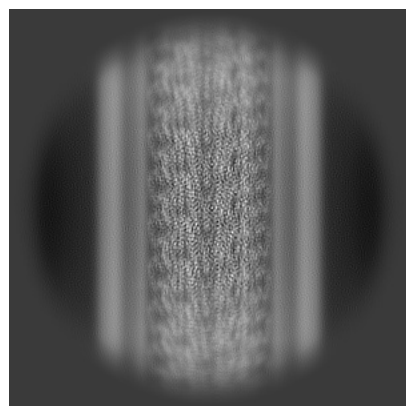
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49125. These allow visual inspection of the internal detail of the map and identification of artifacts.

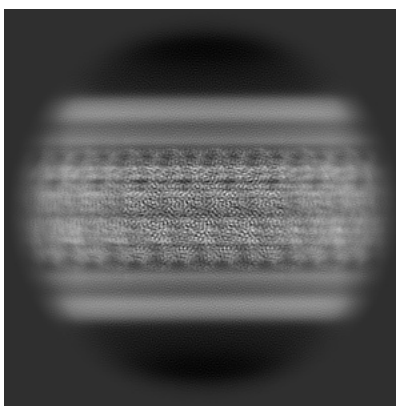
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

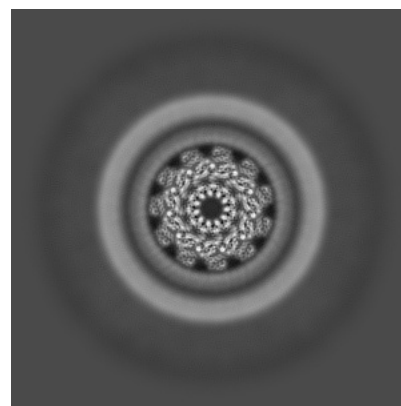
6.1.1 Primary map



X

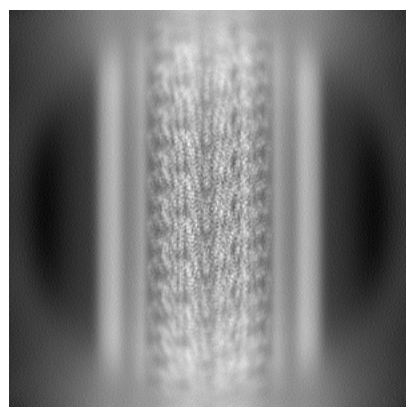


Y

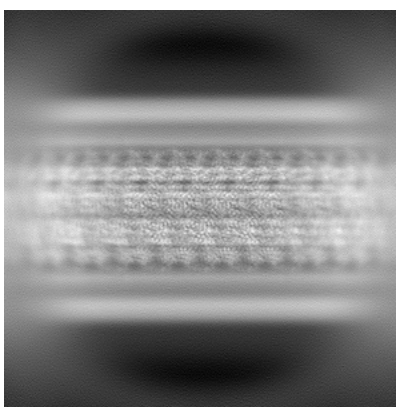


Z

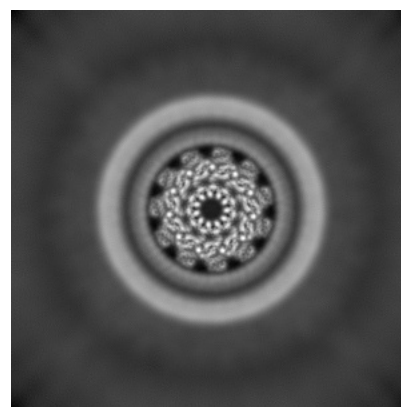
6.1.2 Raw map



X



Y

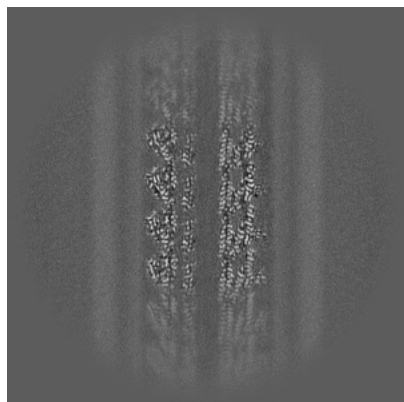


Z

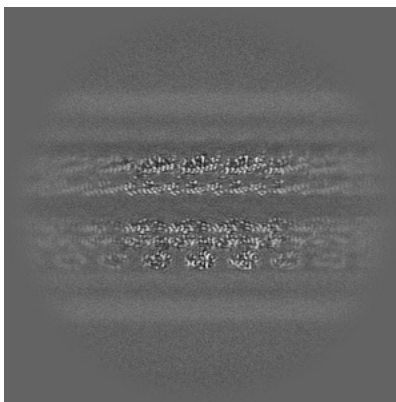
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

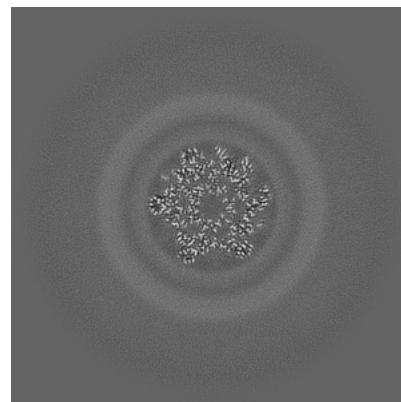
6.2.1 Primary map



X Index: 224

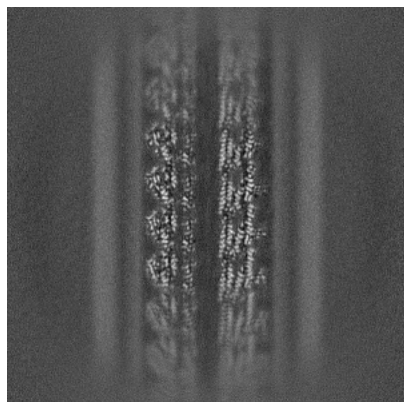


Y Index: 224

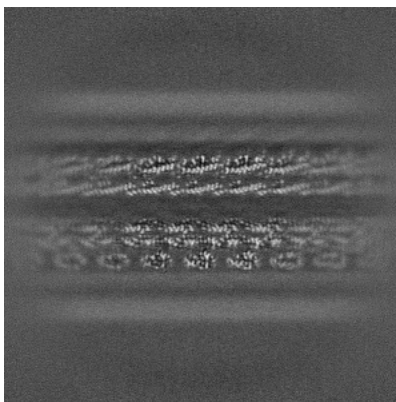


Z Index: 224

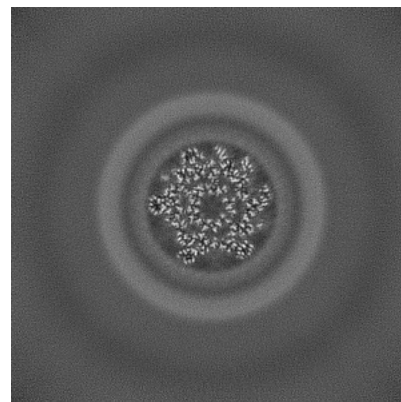
6.2.2 Raw map



X Index: 224



Y Index: 224

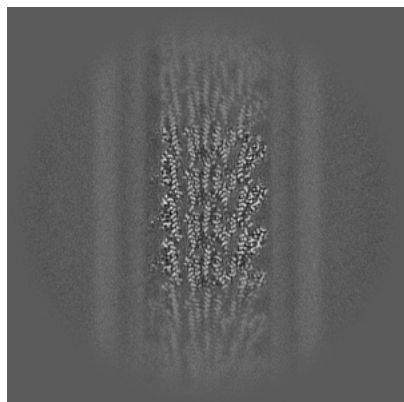


Z Index: 224

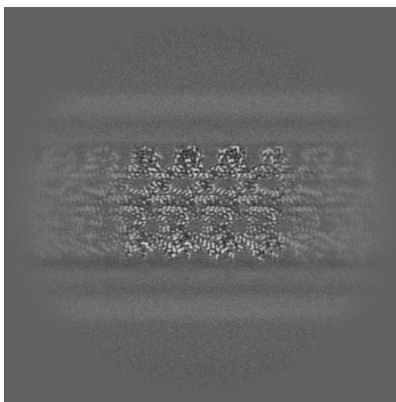
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

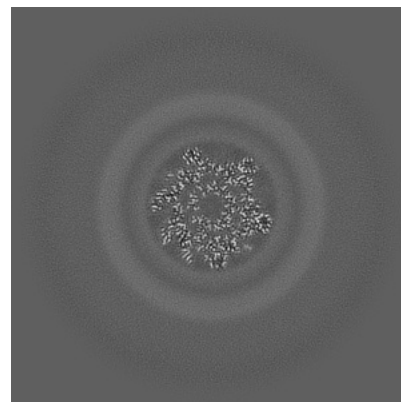
6.3.1 Primary map



X Index: 242

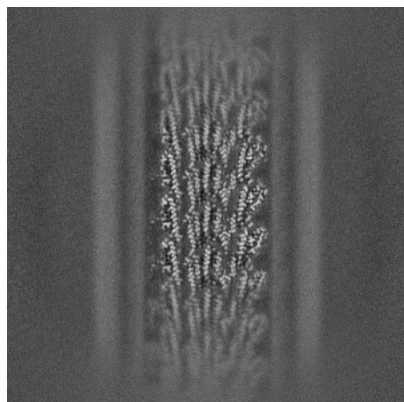


Y Index: 205

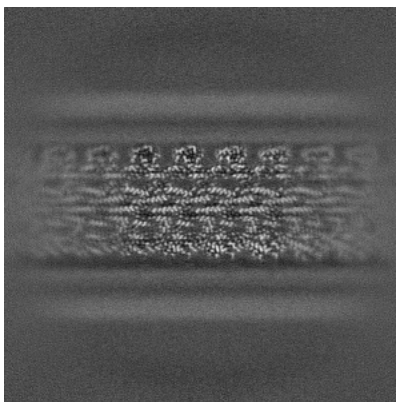


Z Index: 211

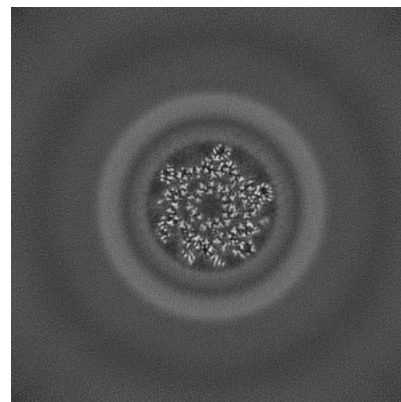
6.3.2 Raw map



X Index: 242



Y Index: 206

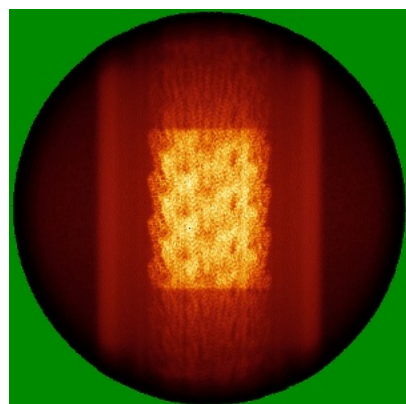


Z Index: 238

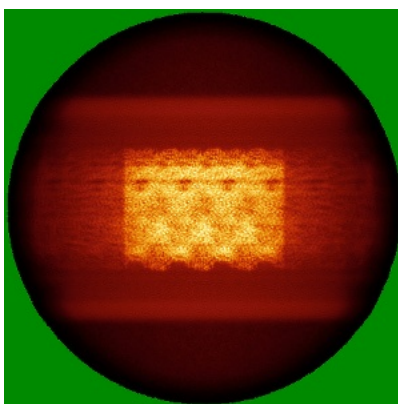
The images above show the largest variance slices of the map in three orthogonal directions.

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

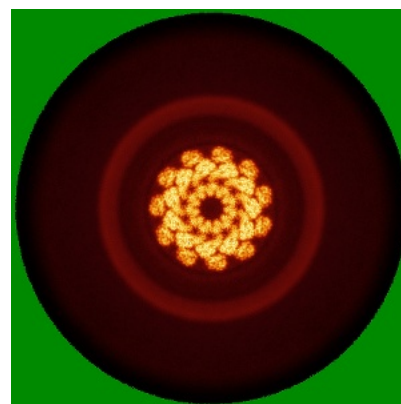
6.4.1 Primary map



X

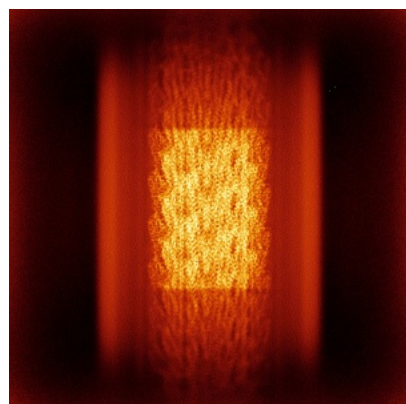


Y

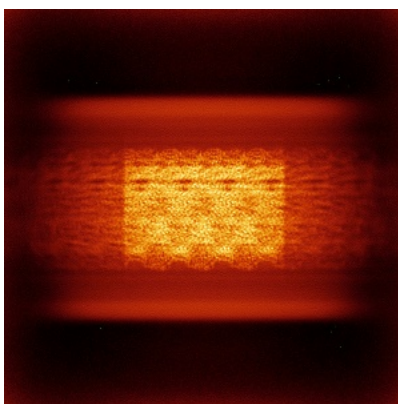


Z

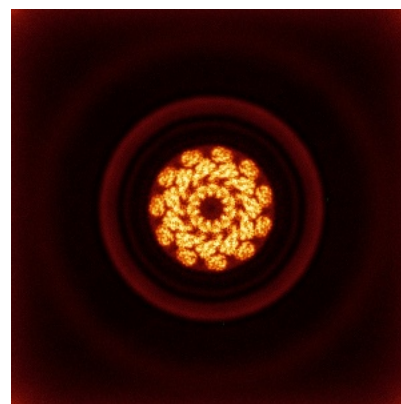
6.4.2 Raw map



X



Y

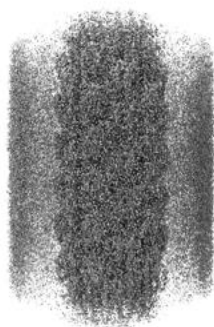


Z

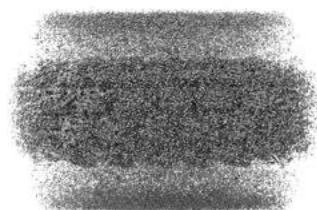
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

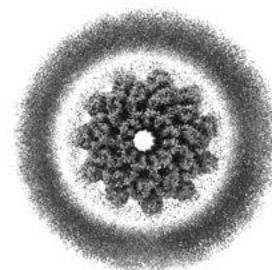
6.5.1 Primary map



X



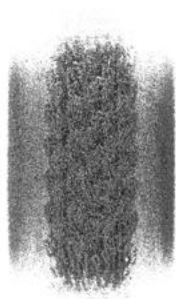
Y



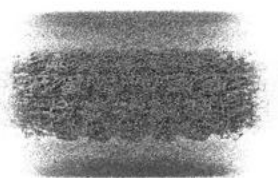
Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

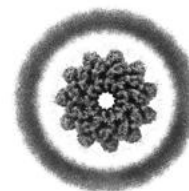
6.5.2 Raw map



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.

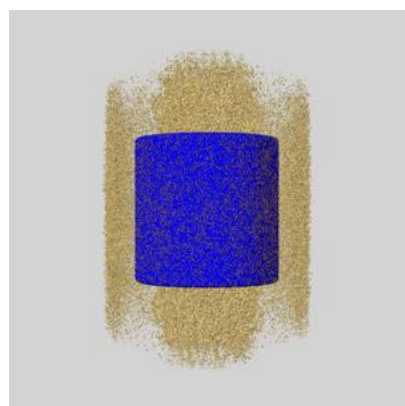
6.6 Mask visualisation [i](#)

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

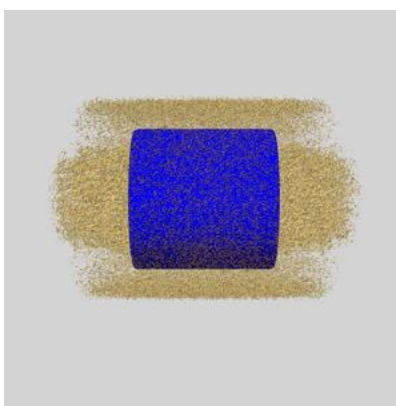
A mask typically either:

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

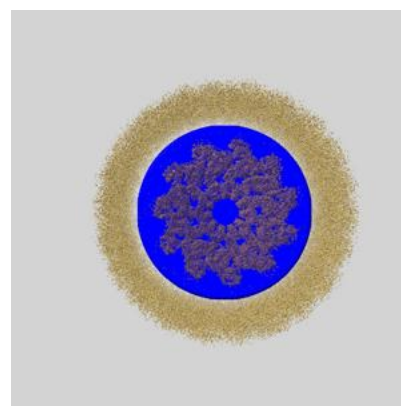
6.6.1 emd_49125_msk_1.map [i](#)



X



Y

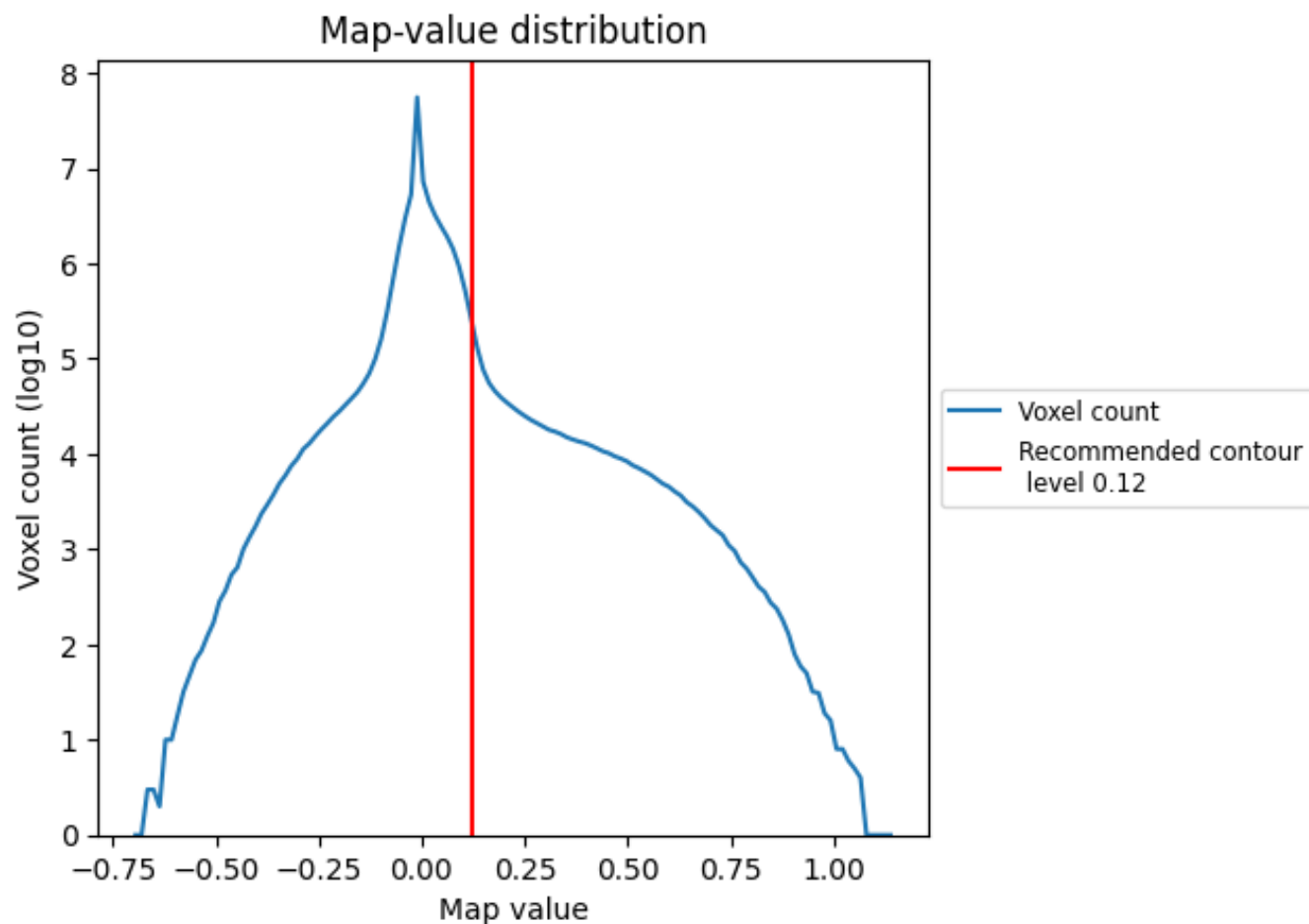


Z

7 Map analysis [i](#)

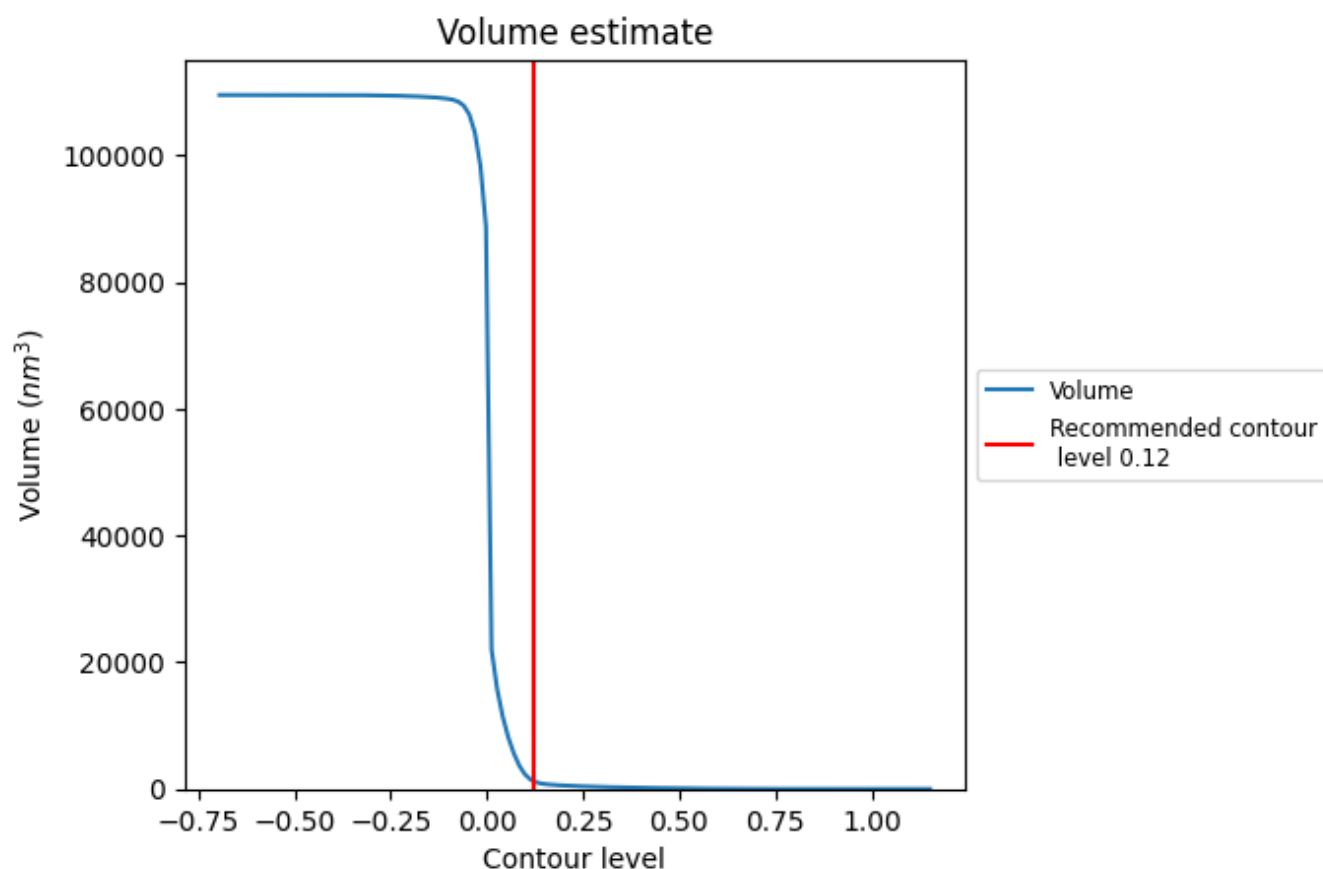
This section contains the results of statistical analysis of the map.

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.

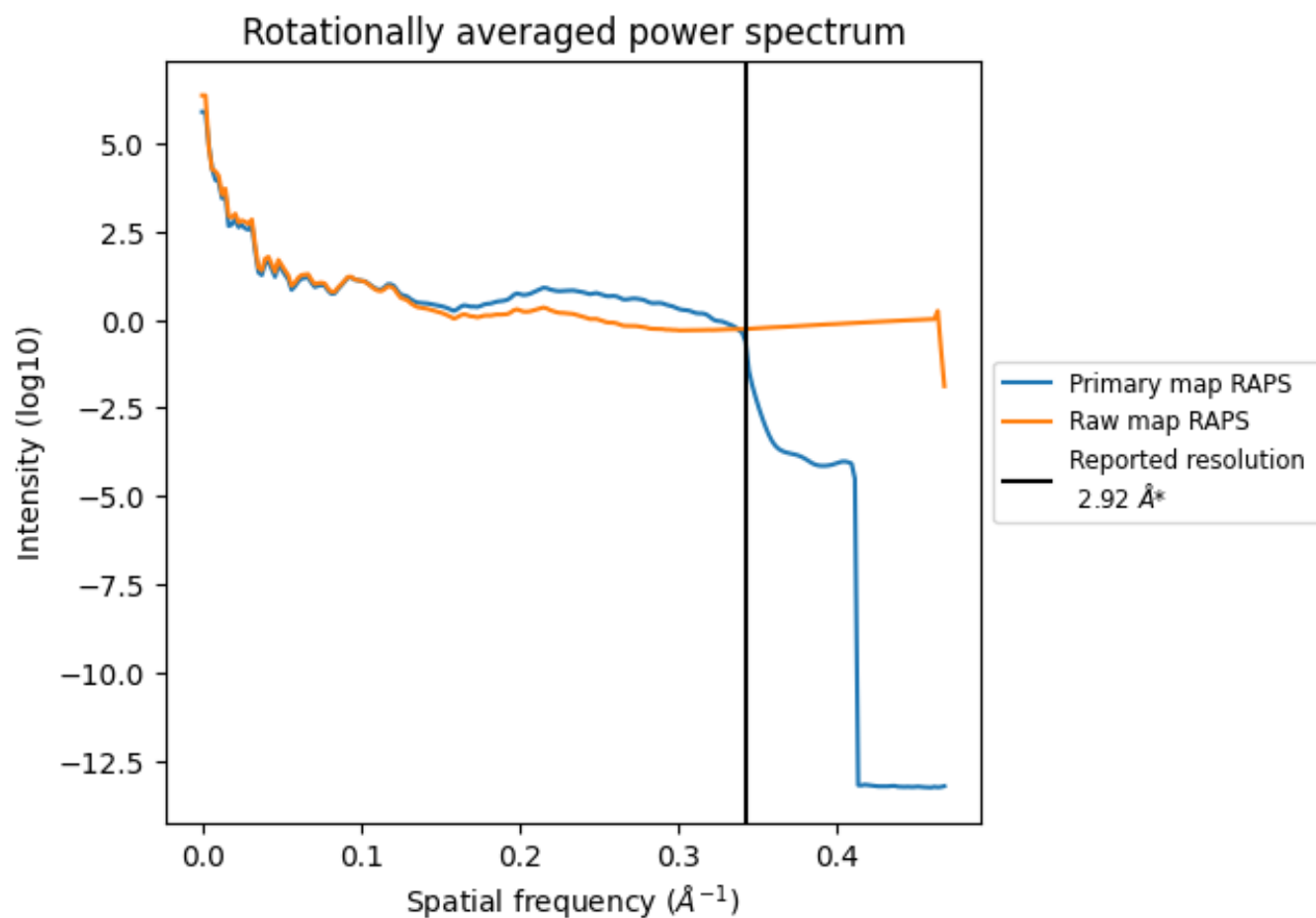
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1301 nm^3 ; this corresponds to an approximate mass of 1175 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 ⓘ

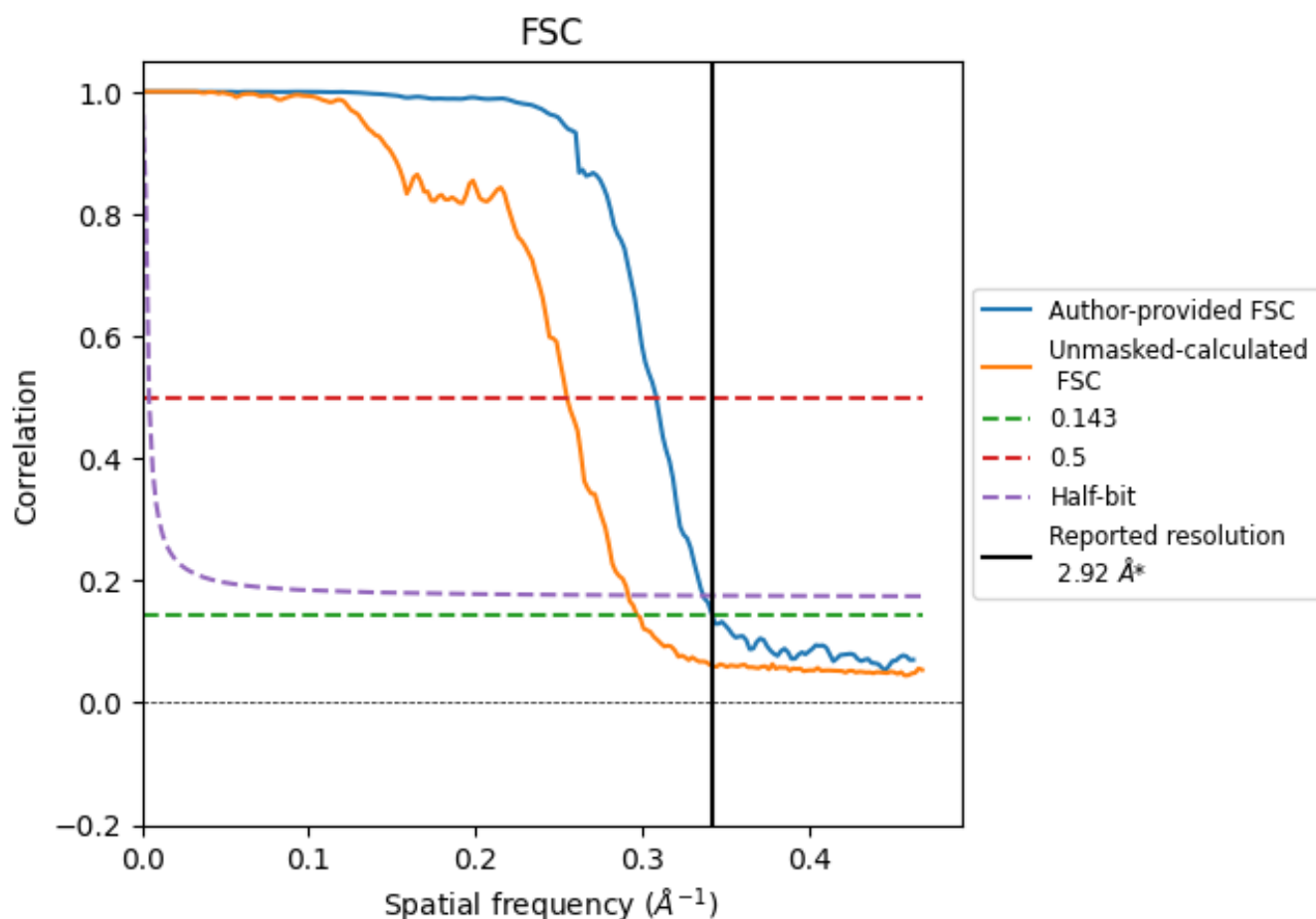


*Reported resolution corresponds to spatial frequency of 0.342 \AA^{-1}

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 0.342 \AA^{-1}

8.2 Resolution estimates [i](#)

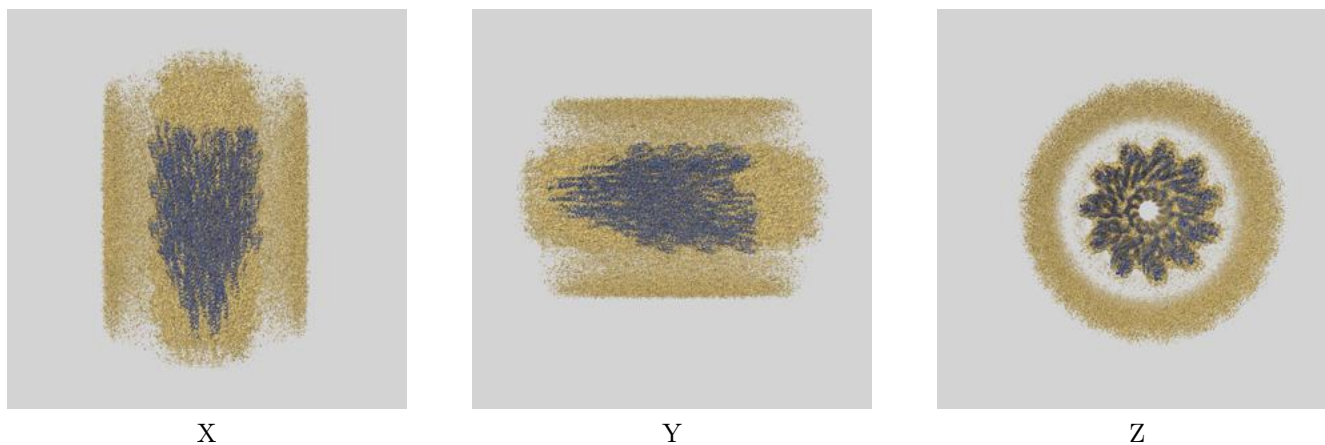
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.92	-	-
Author-provided FSC curve	2.92	3.24	2.97
Unmasked-calculated*	3.36	3.92	3.43

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.36 differs from the reported value 2.92 by more than 10 %

9 Map-model fit [i](#)

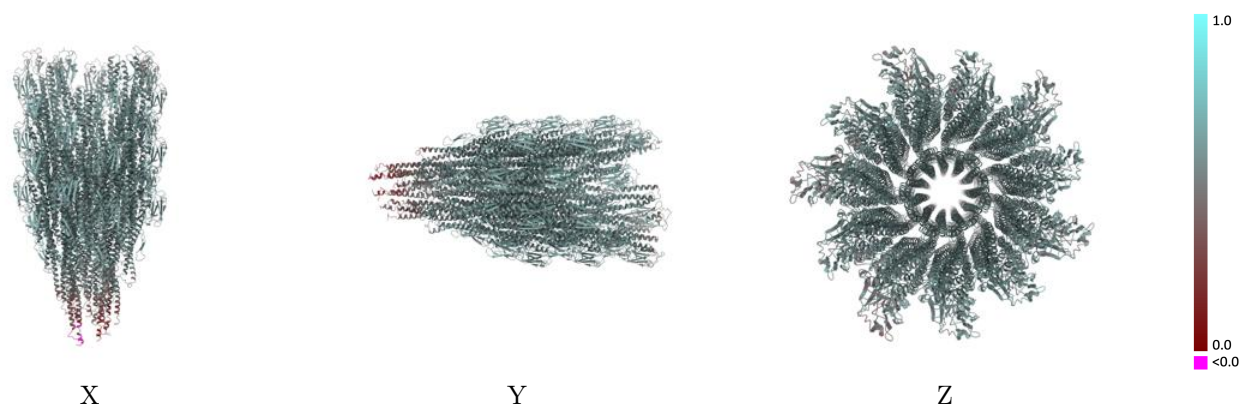
This section contains information regarding the fit between EMDB map EMD-49125 and PDB model 9N8A. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



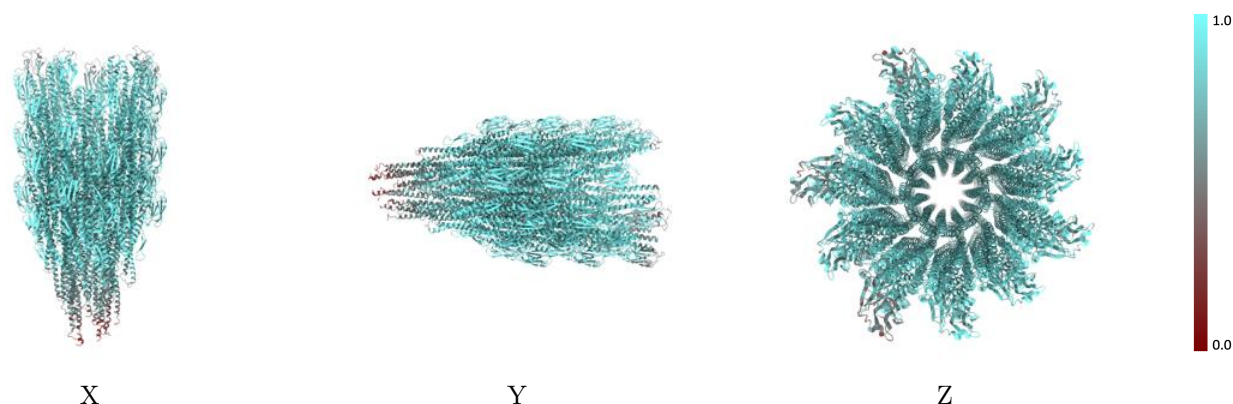
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



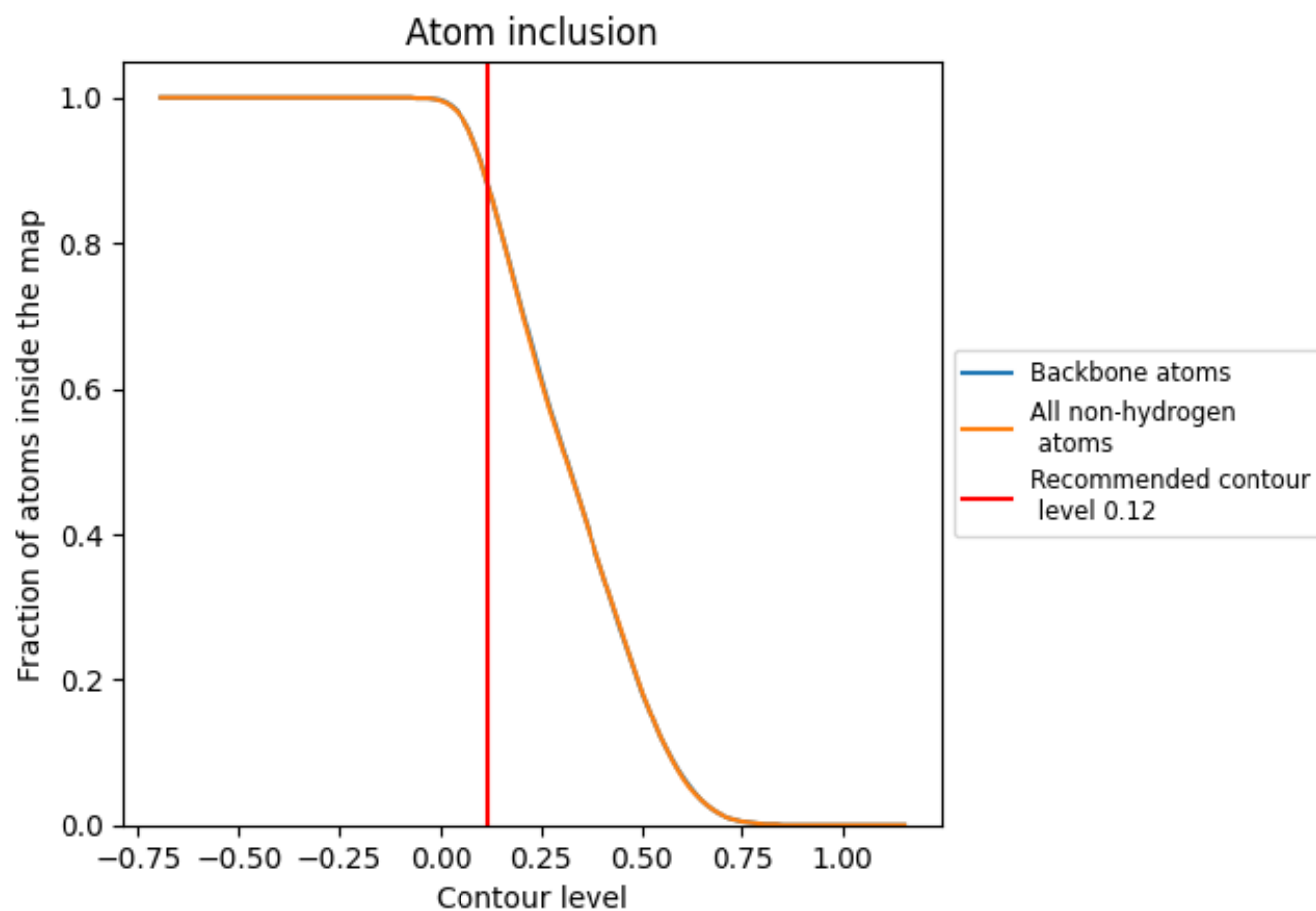
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).





































































9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 88% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8770	 0.5710
A1	 0.9160	 0.5870
A2	 0.8720	 0.5670
A3	 0.8070	 0.5350
B1	 0.8780	 0.5710
B2	 0.8630	 0.5680
B3	 0.9060	 0.5830
C1	 0.8650	 0.5660
C2	 0.9160	 0.5890
C3	 0.9120	 0.5820
D1	 0.9170	 0.5860
E1	 0.8930	 0.5770
F1	 0.8340	 0.5510
G1	 0.9100	 0.5860
H1	 0.8930	 0.5800
I1	 0.7950	 0.5450
J1	 0.8210	 0.5540
K1	 0.9130	 0.5870
L1	 0.8890	 0.5770
M1	 0.8990	 0.5790
N1	 0.9130	 0.5880
O1	 0.8830	 0.5750
P1	 0.8390	 0.5610
Q1	 0.9170	 0.5910
R1	 0.8270	 0.5520
S1	 0.7810	 0.5150
T1	 0.9140	 0.5850
U1	 0.8980	 0.5810
V1	 0.8900	 0.5740
W1	 0.9170	 0.5900
X1	 0.8470	 0.5600
Y1	 0.9130	 0.5840
Z1	 0.7880	 0.5250
a1	 0.8990	 0.5840

