



Full wwPDB EM Validation Report ⓘ

Jun 30, 2026 – 12:46 PM JST

PDB ID : 9X80 / pdb_00009x80
EMDB ID : EMD-66649
Title : sheathed filament of the spirochete periplasmic flagella of *Leptospira biflexa* wild type
Authors : Kawamoto, A.; Nakamura, S.; Koizumi, N.
Deposited on : 2025-10-18
Resolution : 3.24 Å(reported)
Based on initial model : 9LRZ

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.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

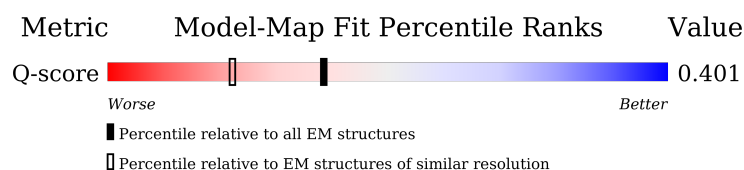
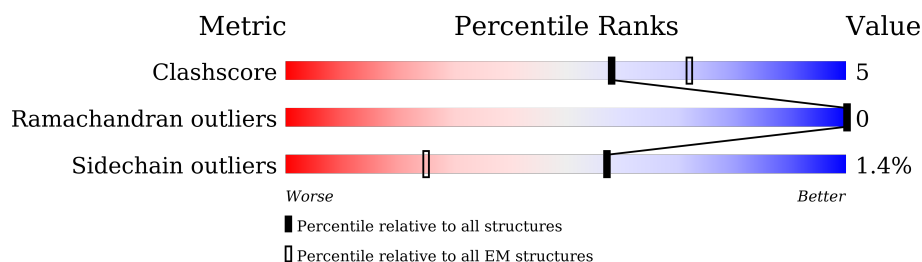
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.24 Å.

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



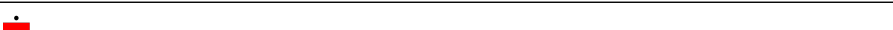
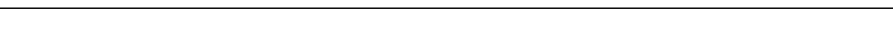
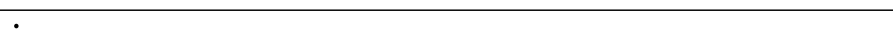
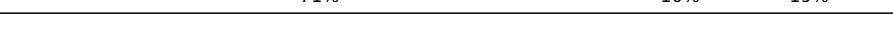
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14594 (2.74 - 3.74)

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	282	
1	D	282	
1	G	282	
1	J	282	

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Mol	Chain	Length	Quality of chain
1	M	282	 89% 10% .
1	P	282	 80% 18% .
1	S	282	 85% 14% .
1	V	282	 82% 16% ..
1	Y	282	 88% 11% ..
1	b	282	 91% 8% .
1	e	282	 84% 14% .
2	K	300	 79% 7% 14%
2	N	300	 78% 8% 14%
2	Q	300	 73% 12% . 14%
2	Z	300	 73% 12% 14%
2	c	300	 79% 6% . 14%
2	f	300	 76% 9% 14%
3	L	277	 71% 10% 19%
3	O	277	 69% 11% . 19%
3	R	277	 18% 66% 15% 19%
3	a	277	 15% 65% 16% 19%
3	d	277	 69% 12% 19%
3	g	277	 69% 12% 19%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 48078 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 Flagellin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	279	Total	C	N	O	S	0	0
			2166	1327	399	424	16		
1	D	279	Total	C	N	O	S	0	0
			2166	1327	399	424	16		
1	G	279	Total	C	N	O	S	0	0
			2166	1327	399	424	16		
1	J	279	Total	C	N	O	S	0	0
			2166	1327	399	424	16		
1	M	279	Total	C	N	O	S	0	0
			2166	1327	399	424	16		
1	P	279	Total	C	N	O	S	0	0
			2166	1327	399	424	16		
1	S	279	Total	C	N	O	S	0	0
			2166	1327	399	424	16		
1	V	279	Total	C	N	O	S	0	0
			2166	1327	399	424	16		
1	Y	279	Total	C	N	O	S	0	0
			2166	1327	399	424	16		
1	b	279	Total	C	N	O	S	0	0
			2166	1327	399	424	16		
1	e	279	Total	C	N	O	S	0	0
			2166	1327	399	424	16		

- Molecule 2 is a protein called Bacterial flagellar sheath protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	257	Total	C	N	O	S	0	0
			2196	1400	379	411	6		
2	N	257	Total	C	N	O	S	0	0
			2196	1400	379	411	6		
2	Q	257	Total	C	N	O	S	0	0
			2196	1400	379	411	6		
2	Z	257	Total	C	N	O	S	0	0
			2196	1400	379	411	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	c	257	Total	C	N	O	S	0	0
			2196	1400	379	411	6		
2	f	257	Total	C	N	O	S	0	0
			2196	1400	379	411	6		

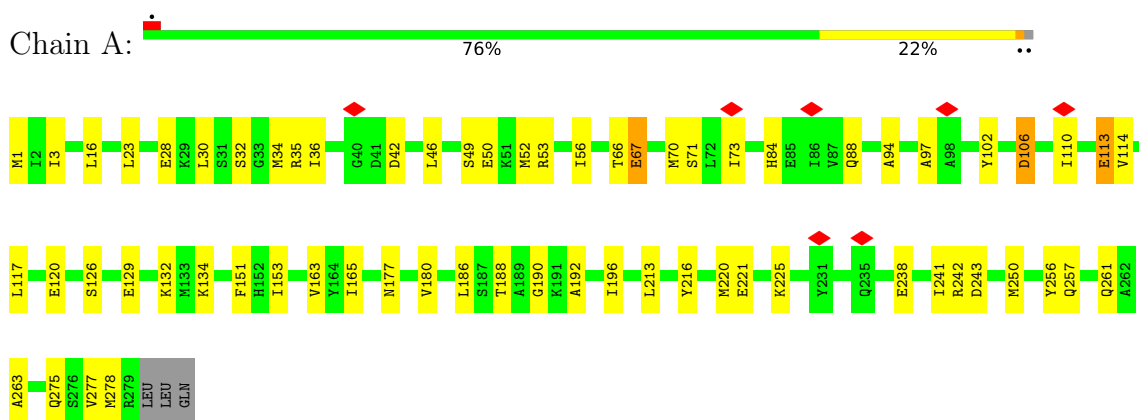
- Molecule 3 is a protein called Bacterial flagellar sheath protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	225	Total	C	N	O	S	0	0
			1846	1174	319	349	4		
3	O	225	Total	C	N	O	S	0	0
			1846	1174	319	349	4		
3	R	225	Total	C	N	O	S	0	0
			1846	1174	319	349	4		
3	a	225	Total	C	N	O	S	0	0
			1846	1174	319	349	4		
3	d	225	Total	C	N	O	S	0	0
			1846	1174	319	349	4		
3	g	225	Total	C	N	O	S	0	0
			1846	1174	319	349	4		

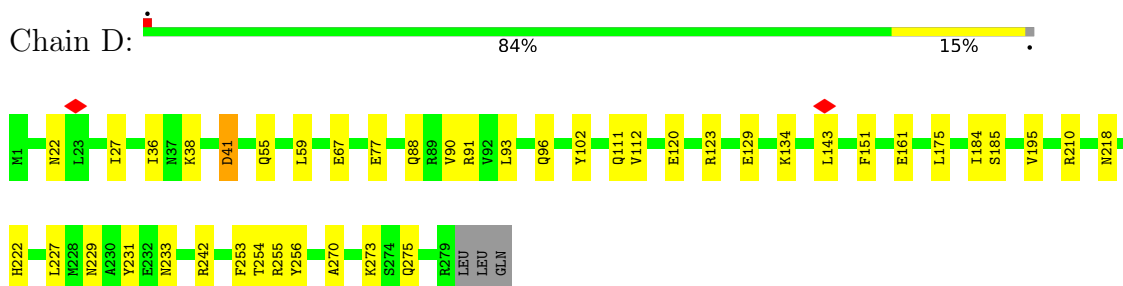
3 Residue-property plots

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.

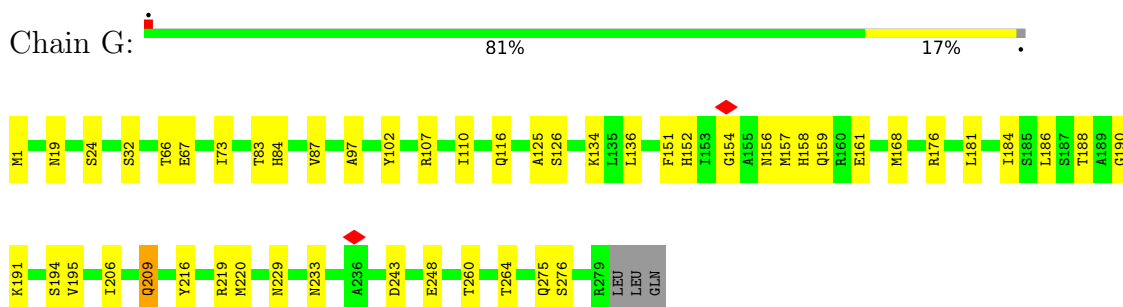
• Molecule 1: Flagellin



• Molecule 1: Flagellin

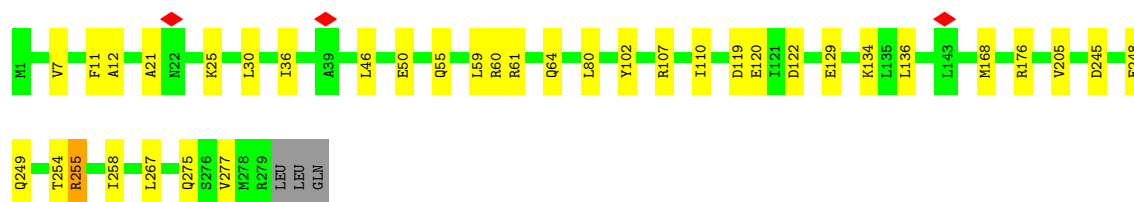


• Molecule 1: Flagellin



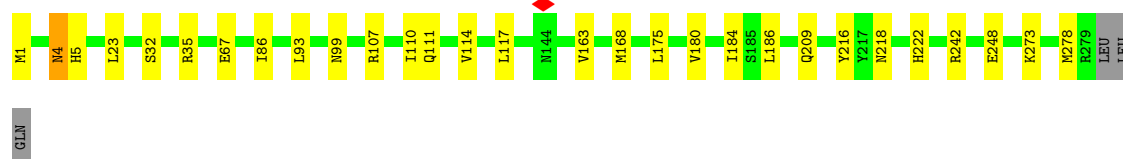
• Molecule 1: Flagellin

Chain J:  86% 12% .



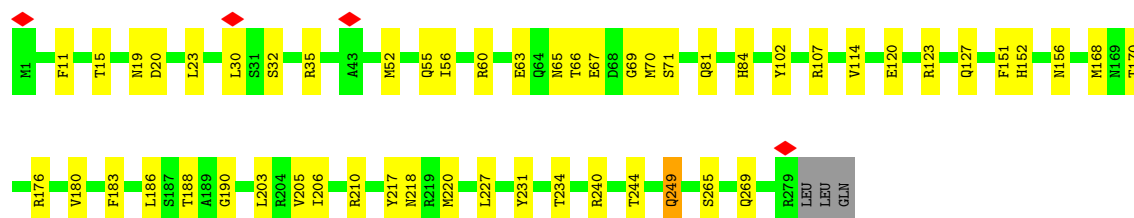
• Molecule 1: Flagellin

Chain M:  89% 10% .



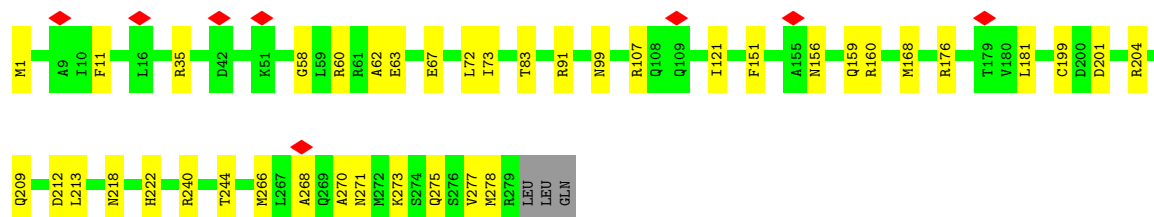
• Molecule 1: Flagellin

Chain P:  80% 18% .



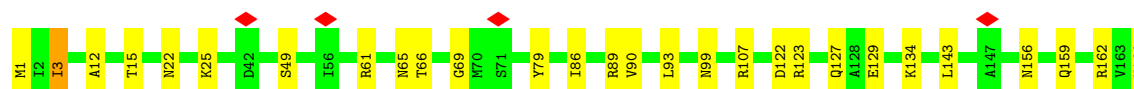
• Molecule 1: Flagellin

Chain S:  85% 14% .



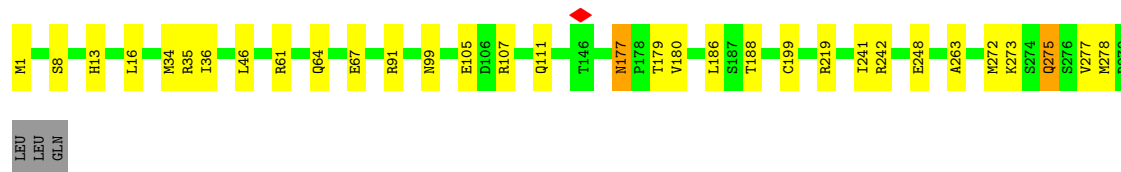
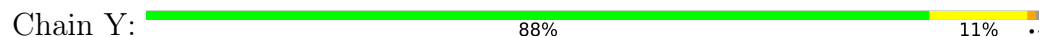
• Molecule 1: Flagellin

Chain V:  82% 16% ..





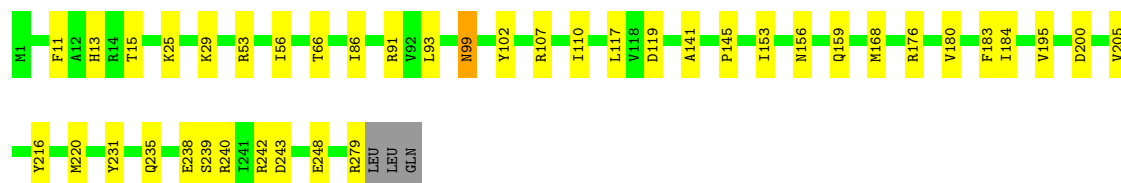
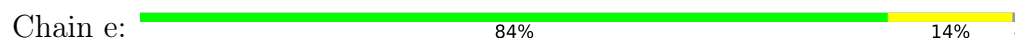
• Molecule 1: Flagellin



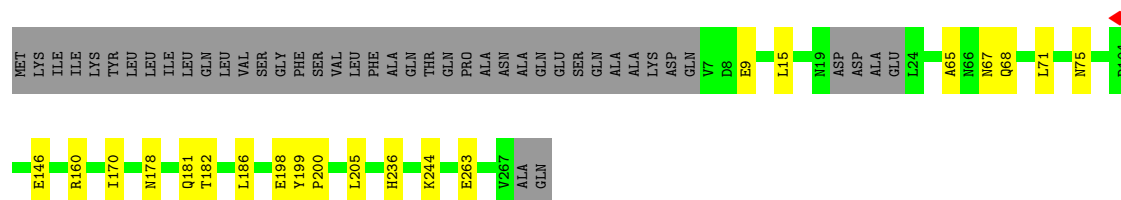
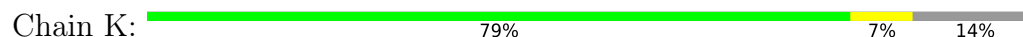
• Molecule 1: Flagellin



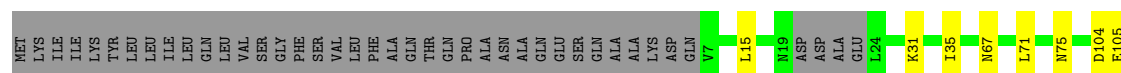
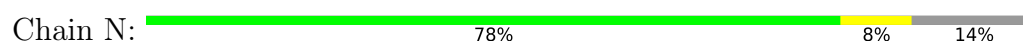
• Molecule 1: Flagellin



• Molecule 2: Bacterial flagellar sheath protein

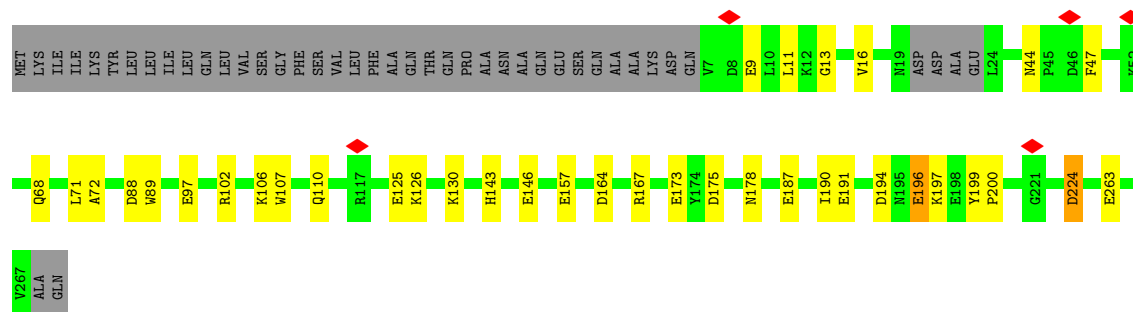
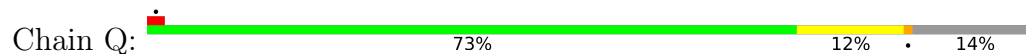


• Molecule 2: Bacterial flagellar sheath protein

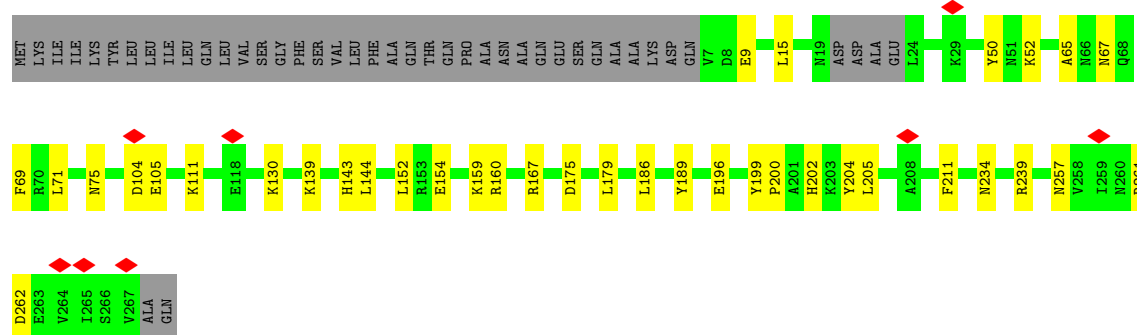




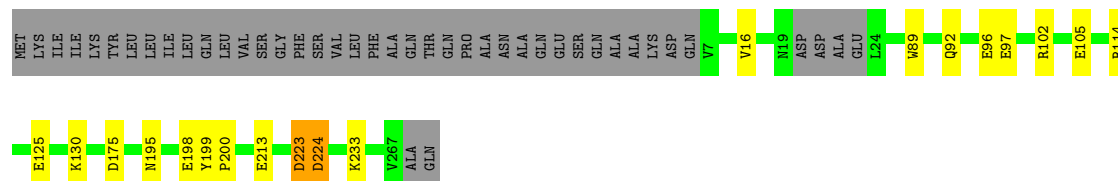
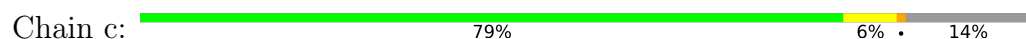
• Molecule 2: Bacterial flagellar sheath protein



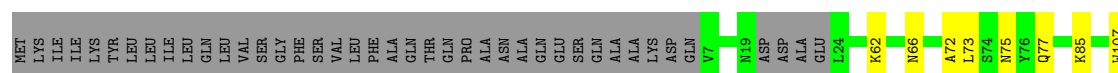
• Molecule 2: Bacterial flagellar sheath protein



• Molecule 2: Bacterial flagellar sheath protein

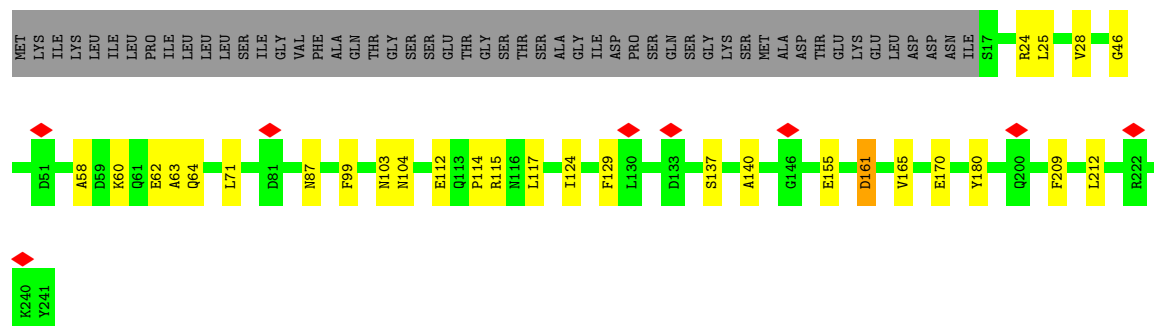


• Molecule 2: Bacterial flagellar sheath protein

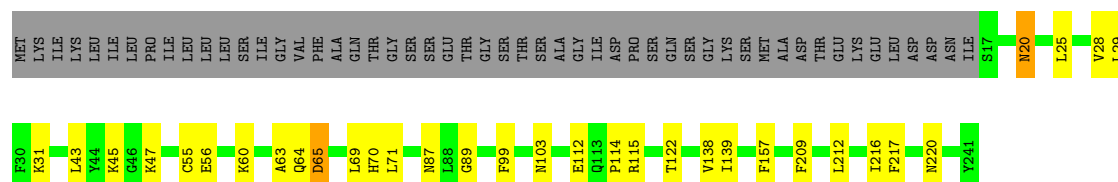




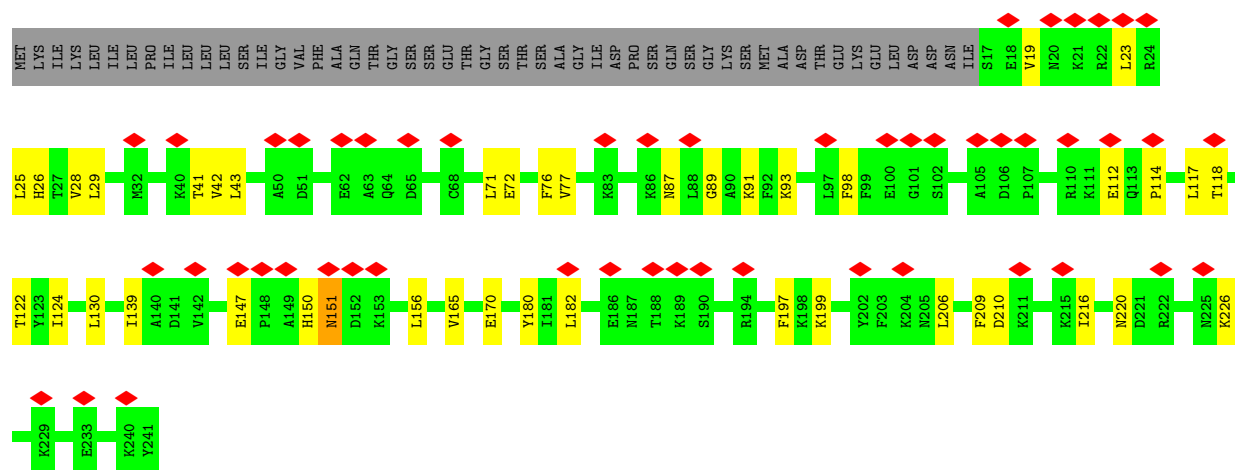
• Molecule 3: Bacterial flagellar sheath protein



• Molecule 3: Bacterial flagellar sheath protein

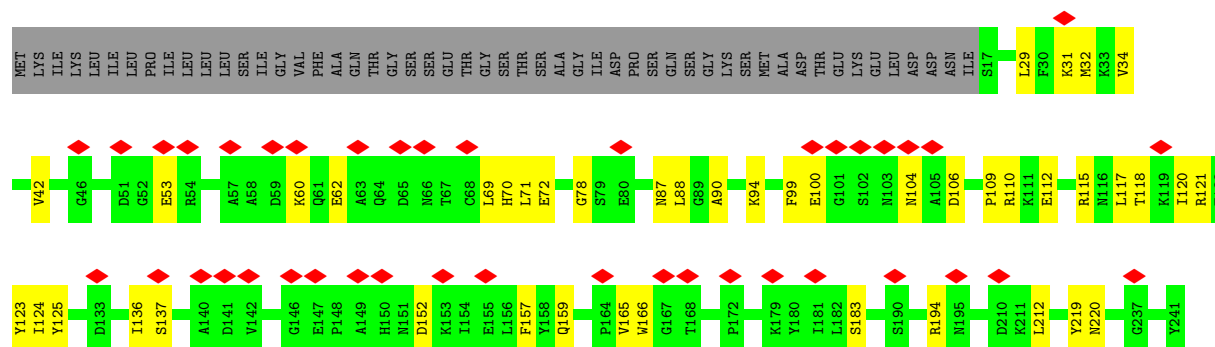


• Molecule 3: Bacterial flagellar sheath protein



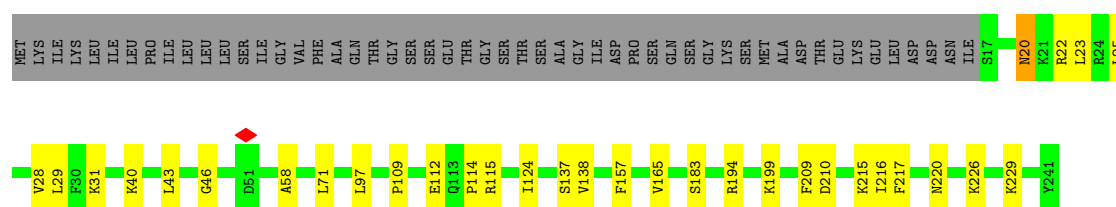
• Molecule 3: Bacterial flagellar sheath protein





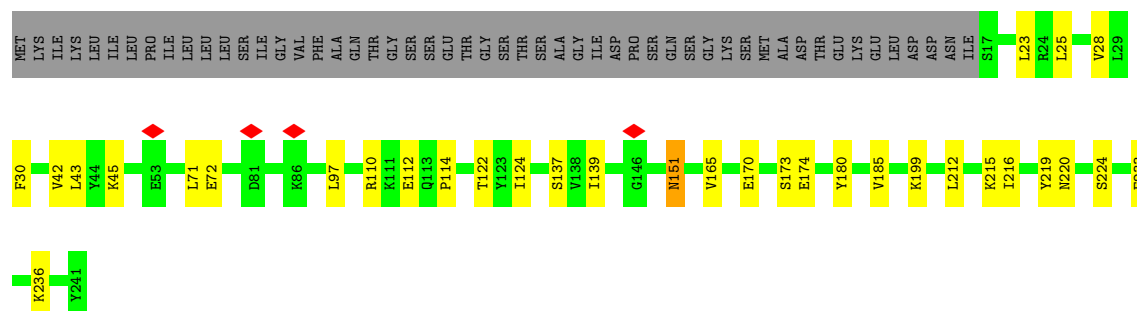
- Molecule 3: Bacterial flagellar sheath protein

Chain d: 69% 12% 19%



- Molecule 3: Bacterial flagellar sheath protein

Chain g: 69% 12% 19%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	163413	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	3.839	Depositor
Minimum map value	-2.697	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.071	Depositor
Recommended contour level	0.273	Depositor
Map size ($\text{\AA}$)	578.56, 578.56, 578.56	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.13, 1.13, 1.13	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.09	0/2188	0.24	0/2944
1	D	0.07	0/2188	0.21	0/2944
1	G	0.08	0/2188	0.23	0/2944
1	J	0.08	0/2188	0.21	0/2944
1	M	0.08	0/2188	0.20	0/2944
1	P	0.09	0/2188	0.23	0/2944
1	S	0.08	0/2188	0.24	0/2944
1	V	0.08	0/2188	0.23	0/2944
1	Y	0.08	0/2188	0.20	0/2944
1	b	0.08	0/2188	0.22	0/2944
1	e	0.08	0/2188	0.22	0/2944
2	K	0.08	0/2242	0.22	0/3010
2	N	0.09	0/2242	0.22	0/3010
2	Q	0.08	0/2242	0.21	0/3010
2	Z	0.08	0/2242	0.20	0/3010
2	c	0.08	0/2242	0.21	0/3010
2	f	0.08	0/2242	0.21	0/3010
3	L	0.07	0/1889	0.20	0/2542
3	O	0.08	0/1889	0.22	0/2542
3	R	0.08	0/1889	0.23	0/2542
3	a	0.07	0/1889	0.19	0/2542
3	d	0.08	0/1889	0.22	0/2542
3	g	0.08	0/1889	0.23	0/2542
All	All	0.08	0/48854	0.22	0/65696

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	A	2166	0	2167	37	0
1	D	2166	0	2167	26	0
1	G	2166	0	2167	31	0
1	J	2166	0	2167	21	0
1	M	2166	0	2167	15	0
1	P	2166	0	2167	33	0
1	S	2166	0	2167	23	0
1	V	2166	0	2167	27	0
1	Y	2166	0	2167	17	0
1	b	2166	0	2167	13	0
1	e	2166	0	2167	25	0
2	K	2196	0	2188	16	0
2	N	2196	0	2188	15	0
2	Q	2196	0	2188	22	0
2	Z	2196	0	2188	21	0
2	c	2196	0	2188	10	0
2	f	2196	0	2188	17	0
3	L	1846	0	1817	19	0
3	O	1846	0	1817	22	0
3	R	1846	0	1817	27	0
3	a	1846	0	1817	26	0
3	d	1846	0	1817	17	0
3	g	1846	0	1817	16	0
All	All	48078	0	47867	453	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (453) 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)
3:R:77:VAL:HB	3:R:89:GLY:HA3	1.67	0.76
3:R:42:VAL:HB	3:R:72:GLU:HB3	1.69	0.74
1:J:245:ASP:HB3	1:J:248:GLU:HB3	1.74	0.70
1:V:1:MET:HB3	1:V:277:VAL:HG12	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:32:SER:HA	1:e:15:THR:HG21	1.76	0.68
3:a:99:PHE:HB3	3:a:115:ARG:HD2	1.75	0.68
1:A:1:MET:HB3	1:A:277:VAL:HG21	1.76	0.68
1:G:73:ILE:HD13	1:G:216:TYR:HB3	1.73	0.67
3:d:138:VAL:HB	3:d:157:PHE:HB3	1.75	0.67
1:A:71:SER:OG	1:P:240:ARG:NH2	2.28	0.66
3:g:28:VAL:HG12	3:g:112:GLU:HB3	1.77	0.66
3:L:99:PHE:HB3	3:L:115:ARG:HD2	1.78	0.65
1:A:23:LEU:HD21	1:A:257:GLN:HG3	1.78	0.65
1:S:218:ASN:O	1:S:222:HIS:ND1	2.31	0.64
2:Q:88:ASP:OD1	3:R:226:LYS:NZ	2.31	0.64
2:Q:68:GLN:NE2	2:Q:146:GLU:OE2	2.32	0.63
1:V:168:MET:HE1	1:V:205:VAL:HG12	1.80	0.63
3:L:64:GLN:O	3:L:103:ASN:ND2	2.27	0.63
2:K:71:LEU:O	2:K:75:ASN:ND2	2.31	0.63
3:L:124:ILE:HB	3:L:137:SER:HB2	1.80	0.63
1:Y:61:ARG:NH1	1:Y:64:GLN:OE1	2.32	0.63
3:a:104:ASN:ND2	3:a:112:GLU:OE2	2.31	0.63
2:c:130:LYS:NZ	2:c:175:ASP:OD2	2.32	0.63
1:e:99:ASN:O	1:e:107:ARG:NH2	2.30	0.63
1:A:102:TYR:HB3	1:A:106:ASP:HB2	1.80	0.63
3:O:28:VAL:HG12	3:O:112:GLU:HB3	1.80	0.63
1:P:66:THR:HG23	1:P:220:MET:HE3	1.80	0.62
1:D:218:ASN:O	1:D:222:HIS:ND1	2.28	0.62
1:A:32:SER:HA	1:P:15:THR:HG21	1.80	0.62
3:a:60:LYS:HG2	3:a:62:GLU:H	1.64	0.62
1:P:35:ARG:HB2	1:P:244:THR:HA	1.80	0.62
3:R:28:VAL:HG12	3:R:112:GLU:HB3	1.81	0.62
3:a:70:HIS:HE1	3:a:72:GLU:HB2	1.64	0.62
1:A:35:ARG:NH2	1:A:42:ASP:OD2	2.32	0.61
1:A:73:ILE:HD13	1:A:216:TYR:HB3	1.81	0.61
1:A:153:ILE:HG21	1:A:220:MET:HE1	1.83	0.61
1:A:106:ASP:OD1	1:A:106:ASP:N	2.32	0.61
2:Q:97:GLU:OE1	2:Q:102:ARG:NH2	2.33	0.61
1:b:156:ASN:ND2	1:b:159:GLN:OE1	2.33	0.61
1:A:67:GLU:HA	1:A:70:MET:HE2	1.82	0.61
3:L:104:ASN:ND2	3:L:112:GLU:OE2	2.33	0.61
3:d:216:ILE:O	3:d:220:ASN:ND2	2.32	0.61
3:a:78:GLY:HA3	3:a:88:LEU:HD12	1.83	0.61
1:A:126:SER:O	1:A:134:LYS:NZ	2.33	0.60
1:S:99:ASN:O	1:S:107:ARG:NH2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:243:ASP:OD2	1:V:255:ARG:NH2	2.34	0.60
1:V:99:ASN:O	1:V:107:ARG:NH2	2.32	0.60
1:Y:1:MET:HE1	1:Y:273:LYS:HG2	1.84	0.60
3:g:216:ILE:O	3:g:220:ASN:ND2	2.35	0.60
1:A:66:THR:HG23	1:A:220:MET:HE3	1.84	0.60
1:J:254:THR:HG21	1:b:271:ASN:HB3	1.82	0.60
1:e:102:TYR:O	1:e:107:ARG:NH1	2.35	0.59
1:V:176:ARG:HA	1:V:183:PHE:HA	1.84	0.59
1:P:30:LEU:HD21	1:P:249:GLN:HB3	1.85	0.59
2:K:67:ASN:ND2	3:L:87:ASN:OD1	2.35	0.59
1:M:23:LEU:HD23	1:b:273:LYS:HE3	1.84	0.58
3:g:233:GLU:HA	3:g:236:LYS:HZ3	1.66	0.58
3:d:124:ILE:HB	3:d:137:SER:HB2	1.84	0.58
2:N:105:GLU:OE2	2:N:114:ARG:NH1	2.36	0.58
2:c:92:GLN:NE2	2:c:96:GLU:OE2	2.35	0.58
2:Z:71:LEU:HD13	2:Z:143:HIS:HD2	1.68	0.58
3:g:122:THR:HB	3:g:139:ILE:HB	1.85	0.58
1:D:229:ASN:O	1:D:233:ASN:ND2	2.37	0.58
3:a:117:LEU:HD13	3:a:120:ILE:HD11	1.84	0.58
3:d:22:ARG:NH2	3:d:210:ASP:OD2	2.35	0.58
3:d:25:LEU:HD23	3:d:114:PRO:HB3	1.86	0.58
1:e:168:MET:HE1	1:e:205:VAL:HG12	1.86	0.57
3:a:124:ILE:HB	3:a:137:SER:HB2	1.86	0.57
1:G:161:GLU:HG3	1:G:219:ARG:HH22	1.69	0.57
3:L:28:VAL:HG12	3:L:112:GLU:HB3	1.86	0.57
1:J:102:TYR:O	1:J:107:ARG:NH1	2.37	0.57
2:f:62:LYS:O	2:f:66:ASN:ND2	2.32	0.57
1:e:25:LYS:O	1:e:29:LYS:NZ	2.37	0.57
1:M:248:GLU:HB2	1:e:13:HIS:CE1	2.40	0.57
2:N:130:LYS:NZ	2:N:175:ASP:OD2	2.37	0.57
2:Q:263:GLU:O	2:f:85:LYS:NZ	2.38	0.57
1:b:126:SER:O	1:b:134:LYS:NZ	2.37	0.57
1:P:176:ARG:HA	1:P:183:PHE:HA	1.87	0.56
2:f:186:LEU:HD13	2:f:205:LEU:HG	1.85	0.56
3:a:53:GLU:O	3:a:121:ARG:NH1	2.37	0.56
3:a:71:LEU:HD21	3:a:212:LEU:HD23	1.87	0.56
3:O:25:LEU:HD23	3:O:114:PRO:HB3	1.86	0.56
1:D:175:LEU:HD22	1:D:184:ILE:HD13	1.86	0.56
3:g:30:PHE:HA	3:g:45:LYS:HE3	1.88	0.56
1:G:126:SER:O	1:G:134:LYS:NZ	2.38	0.56
2:Z:67:ASN:HB2	3:a:90:ALA:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:130:LYS:NZ	2:Z:175:ASP:OD2	2.39	0.56
1:P:188:THR:HG22	1:P:190:GLY:H	1.71	0.55
1:M:218:ASN:O	1:M:222:HIS:ND1	2.37	0.55
1:J:61:ARG:NH1	1:J:64:GLN:OE1	2.40	0.55
3:g:124:ILE:HB	3:g:137:SER:HB2	1.87	0.55
1:D:55:GLN:O	1:D:59:LEU:N	2.32	0.55
1:G:176:ARG:NH2	1:G:181:LEU:O	2.40	0.55
1:J:7:VAL:O	1:J:11:PHE:N	2.38	0.55
1:V:229:ASN:O	1:V:233:ASN:ND2	2.40	0.55
1:A:84:HIS:CE1	1:A:88:GLN:HE21	2.24	0.55
3:a:152:ASP:HA	3:a:183:SER:HB3	1.86	0.55
3:g:151:ASN:N	3:g:151:ASN:OD1	2.40	0.55
2:c:195:ASN:ND2	2:c:198:GLU:OE2	2.40	0.55
2:Z:9:GLU:OE1	2:Z:160:ARG:NH1	2.40	0.55
2:N:167:ARG:NH2	2:N:189:TYR:OH	2.39	0.54
1:V:22:ASN:HA	1:V:25:LYS:HZ3	1.71	0.54
3:d:112:GLU:OE2	3:d:115:ARG:NH2	2.40	0.54
1:A:117:LEU:HA	1:A:120:GLU:HB3	1.88	0.54
1:M:93:LEU:HD22	1:M:110:ILE:HG23	1.90	0.54
1:P:168:MET:HE1	1:P:205:VAL:HG12	1.89	0.54
1:A:261:GLN:HB2	1:S:278:MET:HE1	1.89	0.54
1:G:116:GLN:OE1	1:V:219:ARG:NH1	2.41	0.54
1:J:120:GLU:OE1	1:Y:219:ARG:NE	2.40	0.54
1:M:4:ASN:O	1:M:5:HIS:ND1	2.41	0.54
3:R:25:LEU:HD23	3:R:114:PRO:HB3	1.90	0.54
1:G:168:MET:HE3	1:G:209:GLN:HB2	1.90	0.54
3:O:47:LYS:HE2	3:O:65:ASP:HB2	1.90	0.54
1:P:71:SER:OG	1:e:240:ARG:NH2	2.40	0.54
3:g:215:LYS:NZ	3:g:219:TYR:OH	2.37	0.54
2:K:198:GLU:HG2	2:K:200:PRO:HD2	1.90	0.53
2:f:107:TRP:HB2	2:f:110:GLN:HG3	1.89	0.53
1:G:1:MET:SD	1:G:276:SER:OG	2.61	0.53
1:G:275:GLN:OE1	1:G:275:GLN:N	2.42	0.53
1:Y:177:ASN:HD22	1:Y:179:THR:H	1.55	0.53
1:e:153:ILE:HG21	1:e:220:MET:HE1	1.90	0.53
1:D:275:GLN:OE1	1:D:275:GLN:N	2.41	0.53
1:e:66:THR:HG23	1:e:220:MET:HE3	1.91	0.53
2:Q:9:GLU:HB3	2:Q:157:GLU:HA	1.89	0.53
1:G:229:ASN:OD1	1:G:233:ASN:ND2	2.42	0.53
3:O:71:LEU:HD21	3:O:212:LEU:HD23	1.91	0.53
1:S:91:ARG:HD3	1:S:199:CYS:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:ILE:O	1:D:242:ARG:NE	2.42	0.53
1:J:36:ILE:HG21	1:J:46:LEU:HB2	1.91	0.53
3:R:26:HIS:NE2	3:R:210:ASP:OD1	2.38	0.53
1:Y:8:SER:OG	1:Y:273:LYS:NZ	2.33	0.53
3:a:42:VAL:HB	3:a:72:GLU:HB3	1.91	0.52
3:R:98:PHE:O	3:R:118:THR:N	2.37	0.52
1:e:93:LEU:HD22	1:e:110:ILE:HG23	1.91	0.52
3:R:19:VAL:HG11	3:R:206:LEU:HB3	1.91	0.52
1:S:156:ASN:ND2	1:S:159:GLN:OE1	2.43	0.52
2:Z:154:GLU:HA	2:Z:159:LYS:HE2	1.91	0.52
1:J:60:ARG:NH2	1:Y:248:GLU:OE2	2.41	0.52
1:V:86:ILE:HA	1:V:89:ARG:HB3	1.89	0.52
2:f:73:LEU:HG	2:f:77:GLN:HE21	1.74	0.52
1:A:53:ARG:HA	1:A:56:ILE:HB	1.91	0.52
2:K:263:GLU:OE2	3:a:219:TYR:OH	2.22	0.52
1:e:156:ASN:OD1	1:e:159:GLN:NE2	2.41	0.52
1:D:88:GLN:HA	1:D:91:ARG:HB3	1.92	0.52
1:P:120:GLU:OE2	1:P:123:ARG:NH2	2.38	0.52
1:b:18:SER:O	1:b:22:ASN:ND2	2.38	0.52
2:Z:234:ASN:ND2	2:Z:262:ASP:OD2	2.43	0.52
2:f:199:TYR:CD1	2:f:200:PRO:HD3	2.44	0.52
1:b:28:GLU:O	1:b:32:SER:OG	2.28	0.52
1:b:168:MET:HE1	1:b:205:VAL:HG12	1.91	0.52
1:J:168:MET:HE1	1:J:205:VAL:HG12	1.92	0.51
1:J:21:ALA:O	1:J:25:LYS:NZ	2.43	0.51
1:M:1:MET:HE1	1:M:273:LYS:HG2	1.92	0.51
1:J:119:ASP:OD2	1:Y:219:ARG:NH1	2.39	0.51
1:e:184:ILE:HD12	1:e:195:VAL:HG13	1.92	0.51
2:K:199:TYR:CD2	2:K:200:PRO:HD3	2.45	0.51
1:P:102:TYR:O	1:P:107:ARG:NH1	2.44	0.51
1:V:49:SER:OG	1:V:238:GLU:OE2	2.26	0.51
1:G:67:GLU:HG3	1:V:240:ARG:HD2	1.92	0.51
2:Z:167:ARG:NH2	2:Z:189:TYR:OH	2.44	0.51
3:a:183:SER:O	3:a:194:ARG:NH2	2.44	0.51
3:d:31:LYS:HB2	3:d:109:PRO:HB3	1.92	0.51
3:L:60:LYS:HD2	3:L:63:ALA:HB2	1.93	0.51
1:P:114:VAL:HG21	1:P:186:LEU:HD12	1.93	0.51
3:L:24:ARG:HG2	3:L:117:LEU:HG	1.93	0.50
2:Z:104:ASP:N	2:Z:104:ASP:OD1	2.42	0.50
2:Z:139:LYS:O	2:Z:143:HIS:ND1	2.33	0.50
1:A:50:GLU:OE2	1:A:242:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:205:LEU:HD13	2:f:236:HIS:CD2	2.45	0.50
2:N:71:LEU:O	2:N:75:ASN:ND2	2.44	0.50
3:R:77:VAL:HG22	3:R:91:LYS:HE3	1.93	0.50
3:g:170:GLU:HB2	3:g:180:TYR:HB3	1.93	0.50
3:O:99:PHE:HB3	3:O:115:ARG:HD2	1.92	0.50
3:O:138:VAL:HB	3:O:157:PHE:HB3	1.93	0.50
1:V:3:ILE:HG23	1:V:277:VAL:HG11	1.94	0.50
1:A:114:VAL:HG21	1:A:186:LEU:HD11	1.93	0.50
2:K:170:ILE:HD13	2:K:186:LEU:HG	1.94	0.50
2:Q:130:LYS:NZ	2:Q:175:ASP:OD2	2.31	0.50
2:c:199:TYR:CD2	2:c:200:PRO:HD3	2.46	0.50
3:a:29:LEU:HA	3:a:32:MET:HB3	1.92	0.50
3:L:140:ALA:HB3	3:L:155:GLU:HB2	1.93	0.50
2:N:15:LEU:O	2:N:155:ARG:NE	2.44	0.50
3:O:64:GLN:O	3:O:103:ASN:ND2	2.45	0.50
2:Q:224:ASP:OD1	2:Q:224:ASP:N	2.43	0.49
1:D:90:VAL:HA	1:D:93:LEU:HB2	1.94	0.49
1:b:156:ASN:HB2	1:b:159:GLN:HG3	1.94	0.49
1:M:99:ASN:O	1:M:107:ARG:NH2	2.45	0.49
2:f:170:ILE:HD13	2:f:186:LEU:HG	1.94	0.49
2:Q:199:TYR:CD1	2:Q:200:PRO:HD3	2.46	0.49
1:V:129:GLU:OE2	1:V:134:LYS:NZ	2.44	0.49
3:g:110:ARG:NH2	3:g:224:SER:OG	2.45	0.49
1:A:49:SER:OG	1:A:238:GLU:OE2	2.29	0.49
1:A:73:ILE:HD11	1:A:151:PHE:HE2	1.77	0.49
3:O:31:LYS:NZ	3:O:112:GLU:OE1	2.46	0.49
2:Q:13:GLY:HA3	3:R:42:VAL:HG11	1.94	0.49
1:A:132:LYS:NZ	1:P:55:GLN:OE1	2.33	0.49
1:D:22:ASN:HB3	1:D:256:TYR:CZ	2.47	0.49
1:S:176:ARG:NH2	1:S:181:LEU:O	2.44	0.49
1:S:35:ARG:HB2	1:S:244:THR:HB	1.94	0.49
1:P:32:SER:HB3	1:e:11:PHE:HE1	1.77	0.49
1:A:129:GLU:OE1	1:P:156:ASN:ND2	2.46	0.48
3:O:29:LEU:HD21	3:O:217:PHE:HB2	1.94	0.48
1:b:1:MET:HB3	1:b:277:VAL:HG11	1.93	0.48
1:S:58:GLY:O	1:S:62:ALA:N	2.41	0.48
3:d:46:GLY:HA2	3:d:58:ALA:HB2	1.94	0.48
1:A:97:ALA:HB2	1:A:110:ILE:HG21	1.95	0.48
1:M:111:GLN:OE1	1:M:186:LEU:N	2.41	0.48
3:a:100:GLU:OE1	3:a:118:THR:OG1	2.29	0.48
1:G:24:SER:OG	1:V:273:LYS:NZ	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:164:ASP:OD1	2:Q:167:ARG:NH1	2.41	0.48
1:V:12:ALA:HB3	1:V:267:LEU:HD13	1.95	0.48
1:Y:35:ARG:NH2	1:Y:241:ILE:O	2.37	0.48
3:a:34:VAL:HG13	3:a:220:ASN:HD21	1.78	0.48
3:d:23:LEU:HD23	3:d:97:LEU:HD21	1.95	0.48
3:L:103:ASN:HA	3:L:115:ARG:HH22	1.77	0.48
2:N:199:TYR:CD1	2:N:200:PRO:HD3	2.48	0.48
3:R:151:ASN:OD1	3:R:151:ASN:N	2.45	0.48
2:c:97:GLU:OE1	2:c:102:ARG:NH2	2.43	0.48
1:P:206:ILE:O	1:P:210:ARG:HG3	2.13	0.48
3:g:23:LEU:HD23	3:g:97:LEU:HD21	1.94	0.48
1:A:188:THR:HG22	1:A:190:GLY:H	1.79	0.48
1:A:36:ILE:HG21	1:A:46:LEU:HD13	1.96	0.48
3:d:43:LEU:HD12	3:d:71:LEU:HD13	1.94	0.48
1:A:192:ALA:O	1:A:196:ILE:HG13	2.14	0.48
1:Y:36:ILE:HG21	1:Y:46:LEU:HB2	1.96	0.48
2:c:105:GLU:OE2	2:c:114:ARG:NH1	2.47	0.48
1:S:168:MET:HE3	1:S:209:GLN:HG2	1.95	0.48
1:J:255:ARG:HH22	1:J:258:ILE:HD12	1.80	0.47
1:M:32:SER:HA	1:b:15:THR:HG21	1.96	0.47
3:O:60:LYS:HD2	3:O:63:ALA:HB2	1.95	0.47
1:G:66:THR:HG23	1:G:220:MET:HE3	1.96	0.47
2:Q:194:ASP:HB3	2:Q:197:LYS:HD3	1.96	0.47
1:V:254:THR:O	1:V:258:ILE:N	2.46	0.47
1:G:152:HIS:NE2	1:G:154:GLY:O	2.47	0.47
2:K:67:ASN:HD22	3:L:129:PHE:HE2	1.62	0.47
2:K:186:LEU:HD13	2:K:205:LEU:HG	1.96	0.47
1:P:71:SER:HG	1:e:240:ARG:NH2	2.12	0.47
3:R:71:LEU:HD23	3:R:209:PHE:HD2	1.79	0.47
3:g:71:LEU:HD21	3:g:212:LEU:HD23	1.96	0.47
3:O:55:CYS:SG	3:O:56:GLU:N	2.88	0.47
1:A:30:LEU:HD11	1:A:250:MET:SD	2.55	0.47
1:D:41:ASP:N	1:D:41:ASP:OD1	2.48	0.47
1:J:55:GLN:O	1:J:59:LEU:N	2.35	0.47
2:K:205:LEU:HD13	2:K:236:HIS:CE1	2.50	0.47
3:d:29:LEU:HD21	3:d:217:PHE:HB2	1.97	0.47
3:L:60:LYS:HG2	3:L:62:GLU:H	1.80	0.46
3:O:20:ASN:OD1	3:O:20:ASN:N	2.48	0.46
2:Q:107:TRP:HB2	2:Q:110:GLN:HG3	1.97	0.46
1:V:61:ARG:NH2	1:V:65:ASN:OD1	2.47	0.46
1:e:91:ARG:NE	1:e:200:ASP:OD1	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:168:MET:HE3	1:M:209:GLN:HB2	1.97	0.46
2:N:199:TYR:CG	2:N:200:PRO:HD3	2.51	0.46
2:Q:190:ILE:HB	2:Q:196:GLU:HG2	1.97	0.46
1:D:27:ILE:HD13	1:S:270:ALA:HB2	1.97	0.46
1:G:157:MET:O	1:G:158:HIS:ND1	2.48	0.46
1:J:80:LEU:HD21	1:J:168:MET:HG3	1.97	0.46
1:J:122:ASP:OD2	1:J:176:ARG:NH1	2.46	0.46
1:M:35:ARG:N	1:M:242:ARG:O	2.42	0.46
1:Y:16:LEU:HD13	1:Y:263:ALA:HB3	1.98	0.46
1:A:177:ASN:HB3	1:A:180:VAL:HB	1.98	0.46
1:A:221:GLU:O	1:A:225:LYS:NZ	2.49	0.46
2:f:75:ASN:HB2	2:f:140:ALA:HB2	1.98	0.46
1:G:84:HIS:HB2	1:G:206:ILE:HG21	1.98	0.46
1:G:125:ALA:HA	1:G:136:LEU:HB2	1.98	0.46
3:L:25:LEU:HD23	3:L:114:PRO:HB3	1.98	0.46
2:c:224:ASP:N	2:c:224:ASP:OD1	2.47	0.46
3:a:31:LYS:HB2	3:a:109:PRO:HB3	1.97	0.46
1:A:52:MET:HB2	1:A:238:GLU:HG3	1.97	0.45
2:K:15:LEU:HD23	2:K:65:ALA:HB1	1.98	0.45
2:Z:186:LEU:HD11	2:Z:204:TYR:HB3	1.96	0.45
3:a:87:ASN:ND2	3:a:87:ASN:O	2.49	0.45
2:N:126:LYS:O	2:N:130:LYS:HG2	2.16	0.45
2:Q:173:GLU:HG3	2:Q:178:ASN:HB2	1.99	0.45
2:Z:71:LEU:O	2:Z:75:ASN:ND2	2.45	0.45
1:G:260:THR:O	1:G:264:THR:OG1	2.27	0.45
1:G:102:TYR:O	1:G:107:ARG:NH2	2.49	0.45
3:R:43:LEU:HD12	3:R:71:LEU:HD13	1.99	0.45
1:G:161:GLU:HG3	1:G:219:ARG:NH2	2.31	0.45
1:G:184:ILE:HD12	1:G:195:VAL:HG13	1.98	0.45
3:a:70:HIS:CE1	3:a:72:GLU:HB2	2.47	0.45
1:J:129:GLU:OE2	1:J:134:LYS:NZ	2.39	0.45
1:P:63:GLU:O	1:P:67:GLU:N	2.49	0.45
2:K:68:GLN:NE2	2:K:146:GLU:OE2	2.49	0.45
2:Z:202:HIS:CE1	2:Z:239:ARG:HG2	2.52	0.45
1:A:28:GLU:HA	1:P:11:PHE:CE1	2.51	0.45
1:A:165:ILE:HG12	1:A:213:LEU:HD21	1.99	0.45
2:N:106:LYS:HB3	2:f:181:GLN:CD	2.42	0.45
1:A:113:GLU:OE2	1:P:218:ASN:ND2	2.38	0.44
3:L:46:GLY:HA2	3:L:58:ALA:HB2	1.99	0.44
1:P:265:SER:O	1:P:269:GLN:HG2	2.17	0.44
2:Z:15:LEU:HD21	2:Z:152:LEU:HB3	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:68:GLN:OE1	3:L:87:ASN:ND2	2.50	0.44
2:N:104:ASP:HB3	1:e:180:VAL:O	2.18	0.44
1:G:209:GLN:HE21	1:G:209:GLN:HA	1.82	0.44
3:O:122:THR:N	3:O:139:ILE:O	2.37	0.44
2:Z:199:TYR:CD2	2:Z:200:PRO:HD3	2.53	0.44
1:G:188:THR:HG22	1:G:190:GLY:H	1.83	0.44
2:K:199:TYR:CE1	2:K:244:LYS:HD2	2.53	0.44
3:O:122:THR:HB	3:O:139:ILE:HB	1.99	0.44
1:S:72:LEU:HD22	1:S:151:PHE:HZ	1.82	0.44
2:Z:50:TYR:O	2:Z:52:LYS:NZ	2.51	0.44
2:K:170:ILE:HG23	2:K:182:THR:HB	1.99	0.44
3:R:41:THR:HG21	3:R:216:ILE:HD11	1.99	0.44
1:D:111:GLN:HE22	1:D:185:SER:HA	1.82	0.44
2:Q:68:GLN:OE1	3:R:87:ASN:ND2	2.51	0.44
3:R:156:LEU:HD11	3:R:182:LEU:HD13	1.99	0.44
3:a:110:ARG:H	3:a:110:ARG:HD2	1.82	0.44
3:d:71:LEU:HD23	3:d:209:PHE:HD1	1.83	0.44
3:g:42:VAL:HB	3:g:72:GLU:HB3	2.00	0.44
1:G:156:ASN:HB2	1:G:159:GLN:HG3	1.99	0.44
1:J:46:LEU:O	1:J:50:GLU:HG2	2.18	0.44
2:N:31:LYS:HE2	2:N:35:ILE:HD11	1.99	0.44
1:P:60:ARG:NH2	1:e:248:GLU:OE1	2.49	0.44
3:R:147:GLU:O	3:R:150:HIS:ND1	2.44	0.44
1:V:123:ARG:NH1	1:V:127:GLN:OE1	2.47	0.44
2:Z:179:LEU:HD22	2:Z:211:PHE:HB2	2.00	0.44
1:D:36:ILE:HG23	1:D:41:ASP:HB2	1.99	0.43
3:d:226:LYS:HA	3:d:229:LYS:HD3	2.00	0.43
1:A:34:MET:HA	1:A:243:ASP:HA	1.99	0.43
1:D:151:PHE:N	1:D:161:GLU:O	2.35	0.43
1:D:38:LYS:HE2	1:S:11:PHE:HE1	1.83	0.43
1:V:122:ASP:OD2	1:V:176:ARG:NH1	2.51	0.43
1:V:188:THR:HG22	1:V:190:GLY:H	1.84	0.43
1:P:227:LEU:O	1:P:231:TYR:N	2.49	0.43
3:a:31:LYS:NZ	3:a:106:ASP:O	2.48	0.43
2:c:89:TRP:CH2	2:c:125:GLU:HG3	2.54	0.43
2:f:179:LEU:HD22	2:f:211:PHE:HB2	2.00	0.43
1:P:70:MET:HB3	1:P:217:TYR:CE2	2.53	0.43
1:Y:34:MET:HB3	1:Y:242:ARG:HE	1.84	0.43
1:D:255:ARG:HE	1:D:256:TYR:HE1	1.65	0.43
3:O:71:LEU:HD23	3:O:209:PHE:HD1	1.83	0.43
1:P:81:GLN:OE1	1:P:210:ARG:NH2	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:199:LYS:HE2	3:R:199:LYS:HB3	1.84	0.43
1:D:129:GLU:HG2	1:D:134:LYS:HD3	2.00	0.43
2:N:186:LEU:HD13	2:N:205:LEU:HG	2.01	0.43
3:a:157:PHE:HE1	3:a:159:GLN:HB2	1.83	0.43
1:G:191:LYS:O	1:G:194:SER:OG	2.28	0.43
1:S:270:ALA:O	1:S:273:LYS:HB3	2.19	0.43
1:V:162:ARG:HD3	1:V:164:TYR:CZ	2.53	0.43
1:b:1:MET:HE1	1:b:273:LYS:HG2	2.00	0.43
1:e:53:ARG:HH21	1:e:242:ARG:HG2	1.84	0.43
1:e:216:TYR:O	1:e:220:MET:HG2	2.18	0.43
1:D:96:GLN:HG2	1:D:102:TYR:HE2	1.84	0.43
1:Y:91:ARG:HD3	1:Y:199:CYS:HB2	2.01	0.43
1:P:170:THR:OG1	1:P:176:ARG:HD2	2.19	0.43
2:Z:196:GLU:O	2:Z:202:HIS:NE2	2.50	0.43
1:D:120:GLU:OE2	1:D:123:ARG:NH2	2.39	0.42
2:N:107:TRP:HZ3	2:f:215:MET:HE2	1.84	0.42
3:R:29:LEU:HD13	3:R:43:LEU:HD11	2.00	0.42
1:V:69:GLY:HA3	1:V:220:MET:HE2	2.00	0.42
1:Y:99:ASN:O	1:Y:107:ARG:NH2	2.53	0.42
1:M:175:LEU:HD22	1:M:184:ILE:HD13	2.00	0.42
3:O:87:ASN:O	3:O:87:ASN:ND2	2.53	0.42
1:P:123:ARG:NH1	1:P:127:GLN:OE1	2.53	0.42
2:Q:106:LYS:HG3	2:Q:107:TRP:HD1	1.83	0.42
1:V:66:THR:HG23	1:V:220:MET:HE3	2.01	0.42
3:a:70:HIS:NE2	3:a:94:LYS:HD2	2.34	0.42
1:e:239:SER:OG	1:e:243:ASP:OD2	2.34	0.42
1:D:253:PHE:CZ	1:S:266:MET:HE1	2.54	0.42
1:P:19:ASN:O	1:P:23:LEU:N	2.48	0.42
2:Q:72:ALA:HB2	2:Q:143:HIS:HB2	2.02	0.42
1:e:86:ILE:HG23	1:e:117:LEU:HD22	2.01	0.42
1:D:270:ALA:O	1:D:273:LYS:HG2	2.20	0.42
2:Q:89:TRP:CZ3	2:Q:125:GLU:HG3	2.55	0.42
1:b:73:ILE:HD13	1:b:216:TYR:HB3	2.01	0.42
3:d:28:VAL:HG12	3:d:112:GLU:HB3	2.02	0.42
2:f:126:LYS:O	2:f:130:LYS:HG2	2.18	0.42
2:f:194:ASP:HB3	2:f:197:LYS:HD3	2.01	0.42
2:Q:126:LYS:O	2:Q:130:LYS:HG2	2.19	0.42
1:V:233:ASN:O	1:V:237:SER:OG	2.29	0.42
2:f:72:ALA:HB2	2:f:143:HIS:HB2	2.02	0.42
3:g:43:LEU:HD12	3:g:71:LEU:HD13	2.02	0.42
1:G:83:THR:O	1:G:87:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:216:ILE:O	3:O:220:ASN:ND2	2.42	0.42
1:P:65:ASN:HD22	1:P:152:HIS:HB3	1.85	0.42
2:Q:187:GLU:O	2:Q:191:GLU:HG2	2.19	0.42
1:b:81:GLN:OE1	1:b:210:ARG:NH2	2.53	0.42
2:c:213:GLU:OE1	2:c:233:LYS:NZ	2.48	0.42
1:J:30:LEU:HD21	1:J:249:GLN:HB3	2.01	0.42
1:M:86:ILE:HG23	1:M:117:LEU:HD22	2.00	0.42
2:Q:199:TYR:CG	2:Q:200:PRO:HD3	2.55	0.42
3:d:20:ASN:OD1	3:d:20:ASN:N	2.51	0.42
1:e:56:ILE:HG23	1:e:231:TYR:HE1	1.83	0.42
2:f:249:SER:O	2:f:253:LYS:HG2	2.20	0.42
3:O:43:LEU:HA	3:O:70:HIS:O	2.20	0.42
3:R:23:LEU:HB3	3:R:117:LEU:HD11	2.02	0.42
2:c:223:ASP:OD1	2:c:223:ASP:N	2.51	0.42
3:d:183:SER:HA	3:d:194:ARG:HH21	1.85	0.42
1:G:73:ILE:HD11	1:G:151:PHE:HE2	1.84	0.41
3:L:71:LEU:HD21	3:L:212:LEU:HD23	2.01	0.41
3:O:43:LEU:HD12	3:O:71:LEU:HD13	2.02	0.41
1:S:73:ILE:HG23	1:S:213:LEU:HB3	2.02	0.41
1:S:268:ALA:HA	1:S:271:ASN:HB2	2.02	0.41
1:e:176:ARG:HG3	1:e:183:PHE:HB3	2.02	0.41
2:f:199:TYR:CG	2:f:200:PRO:HD3	2.54	0.41
2:N:67:ASN:ND2	3:O:89:GLY:O	2.52	0.41
1:P:52:MET:O	1:P:56:ILE:N	2.45	0.41
1:S:1:MET:HB3	1:S:277:VAL:HG11	2.02	0.41
2:Z:105:GLU:OE2	2:Z:111:LYS:HG2	2.21	0.41
1:D:227:LEU:O	1:D:231:TYR:N	2.44	0.41
1:G:107:ARG:HG2	1:G:186:LEU:O	2.21	0.41
1:V:90:VAL:HA	1:V:93:LEU:HD12	2.03	0.41
2:K:9:GLU:HB2	2:K:160:ARG:HG2	2.02	0.41
3:L:161:ASP:OD1	3:L:161:ASP:N	2.53	0.41
3:R:170:GLU:HB3	3:R:180:TYR:HB3	2.02	0.41
1:S:83:THR:HG23	1:S:121:ILE:HG12	2.03	0.41
3:a:136:ILE:HG21	3:a:166:TRP:HZ3	1.86	0.41
1:J:136:LEU:HB3	1:J:168:MET:HB2	2.03	0.41
1:P:84:HIS:CE1	1:P:203:LEU:HD22	2.55	0.41
3:R:93:LYS:HG2	3:R:124:ILE:HG23	2.02	0.41
2:Z:257:ASN:HB3	2:Z:261:ARG:HH12	1.86	0.41
3:g:173:SER:OG	3:g:174:GLU:OE1	2.36	0.41
1:D:67:GLU:HB3	1:S:240:ARG:HH11	1.85	0.41
1:G:97:ALA:HB2	1:G:110:ILE:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:60:ARG:HD2	1:S:60:ARG:HA	1.95	0.41
1:D:184:ILE:HD12	1:D:195:VAL:HG13	2.03	0.41
1:G:32:SER:HA	1:V:15:THR:HG21	2.02	0.41
1:J:12:ALA:HB3	1:J:267:LEU:HD13	2.02	0.41
1:Y:105:GLU:OE1	1:Y:105:GLU:N	2.45	0.41
1:Y:111:GLN:OE1	1:Y:186:LEU:N	2.44	0.41
1:e:235:GLN:NE2	1:e:238:GLU:OE1	2.54	0.41
1:D:77:GLU:OE2	1:D:210:ARG:NH2	2.37	0.41
1:M:114:VAL:HG21	1:M:186:LEU:HD12	2.02	0.41
1:M:163:VAL:HG13	1:M:216:TYR:CE2	2.55	0.41
3:O:31:LYS:HE3	3:O:31:LYS:HB2	1.96	0.41
2:Q:44:ASN:ND2	2:Q:47:PHE:HB2	2.36	0.41
3:R:23:LEU:HA	3:R:26:HIS:CD2	2.55	0.41
3:R:122:THR:HB	3:R:139:ILE:HB	2.02	0.41
3:R:139:ILE:HD13	3:R:197:PHE:HZ	1.86	0.41
1:S:60:ARG:NH1	1:S:63:GLU:OE1	2.54	0.41
1:S:201:ASP:OD1	1:S:204:ARG:NH2	2.54	0.41
1:V:156:ASN:ND2	1:V:159:GLN:OE1	2.54	0.41
3:a:123:TYR:HE1	3:a:125:TYR:HB2	1.86	0.41
2:Z:186:LEU:HD13	2:Z:205:LEU:HG	2.02	0.41
3:d:40:LYS:HE3	3:d:40:LYS:HB2	1.90	0.41
1:A:16:LEU:HD13	1:A:263:ALA:HB3	2.02	0.40
3:L:71:LEU:HD23	3:L:209:PHE:HD1	1.84	0.40
1:Y:272:MET:HA	1:Y:275:GLN:NE2	2.36	0.40
1:A:94:ALA:HA	1:A:97:ALA:HB3	2.03	0.40
1:A:163:VAL:HG13	1:A:216:TYR:CE2	2.56	0.40
1:D:112:VAL:HG11	1:S:212:ASP:OD1	2.21	0.40
2:N:147:ILE:HD12	2:N:158:PHE:HE1	1.87	0.40
1:P:69:GLY:HA2	1:P:151:PHE:CZ	2.56	0.40
3:R:216:ILE:O	3:R:220:ASN:ND2	2.51	0.40
3:g:25:LEU:HD23	3:g:114:PRO:HB3	2.02	0.40
1:G:248:GLU:HB2	1:Y:13:HIS:NE2	2.36	0.40
2:K:178:ASN:HB3	2:K:181:GLN:CD	2.47	0.40
2:Z:65:ALA:O	2:Z:69:PHE:N	2.46	0.40
1:e:141:ALA:O	1:e:145:PRO:HB3	2.21	0.40
1:J:129:GLU:HG2	1:J:134:LYS:HD3	2.04	0.40
3:L:170:GLU:HB2	3:L:180:TYR:HB3	2.04	0.40
3:O:45:LYS:HG3	3:O:69:LEU:HD23	2.03	0.40
3:R:226:LYS:HE2	3:R:226:LYS:HB3	1.90	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	277/282 (98%)	270 (98%)	7 (2%)	0	100	100
1	D	277/282 (98%)	275 (99%)	2 (1%)	0	100	100
1	G	277/282 (98%)	272 (98%)	5 (2%)	0	100	100
1	J	277/282 (98%)	274 (99%)	3 (1%)	0	100	100
1	M	277/282 (98%)	273 (99%)	4 (1%)	0	100	100
1	P	277/282 (98%)	273 (99%)	4 (1%)	0	100	100
1	S	277/282 (98%)	270 (98%)	7 (2%)	0	100	100
1	V	277/282 (98%)	272 (98%)	5 (2%)	0	100	100
1	Y	277/282 (98%)	273 (99%)	4 (1%)	0	100	100
1	b	277/282 (98%)	274 (99%)	3 (1%)	0	100	100
1	e	277/282 (98%)	271 (98%)	6 (2%)	0	100	100
2	K	253/300 (84%)	248 (98%)	5 (2%)	0	100	100
2	N	253/300 (84%)	247 (98%)	6 (2%)	0	100	100
2	Q	253/300 (84%)	246 (97%)	7 (3%)	0	100	100
2	Z	253/300 (84%)	251 (99%)	2 (1%)	0	100	100
2	c	253/300 (84%)	251 (99%)	2 (1%)	0	100	100
2	f	253/300 (84%)	247 (98%)	6 (2%)	0	100	100
3	L	223/277 (80%)	221 (99%)	2 (1%)	0	100	100
3	O	223/277 (80%)	217 (97%)	6 (3%)	0	100	100
3	R	223/277 (80%)	221 (99%)	2 (1%)	0	100	100
3	a	223/277 (80%)	221 (99%)	2 (1%)	0	100	100
3	d	223/277 (80%)	218 (98%)	5 (2%)	0	100	100
3	g	223/277 (80%)	218 (98%)	5 (2%)	0	100	100
All	All	5903/6564 (90%)	5803 (98%)	100 (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	A	231/234 (99%)	223 (96%)	8 (4%)	32	60
1	D	231/234 (99%)	228 (99%)	3 (1%)	61	75
1	G	231/234 (99%)	229 (99%)	2 (1%)	70	79
1	J	231/234 (99%)	227 (98%)	4 (2%)	53	72
1	M	231/234 (99%)	227 (98%)	4 (2%)	53	72
1	P	231/234 (99%)	227 (98%)	4 (2%)	53	72
1	S	231/234 (99%)	228 (99%)	3 (1%)	61	75
1	V	231/234 (99%)	227 (98%)	4 (2%)	53	72
1	Y	231/234 (99%)	224 (97%)	7 (3%)	36	63
1	b	231/234 (99%)	228 (99%)	3 (1%)	61	75
1	e	231/234 (99%)	228 (99%)	3 (1%)	61	75
2	K	240/275 (87%)	240 (100%)	0	100	100
2	N	240/275 (87%)	239 (100%)	1 (0%)	84	85
2	Q	240/275 (87%)	235 (98%)	5 (2%)	47	69
2	Z	240/275 (87%)	239 (100%)	1 (0%)	84	85
2	c	240/275 (87%)	237 (99%)	3 (1%)	61	75
2	f	240/275 (87%)	239 (100%)	1 (0%)	84	85
3	L	204/248 (82%)	202 (99%)	2 (1%)	68	78
3	O	204/248 (82%)	202 (99%)	2 (1%)	68	78
3	R	204/248 (82%)	200 (98%)	4 (2%)	48	69
3	a	204/248 (82%)	202 (99%)	2 (1%)	68	78
3	d	204/248 (82%)	200 (98%)	4 (2%)	48	69
3	g	204/248 (82%)	200 (98%)	4 (2%)	48	69
All	All	5205/5712 (91%)	5131 (99%)	74 (1%)	57	74

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	67	GLU
1	A	106	ASP
1	A	113	GLU
1	A	241	ILE
1	A	256	TYR
1	A	275	GLN
1	A	278	MET
1	D	41	ASP
1	D	143	LEU
1	D	254	THR
1	G	19	ASN
1	G	209	GLN
1	J	110	ILE
1	J	255	ARG
1	J	275	GLN
1	J	277	VAL
3	L	161	ASP
3	L	165	VAL
1	M	4	ASN
1	M	67	GLU
1	M	180	VAL
1	M	278	MET
2	N	228	LYS
3	O	20	ASN
3	O	65	ASP
1	P	20	ASP
1	P	180	VAL
1	P	234	THR
1	P	249	GLN
2	Q	11	LEU
2	Q	16	VAL
2	Q	71	LEU
2	Q	196	GLU
2	Q	224	ASP
3	R	76	PHE
3	R	130	LEU
3	R	151	ASN
3	R	165	VAL
1	S	67	GLU
1	S	160	ARG
1	S	275	GLN

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Mol	Chain	Res	Type
1	V	3	ILE
1	V	79	TYR
1	V	143	LEU
1	V	277	VAL
1	Y	67	GLU
1	Y	177	ASN
1	Y	180	VAL
1	Y	188	THR
1	Y	275	GLN
1	Y	277	VAL
1	Y	278	MET
2	Z	144	LEU
3	a	69	LEU
3	a	165	VAL
1	b	4	ASN
1	b	67	GLU
1	b	275	GLN
2	c	16	VAL
2	c	223	ASP
2	c	224	ASP
3	d	20	ASN
3	d	165	VAL
3	d	199	LYS
3	d	215	LYS
1	e	99	ASN
1	e	119	ASP
1	e	279	ARG
2	f	265	ILE
3	g	151	ASN
3	g	165	VAL
3	g	185	VAL
3	g	199	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	55	GLN
1	A	65	ASN
1	A	88	GLN
1	A	144	ASN
1	A	156	ASN

Continued on next page...

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Mol	Chain	Res	Type
1	A	249	GLN
1	A	275	GLN
1	D	127	GLN
1	D	131	ASN
1	D	156	ASN
1	G	37	ASN
1	G	96	GLN
1	G	127	GLN
1	G	209	GLN
1	G	233	ASN
1	J	19	ASN
2	K	58	HIS
2	K	67	ASN
2	K	68	GLN
2	K	81	ASN
3	L	26	HIS
3	L	87	ASN
3	O	66	ASN
1	P	13	HIS
1	P	37	ASN
1	P	64	GLN
1	P	156	ASN
1	P	229	ASN
1	P	249	GLN
2	Q	142	ASN
3	R	64	GLN
3	R	87	ASN
3	R	127	ASN
3	R	184	ASN
1	S	5	HIS
1	S	144	ASN
1	V	22	ASN
1	V	64	GLN
1	V	111	GLN
1	V	156	ASN
1	V	249	GLN
1	Y	65	ASN
1	Y	177	ASN
2	Z	131	GLN
2	Z	135	ASN
3	a	145	ASN
3	a	191	ASN

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Mol	Chain	Res	Type
3	a	225	ASN
3	a	227	HIS
1	b	156	ASN
1	b	159	GLN
2	c	67	ASN
2	c	142	ASN
3	d	39	HIS
3	d	191	ASN
3	d	225	ASN
1	e	88	GLN
1	e	156	ASN
1	e	159	GLN
1	e	209	GLN
1	e	233	ASN
2	f	58	HIS
2	f	86	ASN
3	g	145	ASN
3	g	191	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

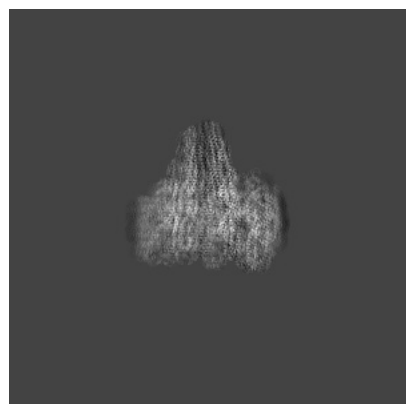
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66649. These allow visual inspection of the internal detail of the map and identification of artifacts.

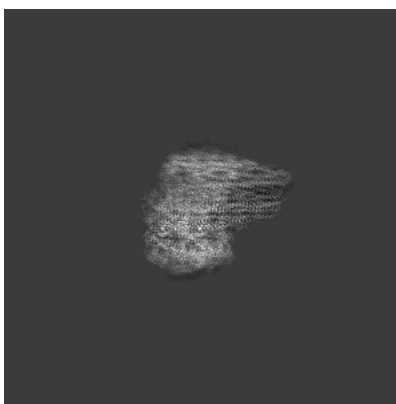
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

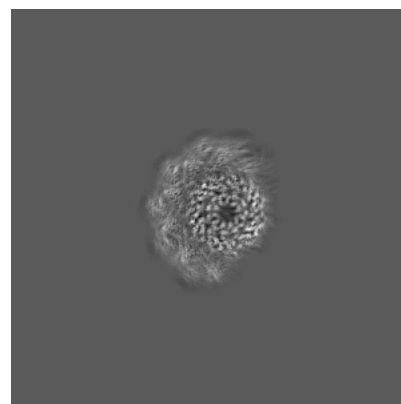
6.1.1 Primary map



X

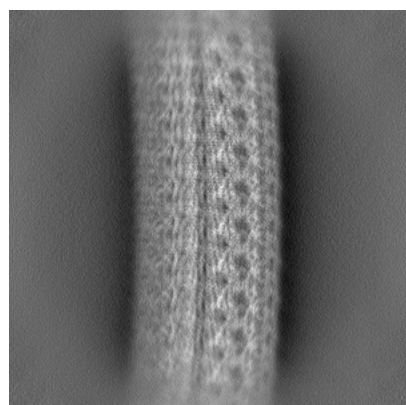


Y

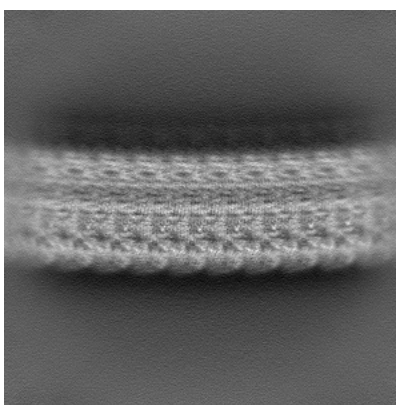


Z

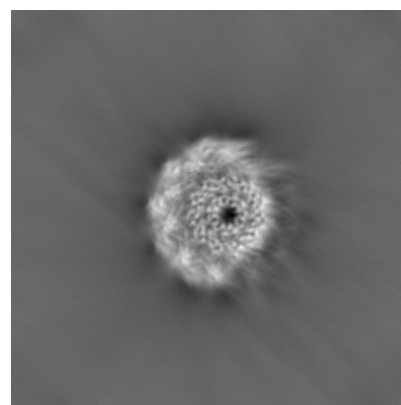
6.1.2 Raw map



X



Y

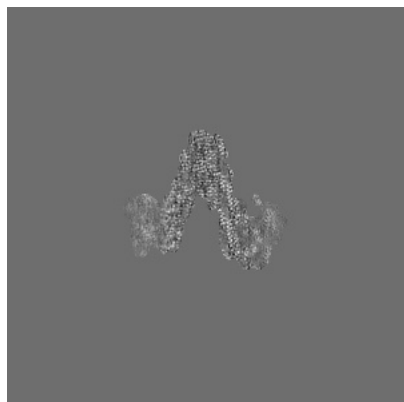


Z

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

6.2 Central slices [i](#)

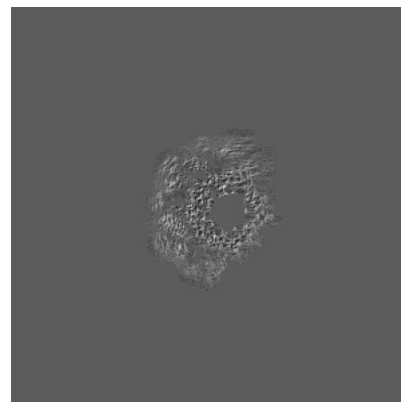
6.2.1 Primary map



X Index: 256

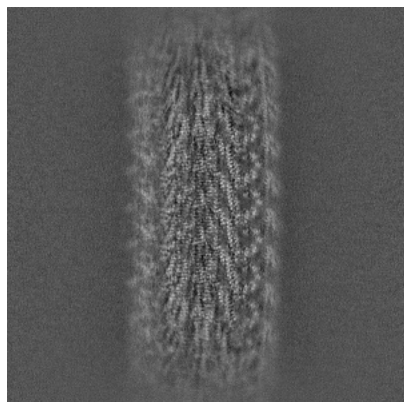


Y Index: 256

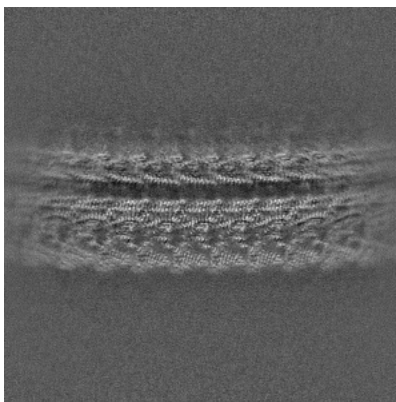


Z Index: 256

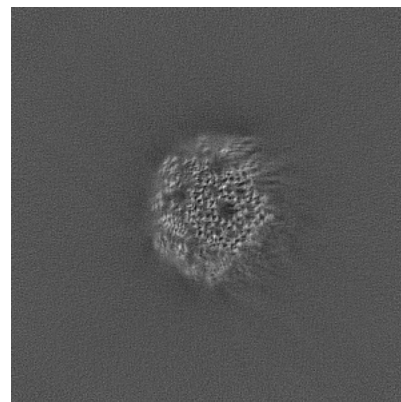
6.2.2 Raw map



X Index: 256



Y Index: 256

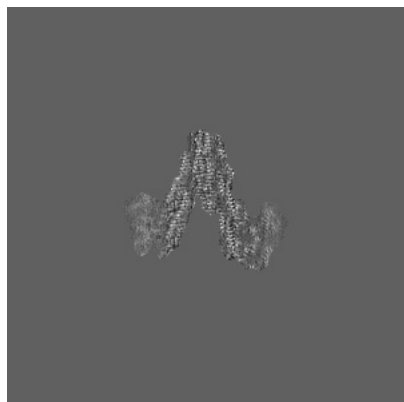


Z Index: 256

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

6.3 Largest variance slices [i](#)

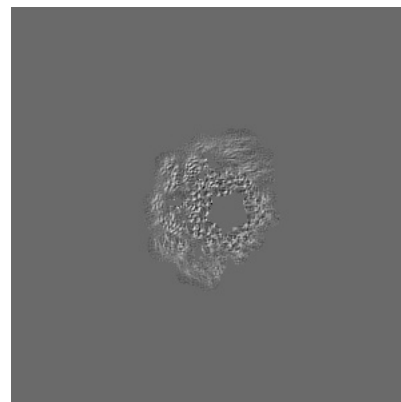
6.3.1 Primary map



X Index: 254

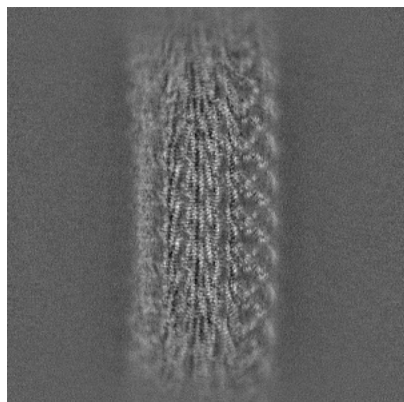


Y Index: 275

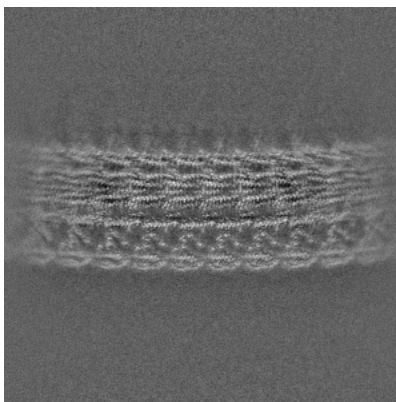


Z Index: 253

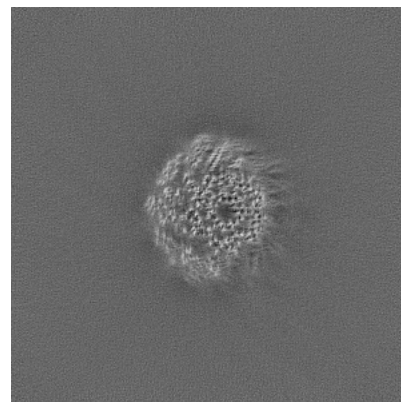
6.3.2 Raw map



X Index: 260



Y Index: 264

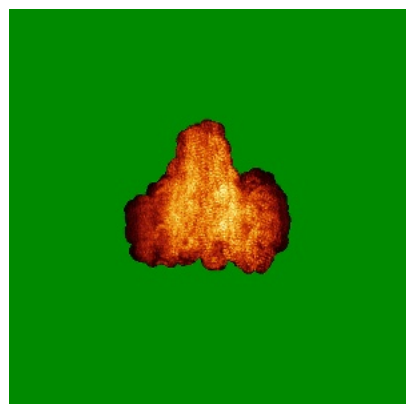


Z Index: 224

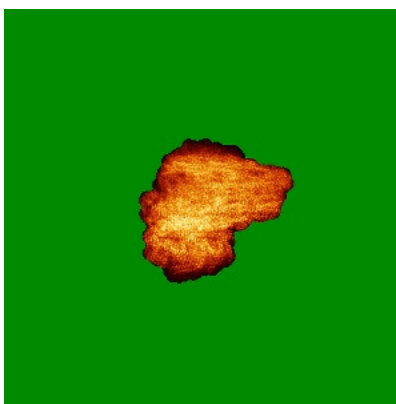
The images above show the largest variance slices of the map in three orthogonal directions.

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

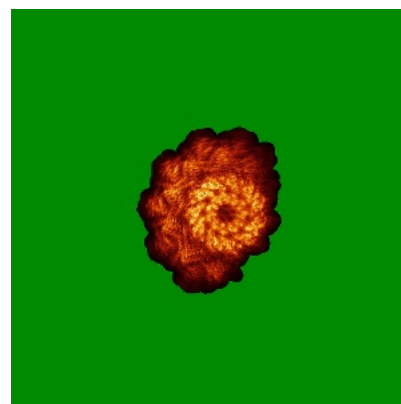
6.4.1 Primary map



X

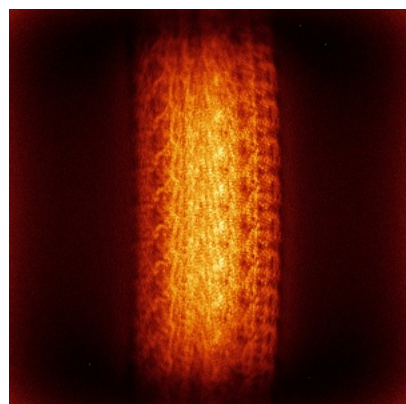


Y

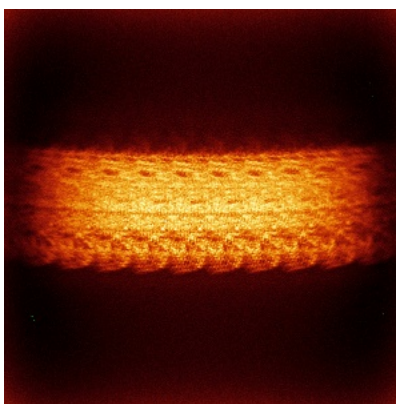


Z

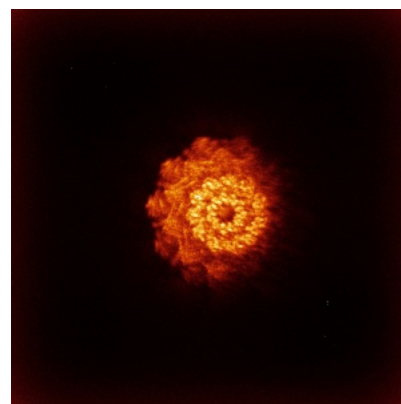
6.4.2 Raw map



X



Y



Z

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

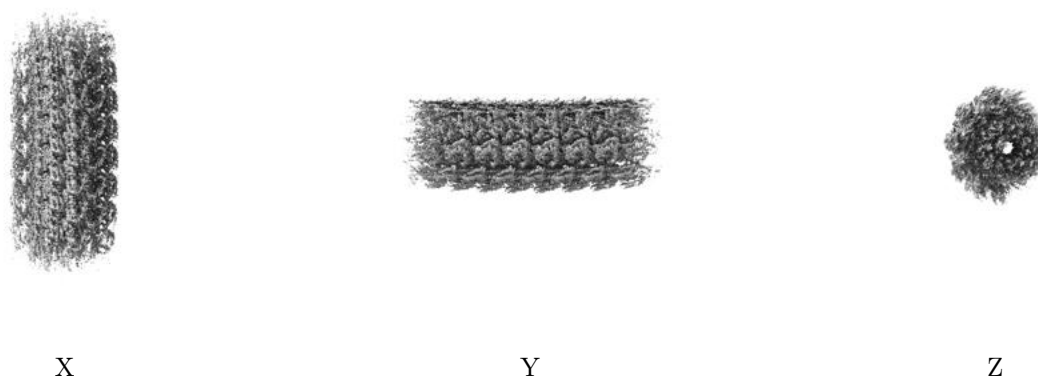
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.273. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

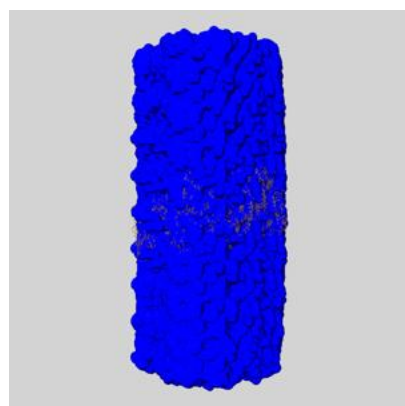
6.6 Mask visualisation [i](#)

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

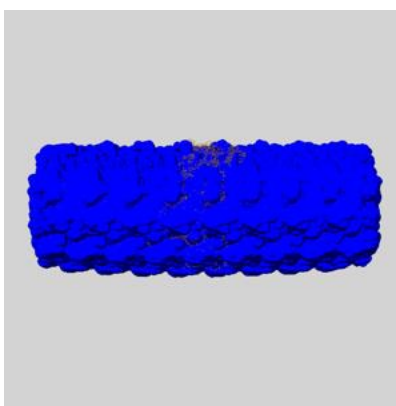
A mask typically either:

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

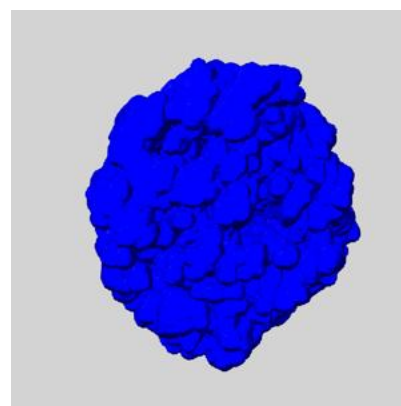
6.6.1 emd_66649_msk_1.map [i](#)



X



Y

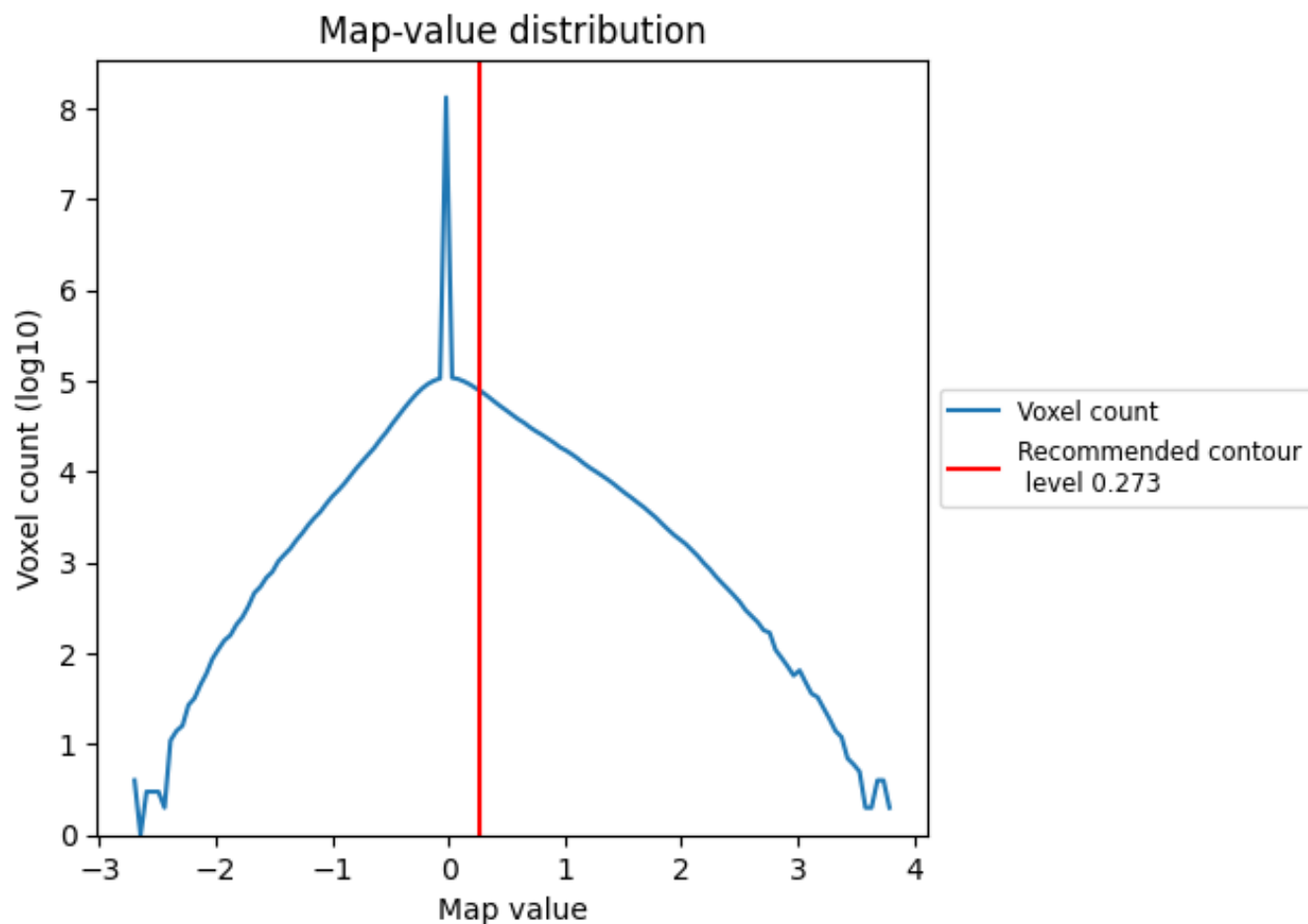


Z

7 Map analysis [i](#)

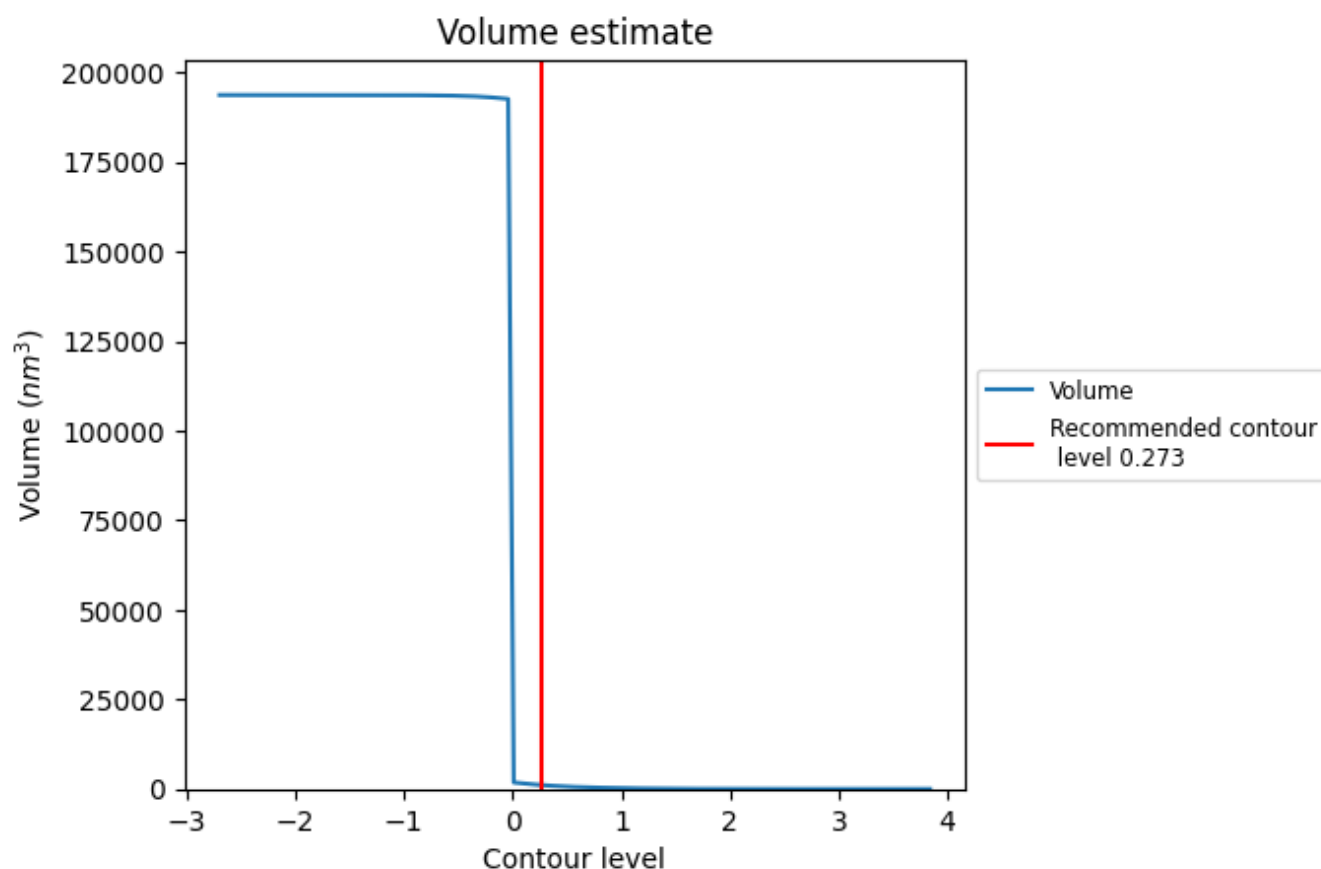
This section contains the results of statistical analysis of the map.

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.

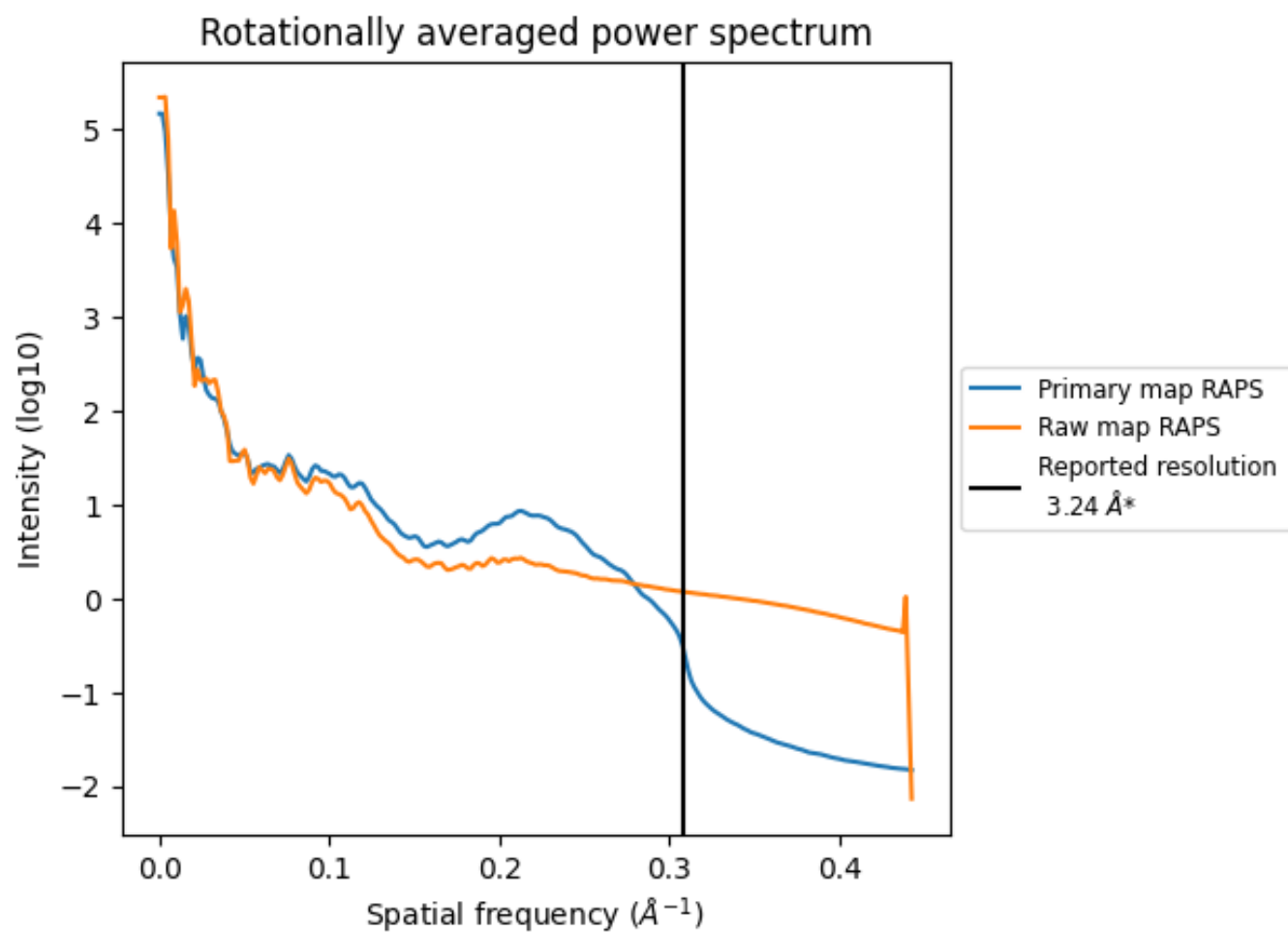
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1074 nm³; this corresponds to an approximate mass of 970 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

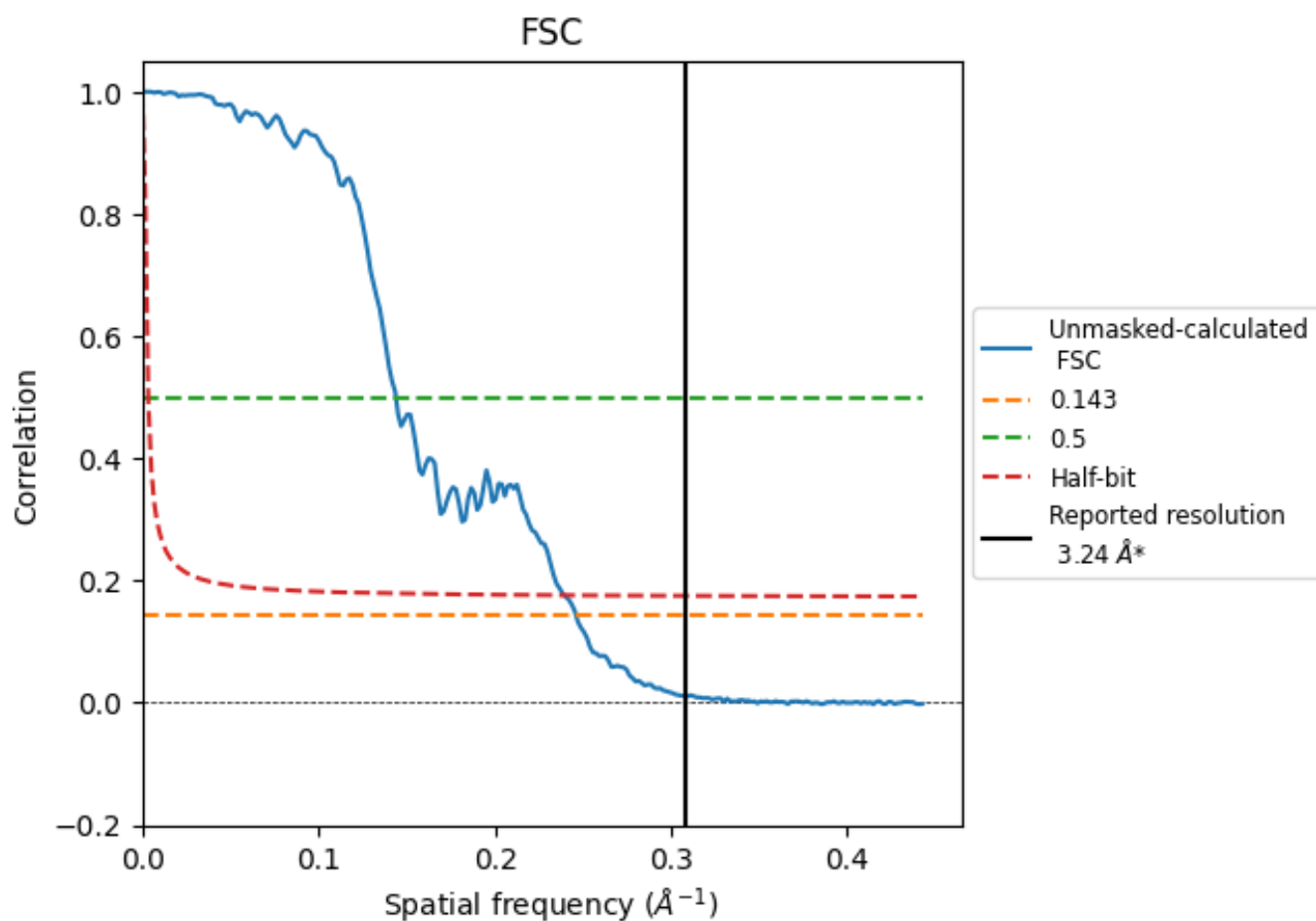


*Reported resolution corresponds to spatial frequency of 0.309 Å⁻¹

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 $0.309 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

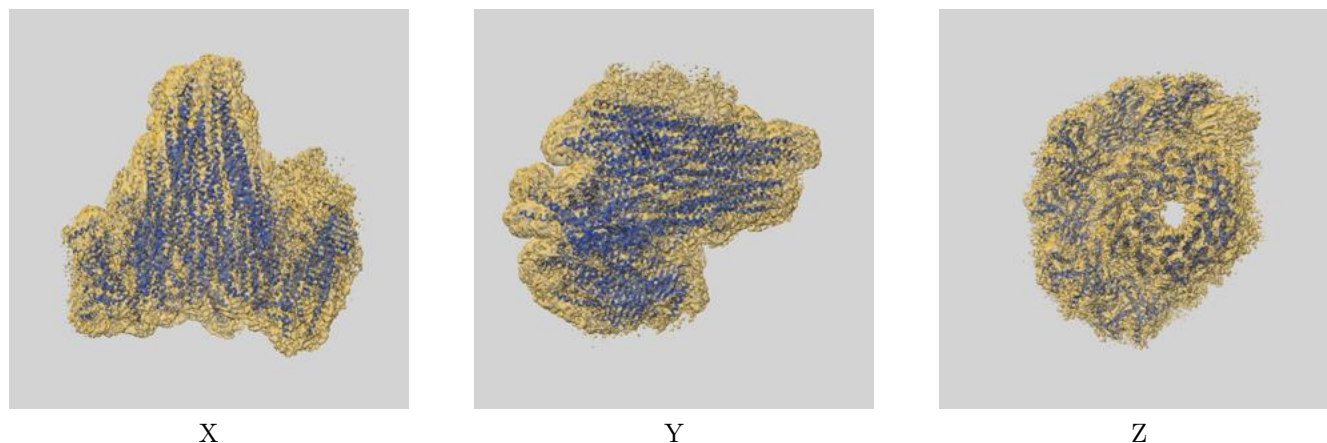
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.24	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.06	6.95	4.18

*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 4.06 differs from the reported value 3.24 by more than 10 %

9 Map-model fit [i](#)

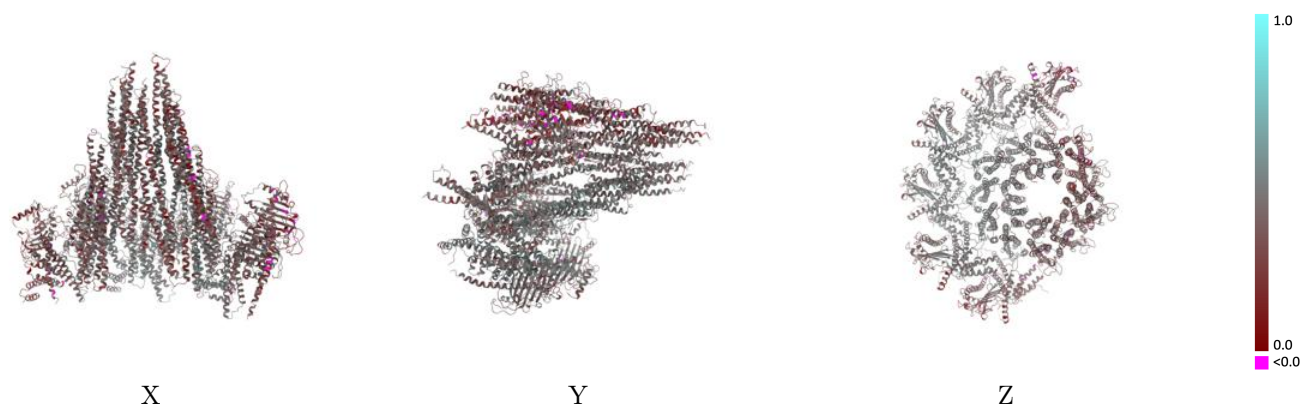
This section contains information regarding the fit between EMDB map EMD-66649 and PDB model 9X80. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



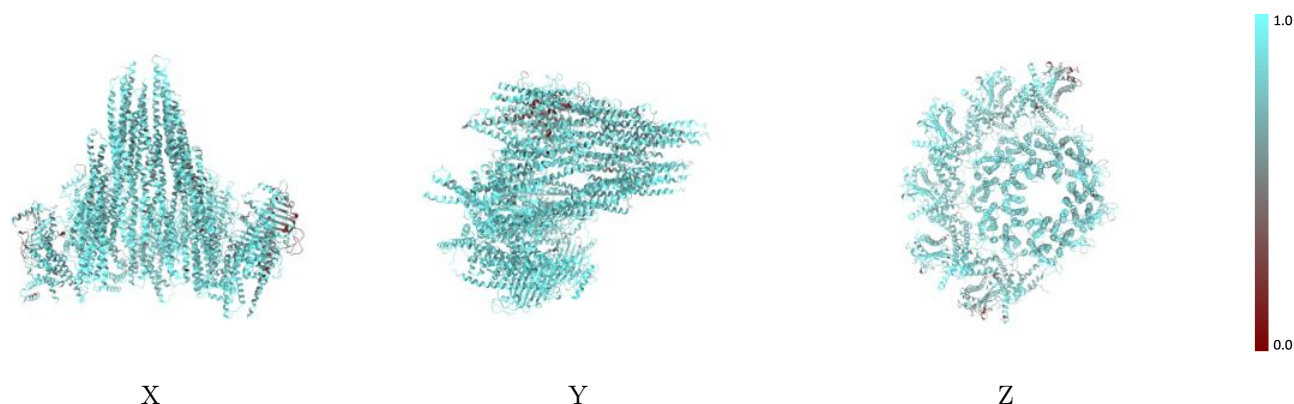
The images above show the 3D surface view of the map at the recommended contour level 0.273 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



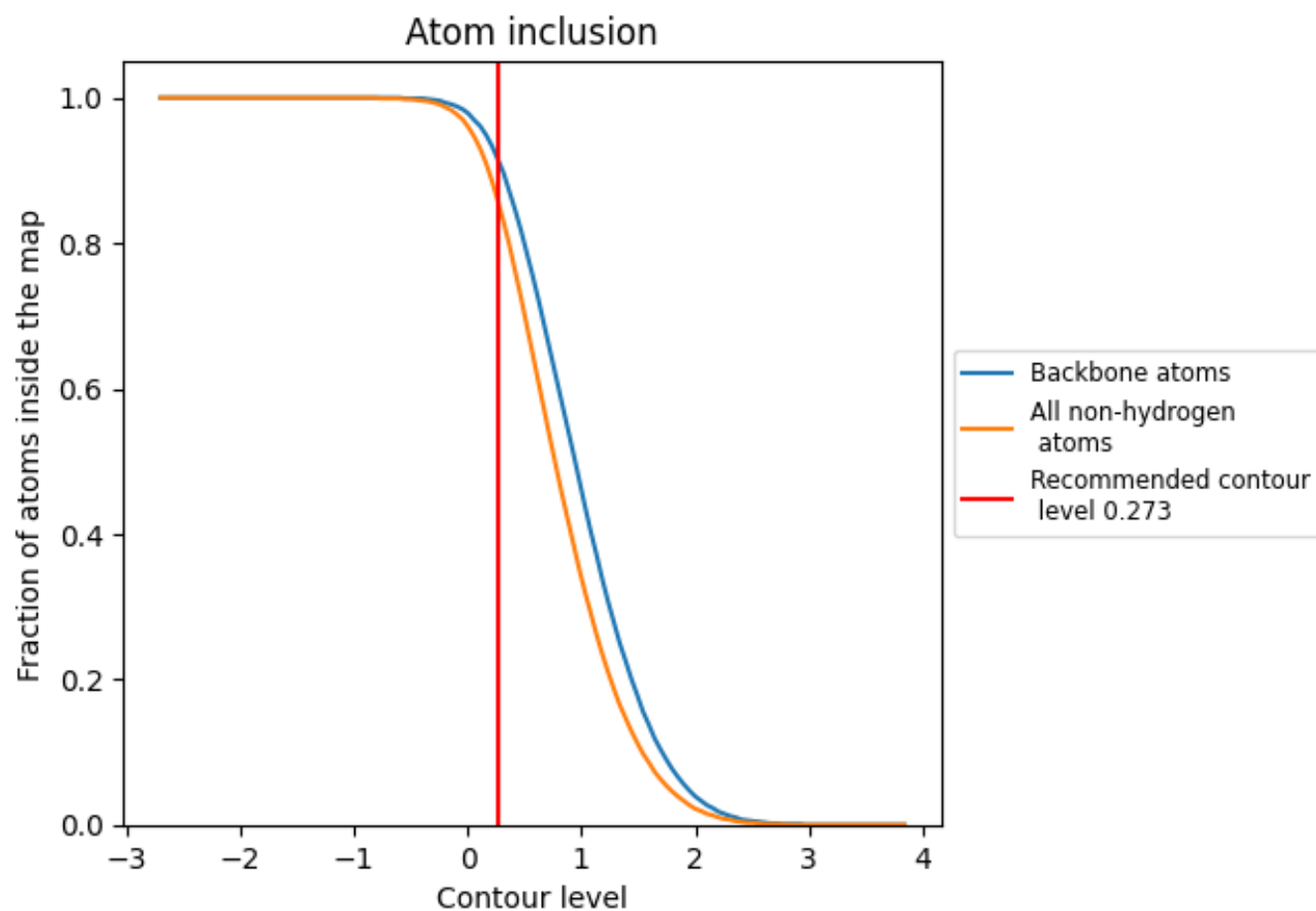
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.273).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.273) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8550	 0.4010
A	 0.8160	 0.3010
D	 0.8490	 0.3700
G	 0.8620	 0.3860
J	 0.8810	 0.4600
K	 0.9170	 0.4360
L	 0.8060	 0.3790
M	 0.8920	 0.4770
N	 0.9160	 0.4760
O	 0.8940	 0.4280
P	 0.8370	 0.3970
Q	 0.8910	 0.3790
R	 0.6130	 0.2740
S	 0.8480	 0.3330
V	 0.8730	 0.3660
Y	 0.8740	 0.4440
Z	 0.8090	 0.3380
a	 0.6470	 0.2850
b	 0.8870	 0.4870
c	 0.9250	 0.4620
d	 0.9160	 0.4250
e	 0.8730	 0.4560
f	 0.9100	 0.4430
g	 0.8690	 0.3860

