



## Full wwPDB EM Validation Report ⓘ

Jun 3, 2026 – 04:54 PM EDT

PDB ID : 9YDX / pdb\_00009ydx  
EMDB ID : EMD-72840  
Title : RBM3 domain of FliF protein in MS-ring of flagellar motor in *Vibrio cholerae*  
Authors : Guo, W.; Yue, J.  
Deposited on : 2025-09-23  
Resolution : 3.75 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](mailto: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>.

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

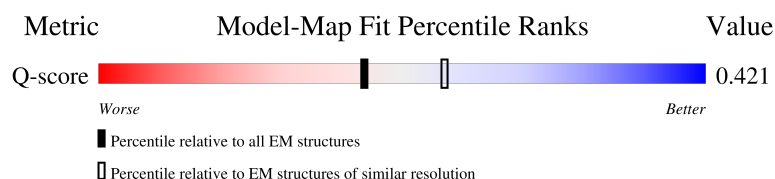
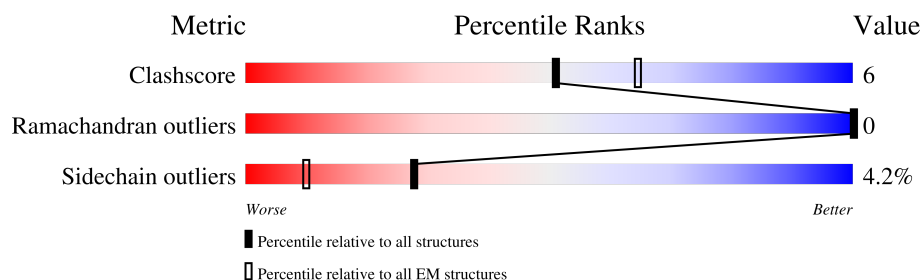
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.75 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	10301 ( 3.25 - 4.25 )

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  $\geq 3$ , 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	Aa	198	<div> <div>8%</div> <div>58%</div> <div>14%</div> <div>27%</div> </div>
1	Ab	198	<div> <div>7%</div> <div>60%</div> <div>12%</div> <div>27%</div> </div>
1	Ac	198	<div> <div>9%</div> <div>61%</div> <div>11%</div> <div>27%</div> </div>
1	Ad	198	<div> <div>8%</div> <div>60%</div> <div>12%</div> <div>27%</div> </div>





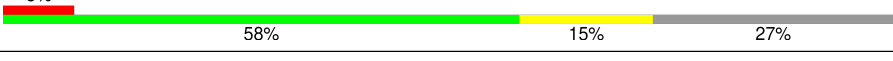
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Mol	Chain	Length	Quality of chain
1	Ae	198	
1	Af	198	
1	Ag	198	
1	Ah	198	
1	Ai	198	
1	Aj	198	
1	Ak	198	
1	Al	198	
1	Am	198	
1	An	198	
1	Ao	198	
1	Ap	198	
1	Aq	198	
1	Ar	198	
1	As	198	
1	At	198	
1	Au	198	
1	Av	198	
1	Aw	198	
1	Ax	198	
1	Ay	198	
1	Az	198	
1	Ba	198	
1	Bb	198	
1	Bc	198	

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Mol	Chain	Length	Quality of chain
1	Bd	198	
1	Be	198	
1	Bf	198	
1	Bg	198	
1	Bh	198	

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 38556 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 Flagellar M-ring protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Aa	144	Total	C	N	O	S	0	0
			1134	702	201	230	1		
1	Ab	144	Total	C	N	O	S	0	0
			1134	702	201	230	1		
1	Ac	144	Total	C	N	O	S	0	0
			1134	702	201	230	1		
1	Ad	144	Total	C	N	O	S	0	0
			1134	702	201	230	1		
1	Ae	144	Total	C	N	O	S	0	0
			1134	702	201	230	1		
1	Af	144	Total	C	N	O	S	0	0
			1134	702	201	230	1		
1	Ag	144	Total	C	N	O	S	0	0
			1134	702	201	230	1		
1	Ah	144	Total	C	N	O	S	0	0
			1134	702	201	230	1		
1	Ai	144	Total	C	N	O	S	0	0
			1134	702	201	230	1		
1	Aj	144	Total	C	N	O	S	0	0
			1134	702	201	230	1		
1	Ak	144	Total	C	N	O	S	0	0
			1134	702	201	230	1		
1	Al	144	Total	C	N	O	S	0	0
			1134	702	201	230	1		
1	Am	144	Total	C	N	O	S	0	0
			1134	702	201	230	1		
1	An	144	Total	C	N	O	S	0	0
			1134	702	201	230	1		
1	Ao	144	Total	C	N	O	S	0	0
			1134	702	201	230	1		
1	Ap	144	Total	C	N	O	S	0	0
			1134	702	201	230	1		
1	Aq	144	Total	C	N	O	S	0	0
			1134	702	201	230	1		

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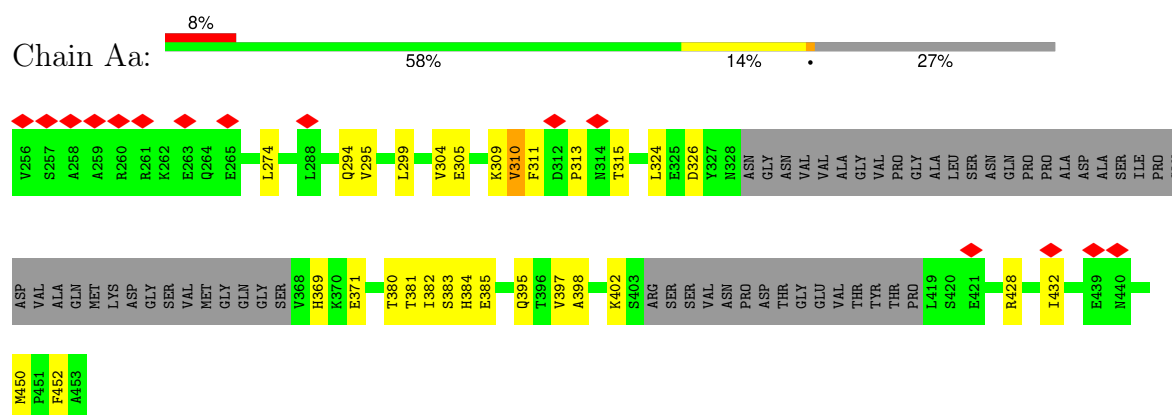
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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Ar	144	Total	C	N	O	S	0	0
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1	As	144	Total	C	N	O	S	0	0
			1134	702	201	230	1		
1	At	144	Total	C	N	O	S	0	0
			1134	702	201	230	1		
1	Au	144	Total	C	N	O	S	0	0
			1134	702	201	230	1		
1	Av	144	Total	C	N	O	S	0	0
			1134	702	201	230	1		
1	Aw	144	Total	C	N	O	S	0	0
			1134	702	201	230	1		
1	Ax	144	Total	C	N	O	S	0	0
			1134	702	201	230	1		
1	Ay	144	Total	C	N	O	S	0	0
			1134	702	201	230	1		
1	Az	144	Total	C	N	O	S	0	0
			1134	702	201	230	1		
1	Ba	144	Total	C	N	O	S	0	0
			1134	702	201	230	1		
1	Bb	144	Total	C	N	O	S	0	0
			1134	702	201	230	1		
1	Bc	144	Total	C	N	O	S	0	0
			1134	702	201	230	1		
1	Bd	144	Total	C	N	O	S	0	0
			1134	702	201	230	1		
1	Be	144	Total	C	N	O	S	0	0
			1134	702	201	230	1		
1	Bf	144	Total	C	N	O	S	0	0
			1134	702	201	230	1		
1	Bg	144	Total	C	N	O	S	0	0
			1134	702	201	230	1		
1	Bh	144	Total	C	N	O	S	0	0
			1134	702	201	230	1		

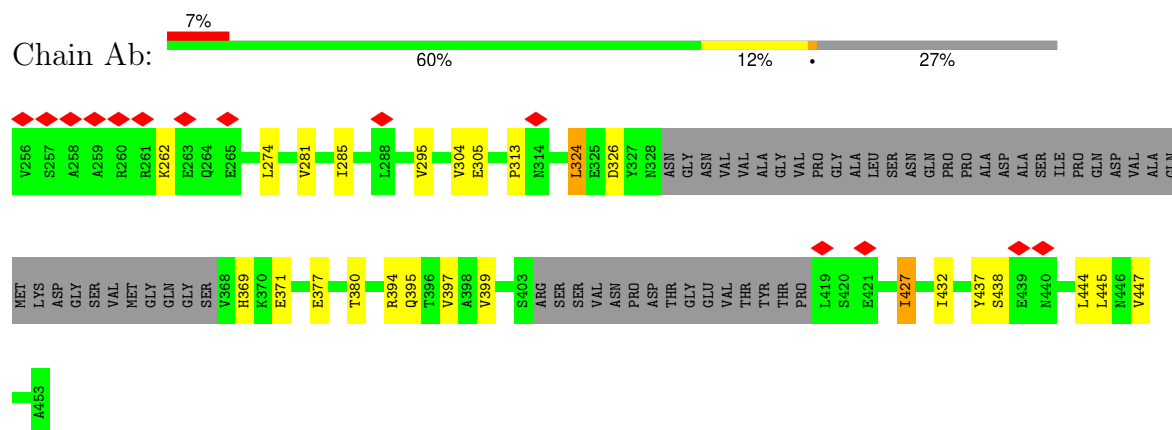
### 3 Residue-property plots

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.

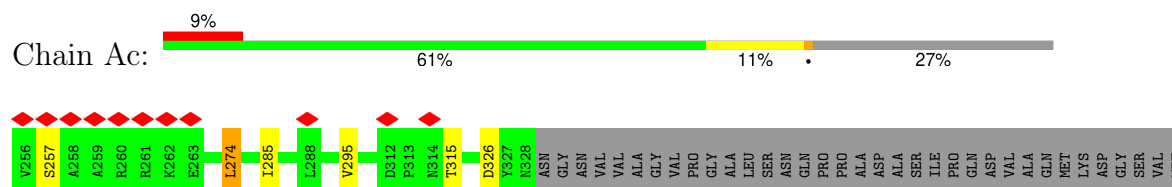
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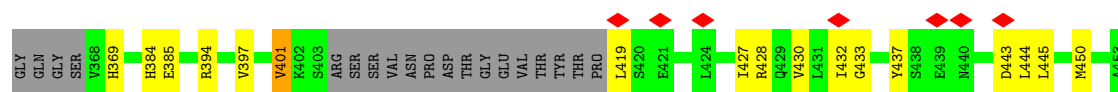


- Molecule 1: Flagellar M-ring protein

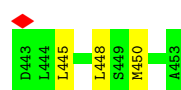
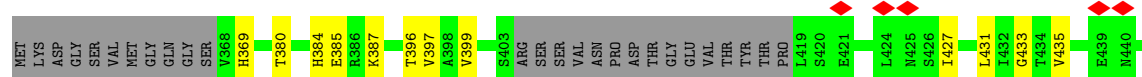
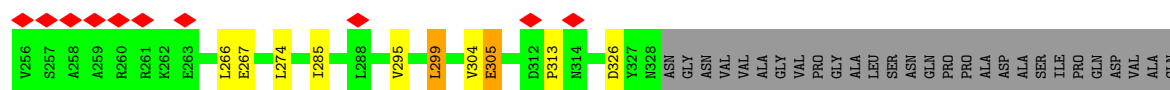


- Molecule 1: Flagellar M-ring protein

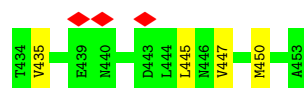
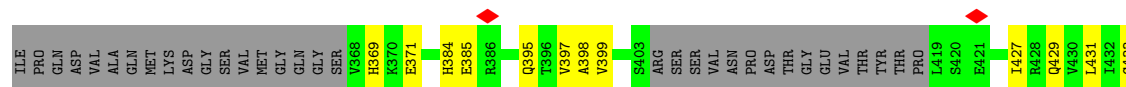




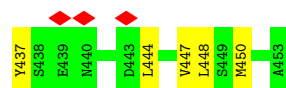
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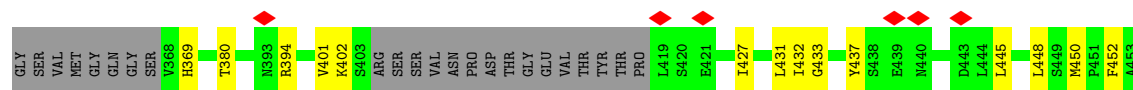
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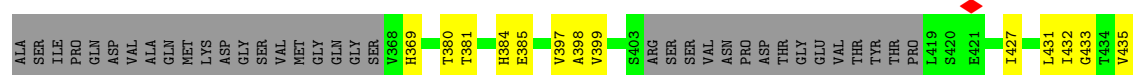
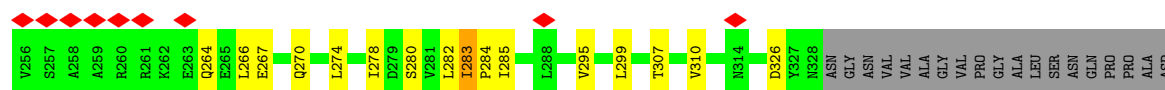
• Molecule 1: Flagellar M-ring protein



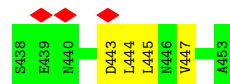
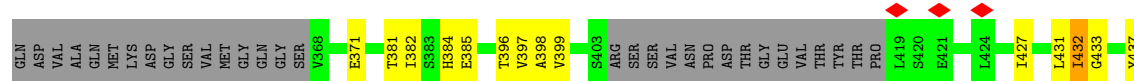
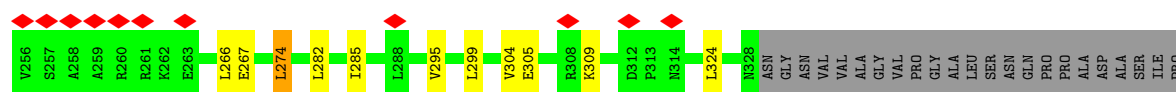




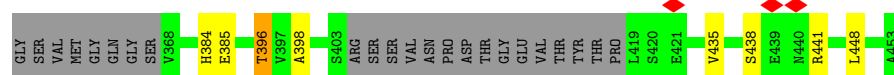
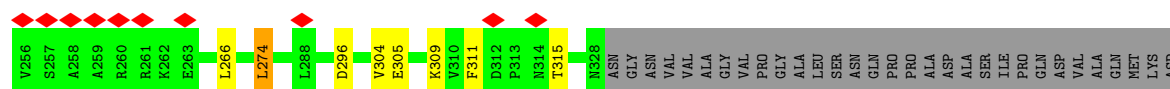
- Molecule 1: Flagellar M-ring protein



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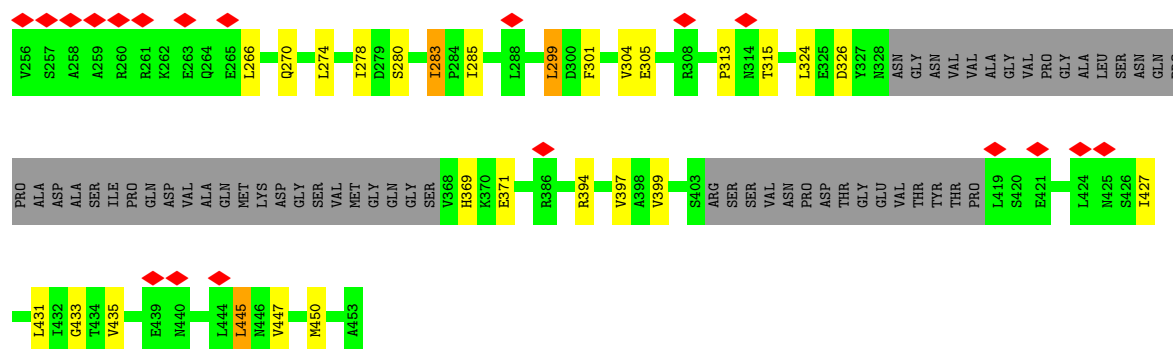


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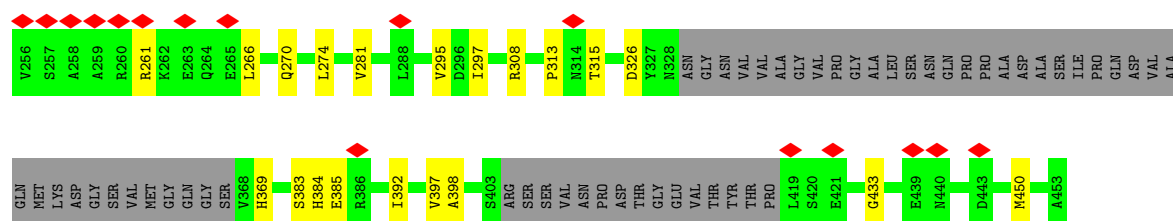


- Molecule 1: Flagellar M-ring protein

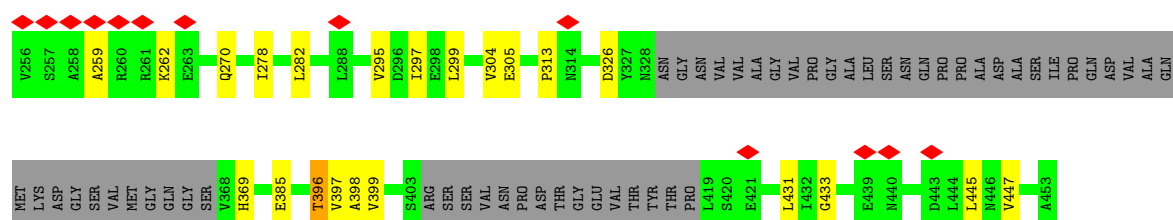




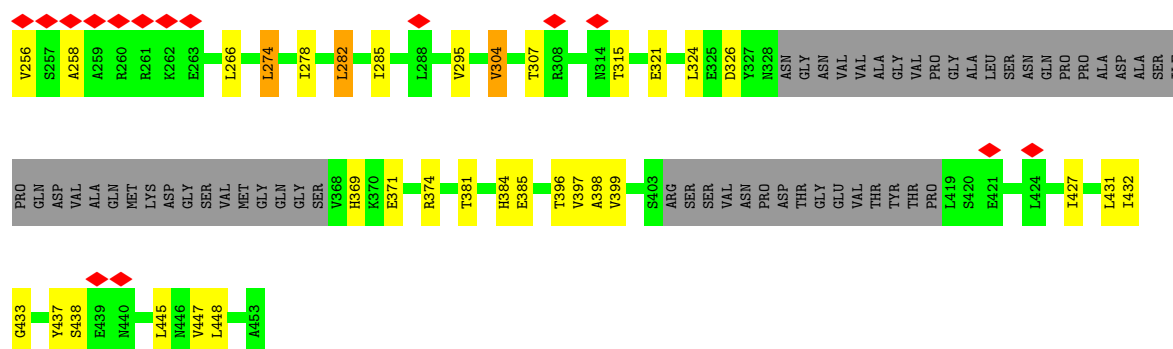
- Molecule 1: Flagellar M-ring protein



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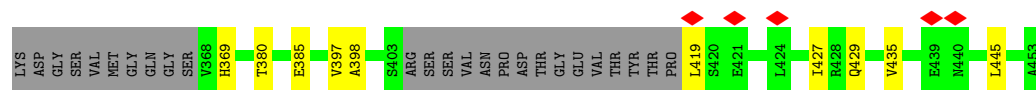


- Molecule 1: Flagellar M-ring protein

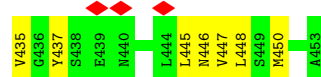
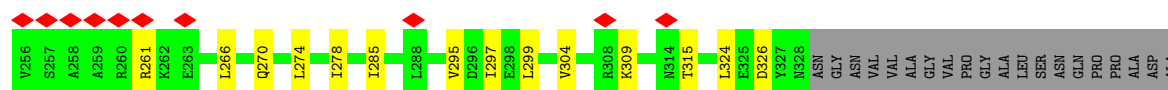


- Molecule 1: Flagellar M-ring protein

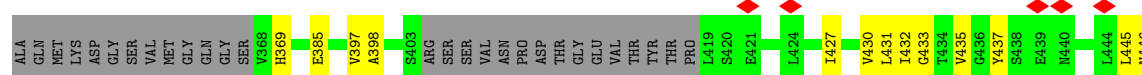
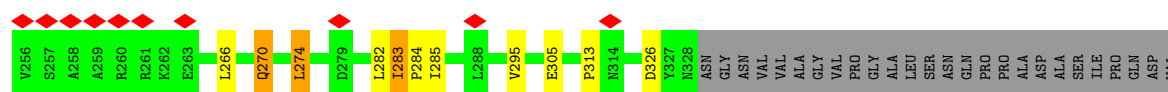




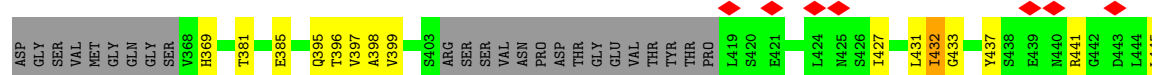
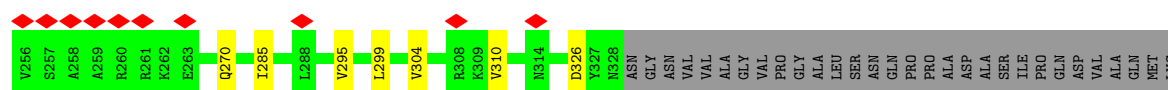
• Molecule 1: Flagellar M-ring protein



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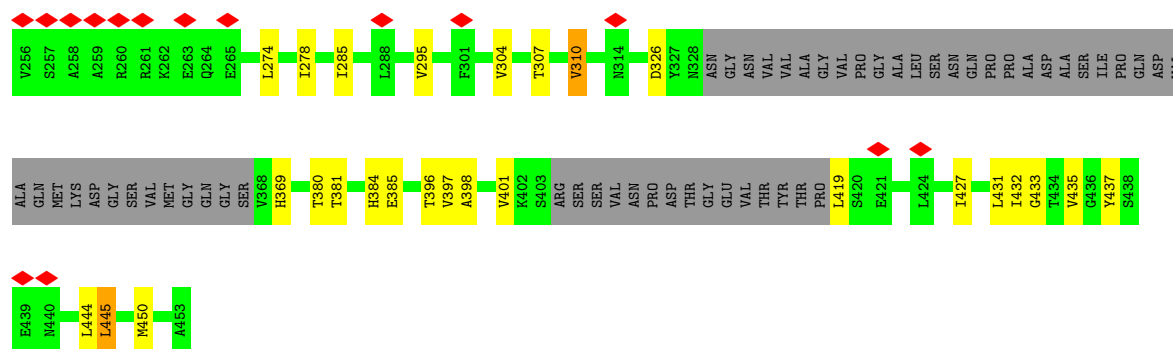


• Molecule 1: Flagellar M-ring protein

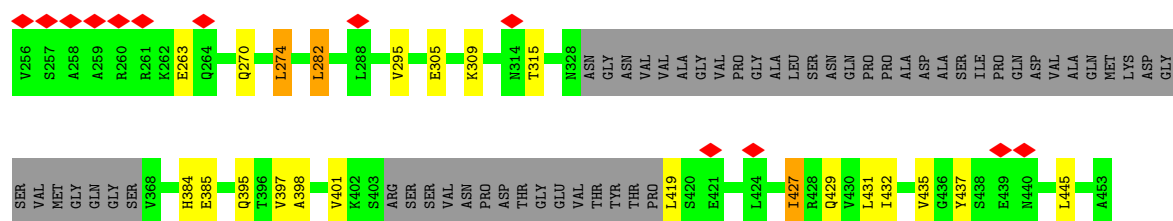


• Molecule 1: Flagellar M-ring protein





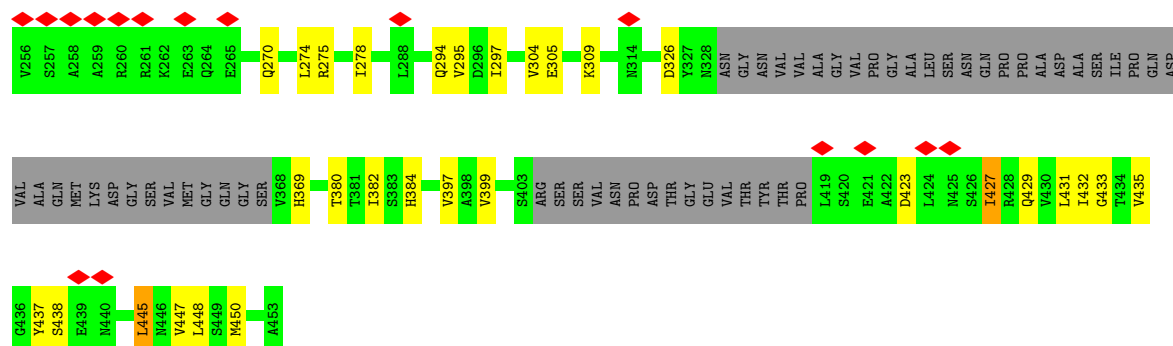
• Molecule 1: Flagellar M-ring protein



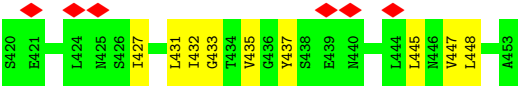
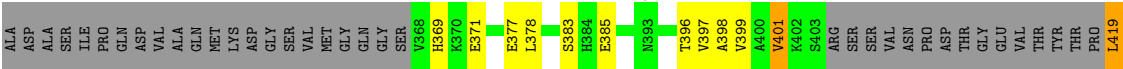
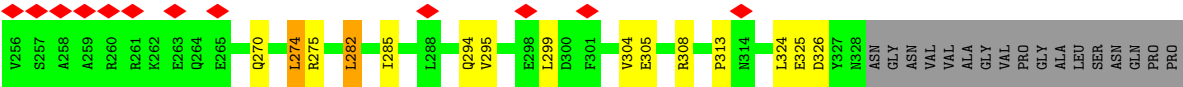
• Molecule 1: Flagellar M-ring protein



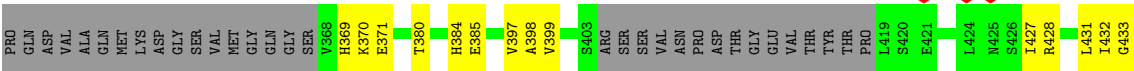
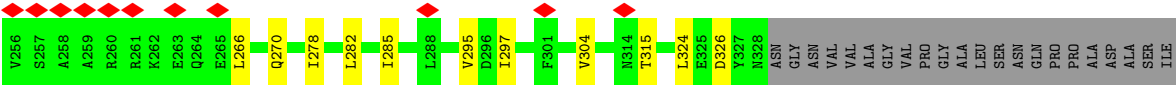
• Molecule 1: Flagellar M-ring protein







• Molecule 1: Flagellar M-ring protein





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C34	Depositor
Number of particles used	44428	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	1.477	Depositor
Minimum map value	-1.249	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	640.63995, 640.63995, 640.63995	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.43, 1.43, 1.43	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	Aa	0.19	0/1145	0.40	0/1546
1	Ab	0.18	0/1145	0.38	0/1546
1	Ac	0.18	0/1145	0.37	0/1546
1	Ad	0.18	0/1145	0.38	0/1546
1	Ae	0.17	0/1145	0.35	0/1546
1	Af	0.18	0/1145	0.35	0/1546
1	Ag	0.18	0/1145	0.41	0/1546
1	Ah	0.17	0/1145	0.37	0/1546
1	Ai	0.18	0/1145	0.38	0/1546
1	Aj	0.17	0/1145	0.38	0/1546
1	Ak	0.19	0/1145	0.38	0/1546
1	Al	0.19	0/1145	0.39	0/1546
1	Am	0.17	0/1145	0.36	0/1546
1	An	0.17	0/1145	0.39	0/1546
1	Ao	0.18	0/1145	0.38	0/1546
1	Ap	0.17	0/1145	0.36	0/1546
1	Aq	0.18	0/1145	0.39	0/1546
1	Ar	0.18	0/1145	0.38	0/1546
1	As	0.18	0/1145	0.38	0/1546
1	At	0.18	0/1145	0.36	0/1546
1	Au	0.19	0/1145	0.41	1/1546 (0.1%)
1	Av	0.17	0/1145	0.35	0/1546
1	Aw	0.17	0/1145	0.39	0/1546
1	Ax	0.19	0/1145	0.42	0/1546
1	Ay	0.18	0/1145	0.37	0/1546
1	Az	0.17	0/1145	0.38	0/1546
1	Ba	0.17	0/1145	0.38	0/1546
1	Bb	0.19	0/1145	0.39	0/1546
1	Bc	0.18	0/1145	0.37	0/1546
1	Bd	0.19	0/1145	0.40	0/1546
1	Be	0.18	0/1145	0.38	0/1546
1	Bf	0.17	0/1145	0.37	0/1546
1	Bg	0.18	0/1145	0.38	0/1546
1	Bh	0.18	0/1145	0.38	0/1546

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.18	0/38930	0.38	1/52564 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Au	281	VAL	N-CA-C	-5.02	108.94	113.71

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	Aa	1134	0	1129	18	0
1	Ab	1134	0	1129	15	0
1	Ac	1134	0	1129	18	0
1	Ad	1134	0	1129	16	0
1	Ae	1134	0	1129	18	0
1	Af	1134	0	1129	17	0
1	Ag	1134	0	1129	17	0
1	Ah	1134	0	1129	14	0
1	Ai	1134	0	1129	12	0
1	Aj	1134	0	1129	12	0
1	Ak	1134	0	1129	18	0
1	Al	1134	0	1129	17	0
1	Am	1134	0	1129	10	0
1	An	1134	0	1129	17	0
1	Ao	1134	0	1129	14	0
1	Ap	1134	0	1129	14	0
1	Aq	1134	0	1129	19	0
1	Ar	1134	0	1129	20	0
1	As	1134	0	1129	19	0
1	At	1134	0	1129	16	0
1	Au	1134	0	1129	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Av	1134	0	1129	22	0
1	Aw	1134	0	1129	16	0
1	Ax	1134	0	1129	14	0
1	Ay	1134	0	1129	16	0
1	Az	1134	0	1129	14	0
1	Ba	1134	0	1129	14	0
1	Bb	1134	0	1129	18	0
1	Bc	1134	0	1129	13	0
1	Bd	1134	0	1129	14	0
1	Be	1134	0	1129	9	0
1	Bf	1134	0	1129	12	0
1	Bg	1134	0	1129	22	0
1	Bh	1134	0	1129	21	0
All	All	38556	0	38386	423	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (423) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bc:384:HIS:HB3	1:Bd:305:GLU:HB2	1.74	0.69
1:Ak:432:ILE:HD12	1:Ak:437:TYR:HB2	1.75	0.67
1:Aw:432:ILE:HD12	1:Aw:437:TYR:HB2	1.78	0.66
1:Ba:432:ILE:HG23	1:Ba:437:TYR:HB3	1.78	0.66
1:Az:282:LEU:HD21	1:Az:431:LEU:HD21	1.77	0.66
1:Ao:270:GLN:HB3	1:Ao:297:ILE:HD12	1.79	0.65
1:Ar:384:HIS:HB3	1:As:305:GLU:HB2	1.79	0.64
1:At:326:ASP:HB3	1:At:369:HIS:HB3	1.80	0.63
1:Ba:326:ASP:HB3	1:Ba:369:HIS:HB3	1.79	0.63
1:Bg:282:LEU:HD21	1:Bg:431:LEU:HD21	1.81	0.63
1:Ad:326:ASP:HB3	1:Ad:369:HIS:HB3	1.81	0.62
1:Az:432:ILE:HD12	1:Az:437:TYR:HB2	1.80	0.62
1:Ay:384:HIS:HB3	1:Az:305:GLU:HB2	1.81	0.62
1:Au:274:LEU:HD21	1:Au:435:VAL:HG13	1.82	0.62
1:Ab:285:ILE:HG21	1:Ab:427:ILE:HD11	1.81	0.62
1:Bc:432:ILE:HG23	1:Bc:437:TYR:HB3	1.82	0.62
1:Al:384:HIS:HB3	1:Am:305:GLU:HB2	1.81	0.61
1:Bc:326:ASP:HB3	1:Bc:369:HIS:HB3	1.80	0.61
1:Al:432:ILE:HD12	1:Al:437:TYR:HB2	1.81	0.61
1:Ax:432:ILE:HD12	1:Ax:437:TYR:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ak:326:ASP:HB3	1:Ak:369:HIS:HB3	1.82	0.60
1:Ae:384:HIS:HB3	1:Af:305:GLU:HB2	1.82	0.60
1:Al:267:GLU:HG2	1:Al:299:LEU:HD23	1.82	0.60
1:Aj:283:ILE:HG13	1:Aj:284:PRO:HD3	1.83	0.60
1:Bb:384:HIS:HB3	1:Bc:305:GLU:HB2	1.83	0.60
1:Ah:432:ILE:HG23	1:Ah:437:TYR:HB3	1.84	0.59
1:Ak:270:GLN:HG3	1:Ak:299:LEU:HD21	1.83	0.59
1:An:326:ASP:HB3	1:An:369:HIS:HB3	1.83	0.59
1:Bg:432:ILE:HD12	1:Bg:437:TYR:HB2	1.83	0.59
1:Ar:326:ASP:HB3	1:Ar:369:HIS:HB3	1.83	0.59
1:Bg:326:ASP:HB3	1:Bg:369:HIS:HB3	1.83	0.59
1:Be:274:LEU:HD21	1:Be:435:VAL:HG13	1.85	0.59
1:Aw:326:ASP:HB3	1:Aw:369:HIS:HB3	1.85	0.59
1:Ap:295:VAL:HG12	1:Ap:397:VAL:HG22	1.85	0.58
1:Aj:282:LEU:HD21	1:Aj:431:LEU:HD11	1.85	0.58
1:At:274:LEU:HD12	1:At:295:VAL:HG11	1.86	0.58
1:Aa:294:GLN:HB2	1:Bh:434:THR:HG22	1.86	0.58
1:Av:326:ASP:HB3	1:Av:369:HIS:HB3	1.86	0.58
1:Ab:438:SER:HB3	1:Ac:394:ARG:HH12	1.67	0.58
1:Am:274:LEU:HD21	1:Am:435:VAL:HG13	1.84	0.58
1:Ag:285:ILE:HG21	1:Ag:427:ILE:HD11	1.86	0.57
1:Ai:384:HIS:HB3	1:Aj:305:GLU:HB2	1.85	0.57
1:Aq:321:GLU:HG2	1:Aq:374:ARG:HG3	1.86	0.57
1:Ba:385:GLU:HG2	1:Bb:304:VAL:HG22	1.86	0.57
1:Ab:432:ILE:HG23	1:Ab:437:TYR:HB3	1.86	0.57
1:Ak:385:GLU:HG2	1:Al:304:VAL:HG22	1.87	0.57
1:Al:399:VAL:HB	1:Al:447:VAL:HG22	1.86	0.57
1:As:309:LYS:HB3	1:As:382:ILE:HG12	1.87	0.57
1:Be:274:LEU:HD22	1:Be:295:VAL:HG11	1.86	0.57
1:Ah:385:GLU:HG2	1:Ai:304:VAL:HG22	1.87	0.57
1:Be:432:ILE:HD12	1:Be:437:TYR:HB2	1.86	0.56
1:Ak:267:GLU:HG2	1:Ak:299:LEU:HD23	1.87	0.56
1:At:385:GLU:HG2	1:Au:304:VAL:HG22	1.88	0.56
1:Af:326:ASP:HB3	1:Af:369:HIS:HB3	1.88	0.56
1:Ad:274:LEU:HD11	1:Ad:435:VAL:HG13	1.87	0.56
1:Ah:283:ILE:HG13	1:Ah:284:PRO:HD3	1.86	0.56
1:Ac:326:ASP:HB3	1:Ac:369:HIS:HB3	1.86	0.55
1:Bh:324:LEU:HB3	1:Bh:371:GLU:HB2	1.87	0.55
1:Ak:274:LEU:HD11	1:Ak:435:VAL:HG13	1.88	0.55
1:Av:309:LYS:HG3	1:Av:382:ILE:HG12	1.88	0.55
1:Ae:399:VAL:HB	1:Ae:447:VAL:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ba:285:ILE:HD13	1:Bb:450:MET:HE3	1.88	0.55
1:Az:385:GLU:HG2	1:Ba:304:VAL:HG22	1.88	0.55
1:Ar:262:LYS:HE3	1:As:261:ARG:HH11	1.72	0.55
1:Ah:270:GLN:HG3	1:Ah:299:LEU:HD11	1.88	0.55
1:Ai:432:ILE:HG23	1:Ai:437:TYR:HB3	1.87	0.55
1:Ae:274:LEU:HD11	1:Ae:435:VAL:HG13	1.89	0.55
1:Af:385:GLU:HG2	1:Ag:304:VAL:HG22	1.89	0.55
1:Ap:326:ASP:HB3	1:Ap:369:HIS:HB3	1.89	0.55
1:Ap:399:VAL:HB	1:Ap:447:VAL:HG22	1.88	0.55
1:Az:429:GLN:HB3	1:Ba:448:LEU:HD11	1.90	0.55
1:Ax:399:VAL:HB	1:Ax:447:VAL:HG22	1.88	0.54
1:Bg:274:LEU:HB3	1:Bg:295:VAL:HG21	1.89	0.54
1:Bb:438:SER:HB3	1:Bc:394:ARG:HH12	1.72	0.54
1:Aq:315:THR:HB	1:Ar:313:PRO:HG3	1.90	0.54
1:Aq:385:GLU:HG2	1:Ar:304:VAL:HG22	1.88	0.54
1:Av:384:HIS:HB3	1:Aw:305:GLU:HB2	1.90	0.54
1:Az:274:LEU:HD11	1:Az:435:VAL:HG13	1.89	0.54
1:Bh:326:ASP:HB3	1:Bh:369:HIS:HB3	1.88	0.54
1:Ao:384:HIS:HB3	1:Ap:305:GLU:HB3	1.90	0.54
1:Bd:384:HIS:HB3	1:Be:305:GLU:HB2	1.89	0.54
1:Ah:324:LEU:HB3	1:Ah:371:GLU:HB3	1.88	0.54
1:An:433:GLY:HA3	1:Ao:398:ALA:HB2	1.90	0.54
1:Ao:385:GLU:HG2	1:Ap:304:VAL:HG22	1.89	0.54
1:Ar:286:LEU:HD12	1:Ar:291:TYR:HB3	1.88	0.54
1:Ar:402:LYS:HD3	1:Ar:452:PHE:HB2	1.88	0.54
1:Ay:326:ASP:HB3	1:Ay:369:HIS:HB3	1.89	0.54
1:Bg:274:LEU:HD12	1:Bg:295:VAL:HG11	1.88	0.53
1:Ak:399:VAL:HB	1:Ak:447:VAL:HG22	1.88	0.53
1:Ar:385:GLU:HG2	1:As:304:VAL:HG22	1.90	0.53
1:Ag:385:GLU:HG2	1:Ah:304:VAL:HG22	1.91	0.53
1:Ak:283:ILE:HG13	1:Ak:284:PRO:HD3	1.90	0.53
1:Av:432:ILE:HD12	1:Av:437:TYR:HB2	1.91	0.53
1:Ay:274:LEU:HD11	1:Ay:435:VAL:HG13	1.90	0.53
1:Aa:295:VAL:HG12	1:Aa:397:VAL:HG22	1.90	0.53
1:Ag:384:HIS:HB3	1:Ah:305:GLU:HB3	1.91	0.53
1:Bg:274:LEU:HD11	1:Bg:435:VAL:HG13	1.91	0.53
1:Aq:285:ILE:HG21	1:Aq:427:ILE:HD11	1.91	0.52
1:Ba:274:LEU:HD11	1:Ba:435:VAL:HG13	1.91	0.52
1:Bg:385:GLU:HG2	1:Bh:304:VAL:HG22	1.91	0.52
1:Aa:398:ALA:HB2	1:Bh:433:GLY:HA3	1.90	0.52
1:Ad:385:GLU:HG2	1:Ae:304:VAL:HG13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bh:432:ILE:HG23	1:Bh:437:TYR:HB3	1.90	0.52
1:Aq:282:LEU:HD21	1:Aq:431:LEU:HD21	1.91	0.52
1:Am:385:GLU:HG2	1:An:304:VAL:HG22	1.91	0.52
1:Aq:324:LEU:HB3	1:Aq:371:GLU:HB2	1.92	0.52
1:Ah:399:VAL:HB	1:Ah:447:VAL:HG22	1.92	0.52
1:Bc:397:VAL:HB	1:Bc:445:LEU:HD12	1.92	0.52
1:At:282:LEU:HD11	1:At:431:LEU:HD21	1.92	0.52
1:Bg:324:LEU:HB2	1:Bg:371:GLU:HB2	1.91	0.52
1:An:285:ILE:HG21	1:An:427:ILE:HD11	1.92	0.51
1:As:399:VAL:HB	1:As:447:VAL:HG22	1.91	0.51
1:Au:326:ASP:HB3	1:Au:369:HIS:HB3	1.91	0.51
1:Bf:326:ASP:HB3	1:Bf:369:HIS:HB3	1.93	0.51
1:Ay:432:ILE:HG13	1:Ay:445:LEU:HD22	1.92	0.51
1:Be:326:ASP:HB3	1:Be:369:HIS:HB3	1.91	0.51
1:Ai:326:ASP:HB3	1:Ai:369:HIS:HB3	1.93	0.51
1:Ax:385:GLU:HG2	1:Ay:304:VAL:HG22	1.91	0.51
1:Bd:282:LEU:HD21	1:Bd:431:LEU:HD11	1.92	0.51
1:Bf:283:ILE:HG13	1:Bf:284:PRO:HD3	1.91	0.51
1:Aq:278:ILE:HG23	1:Aq:282:LEU:HD23	1.93	0.51
1:Au:429:GLN:HB3	1:Av:448:LEU:HD11	1.92	0.51
1:Bg:285:ILE:HG21	1:Bg:427:ILE:HD11	1.92	0.51
1:Ab:295:VAL:HG12	1:Ab:397:VAL:HG22	1.92	0.51
1:Ac:385:GLU:HG2	1:Ad:304:VAL:HG22	1.92	0.51
1:Ah:295:VAL:HG22	1:Ah:397:VAL:HG22	1.92	0.51
1:Bc:285:ILE:HG21	1:Bc:427:ILE:HD11	1.93	0.51
1:Ai:399:VAL:HB	1:Ai:447:VAL:HG22	1.91	0.51
1:Ag:432:ILE:HD12	1:Ag:437:TYR:HB2	1.92	0.51
1:Aw:274:LEU:HD21	1:Aw:435:VAL:HG13	1.93	0.51
1:Bg:270:GLN:HG3	1:Bg:299:LEU:HD11	1.93	0.51
1:Ab:324:LEU:HB3	1:Ab:371:GLU:HB2	1.93	0.51
1:Aj:270:GLN:HG3	1:Aj:299:LEU:HD11	1.93	0.51
1:Ag:399:VAL:HB	1:Ag:447:VAL:HG22	1.92	0.50
1:Ar:285:ILE:HG21	1:Ar:427:ILE:HD11	1.92	0.50
1:Ax:433:GLY:HA3	1:Ay:398:ALA:HB2	1.94	0.50
1:Bb:309:LYS:HG2	1:Bb:382:ILE:HG12	1.93	0.50
1:Ay:295:VAL:HG12	1:Ay:397:VAL:HG22	1.93	0.50
1:Ao:433:GLY:HA3	1:Ap:398:ALA:HB2	1.93	0.50
1:Aa:309:LYS:HG3	1:Aa:382:ILE:HG12	1.93	0.50
1:Aq:397:VAL:HB	1:Aq:445:LEU:HD12	1.93	0.50
1:Bg:433:GLY:HA3	1:Bh:398:ALA:HB2	1.94	0.50
1:Ab:399:VAL:HB	1:Ab:447:VAL:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Az:384:HIS:HB3	1:Ba:305:GLU:HB2	1.94	0.50
1:An:315:THR:HB	1:Ao:313:PRO:HG3	1.92	0.50
1:Bb:274:LEU:HD11	1:Bb:435:VAL:HG13	1.94	0.50
1:Bf:385:GLU:HG2	1:Bg:304:VAL:HG22	1.93	0.50
1:Ae:427:ILE:HG12	1:Af:450:MET:HE1	1.93	0.50
1:Al:396:THR:HG22	1:Al:444:LEU:HB2	1.92	0.50
1:Aq:433:GLY:HA3	1:Ar:398:ALA:HB2	1.93	0.50
1:An:324:LEU:HB3	1:An:371:GLU:HB3	1.93	0.50
1:Ao:308:ARG:HB2	1:Ao:383:SER:HB3	1.94	0.49
1:Bf:384:HIS:HB3	1:Bg:305:GLU:HB2	1.94	0.49
1:Af:278:ILE:HG23	1:Af:431:LEU:HD11	1.94	0.49
1:Ai:285:ILE:HG21	1:Ai:427:ILE:HD11	1.93	0.49
1:Ar:399:VAL:HB	1:Ar:447:VAL:HG22	1.93	0.49
1:Aw:283:ILE:HG13	1:Aw:284:PRO:HD3	1.94	0.49
1:An:270:GLN:HG3	1:An:299:LEU:HD21	1.94	0.49
1:Ar:310:VAL:HG22	1:Ar:381:THR:HB	1.93	0.49
1:Aa:304:VAL:HG22	1:Bh:385:GLU:HG2	1.94	0.49
1:Ai:394:ARG:HH12	1:Ai:444:LEU:HD13	1.77	0.49
1:Av:285:ILE:HG21	1:Av:427:ILE:HD11	1.94	0.49
1:Bh:432:ILE:HG13	1:Bh:445:LEU:HD22	1.94	0.49
1:Av:274:LEU:HD11	1:Av:435:VAL:HG13	1.94	0.49
1:Aw:432:ILE:HD13	1:Aw:445:LEU:HD13	1.95	0.49
1:Ay:310:VAL:HG13	1:Ay:381:THR:HB	1.95	0.49
1:Ba:399:VAL:HB	1:Ba:447:VAL:HG22	1.94	0.49
1:Aj:326:ASP:HB3	1:Aj:369:HIS:HB3	1.94	0.49
1:Ac:384:HIS:HB3	1:Ad:305:GLU:HB2	1.95	0.49
1:Al:282:LEU:HD11	1:Al:431:LEU:HD11	1.95	0.49
1:Af:308:ARG:HB2	1:Af:383:SER:HB3	1.94	0.49
1:Ay:278:ILE:HG23	1:Ay:431:LEU:HD11	1.94	0.49
1:Bc:315:THR:HB	1:Bd:313:PRO:HG3	1.95	0.49
1:Aa:315:THR:HB	1:Ab:313:PRO:HG3	1.95	0.48
1:Ad:295:VAL:HG12	1:Ad:397:VAL:HG22	1.95	0.48
1:Am:384:HIS:HB3	1:An:305:GLU:HB2	1.95	0.48
1:As:285:ILE:HG21	1:As:427:ILE:HD11	1.94	0.48
1:Bg:325:GLU:HB2	1:Bh:370:LYS:HB2	1.95	0.48
1:Al:433:GLY:HA3	1:Am:398:ALA:HB2	1.95	0.48
1:Av:297:ILE:HG23	1:Av:392:ILE:HG23	1.94	0.48
1:Aj:433:GLY:HA3	1:Ak:398:ALA:HB2	1.95	0.48
1:Ap:278:ILE:HG23	1:Ap:431:LEU:HD11	1.96	0.48
1:As:326:ASP:HB3	1:As:369:HIS:HB3	1.94	0.48
1:Au:325:GLU:HB3	1:Av:370:LYS:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bd:326:ASP:HB3	1:Bd:369:HIS:HB3	1.95	0.48
1:Ac:433:GLY:HA2	1:Ad:396:THR:HB	1.94	0.48
1:Ak:384:HIS:HB3	1:Al:305:GLU:HB2	1.95	0.48
1:Av:315:THR:HB	1:Aw:313:PRO:HG3	1.96	0.48
1:Ay:432:ILE:HG23	1:Ay:437:TYR:HB3	1.95	0.48
1:An:397:VAL:HB	1:An:445:LEU:HD12	1.95	0.48
1:Ao:315:THR:HB	1:Ap:313:PRO:HG3	1.96	0.48
1:Ah:384:HIS:HB3	1:Ai:305:GLU:HB3	1.95	0.48
1:Ao:295:VAL:HG22	1:Ao:397:VAL:HG22	1.96	0.48
1:Ap:433:GLY:HA3	1:Aq:398:ALA:HB2	1.95	0.48
1:Bb:278:ILE:HG23	1:Bb:431:LEU:HD11	1.95	0.48
1:Bd:320:SER:HB2	1:Bd:375:ASN:HB2	1.95	0.48
1:Ad:433:GLY:HA3	1:Ae:398:ALA:HB2	1.96	0.48
1:Aj:285:ILE:HG21	1:Aj:427:ILE:HD11	1.96	0.48
1:Ax:285:ILE:HG21	1:Ax:427:ILE:HD11	1.96	0.48
1:Ae:324:LEU:HB3	1:Ae:371:GLU:HB3	1.94	0.47
1:Ak:278:ILE:HG23	1:Ak:431:LEU:HD11	1.96	0.47
1:Al:385:GLU:HG2	1:Am:304:VAL:HG22	1.96	0.47
1:Au:427:ILE:HG12	1:Av:450:MET:HE1	1.95	0.47
1:Bd:397:VAL:HB	1:Bd:445:LEU:HD12	1.96	0.47
1:Ab:262:LYS:HE2	1:Ac:257:SER:HA	1.97	0.47
1:Al:309:LYS:HG3	1:Al:382:ILE:HG12	1.95	0.47
1:Aq:432:ILE:HG23	1:Aq:437:TYR:HB3	1.95	0.47
1:Au:397:VAL:HG21	1:Au:435:VAL:HG11	1.96	0.47
1:Ba:396:THR:HG22	1:Ba:444:LEU:HB2	1.95	0.47
1:Ar:381:THR:HG23	1:As:308:ARG:HG2	1.96	0.47
1:Aa:313:PRO:HG3	1:Bh:315:THR:HB	1.96	0.47
1:Al:274:LEU:HD22	1:Al:295:VAL:HG11	1.96	0.47
1:Aa:402:LYS:HD3	1:Aa:452:PHE:HB2	1.95	0.47
1:Ac:428:ARG:HG3	1:Ac:445:LEU:HD23	1.97	0.47
1:Bb:275:ARG:HH21	1:Bb:294:GLN:HE22	1.63	0.47
1:Bg:399:VAL:HB	1:Bg:447:VAL:HG22	1.95	0.47
1:Ak:310:VAL:HG22	1:Ak:381:THR:HB	1.95	0.47
1:At:285:ILE:HG21	1:At:427:ILE:HD11	1.96	0.47
1:Ac:274:LEU:HD12	1:Ac:295:VAL:HG11	1.97	0.47
1:Ag:274:LEU:HD23	1:Ag:295:VAL:HG11	1.97	0.47
1:Av:295:VAL:HG12	1:Av:397:VAL:HG22	1.96	0.47
1:Av:399:VAL:HB	1:Av:447:VAL:HG22	1.97	0.47
1:Ba:295:VAL:HG12	1:Ba:397:VAL:HG22	1.96	0.47
1:Aq:399:VAL:HB	1:Aq:447:VAL:HG22	1.96	0.47
1:Ay:433:GLY:HA3	1:Az:398:ALA:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aa:326:ASP:HB3	1:Aa:369:HIS:HB3	1.96	0.47
1:Ag:326:ASP:HB3	1:Ag:369:HIS:HB3	1.95	0.47
1:At:266:LEU:HD23	1:At:301:PHE:HZ	1.80	0.47
1:Ae:385:GLU:HG2	1:Af:304:VAL:HG22	1.96	0.46
1:Ap:282:LEU:HD11	1:Ap:431:LEU:HD21	1.98	0.46
1:Aw:274:LEU:HD22	1:Aw:295:VAL:HG11	1.97	0.46
1:Bb:433:GLY:HA3	1:Bc:398:ALA:HB2	1.97	0.46
1:Af:399:VAL:HB	1:Af:447:VAL:HG22	1.97	0.46
1:Aw:385:GLU:HG2	1:Ax:304:VAL:HG22	1.97	0.46
1:Al:285:ILE:HG21	1:Al:427:ILE:HD11	1.97	0.46
1:Ac:428:ARG:O	1:Ac:432:ILE:HG12	2.16	0.46
1:Ae:270:GLN:HG3	1:Ae:299:LEU:HD21	1.98	0.46
1:Ap:270:GLN:HG2	1:Ap:297:ILE:HG21	1.98	0.46
1:Ag:274:LEU:HD11	1:Ag:435:VAL:HG13	1.98	0.46
1:Am:438:SER:HB3	1:An:394:ARG:HH12	1.79	0.46
1:Aq:274:LEU:HD22	1:Aq:295:VAL:HG11	1.97	0.46
1:Ac:295:VAL:HG12	1:Ac:397:VAL:HG22	1.98	0.46
1:Ag:262:LYS:HB3	1:Ag:262:LYS:HE2	1.80	0.46
1:Ae:295:VAL:HG12	1:Ae:397:VAL:HG22	1.97	0.46
1:Al:295:VAL:HG12	1:Al:397:VAL:HG22	1.97	0.46
1:Ap:385:GLU:HG2	1:Aq:304:VAL:HB	1.98	0.46
1:Ad:450:MET:HE2	1:Ad:450:MET:HB3	1.88	0.45
1:Aw:285:ILE:HG21	1:Aw:427:ILE:HD11	1.98	0.45
1:Az:274:LEU:HD12	1:Az:295:VAL:HG21	1.97	0.45
1:Bb:274:LEU:HD22	1:Bb:297:ILE:HD11	1.97	0.45
1:Ar:282:LEU:HD11	1:Ar:431:LEU:HD21	1.98	0.45
1:Ae:326:ASP:HB3	1:Ae:369:HIS:HB3	1.98	0.45
1:Ar:438:SER:HB3	1:As:394:ARG:HH12	1.80	0.45
1:Ak:433:GLY:HA3	1:Al:398:ALA:HB2	1.99	0.45
1:At:432:ILE:HG23	1:At:437:TYR:HB3	1.98	0.45
1:Aw:282:LEU:HD11	1:Aw:431:LEU:HD11	1.97	0.45
1:As:430:VAL:HG23	1:At:448:LEU:HD12	1.98	0.45
1:Bf:315:THR:HB	1:Bg:313:PRO:HG3	1.99	0.45
1:Bh:397:VAL:HB	1:Bh:445:LEU:HD12	1.98	0.45
1:Ad:384:HIS:HB3	1:Ae:305:GLU:HB2	1.99	0.45
1:Ai:304:VAL:HB	1:Ai:387:LYS:HB2	1.98	0.45
1:At:433:GLY:HA3	1:Au:398:ALA:HB2	1.97	0.45
1:Au:385:GLU:HG2	1:Av:304:VAL:HG22	1.98	0.45
1:Ah:285:ILE:HG21	1:Ah:427:ILE:HD11	1.99	0.45
1:As:429:GLN:HB3	1:At:448:LEU:HD11	1.99	0.45
1:Aw:430:VAL:HG23	1:Ax:448:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bh:399:VAL:HB	1:Bh:447:VAL:HG22	1.98	0.45
1:Aj:432:ILE:HG23	1:Aj:437:TYR:HB3	1.99	0.45
1:Ay:396:THR:HG22	1:Ay:444:LEU:HB2	1.98	0.45
1:Ax:295:VAL:HG13	1:Ax:397:VAL:HG22	1.99	0.44
1:Az:315:THR:HB	1:Ba:313:PRO:HG3	1.99	0.44
1:Bd:432:ILE:HG13	1:Bd:445:LEU:HD22	1.99	0.44
1:Be:288:LEU:HA	1:Be:291:TYR:HE1	1.82	0.44
1:Be:433:GLY:HA3	1:Bf:398:ALA:HB2	1.99	0.44
1:Av:432:ILE:HD13	1:Av:445:LEU:HD13	1.99	0.44
1:Aw:433:GLY:HA3	1:Ax:398:ALA:HB2	2.00	0.44
1:Aq:432:ILE:HG13	1:Aq:445:LEU:HD22	1.98	0.44
1:Ao:274:LEU:HD23	1:Ao:295:VAL:HG11	2.00	0.44
1:As:295:VAL:HG12	1:As:397:VAL:HG22	2.00	0.44
1:As:385:GLU:HG2	1:At:304:VAL:HG22	1.98	0.44
1:Ax:399:VAL:HG21	1:Ax:431:LEU:HD13	1.99	0.44
1:Bg:295:VAL:HG12	1:Bg:397:VAL:HG22	1.99	0.44
1:Aq:438:SER:HB3	1:Ar:394:ARG:HH12	1.82	0.44
1:As:397:VAL:HB	1:As:445:LEU:HD12	1.99	0.44
1:Av:433:GLY:HA3	1:Aw:398:ALA:HB2	2.00	0.44
1:Ba:274:LEU:HB3	1:Ba:295:VAL:HG21	1.99	0.44
1:Bg:401:VAL:HG21	1:Bg:419:LEU:HD22	1.99	0.44
1:Ak:295:VAL:HG12	1:Ak:397:VAL:HG22	2.00	0.44
1:Bf:432:ILE:HG23	1:Bf:437:TYR:HB3	1.99	0.44
1:Bh:285:ILE:HG21	1:Bh:427:ILE:HD11	1.99	0.44
1:Bh:428:ARG:HG3	1:Bh:445:LEU:HD23	2.00	0.44
1:Af:429:GLN:HB2	1:Ag:448:LEU:HD11	1.99	0.44
1:Bf:399:VAL:HB	1:Bf:447:VAL:HG22	1.98	0.44
1:Bf:433:GLY:HA3	1:Bg:398:ALA:HB2	2.00	0.44
1:Aq:326:ASP:HB3	1:Aq:369:HIS:HB3	2.00	0.44
1:Af:433:GLY:HA3	1:Ag:398:ALA:HB2	1.99	0.43
1:Af:432:ILE:HG23	1:Af:437:TYR:HB3	1.99	0.43
1:Am:315:THR:HB	1:An:313:PRO:HG3	2.01	0.43
1:At:399:VAL:HB	1:At:447:VAL:HG22	2.00	0.43
1:Ay:401:VAL:HG21	1:Ay:419:LEU:HD22	2.00	0.43
1:Az:309:LYS:HE2	1:Az:309:LYS:HB3	1.91	0.43
1:Ab:394:ARG:HH21	1:Ab:444:LEU:HD13	1.83	0.43
1:Bg:308:ARG:HB2	1:Bg:383:SER:HB3	2.00	0.43
1:Aa:385:GLU:HG2	1:Ab:304:VAL:HG13	1.99	0.43
1:Ai:295:VAL:HG22	1:Ai:397:VAL:HG22	2.01	0.43
1:Ax:326:ASP:HB3	1:Ax:369:HIS:HB3	1.99	0.43
1:Bc:433:GLY:HA2	1:Bd:396:THR:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Be:285:ILE:HD13	1:Bf:450:MET:HE3	2.00	0.43
1:Ab:326:ASP:HB3	1:Ab:369:HIS:HB3	2.00	0.43
1:Aw:295:VAL:HG12	1:Aw:397:VAL:HG22	2.01	0.43
1:Ax:395:GLN:HG3	1:Ax:441:ARG:HH22	1.83	0.43
1:Bb:399:VAL:HB	1:Bb:447:VAL:HG22	1.99	0.43
1:Bh:282:LEU:HD11	1:Bh:431:LEU:HD21	2.01	0.43
1:Ab:274:LEU:HD21	1:Ab:395:GLN:HE22	1.84	0.43
1:Ad:267:GLU:HG2	1:Ad:299:LEU:HD23	2.00	0.43
1:Ae:267:GLU:HG2	1:Ae:299:LEU:HD23	2.00	0.43
1:Aq:384:HIS:HB3	1:Ar:305:GLU:HB3	2.01	0.43
1:As:433:GLY:HA3	1:At:398:ALA:HB2	2.00	0.43
1:Ba:384:HIS:HB3	1:Bb:305:GLU:HB2	2.00	0.43
1:Be:402:LYS:HE2	1:Be:452:PHE:HB2	2.01	0.43
1:Am:309:LYS:HG2	1:Am:311:PHE:HE1	1.84	0.43
1:Bc:385:GLU:HG2	1:Bd:304:VAL:HG22	2.00	0.43
1:Bh:270:GLN:HB3	1:Bh:297:ILE:HD12	2.00	0.43
1:Ag:295:VAL:HG22	1:Ag:397:VAL:HG22	1.99	0.43
1:Aj:402:LYS:HD3	1:Aj:452:PHE:HB2	2.00	0.43
1:An:278:ILE:HG23	1:An:431:LEU:HD11	1.99	0.43
1:Aa:305:GLU:HB3	1:Bh:384:HIS:HB3	2.01	0.43
1:Af:266:LEU:HD23	1:Af:301:PHE:HZ	1.84	0.43
1:As:438:SER:HB2	1:As:441:ARG:HG2	2.01	0.43
1:Ae:278:ILE:HG23	1:Ae:431:LEU:HD11	2.00	0.42
1:Af:285:ILE:HD13	1:Ag:450:MET:HE3	2.01	0.42
1:Am:296:ASP:HB3	1:Am:396:THR:HG23	2.00	0.42
1:Aa:309:LYS:HE2	1:Aa:311:PHE:HZ	1.85	0.42
1:Ak:450:MET:HE3	1:Ak:450:MET:HB3	1.77	0.42
1:Ao:326:ASP:HB3	1:Ao:369:HIS:HB3	2.01	0.42
1:Aq:256:VAL:HG13	1:Aq:258:ALA:H	1.84	0.42
1:Ac:285:ILE:HG21	1:Ac:427:ILE:HD11	2.00	0.42
1:Ah:450:MET:HE2	1:Ah:450:MET:HB2	1.72	0.42
1:Aa:274:LEU:HD21	1:Aa:395:GLN:HE22	1.84	0.42
1:Ab:427:ILE:HG12	1:Ac:450:MET:HE1	2.01	0.42
1:Ak:280:SER:HA	1:Ak:283:ILE:HD11	2.00	0.42
1:Av:278:ILE:HG23	1:Av:431:LEU:HD11	2.01	0.42
1:Bc:395:GLN:HE21	1:Bc:395:GLN:HB2	1.70	0.42
1:Af:274:LEU:HD11	1:Af:435:VAL:HG13	2.00	0.42
1:Ao:450:MET:HE2	1:Ao:450:MET:HB3	1.88	0.42
1:Ar:437:TYR:HD1	1:Ar:443:ASP:HB2	1.84	0.42
1:Bg:275:ARG:HH21	1:Bg:294:GLN:HE22	1.67	0.42
1:Ae:433:GLY:HA3	1:Af:398:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aj:263:GLU:H	1:Aj:263:GLU:HG2	1.69	0.42
1:Av:432:ILE:HG23	1:Av:437:TYR:HB3	2.01	0.42
1:Ai:427:ILE:HG12	1:Aj:450:MET:HE1	2.01	0.42
1:As:285:ILE:HD13	1:At:450:MET:HE3	2.01	0.42
1:Bf:397:VAL:HB	1:Bf:445:LEU:HG	2.02	0.42
1:Ak:282:LEU:HD11	1:Ak:431:LEU:HD21	2.01	0.42
1:Bb:326:ASP:HB3	1:Bb:369:HIS:HB3	2.02	0.42
1:Ac:432:ILE:HG23	1:Ac:437:TYR:HB3	2.02	0.42
1:An:280:SER:HA	1:An:283:ILE:HD11	2.02	0.42
1:As:300:ASP:HB2	1:As:393:ASN:HD22	1.85	0.42
1:Bd:260:ARG:H	1:Bd:260:ARG:HG2	1.59	0.42
1:Aa:428:ARG:O	1:Aa:432:ILE:HG12	2.20	0.41
1:An:274:LEU:HD12	1:An:435:VAL:HG13	2.01	0.41
1:An:399:VAL:HB	1:An:447:VAL:HG22	2.01	0.41
1:At:274:LEU:HB3	1:At:295:VAL:HG21	2.02	0.41
1:Az:295:VAL:HG22	1:Az:397:VAL:HG22	2.01	0.41
1:Bd:402:LYS:HD3	1:Bd:452:PHE:HB2	2.01	0.41
1:Bf:282:LEU:HD13	1:Bf:282:LEU:HA	1.92	0.41
1:Aa:310:VAL:HG22	1:Aa:381:THR:HB	2.03	0.41
1:Ad:304:VAL:HB	1:Ad:387:LYS:HB2	2.02	0.41
1:Ae:429:GLN:HB2	1:Af:448:LEU:HD11	2.02	0.41
1:An:266:LEU:HD23	1:An:301:PHE:HZ	1.85	0.41
1:Ac:427:ILE:HG12	1:Ad:450:MET:HE1	2.01	0.41
1:Ad:399:VAL:HG21	1:Ad:431:LEU:HD13	2.03	0.41
1:Ag:310:VAL:HG22	1:Ag:381:THR:HB	2.02	0.41
1:Ah:427:ILE:HG12	1:Ai:450:MET:HE1	2.02	0.41
1:Al:432:ILE:HG23	1:Al:437:TYR:HB3	2.01	0.41
1:Av:370:LYS:HE2	1:Av:370:LYS:HB2	1.93	0.41
1:Aw:270:GLN:HE21	1:Aw:270:GLN:HB3	1.62	0.41
1:Ax:310:VAL:HG23	1:Ax:381:THR:HB	2.01	0.41
1:Aa:384:HIS:HB3	1:Ab:305:GLU:HB2	2.01	0.41
1:Az:427:ILE:HD13	1:Az:427:ILE:HA	1.95	0.41
1:Bd:397:VAL:HG21	1:Bd:435:VAL:HG11	2.02	0.41
1:Bh:278:ILE:HG23	1:Bh:431:LEU:HD11	2.02	0.41
1:Bh:295:VAL:HG12	1:Bh:397:VAL:HG22	2.03	0.41
1:Aa:324:LEU:HB3	1:Aa:371:GLU:HB3	2.03	0.41
1:Ap:259:ALA:HA	1:Ap:262:LYS:HG2	2.02	0.41
1:Bc:429:GLN:HB2	1:Bd:448:LEU:HD11	2.03	0.41
1:Ab:427:ILE:HD13	1:Ab:427:ILE:HA	1.79	0.41
1:Ac:401:VAL:HG21	1:Ac:419:LEU:HD22	2.03	0.41
1:Ar:278:ILE:HG13	1:Ar:431:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:As:282:LEU:HD21	1:As:431:LEU:HD21	2.02	0.41
1:Ax:270:GLN:HG3	1:Ax:299:LEU:HD11	2.02	0.41
1:Bb:270:GLN:HB3	1:Bb:297:ILE:HD12	2.03	0.41
1:Aa:450:MET:HE3	1:Bh:285:ILE:HD13	2.02	0.41
1:Af:384:HIS:HB3	1:Ag:305:GLU:HB3	2.03	0.41
1:Ar:309:LYS:HE2	1:Ar:311:PHE:HZ	1.85	0.41
1:Ay:450:MET:HE2	1:Ay:450:MET:HB3	1.83	0.41
1:Az:282:LEU:HD13	1:Az:282:LEU:HA	1.91	0.41
1:Aj:394:ARG:HD2	1:Aj:394:ARG:HA	1.80	0.41
1:An:450:MET:HE2	1:An:450:MET:HB3	1.89	0.41
1:Ao:433:GLY:HA2	1:Ap:396:THR:HG22	2.02	0.41
1:At:427:ILE:HD13	1:At:427:ILE:HA	1.95	0.41
1:Av:270:GLN:HG3	1:Av:299:LEU:HD11	2.03	0.41
1:Ay:274:LEU:HB3	1:Ay:295:VAL:HG21	2.03	0.41
1:Bg:427:ILE:HD13	1:Bg:427:ILE:HA	1.98	0.41
1:Ac:427:ILE:HA	1:Ac:430:VAL:HG22	2.02	0.40
1:Ae:427:ILE:HD13	1:Ae:427:ILE:HA	1.95	0.40
1:Ae:450:MET:HE3	1:Ae:450:MET:HB3	1.90	0.40
1:Ag:309:LYS:HG3	1:Ag:382:ILE:HG13	2.03	0.40
1:Ak:285:ILE:HG21	1:Ak:427:ILE:HD11	2.02	0.40
1:Al:324:LEU:HB3	1:Al:371:GLU:HB3	2.03	0.40
1:Bb:295:VAL:HG12	1:Bb:397:VAL:HG22	2.03	0.40
1:Bb:427:ILE:HD13	1:Bb:427:ILE:HA	1.93	0.40
1:Ah:326:ASP:HB3	1:Ah:369:HIS:HB3	2.02	0.40
1:Ao:297:ILE:HG23	1:Ao:392:ILE:HG23	2.03	0.40
1:Au:285:ILE:HG21	1:Au:427:ILE:HD11	2.03	0.40
1:Av:324:LEU:HB3	1:Av:371:GLU:HB3	2.04	0.40
1:Ac:394:ARG:HH21	1:Ac:444:LEU:HD13	1.86	0.40
1:Ad:285:ILE:HG21	1:Ad:427:ILE:HD11	2.04	0.40
1:Av:427:ILE:HD13	1:Av:427:ILE:HA	1.98	0.40
1:Ac:315:THR:HB	1:Ad:313:PRO:HG3	2.04	0.40
1:Ay:285:ILE:HG21	1:Ay:427:ILE:HD11	2.02	0.40
1:Bb:432:ILE:HG23	1:Bb:437:TYR:HB3	2.03	0.40
1:Bb:432:ILE:HG13	1:Bb:445:LEU:HD22	2.03	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	Aa	138/198 (70%)	135 (98%)	3 (2%)	0	100	100
1	Ab	138/198 (70%)	135 (98%)	3 (2%)	0	100	100
1	Ac	138/198 (70%)	134 (97%)	4 (3%)	0	100	100
1	Ad	138/198 (70%)	137 (99%)	1 (1%)	0	100	100
1	Ae	138/198 (70%)	137 (99%)	1 (1%)	0	100	100
1	Af	138/198 (70%)	134 (97%)	4 (3%)	0	100	100
1	Ag	138/198 (70%)	137 (99%)	1 (1%)	0	100	100
1	Ah	138/198 (70%)	138 (100%)	0	0	100	100
1	Ai	138/198 (70%)	136 (99%)	2 (1%)	0	100	100
1	Aj	138/198 (70%)	133 (96%)	5 (4%)	0	100	100
1	Ak	138/198 (70%)	134 (97%)	4 (3%)	0	100	100
1	Al	138/198 (70%)	137 (99%)	1 (1%)	0	100	100
1	Am	138/198 (70%)	135 (98%)	3 (2%)	0	100	100
1	An	138/198 (70%)	137 (99%)	1 (1%)	0	100	100
1	Ao	138/198 (70%)	135 (98%)	3 (2%)	0	100	100
1	Ap	138/198 (70%)	137 (99%)	1 (1%)	0	100	100
1	Aq	138/198 (70%)	137 (99%)	1 (1%)	0	100	100
1	Ar	138/198 (70%)	131 (95%)	7 (5%)	0	100	100
1	As	138/198 (70%)	134 (97%)	4 (3%)	0	100	100
1	At	138/198 (70%)	136 (99%)	2 (1%)	0	100	100
1	Au	138/198 (70%)	135 (98%)	3 (2%)	0	100	100
1	Av	138/198 (70%)	136 (99%)	2 (1%)	0	100	100
1	Aw	138/198 (70%)	135 (98%)	3 (2%)	0	100	100
1	Ax	138/198 (70%)	137 (99%)	1 (1%)	0	100	100
1	Ay	138/198 (70%)	136 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Az	138/198 (70%)	134 (97%)	4 (3%)	0	100	100
1	Ba	138/198 (70%)	137 (99%)	1 (1%)	0	100	100
1	Bb	138/198 (70%)	135 (98%)	3 (2%)	0	100	100
1	Bc	138/198 (70%)	135 (98%)	3 (2%)	0	100	100
1	Bd	138/198 (70%)	132 (96%)	6 (4%)	0	100	100
1	Be	138/198 (70%)	135 (98%)	3 (2%)	0	100	100
1	Bf	138/198 (70%)	132 (96%)	6 (4%)	0	100	100
1	Bg	138/198 (70%)	136 (99%)	2 (1%)	0	100	100
1	Bh	138/198 (70%)	135 (98%)	3 (2%)	0	100	100
All	All	4692/6732 (70%)	4599 (98%)	93 (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	Aa	126/168 (75%)	122 (97%)	4 (3%)	34	55
1	Ab	126/168 (75%)	120 (95%)	6 (5%)	23	47
1	Ac	126/168 (75%)	123 (98%)	3 (2%)	43	61
1	Ad	126/168 (75%)	120 (95%)	6 (5%)	23	47
1	Ae	126/168 (75%)	121 (96%)	5 (4%)	28	51
1	Af	126/168 (75%)	121 (96%)	5 (4%)	28	51
1	Ag	126/168 (75%)	120 (95%)	6 (5%)	23	47
1	Ah	126/168 (75%)	119 (94%)	7 (6%)	19	44
1	Ai	126/168 (75%)	122 (97%)	4 (3%)	34	55
1	Aj	126/168 (75%)	119 (94%)	7 (6%)	19	44
1	Ak	126/168 (75%)	120 (95%)	6 (5%)	23	47
1	Al	126/168 (75%)	120 (95%)	6 (5%)	23	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Am	126/168 (75%)	121 (96%)	5 (4%)	28	51
1	An	126/168 (75%)	123 (98%)	3 (2%)	43	61
1	Ao	126/168 (75%)	123 (98%)	3 (2%)	43	61
1	Ap	126/168 (75%)	123 (98%)	3 (2%)	43	61
1	Aq	126/168 (75%)	118 (94%)	8 (6%)	16	42
1	Ar	126/168 (75%)	119 (94%)	7 (6%)	19	44
1	As	126/168 (75%)	121 (96%)	5 (4%)	28	51
1	At	126/168 (75%)	118 (94%)	8 (6%)	16	42
1	Au	126/168 (75%)	119 (94%)	7 (6%)	19	44
1	Av	126/168 (75%)	123 (98%)	3 (2%)	43	61
1	Aw	126/168 (75%)	121 (96%)	5 (4%)	28	51
1	Ax	126/168 (75%)	123 (98%)	3 (2%)	43	61
1	Ay	126/168 (75%)	121 (96%)	5 (4%)	28	51
1	Az	126/168 (75%)	117 (93%)	9 (7%)	13	39
1	Ba	126/168 (75%)	123 (98%)	3 (2%)	43	61
1	Bb	126/168 (75%)	120 (95%)	6 (5%)	23	47
1	Bc	126/168 (75%)	124 (98%)	2 (2%)	55	68
1	Bd	126/168 (75%)	123 (98%)	3 (2%)	43	61
1	Be	126/168 (75%)	119 (94%)	7 (6%)	19	44
1	Bf	126/168 (75%)	118 (94%)	8 (6%)	16	42
1	Bg	126/168 (75%)	117 (93%)	9 (7%)	13	39
1	Bh	126/168 (75%)	124 (98%)	2 (2%)	55	68
All	All	4284/5712 (75%)	4105 (96%)	179 (4%)	28	50

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Aa	299	LEU
1	Aa	310	VAL
1	Aa	380	THR
1	Aa	383	SER
1	Ab	281	VAL
1	Ab	324	LEU
1	Ab	377	GLU

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Mol	Chain	Res	Type
1	Ab	380	THR
1	Ab	427	ILE
1	Ab	445	LEU
1	Ac	274	LEU
1	Ac	401	VAL
1	Ac	443	ASP
1	Ad	266	LEU
1	Ad	299	LEU
1	Ad	305	GLU
1	Ad	380	THR
1	Ad	445	LEU
1	Ad	448	LEU
1	Ae	266	LEU
1	Ae	294	GLN
1	Ae	307	THR
1	Ae	395	GLN
1	Ae	445	LEU
1	Af	270	GLN
1	Af	299	LEU
1	Af	310	VAL
1	Af	378	LEU
1	Af	444	LEU
1	Ag	266	LEU
1	Ag	282	LEU
1	Ag	380	THR
1	Ag	395	GLN
1	Ag	401	VAL
1	Ag	445	LEU
1	Ah	266	LEU
1	Ah	282	LEU
1	Ah	283	ILE
1	Ah	319	ARG
1	Ah	427	ILE
1	Ah	445	LEU
1	Ah	450	MET
1	Ai	266	LEU
1	Ai	377	GLU
1	Ai	380	THR
1	Ai	445	LEU
1	Aj	263	GLU
1	Aj	282	LEU
1	Aj	283	ILE

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Mol	Chain	Res	Type
1	Aj	380	THR
1	Aj	401	VAL
1	Aj	445	LEU
1	Aj	448	LEU
1	Ak	264	GLN
1	Ak	266	LEU
1	Ak	283	ILE
1	Ak	307	THR
1	Ak	380	THR
1	Ak	445	LEU
1	Al	266	LEU
1	Al	274	LEU
1	Al	381	THR
1	Al	432	ILE
1	Al	443	ASP
1	Al	445	LEU
1	Am	266	LEU
1	Am	274	LEU
1	Am	396	THR
1	Am	441	ARG
1	Am	448	LEU
1	An	283	ILE
1	An	299	LEU
1	An	445	LEU
1	Ao	261	ARG
1	Ao	266	LEU
1	Ao	281	VAL
1	Ap	299	LEU
1	Ap	396	THR
1	Ap	445	LEU
1	Aq	266	LEU
1	Aq	274	LEU
1	Aq	282	LEU
1	Aq	304	VAL
1	Aq	307	THR
1	Aq	381	THR
1	Aq	396	THR
1	Aq	448	LEU
1	Ar	266	LEU
1	Ar	270	GLN
1	Ar	278	ILE
1	Ar	380	THR

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Mol	Chain	Res	Type
1	Ar	429	GLN
1	Ar	431	LEU
1	Ar	445	LEU
1	As	266	LEU
1	As	381	THR
1	As	395	GLN
1	As	431	LEU
1	As	445	LEU
1	At	274	LEU
1	At	307	THR
1	At	381	THR
1	At	396	THR
1	At	424	LEU
1	At	429	GLN
1	At	439	GLU
1	At	446	ASN
1	Au	266	LEU
1	Au	274	LEU
1	Au	282	LEU
1	Au	283	ILE
1	Au	380	THR
1	Au	419	LEU
1	Au	445	LEU
1	Av	261	ARG
1	Av	266	LEU
1	Av	446	ASN
1	Aw	266	LEU
1	Aw	270	GLN
1	Aw	274	LEU
1	Aw	283	ILE
1	Aw	446	ASN
1	Ax	396	THR
1	Ax	432	ILE
1	Ax	445	LEU
1	Ay	307	THR
1	Ay	310	VAL
1	Ay	380	THR
1	Ay	385	GLU
1	Ay	445	LEU
1	Az	263	GLU
1	Az	270	GLN
1	Az	274	LEU

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Mol	Chain	Res	Type
1	Az	282	LEU
1	Az	395	GLN
1	Az	401	VAL
1	Az	419	LEU
1	Az	427	ILE
1	Az	445	LEU
1	Ba	283	ILE
1	Ba	299	LEU
1	Ba	377	GLU
1	Bb	380	THR
1	Bb	423	ASP
1	Bb	427	ILE
1	Bb	429	GLN
1	Bb	445	LEU
1	Bb	448	LEU
1	Bc	274	LEU
1	Bc	281	VAL
1	Bd	282	LEU
1	Bd	380	THR
1	Bd	396	THR
1	Be	274	LEU
1	Be	286	LEU
1	Be	319	ARG
1	Be	385	GLU
1	Be	395	GLN
1	Be	432	ILE
1	Be	446	ASN
1	Bf	266	LEU
1	Bf	274	LEU
1	Bf	281	VAL
1	Bf	282	LEU
1	Bf	283	ILE
1	Bf	380	THR
1	Bf	396	THR
1	Bf	446	ASN
1	Bg	274	LEU
1	Bg	282	LEU
1	Bg	377	GLU
1	Bg	378	LEU
1	Bg	396	THR
1	Bg	401	VAL
1	Bg	419	LEU

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Mol	Chain	Res	Type
1	Bg	445	LEU
1	Bg	448	LEU
1	Bh	266	LEU
1	Bh	380	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	Aa	264	GLN
1	Ab	290	ASN
1	Ac	290	ASN
1	Ac	314	ASN
1	Ad	290	ASN
1	Ad	314	ASN
1	Ad	395	GLN
1	Ae	375	ASN
1	Ae	446	ASN
1	Af	270	GLN
1	Af	290	ASN
1	Af	395	GLN
1	Af	429	GLN
1	Af	446	ASN
1	Ag	294	GLN
1	Ah	290	ASN
1	Ah	314	ASN
1	Ah	446	ASN
1	Ai	290	ASN
1	Ai	440	ASN
1	Ai	446	ASN
1	Aj	393	ASN
1	Aj	395	GLN
1	Aj	425	ASN
1	Aj	446	ASN
1	Ak	264	GLN
1	Ak	290	ASN
1	Ak	314	ASN
1	Al	290	ASN
1	Al	314	ASN
1	Al	446	ASN
1	Am	290	ASN
1	Am	294	GLN
1	Am	395	GLN

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Mol	Chain	Res	Type
1	An	290	ASN
1	An	375	ASN
1	An	395	GLN
1	An	429	GLN
1	Ao	270	GLN
1	Ao	290	ASN
1	Ao	314	ASN
1	Ap	314	ASN
1	Aq	290	ASN
1	Aq	395	GLN
1	Ar	270	GLN
1	Ar	328	ASN
1	Ar	375	ASN
1	Ar	446	ASN
1	As	290	ASN
1	As	328	ASN
1	As	369	HIS
1	As	375	ASN
1	As	393	ASN
1	As	446	ASN
1	At	314	ASN
1	At	429	GLN
1	At	446	ASN
1	Av	328	ASN
1	Av	395	GLN
1	Av	446	ASN
1	Aw	270	GLN
1	Aw	290	ASN
1	Aw	314	ASN
1	Ax	290	ASN
1	Ax	446	ASN
1	Ay	290	ASN
1	Ay	314	ASN
1	Ay	425	ASN
1	Az	270	GLN
1	Az	290	ASN
1	Az	395	GLN
1	Az	429	GLN
1	Az	440	ASN
1	Ba	393	ASN
1	Ba	429	GLN
1	Ba	446	ASN

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Mol	Chain	Res	Type
1	Bb	294	GLN
1	Bb	314	ASN
1	Bb	328	ASN
1	Bb	369	HIS
1	Bb	446	ASN
1	Bc	395	GLN
1	Bc	425	ASN
1	Bc	429	GLN
1	Bd	328	ASN
1	Bd	395	GLN
1	Bd	446	ASN
1	Be	290	ASN
1	Be	395	GLN
1	Be	429	GLN
1	Bf	290	ASN
1	Bf	314	ASN
1	Bf	393	ASN
1	Bf	446	ASN
1	Bg	290	ASN
1	Bg	294	GLN
1	Bg	314	ASN
1	Bg	395	GLN
1	Bg	446	ASN
1	Bh	290	ASN
1	Bh	369	HIS
1	Bh	446	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.



## 5.6 Ligand geometry [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 [i](#)

There are no chain breaks in this entry.

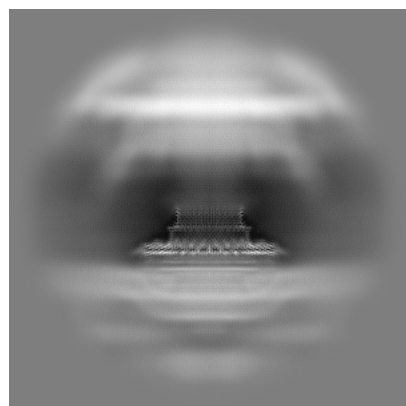
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72840. These allow visual inspection of the internal detail of the map and identification of artifacts.

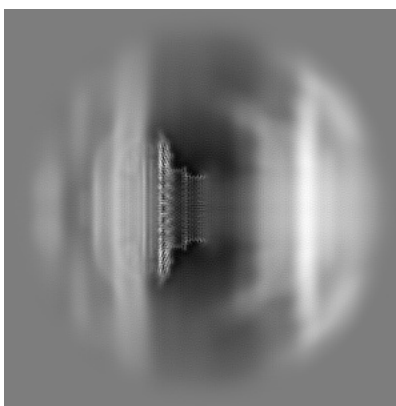
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

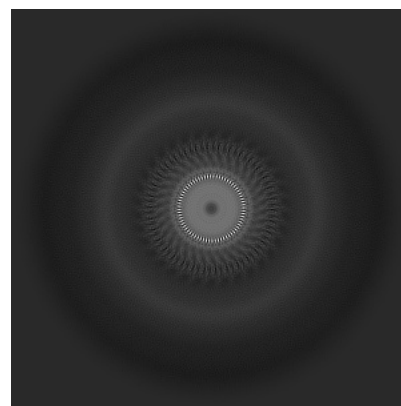
#### 6.1.1 Primary map



X

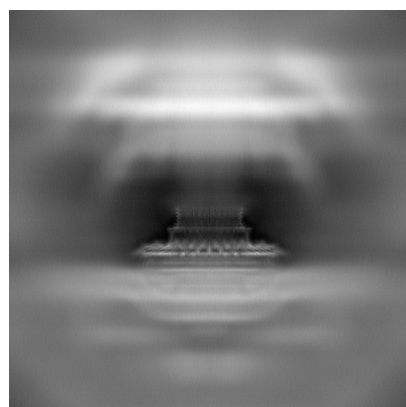


Y

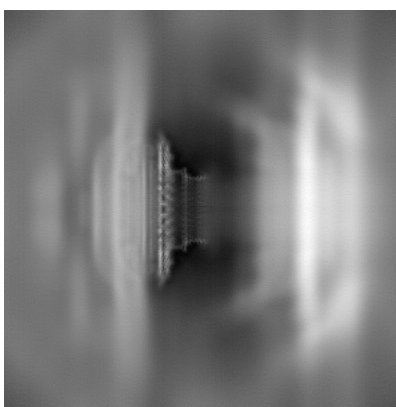


Z

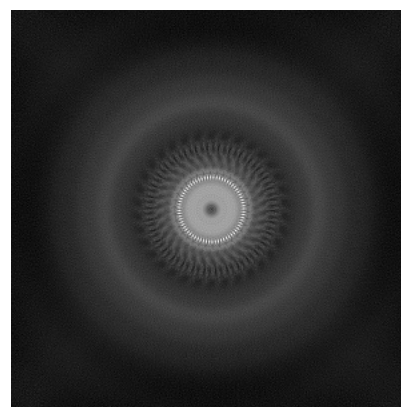
#### 6.1.2 Raw map



X



Y

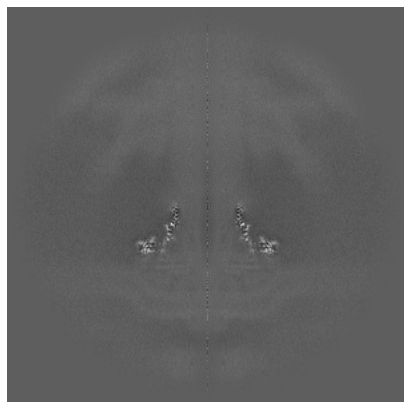


Z

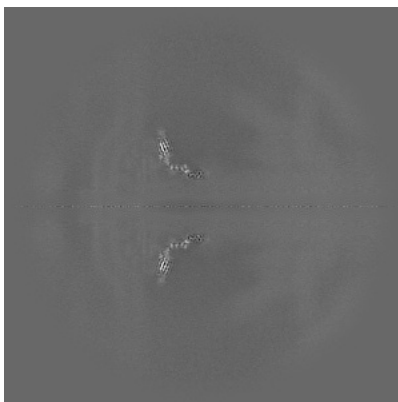
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

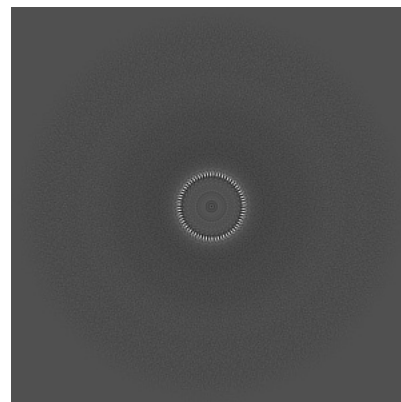
### 6.2.1 Primary map



X Index: 224

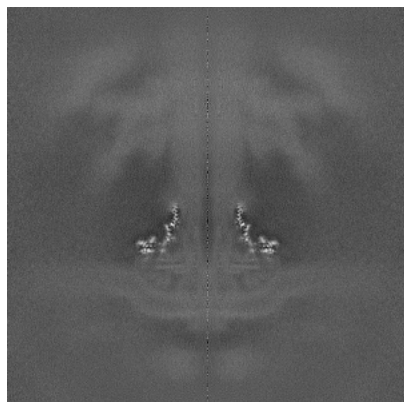


Y Index: 224

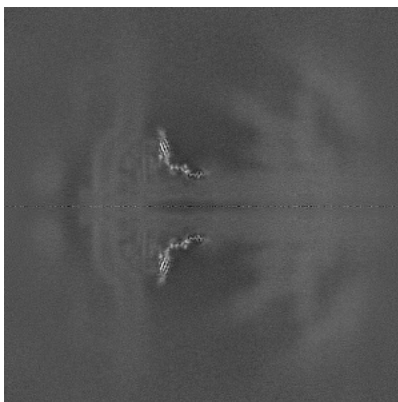


Z Index: 224

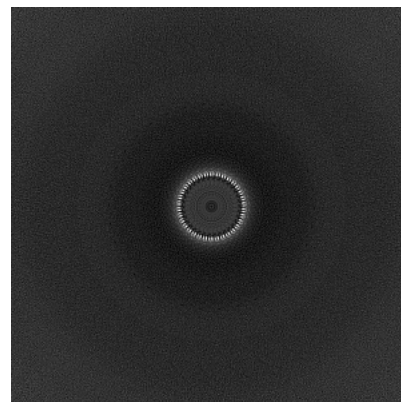
### 6.2.2 Raw map



X Index: 224



Y Index: 224

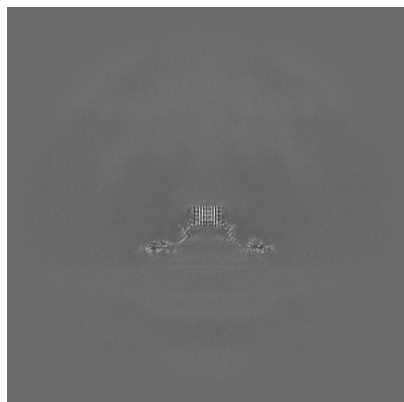


Z Index: 224

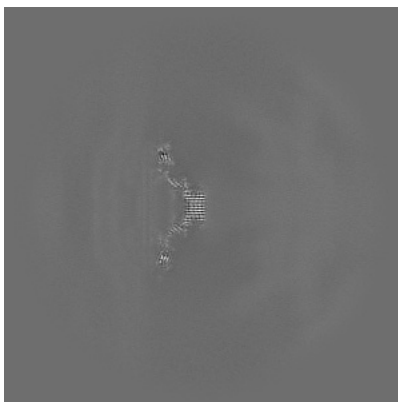
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

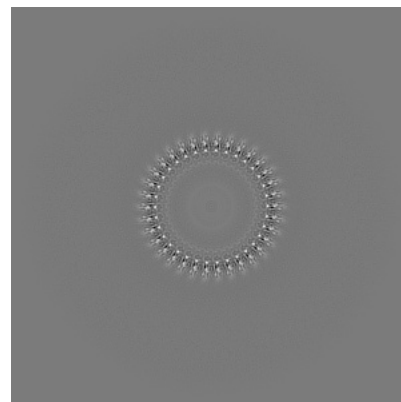
### 6.3.1 Primary map



X Index: 259

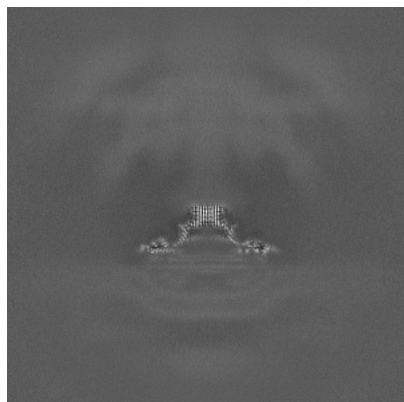


Y Index: 259

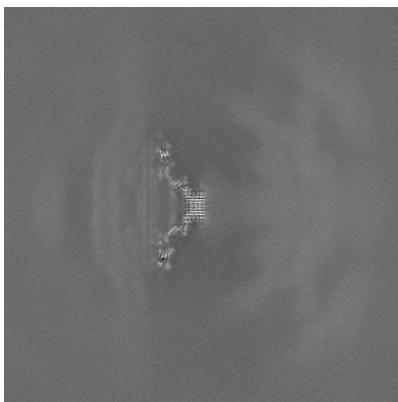


Z Index: 178

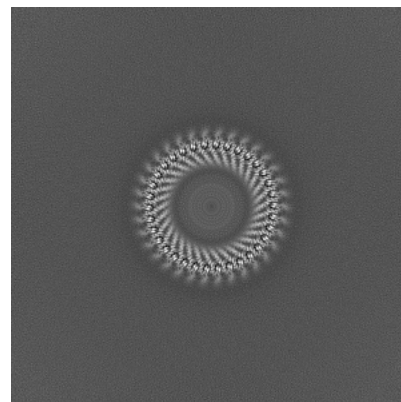
### 6.3.2 Raw map



X Index: 189



Y Index: 189

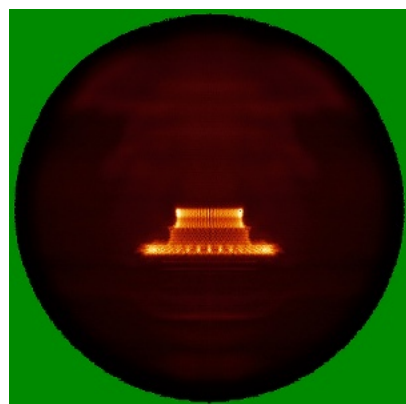


Z Index: 175

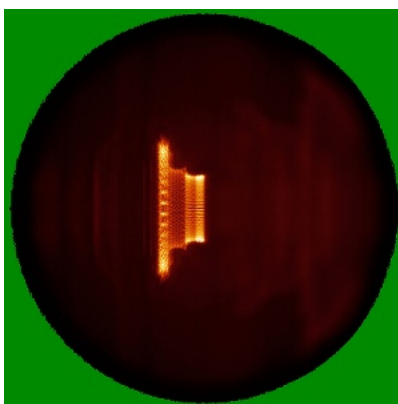
The images above show the largest variance slices of the map in three orthogonal directions.

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

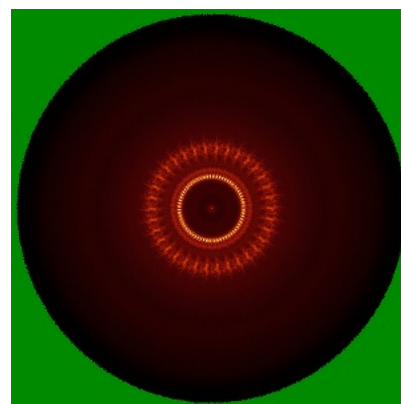
### 6.4.1 Primary map



X

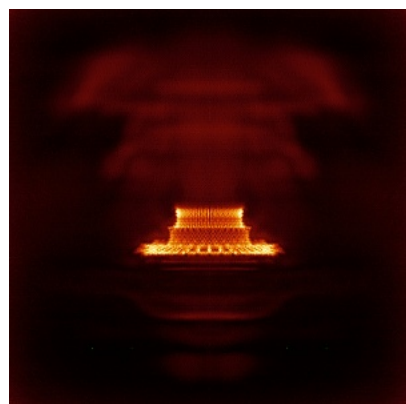


Y

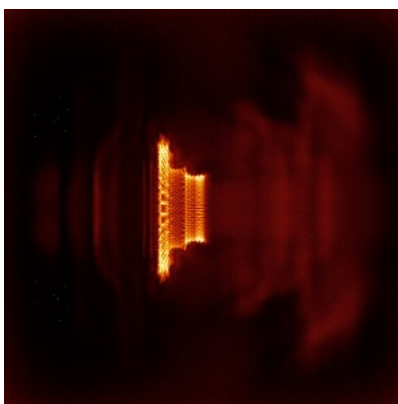


Z

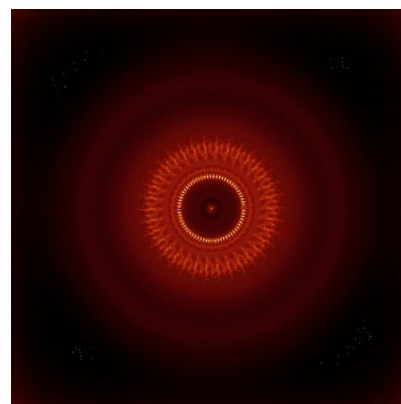
### 6.4.2 Raw map



X



Y

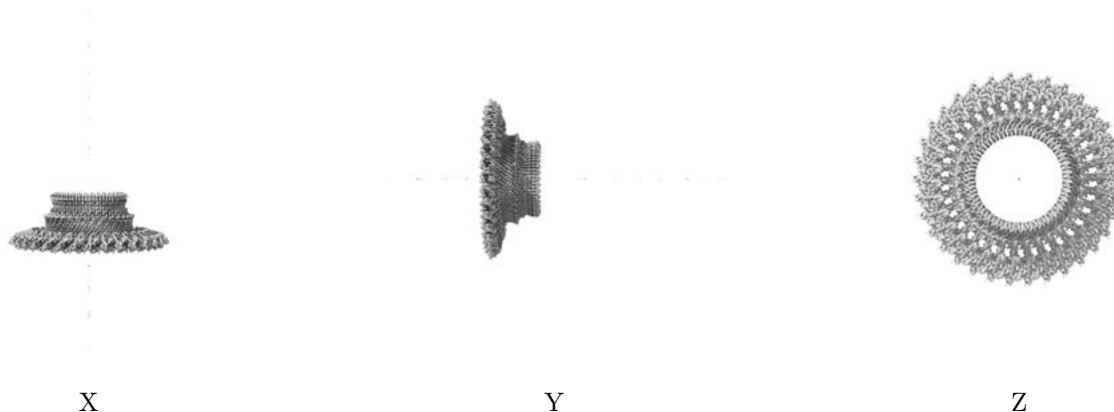


Z

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 0.15. 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.

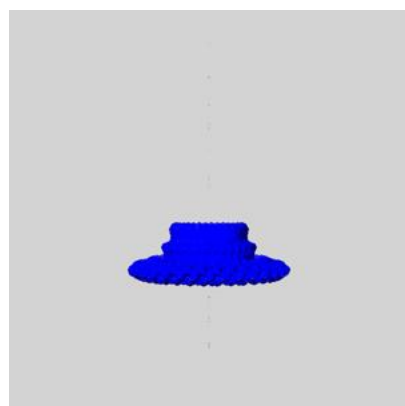
## 6.6 Mask visualisation [i](#)

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

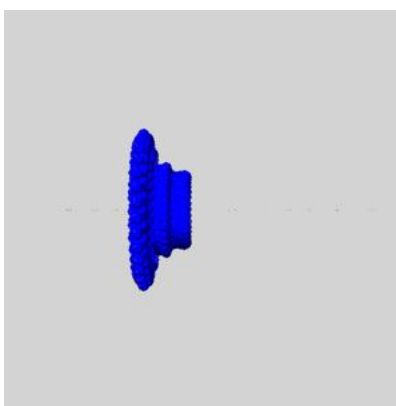
A mask typically either:

- 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\_72840\_msk\_1.map [i](#)



X



Y

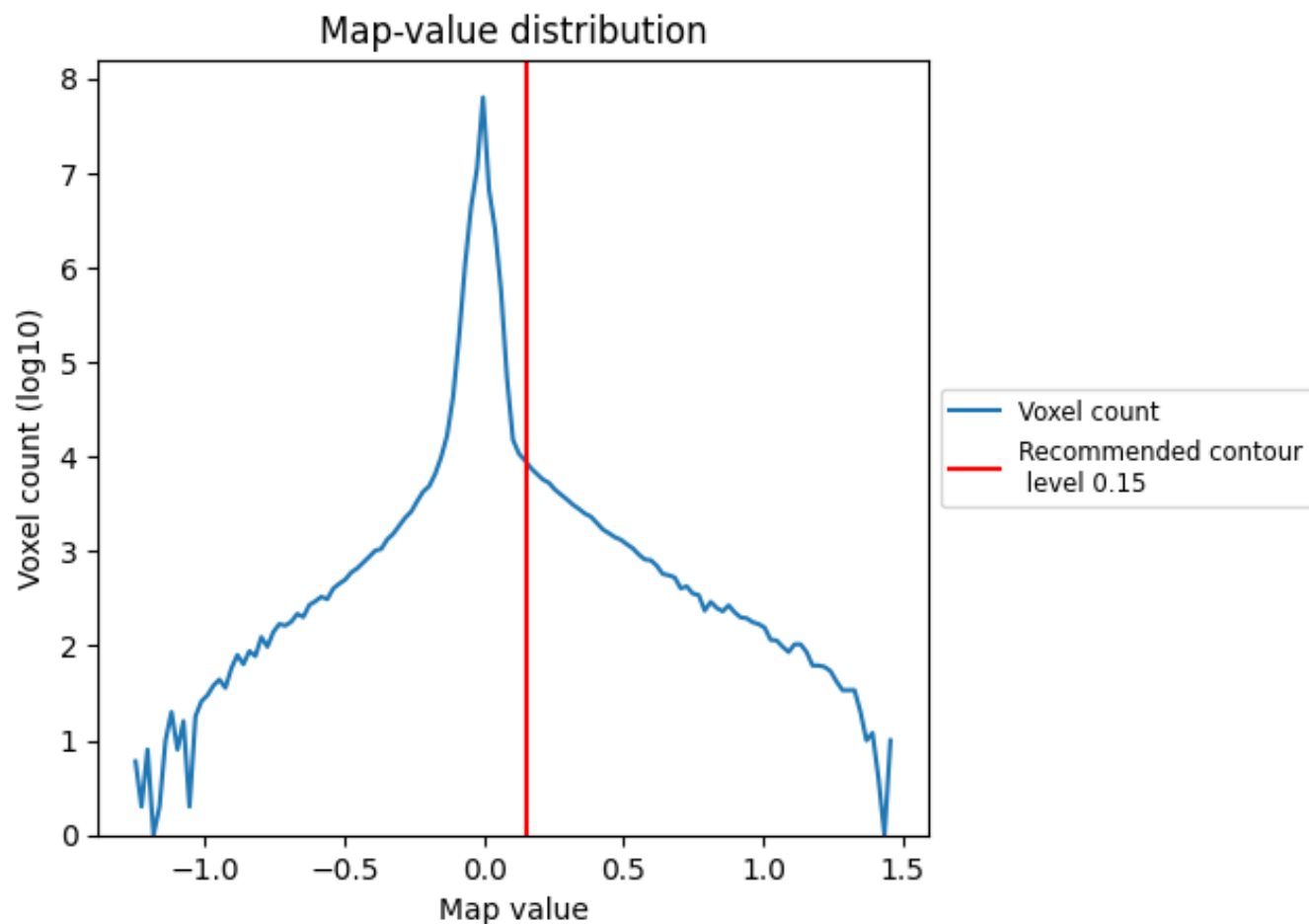


Z

## 7 Map analysis [i](#)

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

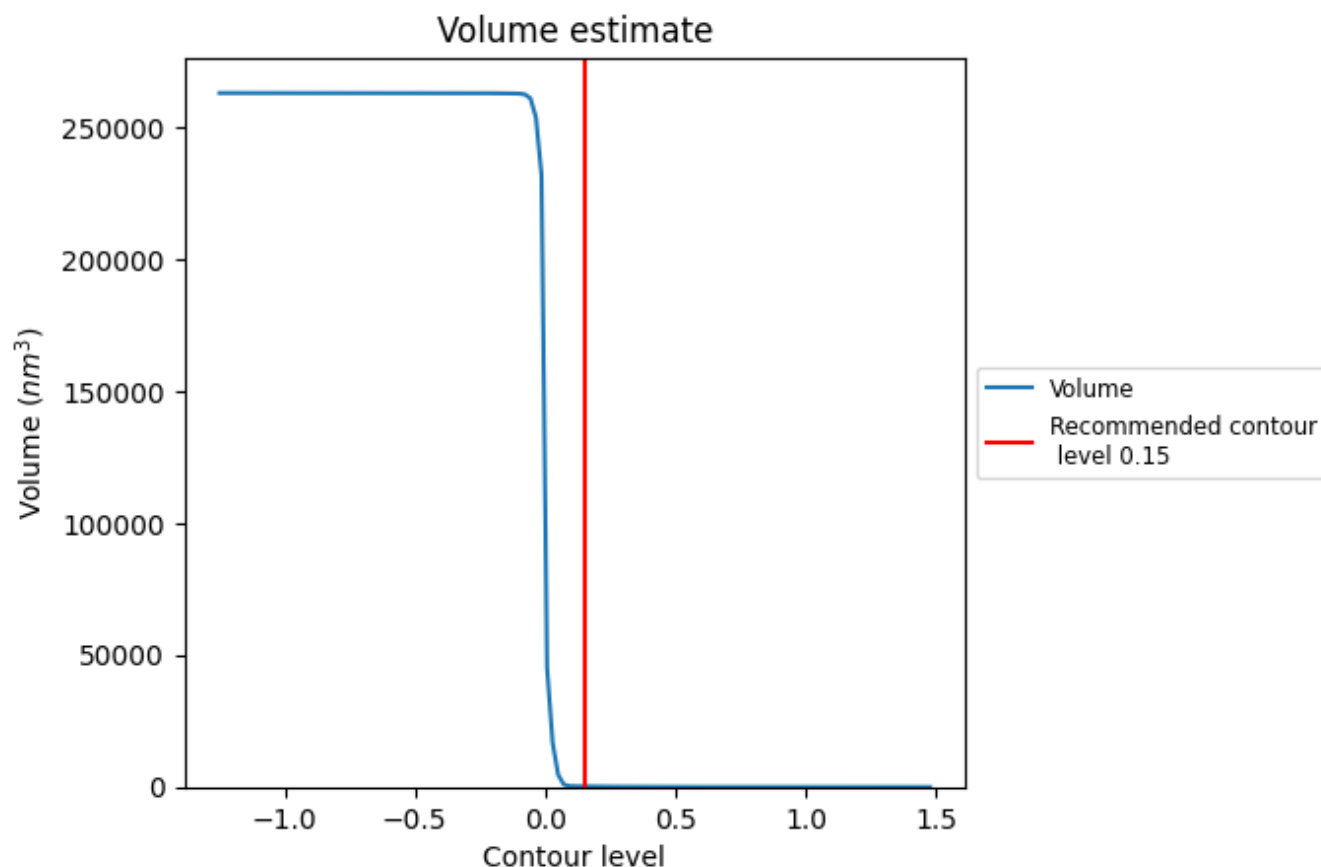
### 7.1 Map-value distribution [i](#)



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.



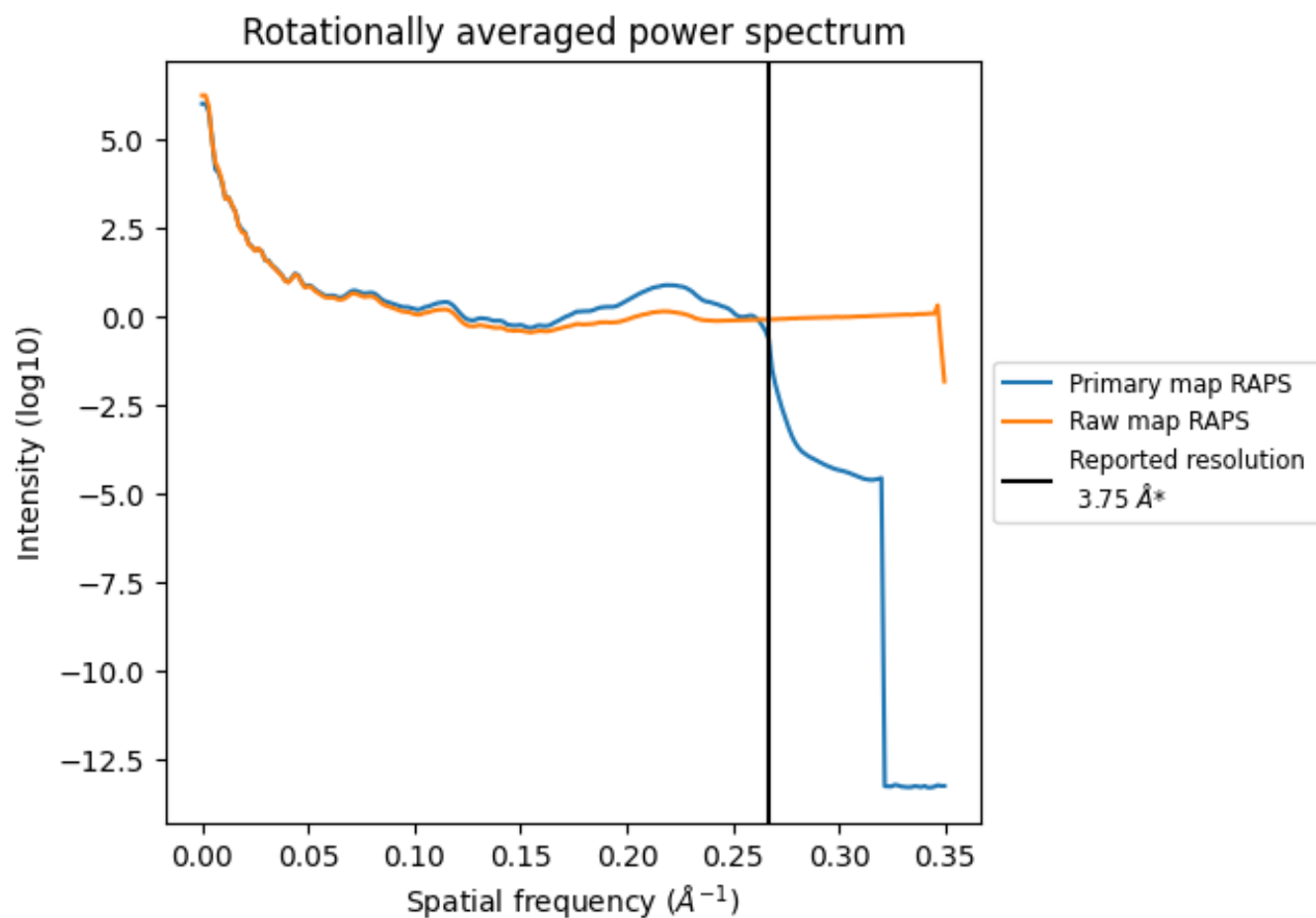
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 221  $\text{nm}^3$ ; this corresponds to an approximate mass of 200 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 ⓘ

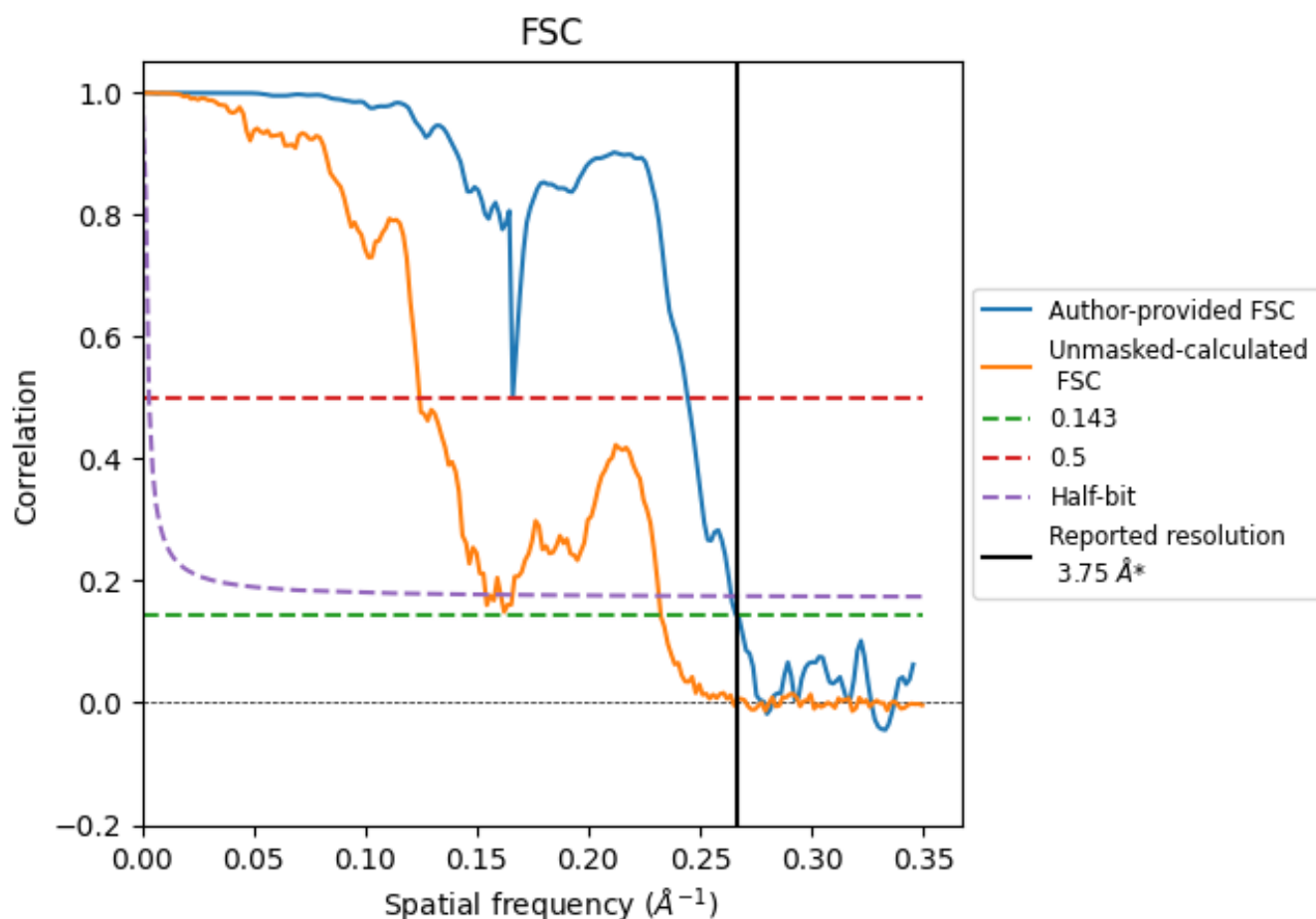


\*Reported resolution corresponds to spatial frequency of 0.267 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

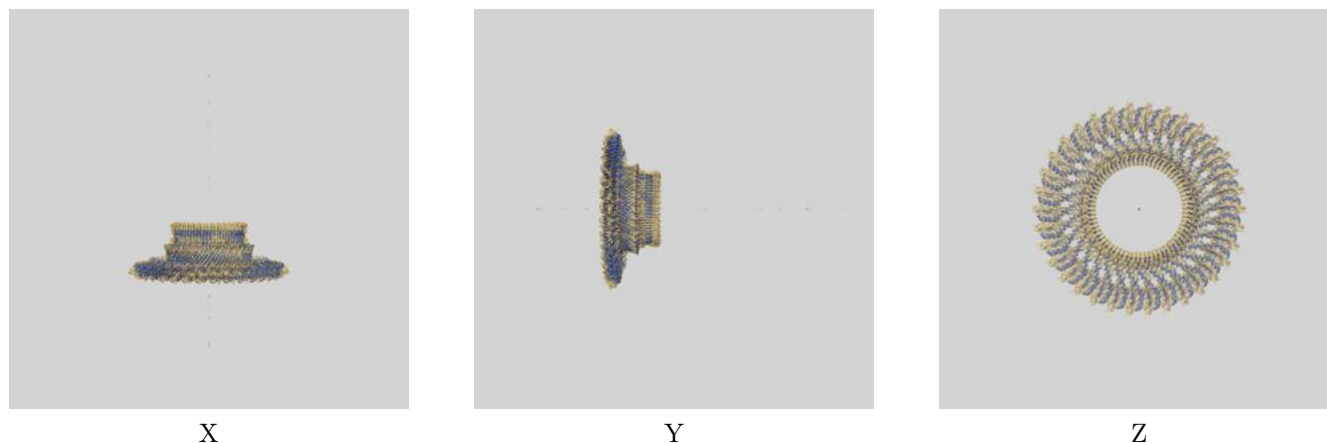
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.75	-	-
Author-provided FSC curve	3.75	4.09	3.79
Unmasked-calculated*	4.30	8.04	6.49

\*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 4.30 differs from the reported value 3.75 by more than 10 %

## 9 Map-model fit [i](#)

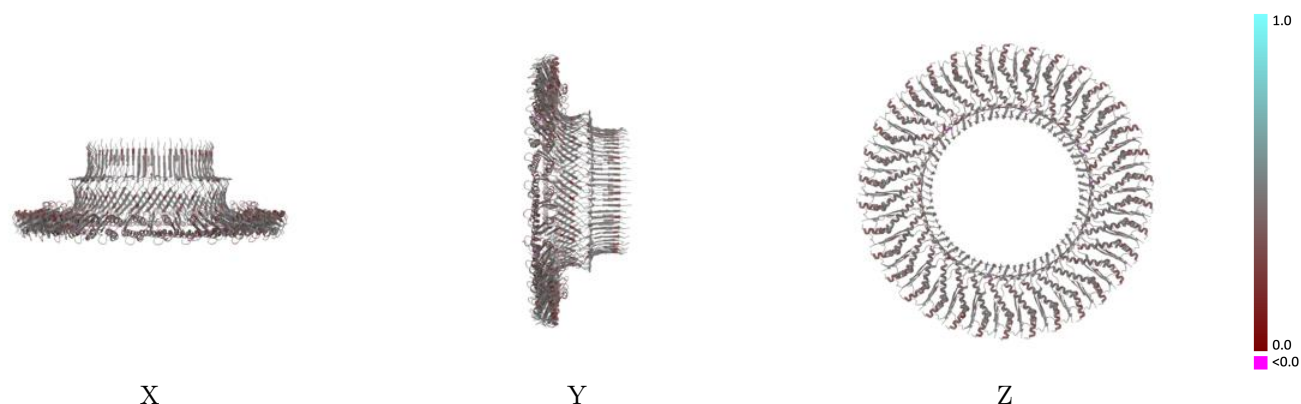
This section contains information regarding the fit between EMDB map EMD-72840 and PDB model 9YDX. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

### 9.1 Map-model overlay [i](#)



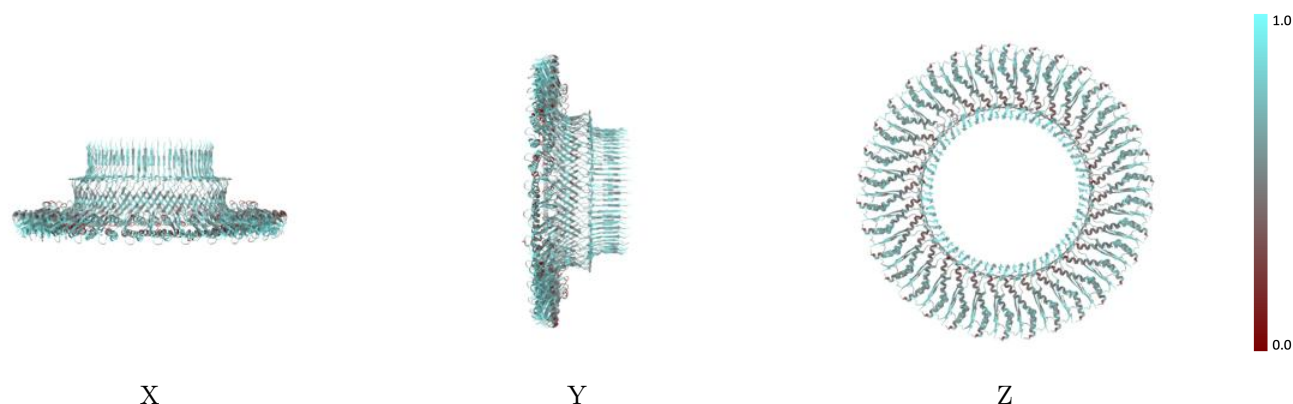
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



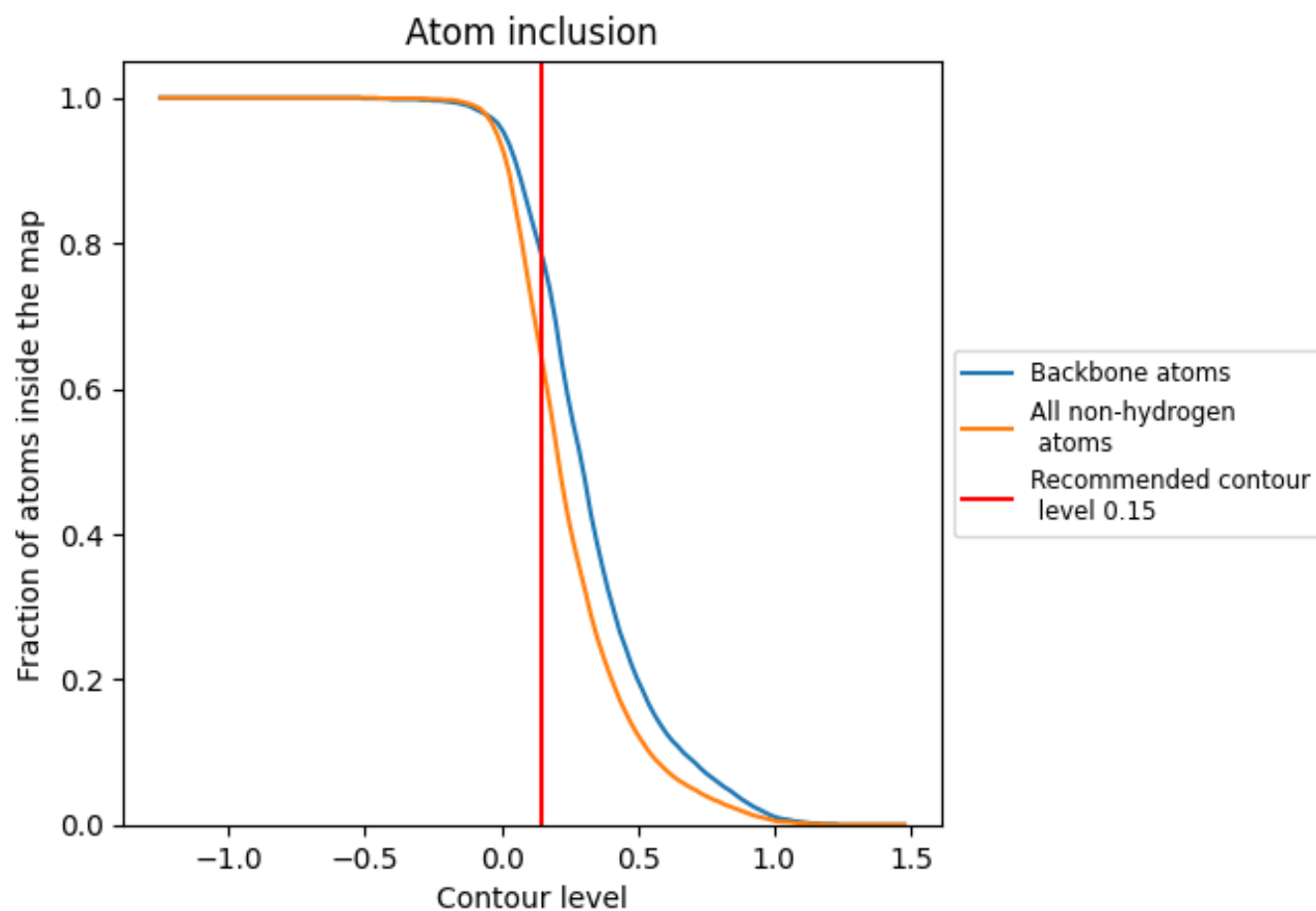
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 64% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6360	 0.4210
Aa	 0.6290	 0.4220
Ab	 0.6310	 0.4210
Ac	 0.6320	 0.4210
Ad	 0.6390	 0.4290
Ae	 0.6370	 0.4220
Af	 0.6360	 0.4270
Ag	 0.6330	 0.4160
Ah	 0.6460	 0.4230
Ai	 0.6310	 0.4210
Aj	 0.6340	 0.4190
Ak	 0.6370	 0.4170
Al	 0.6440	 0.4270
Am	 0.6440	 0.4220
An	 0.6370	 0.4260
Ao	 0.6360	 0.4180
Ap	 0.6400	 0.4120
Aq	 0.6400	 0.4130
Ar	 0.6330	 0.4170
As	 0.6370	 0.4230
At	 0.6380	 0.4210
Au	 0.6280	 0.4200
Av	 0.6400	 0.4180
Aw	 0.6410	 0.4210
Ax	 0.6280	 0.4140
Ay	 0.6370	 0.4240
Az	 0.6400	 0.4130
Ba	 0.6360	 0.4090
Bb	 0.6370	 0.4180
Bc	 0.6400	 0.4290
Bd	 0.6340	 0.4230
Be	 0.6310	 0.4180
Bf	 0.6400	 0.4250
Bg	 0.6390	 0.4270
Bh	 0.6280	 0.4260

