



Full wwPDB EM Validation Report ⓘ

Jul 13, 2026 – 08:27 PM JST

PDB ID : 9V96 / pdb_00009v96
EMDB ID : EMD-64862
Title : Cryo-EM structure of the inner core of ArlA2 filament of *Haloarcula marismortui*
Authors : Meshcheryakov, V.A.; Hyun, J.; Syutkin, A.S.; Pyatibratov, M.G.; Wolf, M.
Deposited on : 2025-05-30
Resolution : 3.14 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

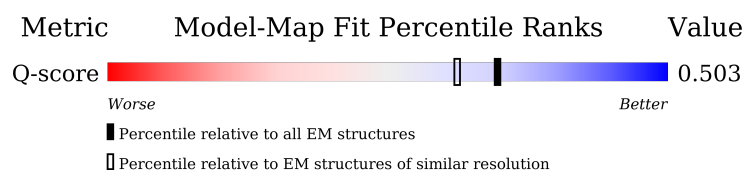
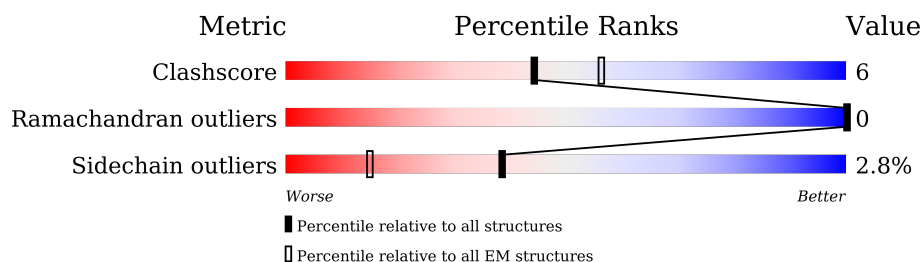
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.14 Å.

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



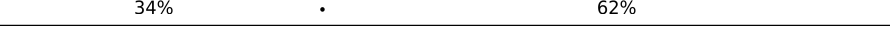
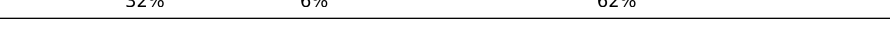
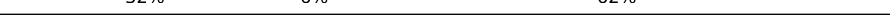
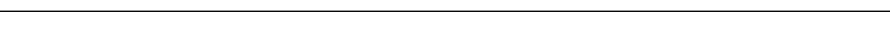
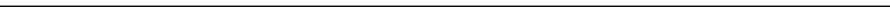
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14483 (2.64 - 3.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	463	
1	B	463	
1	C	463	
1	D	463	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	463	
1	G	463	
1	H	463	
1	I	463	
1	J	463	
1	K	463	
1	L	463	
1	M	463	
1	N	463	
1	O	463	
1	P	463	
1	R	463	
1	S	463	
1	T	463	
1	U	463	
1	V	463	
1	W	463	
1	X	463	
1	Y	463	
1	Z	463	
1	a	463	
1	b	463	
1	d	463	
1	e	463	
1	f	463	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	g	463	
1	i	463	
1	j	463	
1	k	463	
1	l	463	
1	m	463	
1	n	463	
1	o	463	
1	p	463	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 48061 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	176	Total	C	N	O	S	0	0
			1264	775	204	281	4		
1	C	176	Total	C	N	O	S	0	0
			1264	775	204	281	4		
1	D	176	Total	C	N	O	S	0	0
			1264	775	204	281	4		
1	E	176	Total	C	N	O	S	0	0
			1264	775	204	281	4		
1	G	176	Total	C	N	O	S	0	0
			1264	775	204	281	4		
1	H	176	Total	C	N	O	S	0	0
			1264	775	204	281	4		
1	I	176	Total	C	N	O	S	0	0
			1264	775	204	281	4		
1	J	176	Total	C	N	O	S	0	0
			1264	775	204	281	4		
1	K	176	Total	C	N	O	S	0	0
			1264	775	204	281	4		
1	L	176	Total	C	N	O	S	0	0
			1264	775	204	281	4		
1	M	176	Total	C	N	O	S	0	0
			1264	775	204	281	4		
1	N	176	Total	C	N	O	S	0	0
			1264	775	204	281	4		
1	O	176	Total	C	N	O	S	0	0
			1264	775	204	281	4		
1	P	176	Total	C	N	O	S	0	0
			1264	775	204	281	4		
1	R	176	Total	C	N	O	S	0	0
			1264	775	204	281	4		
1	S	176	Total	C	N	O	S	0	0
			1264	775	204	281	4		
1	T	176	Total	C	N	O	S	0	0
			1264	775	204	281	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	U	176	Total 1264	C 775	N 204	O 281	S 4	0	0
1	V	176	Total 1264	C 775	N 204	O 281	S 4	0	0
1	W	176	Total 1264	C 775	N 204	O 281	S 4	0	0
1	X	176	Total 1264	C 775	N 204	O 281	S 4	0	0
1	Y	176	Total 1264	C 775	N 204	O 281	S 4	0	0
1	Z	176	Total 1264	C 775	N 204	O 281	S 4	0	0
1	a	176	Total 1264	C 775	N 204	O 281	S 4	0	0
1	b	176	Total 1264	C 775	N 204	O 281	S 4	0	0
1	d	176	Total 1264	C 775	N 204	O 281	S 4	0	0
1	e	176	Total 1264	C 775	N 204	O 281	S 4	0	0
1	f	176	Total 1264	C 775	N 204	O 281	S 4	0	0
1	g	176	Total 1264	C 775	N 204	O 281	S 4	0	0
1	i	175	Total 1255	C 770	N 202	O 279	S 4	0	0
1	j	176	Total 1264	C 775	N 204	O 281	S 4	0	0
1	k	176	Total 1264	C 775	N 204	O 281	S 4	0	0
1	l	176	Total 1264	C 775	N 204	O 281	S 4	0	0
1	m	176	Total 1264	C 775	N 204	O 281	S 4	0	0
1	n	176	Total 1264	C 775	N 204	O 281	S 4	0	0
1	o	176	Total 1264	C 775	N 204	O 281	S 4	0	0
1	p	176	Total 1264	C 775	N 204	O 281	S 4	0	0
1	B	176	Total 1264	C 775	N 204	O 281	S 4	0	0

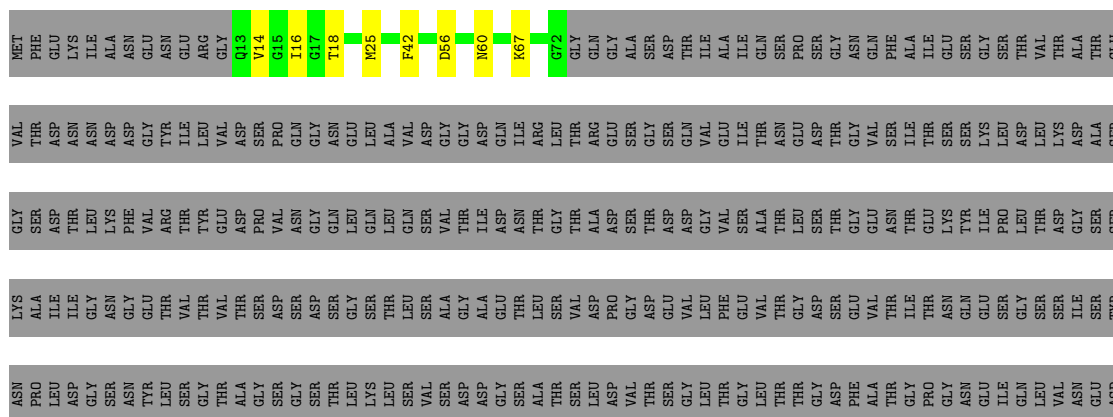
- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total 1	Na 1	0
2	C	1	Total 1	Na 1	0
2	D	1	Total 1	Na 1	0
2	E	1	Total 1	Na 1	0
2	G	1	Total 1	Na 1	0
2	H	1	Total 1	Na 1	0
2	I	1	Total 1	Na 1	0
2	J	1	Total 1	Na 1	0
2	K	1	Total 1	Na 1	0
2	L	1	Total 1	Na 1	0
2	M	1	Total 1	Na 1	0
2	N	1	Total 1	Na 1	0
2	O	1	Total 1	Na 1	0
2	P	1	Total 1	Na 1	0
2	R	1	Total 1	Na 1	0
2	S	1	Total 1	Na 1	0
2	T	1	Total 1	Na 1	0
2	U	1	Total 1	Na 1	0
2	V	1	Total 1	Na 1	0
2	W	1	Total 1	Na 1	0
2	X	1	Total 1	Na 1	0

Continued on next page...

Continued from previous page...

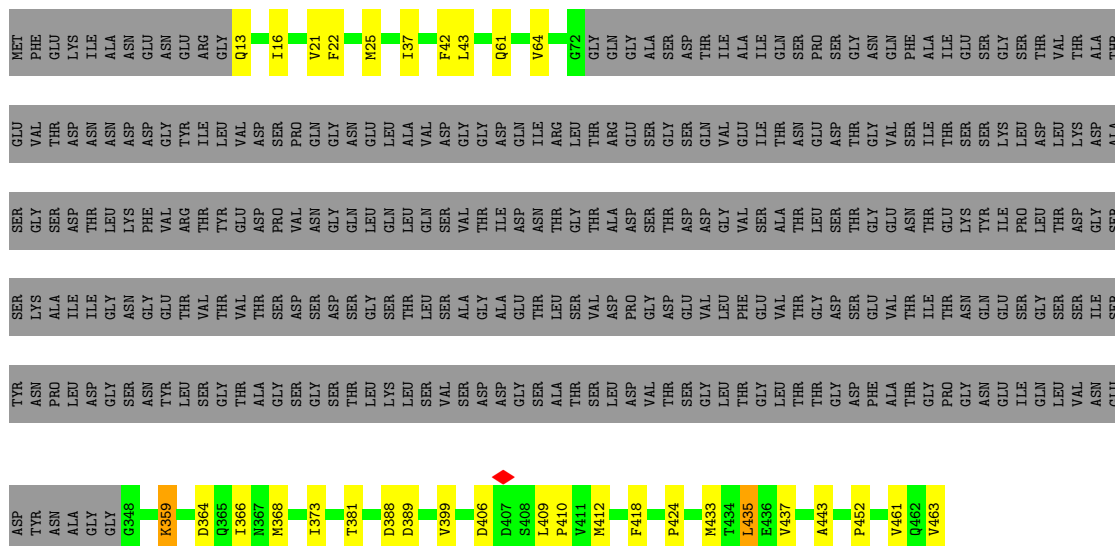
Mol	Chain	Residues	Atoms		AltConf
2	Y	1	Total 1	Na 1	0
2	Z	1	Total 1	Na 1	0
2	a	1	Total 1	Na 1	0
2	b	1	Total 1	Na 1	0
2	d	1	Total 1	Na 1	0
2	e	1	Total 1	Na 1	0
2	f	1	Total 1	Na 1	0
2	g	1	Total 1	Na 1	0
2	i	1	Total 1	Na 1	0
2	j	1	Total 1	Na 1	0
2	k	1	Total 1	Na 1	0
2	l	1	Total 1	Na 1	0
2	m	1	Total 1	Na 1	0
2	n	1	Total 1	Na 1	0
2	o	1	Total 1	Na 1	0
2	p	1	Total 1	Na 1	0
2	B	1	Total 1	Na 1	0





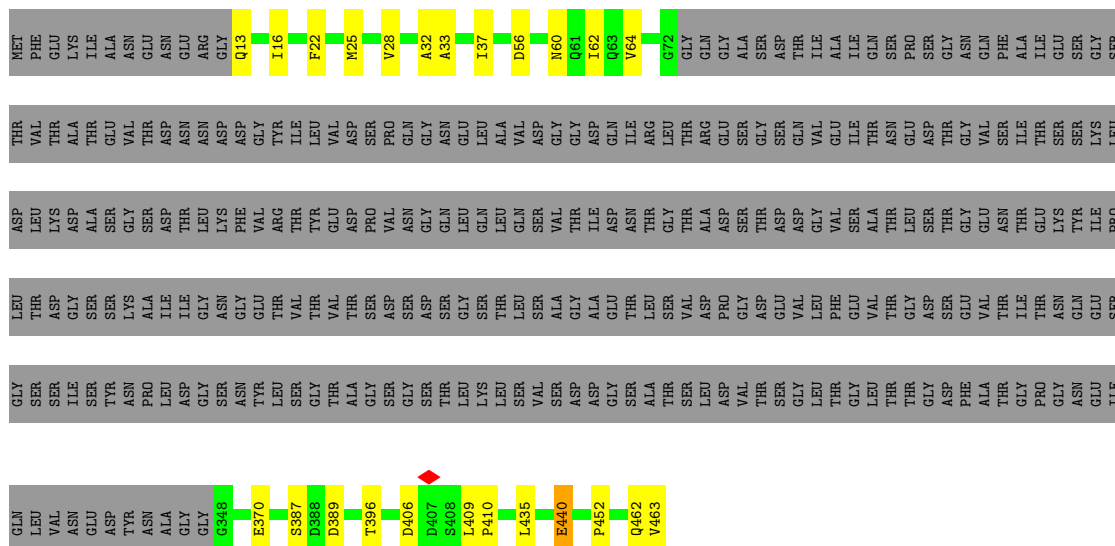
● Molecule 1: Flagellin

Chain D: 31% 6% 62%



● Molecule 1: Flagellin

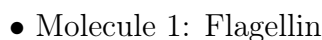
Chain E: 33% 5% 62%



● Molecule 1: Flagellin

Chain G: 33% 5% 62%





Response	Percentage
Yes	32%
No	6%
Don't know	62%

- Molecule 1: Flagellin

Response	Percentage
Yes	32%
No	6%
Don't know	62%

- Molecule 1: Flagellin

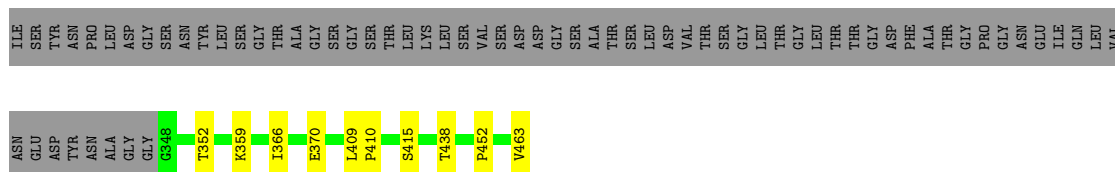
Response	Percentage
Best for the country	32%
Not the best for the country	5%
Don't know	62%



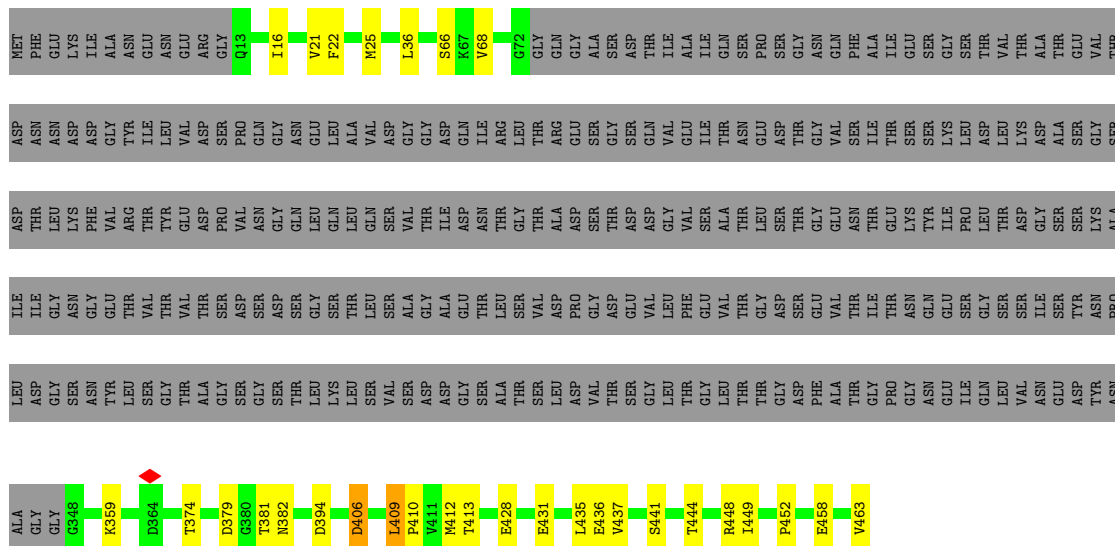
WORLDWIDE
PDB
PROTEIN DATA BANK



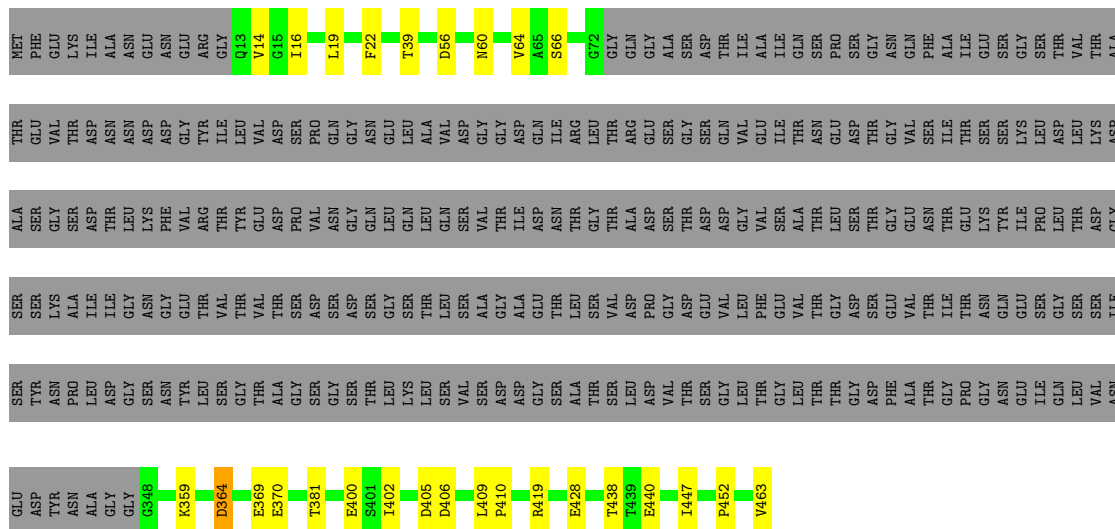




- Molecule 1: Flagellin



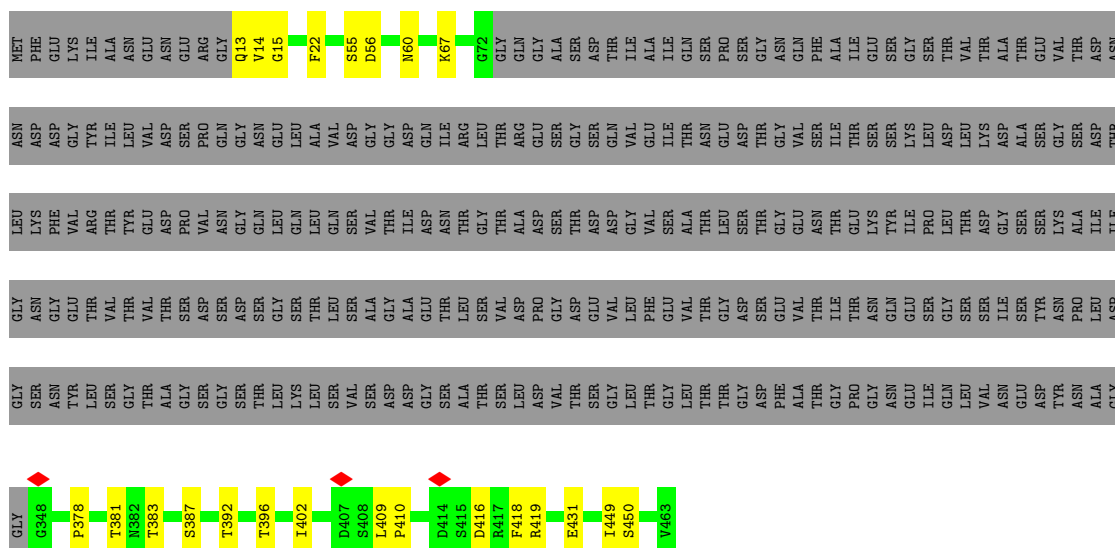
- Molecule 1: Flagellin



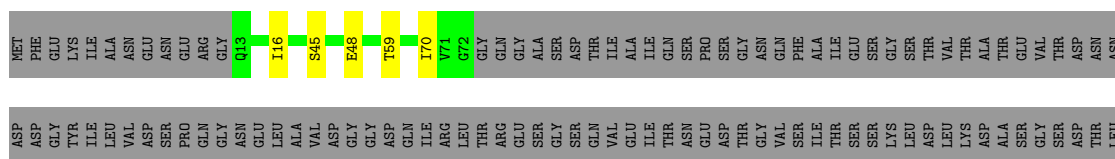
- Molecule 1: Flagellin

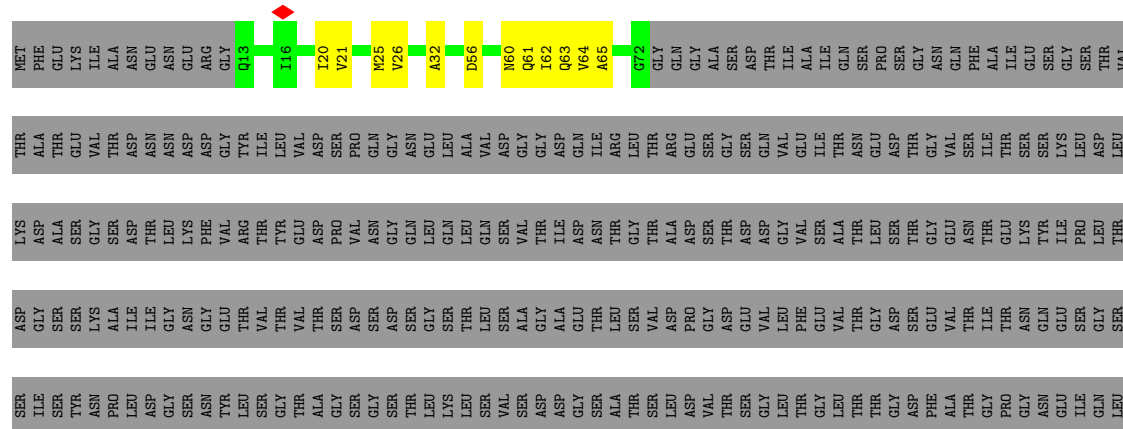


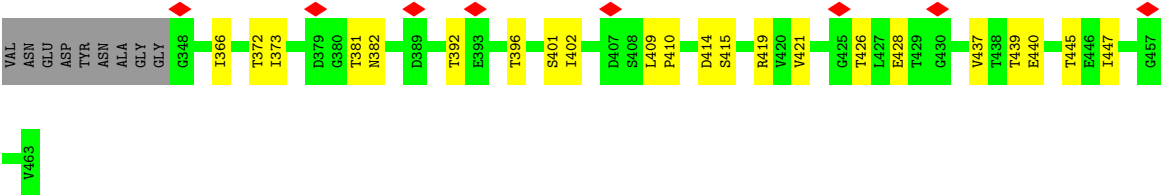
- Molecule 1: Flagellin



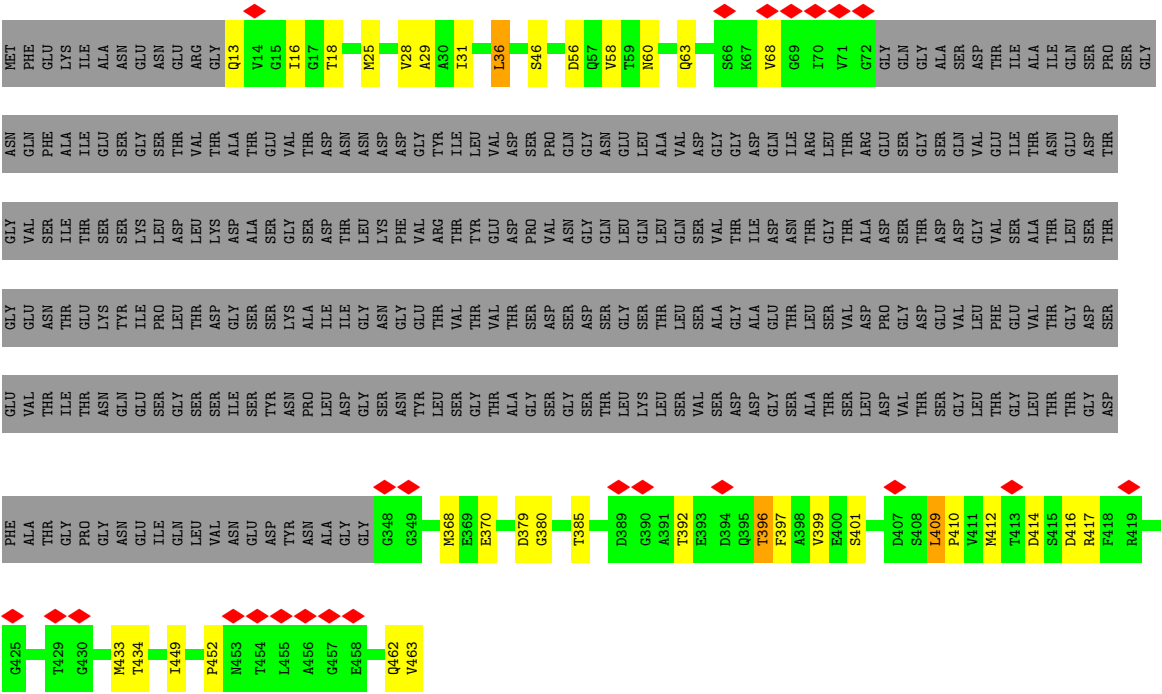
- Molecule 1: Flagellin



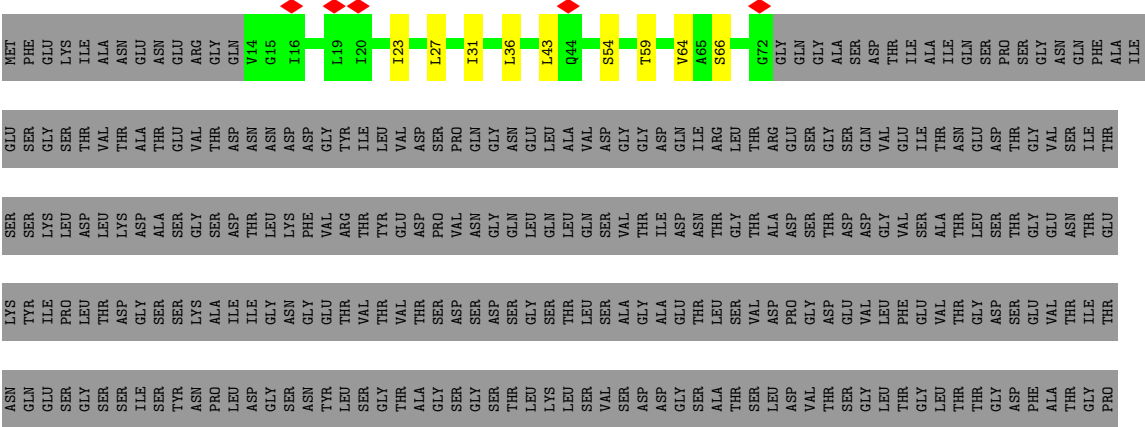


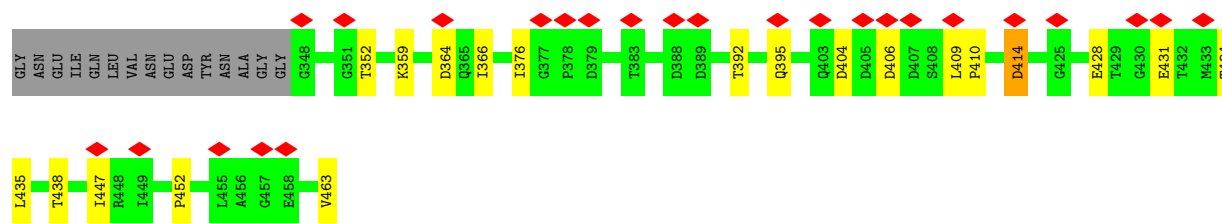


• Molecule 1: Flagellin

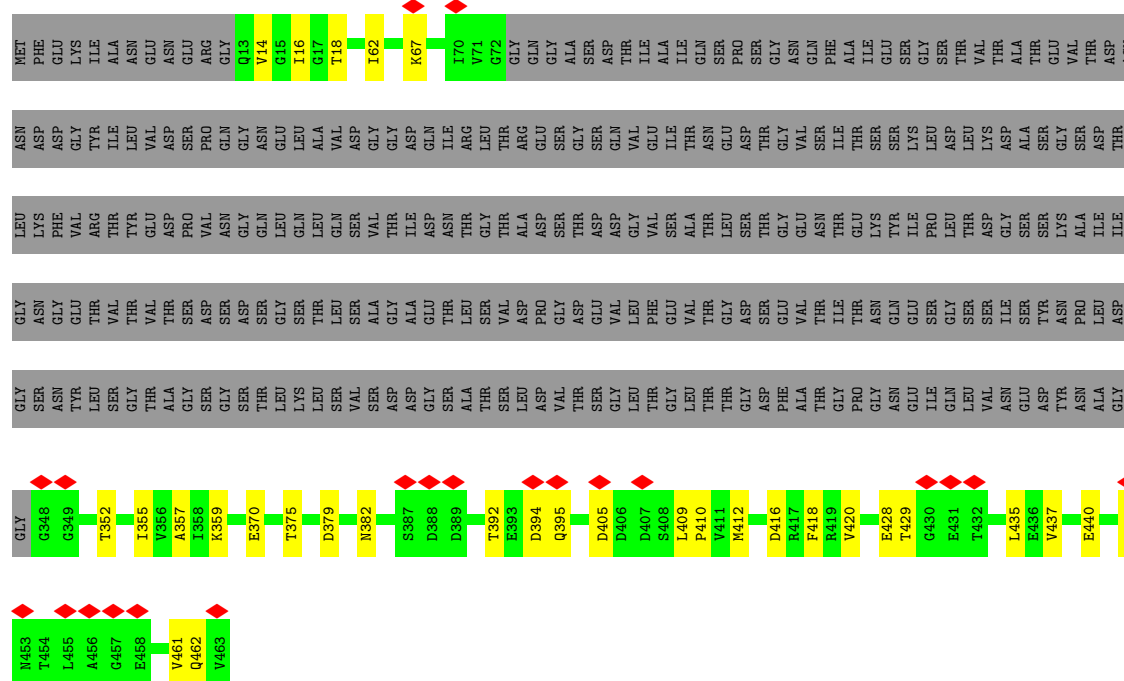


• Molecule 1: Flagellin

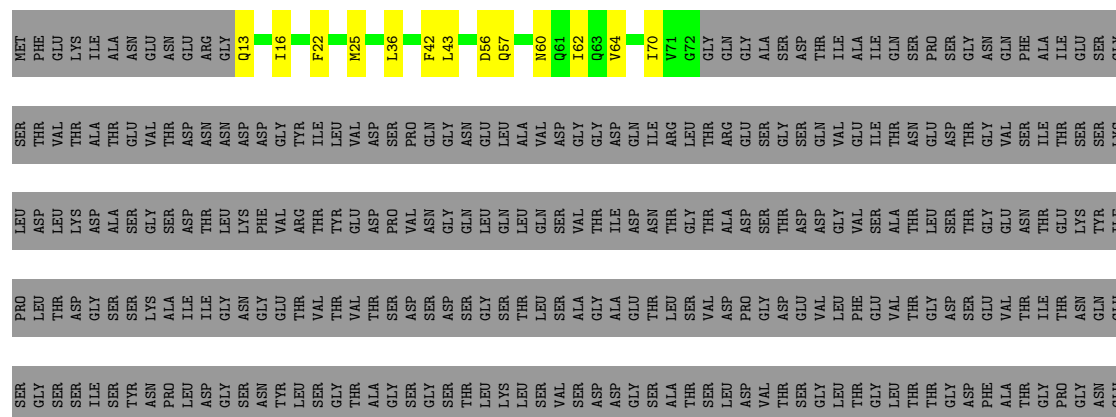


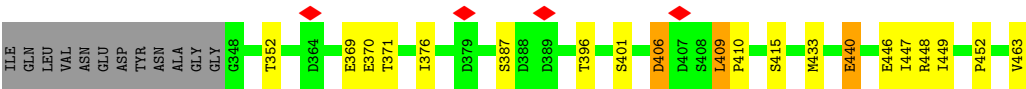


• Molecule 1: Flagellin

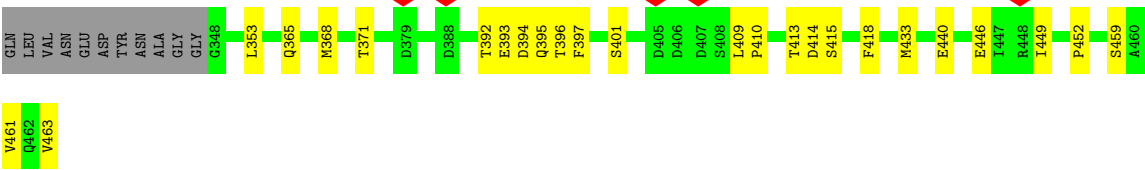
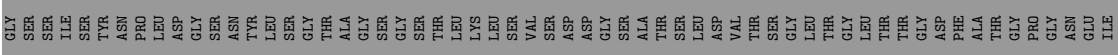
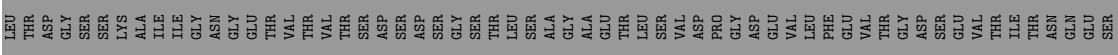
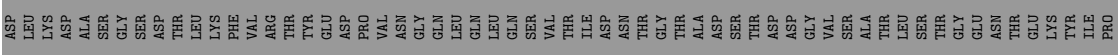
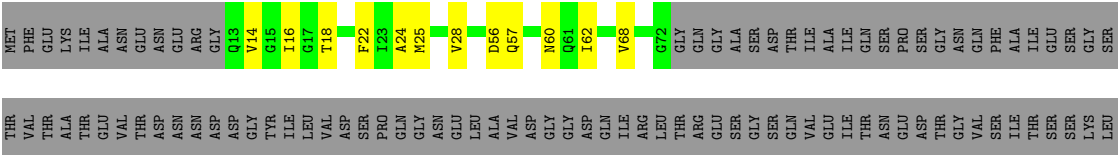


• Molecule 1: Flagellin

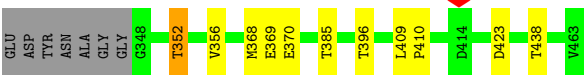
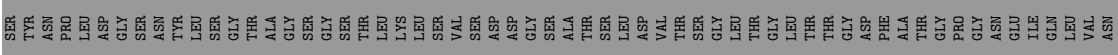
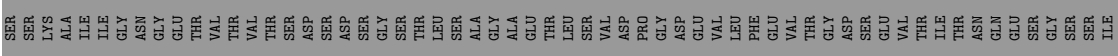
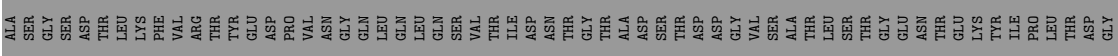
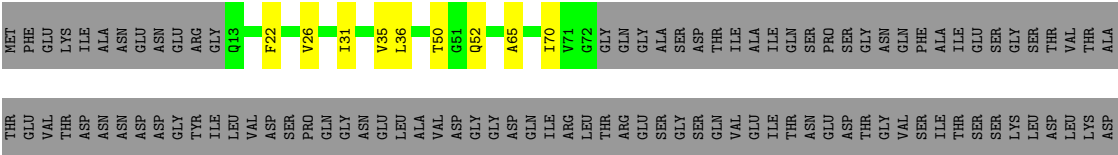




• Molecule 1: Flagellin

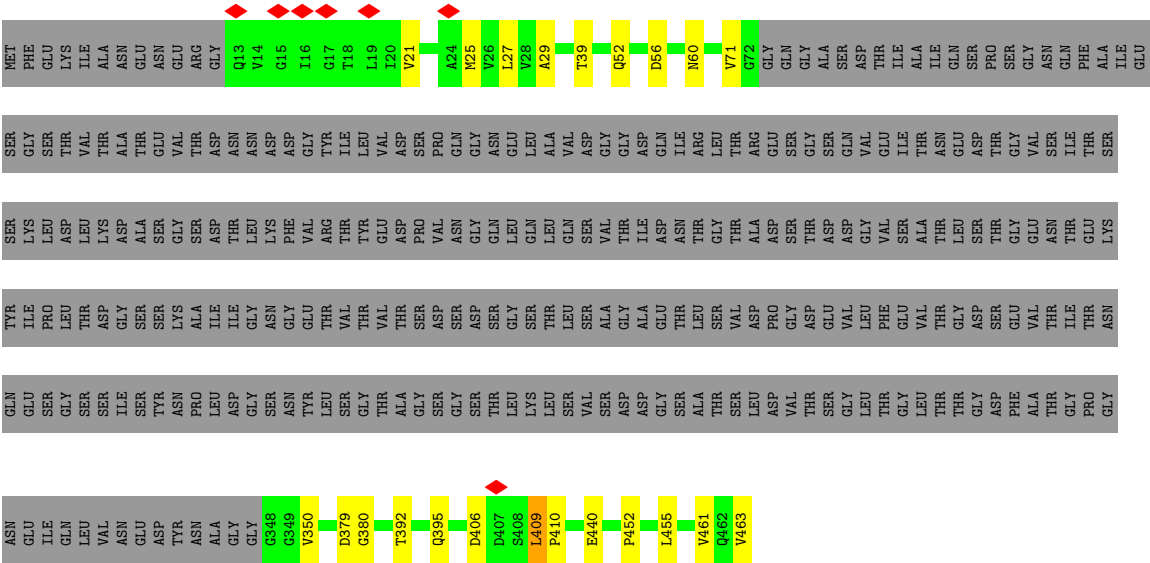


• Molecule 1: Flagellin

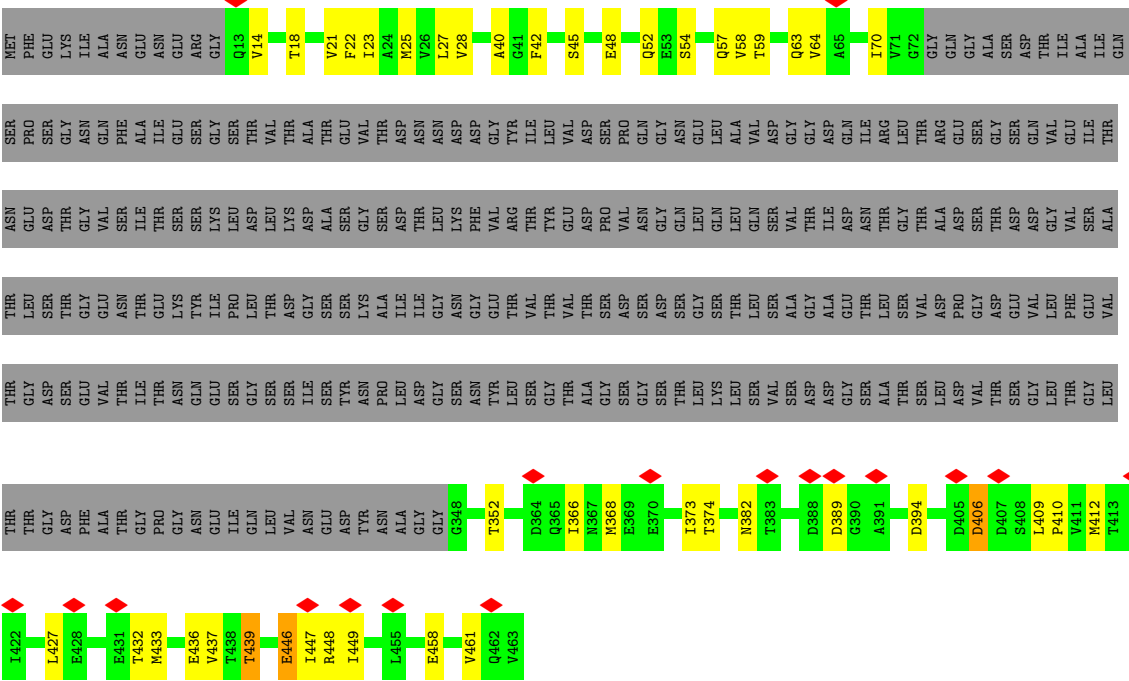


• Molecule 1: Flagellin





● Molecule 1: Flagellin



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	309194	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.801	Depositor
Minimum map value	-1.719	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.088	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	433.19998, 433.19998, 433.19998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.083, 1.083, 1.083	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.12	0/1271	0.33	0/1733
1	B	0.13	0/1271	0.36	0/1733
1	C	0.13	0/1271	0.36	0/1733
1	D	0.11	0/1271	0.30	0/1733
1	E	0.11	0/1271	0.30	0/1733
1	G	0.12	0/1271	0.30	0/1733
1	H	0.12	0/1271	0.29	0/1733
1	I	0.11	0/1271	0.31	0/1733
1	J	0.12	0/1271	0.29	0/1733
1	K	0.11	0/1271	0.29	0/1733
1	L	0.11	0/1271	0.29	0/1733
1	M	0.11	0/1271	0.31	0/1733
1	N	0.12	0/1271	0.33	0/1733
1	O	0.11	0/1271	0.30	0/1733
1	P	0.11	0/1271	0.29	0/1733
1	R	0.10	0/1271	0.29	0/1733
1	S	0.12	0/1271	0.32	0/1733
1	T	0.11	0/1271	0.34	0/1733
1	U	0.12	0/1271	0.32	0/1733
1	V	0.12	0/1271	0.30	0/1733
1	W	0.12	0/1271	0.31	0/1733
1	X	0.13	0/1271	0.35	0/1733
1	Y	0.11	0/1271	0.32	0/1733
1	Z	0.13	0/1271	0.34	0/1733
1	a	0.10	0/1271	0.28	0/1733
1	b	0.13	0/1271	0.34	0/1733
1	d	0.13	0/1271	0.35	0/1733
1	e	0.12	0/1271	0.33	0/1733
1	f	0.12	0/1271	0.36	0/1733
1	g	0.12	0/1271	0.36	0/1733
1	i	0.15	0/1262	0.42	0/1721
1	j	0.13	0/1271	0.36	0/1733

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	k	0.11	0/1271	0.33	0/1733
1	l	0.12	0/1271	0.33	0/1733
1	m	0.12	0/1271	0.30	0/1733
1	n	0.12	0/1271	0.33	0/1733
1	o	0.12	0/1271	0.35	0/1733
1	p	0.11	0/1271	0.31	0/1733
All	All	0.12	0/48289	0.32	0/65842

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1264	0	1241	15	0
1	B	1264	0	1240	30	0
1	C	1264	0	1241	19	0
1	D	1264	0	1242	18	0
1	E	1264	0	1241	14	0
1	G	1264	0	1241	14	0
1	H	1264	0	1241	17	0
1	I	1264	0	1241	19	0
1	J	1264	0	1241	12	0
1	K	1264	0	1241	19	0
1	L	1264	0	1241	16	0
1	M	1264	0	1241	16	0
1	N	1264	0	1240	16	0
1	O	1264	0	1241	9	0
1	P	1264	0	1240	21	0
1	R	1264	0	1241	21	0
1	S	1264	0	1241	17	0
1	T	1264	0	1241	20	0
1	U	1264	0	1240	23	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	V	1264	0	1241	16	0
1	W	1264	0	1241	21	0
1	X	1264	0	1240	19	0
1	Y	1264	0	1240	22	0
1	Z	1264	0	1241	13	0
1	a	1264	0	1241	13	0
1	b	1264	0	1240	17	0
1	d	1264	0	1241	22	0
1	e	1264	0	1241	23	0
1	f	1264	0	1240	20	0
1	g	1264	0	1240	22	0
1	i	1255	0	1232	21	0
1	j	1264	0	1241	31	0
1	k	1264	0	1241	26	0
1	l	1264	0	1241	19	0
1	m	1264	0	1241	21	0
1	n	1264	0	1242	25	0
1	o	1264	0	1241	15	0
1	p	1264	0	1241	12	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
2	R	1	0	0	0	0
2	S	1	0	0	0	0
2	T	1	0	0	0	0
2	U	1	0	0	0	0
2	V	1	0	0	0	0
2	W	1	0	0	0	0
2	X	1	0	0	0	0
2	Y	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Z	1	0	0	0	0
2	a	1	0	0	0	0
2	b	1	0	0	0	0
2	d	1	0	0	0	0
2	e	1	0	0	0	0
2	f	1	0	0	0	0
2	g	1	0	0	0	0
2	i	1	0	0	0	0
2	j	1	0	0	0	0
2	k	1	0	0	0	0
2	l	1	0	0	0	0
2	m	1	0	0	0	0
2	n	1	0	0	0	0
2	o	1	0	0	0	0
2	p	1	0	0	0	0
All	All	48061	0	47142	613	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 (613) 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:Y:14:VAL:HB	1:k:21:VAL:HG11	1.65	0.79
1:B:373:ILE:HG12	1:B:437:VAL:HG22	1.64	0.79
1:j:63:GLN:OE1	1:m:57:GLN:NE2	2.18	0.77
1:B:382:ASN:ND2	1:B:394:ASP:OD2	2.18	0.76
1:P:68:VAL:HG21	1:U:381:THR:HG21	1.71	0.72
1:H:382:ASN:ND2	1:H:394:ASP:OD2	2.23	0.71
1:m:446:GLU:HB3	1:m:448:ARG:HH12	1.56	0.69
1:T:14:VAL:HG11	1:j:13:GLN:HE21	1.56	0.68
1:f:63:GLN:HE22	1:f:65:ALA:HB2	1.59	0.68
1:g:412:MET:HG3	1:g:416:ASP:HB2	1.75	0.68
1:f:26:VAL:HG12	1:j:20:ILE:HG21	1.76	0.67
1:e:36:LEU:HD13	1:B:28:VAL:HG11	1.76	0.67
1:f:20:ILE:HD12	1:f:20:ILE:H	1.60	0.66
1:U:382:ASN:ND2	1:U:394:ASP:OD1	2.30	0.65
1:l:416:ASP:HB3	1:l:418:PHE:HE1	1.62	0.65
1:Y:458:GLU:OE2	1:Y:458:GLU:N	2.30	0.64
1:U:370:GLU:OE2	1:U:370:GLU:N	2.30	0.64
1:e:373:ILE:HG12	1:e:437:VAL:HG12	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:417:ARG:NH2	1:k:438:THR:OG1	2.31	0.63
1:W:359:LYS:NZ	1:W:413:THR:O	2.27	0.63
1:Z:15:GLY:HA2	1:i:36:LEU:HD11	1.81	0.63
1:d:417:ARG:NH2	1:i:438:THR:OG1	2.32	0.63
1:T:359:LYS:NZ	1:T:413:THR:O	2.30	0.63
1:W:382:ASN:ND2	1:W:394:ASP:OD1	2.32	0.62
1:e:63:GLN:OE1	1:e:63:GLN:N	2.32	0.62
1:S:370:GLU:HB2	1:S:440:GLU:HG3	1.81	0.62
1:d:64:VAL:HG21	1:d:447:ILE:HD11	1.82	0.62
1:B:427:LEU:HD21	1:B:433:MET:HE3	1.82	0.62
1:K:13:GLN:HG2	1:S:25:MET:HE1	1.82	0.61
1:L:458:GLU:N	1:L:458:GLU:OE1	2.32	0.61
1:k:435:LEU:HB2	1:k:447:ILE:HB	1.81	0.61
1:Z:22:PHE:HZ	1:i:43:LEU:HG	1.65	0.61
1:B:14:VAL:O	1:B:18:THR:OG1	2.17	0.60
1:G:67:LYS:NZ	1:G:448:ARG:O	2.34	0.60
1:X:14:VAL:HB	1:j:21:VAL:HG11	1.82	0.60
1:f:62:ILE:HG22	1:f:366:ILE:HD13	1.84	0.60
1:k:14:VAL:O	1:k:18:THR:OG1	2.17	0.60
1:m:433:MET:HG2	1:m:449:ILE:HD12	1.82	0.60
1:K:382:ASN:ND2	1:K:394:ASP:OD2	2.34	0.60
1:l:382:ASN:ND2	1:l:394:ASP:OD2	2.34	0.60
1:P:387:SER:HB2	1:P:396:THR:HB	1.84	0.60
1:W:359:LYS:HG3	1:W:412:MET:HE3	1.84	0.60
1:Y:370:GLU:HB2	1:Y:440:GLU:HG3	1.84	0.60
1:E:16:ILE:HG13	1:m:22:PHE:HE1	1.66	0.59
1:b:373:ILE:HG12	1:b:437:VAL:HG12	1.83	0.59
1:d:452:PRO:HD3	1:d:463:VAL:HG12	1.85	0.59
1:m:64:VAL:HG21	1:m:447:ILE:HD11	1.83	0.59
1:Y:393:GLU:OE1	1:Y:394:ASP:HB2	2.02	0.59
1:L:392:THR:HB	1:L:395:GLN:HB2	1.85	0.59
1:U:458:GLU:N	1:U:458:GLU:OE2	2.35	0.59
1:X:66:SER:OG	1:b:436:GLU:OE1	2.19	0.59
1:l:375:THR:OG1	1:l:382:ASN:OD1	2.21	0.59
1:o:70:ILE:HB	1:o:352:THR:HG23	1.85	0.59
1:g:433:MET:HB2	1:g:449:ILE:HG12	1.85	0.59
1:j:17:GLY:HA2	1:j:20:ILE:HD12	1.85	0.58
1:f:401:SER:HB2	1:f:409:LEU:HD23	1.85	0.58
1:k:452:PRO:HD3	1:k:463:VAL:HG12	1.85	0.58
1:M:393:GLU:OE2	1:M:394:ASP:HB2	2.03	0.58
1:U:359:LYS:NZ	1:U:413:THR:O	2.32	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:370:GLU:HB2	1:N:440:GLU:HG3	1.85	0.58
1:R:406:ASP:OD1	1:R:406:ASP:N	2.33	0.58
1:U:452:PRO:HD3	1:U:463:VAL:HG12	1.86	0.58
1:X:370:GLU:HB2	1:X:440:GLU:HG3	1.83	0.58
1:W:374:THR:HB	1:W:436:GLU:HB2	1.86	0.57
1:k:359:LYS:HG2	1:k:366:ILE:HD12	1.86	0.57
1:d:375:THR:OG1	1:d:382:ASN:OD1	2.20	0.57
1:Y:387:SER:HB2	1:Y:396:THR:HB	1.85	0.57
1:G:22:PHE:HE1	1:J:16:ILE:HG13	1.69	0.57
1:n:413:THR:OG1	1:n:414:ASP:OD1	2.22	0.57
1:l:355:ILE:HG22	1:l:420:VAL:HB	1.86	0.57
1:m:387:SER:HB2	1:m:396:THR:HB	1.87	0.56
1:D:373:ILE:HG12	1:D:437:VAL:HG12	1.87	0.56
1:J:364:ASP:OD1	1:J:364:ASP:N	2.35	0.56
1:W:428:GLU:HB2	1:W:431:GLU:HG3	1.87	0.56
1:J:359:LYS:HG2	1:J:366:ILE:HD12	1.86	0.56
1:j:14:VAL:O	1:j:18:THR:OG1	2.21	0.56
1:J:392:THR:HB	1:J:395:GLN:HB2	1.87	0.56
1:e:20:ILE:H	1:e:20:ILE:HD12	1.69	0.56
1:g:452:PRO:HD3	1:g:463:VAL:HG12	1.87	0.56
1:A:67:LYS:NZ	1:A:448:ARG:O	2.38	0.55
1:T:452:PRO:HD3	1:T:463:VAL:HG12	1.89	0.55
1:e:428:GLU:HB2	1:e:431:GLU:HG2	1.88	0.55
1:g:462:GLN:HG3	1:g:462:GLN:O	2.05	0.55
1:d:432:THR:OG1	1:d:449:ILE:O	2.21	0.55
1:K:68:VAL:HG11	1:O:381:THR:HG21	1.89	0.55
1:f:428:GLU:OE1	1:f:428:GLU:N	2.40	0.55
1:n:446:GLU:N	1:n:446:GLU:OE1	2.40	0.55
1:f:381:THR:O	1:f:382:ASN:ND2	2.40	0.54
1:o:423:ASP:OD2	1:o:423:ASP:N	2.40	0.54
1:d:403:GLN:NE2	1:i:372:THR:HG21	2.23	0.54
1:f:61:GLN:OE1	1:f:445:THR:OG1	2.25	0.54
1:g:63:GLN:OE1	1:g:63:GLN:N	2.40	0.54
1:T:22:PHE:HE1	1:X:16:ILE:HG13	1.71	0.54
1:i:353:LEU:HD13	1:i:449:ILE:HD13	1.90	0.54
1:O:379:ASP:OD1	1:O:380:GLY:N	2.41	0.54
1:W:66:SER:O	1:W:66:SER:OG	2.25	0.54
1:j:414:ASP:OD1	1:j:414:ASP:N	2.40	0.54
1:N:452:PRO:HD3	1:N:463:VAL:HG12	1.89	0.54
1:G:379:ASP:OD1	1:G:380:GLY:N	2.41	0.54
1:I:417:ARG:HH22	1:M:440:GLU:HA	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:22:PHE:HZ	1:V:39:THR:HG21	1.73	0.54
1:T:359:LYS:HG2	1:T:366:ILE:HD12	1.89	0.54
1:e:387:SER:HB2	1:e:396:THR:HB	1.90	0.54
1:C:67:LYS:NZ	1:C:448:ARG:O	2.41	0.53
1:Y:370:GLU:N	1:Y:370:GLU:OE2	2.41	0.53
1:d:392:THR:OG1	1:d:396:THR:OG1	2.25	0.53
1:A:458:GLU:OE1	1:A:458:GLU:N	2.42	0.53
1:J:14:VAL:O	1:J:18:THR:OG1	2.27	0.53
1:Z:409:LEU:HB3	1:Z:410:PRO:HD3	1.91	0.53
1:d:403:GLN:HE22	1:i:372:THR:HG21	1.71	0.53
1:g:396:THR:OG1	1:g:397:PHE:N	2.41	0.53
1:m:452:PRO:HD3	1:m:463:VAL:HG12	1.90	0.53
1:U:370:GLU:HB2	1:U:440:GLU:HG3	1.90	0.53
1:e:446:GLU:HG2	1:e:448:ARG:HH12	1.73	0.53
1:X:402:ILE:HD11	1:X:419:ARG:NH2	2.24	0.53
1:Z:387:SER:HB2	1:Z:396:THR:HB	1.89	0.53
1:L:61:GLN:HG2	1:L:443:ALA:HB1	1.90	0.53
1:Y:451:VAL:HA	1:Y:463:VAL:HG12	1.90	0.53
1:a:70:ILE:HB	1:a:352:THR:HG22	1.90	0.53
1:f:414:ASP:N	1:f:414:ASP:OD1	2.41	0.53
1:g:414:ASP:OD2	1:g:414:ASP:N	2.40	0.53
1:S:22:PHE:HE1	1:W:16:ILE:HG13	1.73	0.53
1:T:382:ASN:ND2	1:T:394:ASP:OD1	2.42	0.53
1:i:433:MET:HB3	1:i:449:ILE:HB	1.91	0.53
1:n:452:PRO:HD3	1:n:463:VAL:HG12	1.91	0.53
1:X:452:PRO:HD3	1:X:463:VAL:HG12	1.91	0.53
1:S:458:GLU:OE2	1:S:458:GLU:N	2.41	0.53
1:U:22:PHE:HE1	1:Y:16:ILE:HG13	1.74	0.53
1:D:16:ILE:HG13	1:n:22:PHE:HE1	1.73	0.52
1:j:366:ILE:HB	1:j:412:MET:HB2	1.91	0.52
1:p:52:GLN:HA	1:p:52:GLN:OE1	2.10	0.52
1:U:14:VAL:HG11	1:k:13:GLN:HE21	1.74	0.52
1:M:70:ILE:HB	1:M:352:THR:HG22	1.91	0.52
1:G:414:ASP:OD1	1:G:414:ASP:N	2.43	0.52
1:V:415:SER:OG	1:V:415:SER:O	2.23	0.52
1:O:392:THR:HB	1:O:395:GLN:HB2	1.91	0.52
1:b:433:MET:HE2	1:b:435:LEU:HD11	1.92	0.52
1:g:68:VAL:HG21	1:k:376:ILE:HG21	1.91	0.52
1:p:392:THR:HB	1:p:395:GLN:HB2	1.90	0.52
1:A:414:ASP:N	1:A:414:ASP:OD1	2.43	0.52
1:D:22:PHE:HE1	1:H:16:ILE:HG13	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:452:PRO:HD3	1:E:463:VAL:HG12	1.90	0.52
1:R:414:ASP:N	1:R:414:ASP:OD1	2.41	0.52
1:O:70:ILE:HB	1:O:352:THR:HG22	1.92	0.51
1:R:387:SER:HB3	1:R:396:THR:HB	1.92	0.51
1:M:403:GLN:HB3	1:M:417:ARG:HG3	1.93	0.51
1:f:402:ILE:HD11	1:f:419:ARG:HB2	1.90	0.51
1:I:13:GLN:HG2	1:P:25:MET:HE1	1.91	0.51
1:n:415:SER:O	1:n:415:SER:OG	2.22	0.51
1:C:42:PHE:CE2	1:o:52:GLN:HA	2.45	0.51
1:E:25:MET:HG3	1:I:13:GLN:HB3	1.92	0.51
1:d:387:SER:HB2	1:d:396:THR:HB	1.93	0.51
1:C:414:ASP:OD1	1:C:414:ASP:N	2.41	0.51
1:Y:67:LYS:HG2	1:Y:355:ILE:HD12	1.93	0.51
1:i:23:ILE:H	1:i:23:ILE:HD12	1.75	0.51
1:L:22:PHE:HZ	1:T:39:THR:HG21	1.75	0.51
1:N:14:VAL:O	1:N:18:THR:OG1	2.27	0.51
1:W:452:PRO:HD3	1:W:463:VAL:HG12	1.93	0.51
1:j:415:SER:O	1:j:415:SER:OG	2.23	0.51
1:H:25:MET:HE1	1:m:13:GLN:HG2	1.93	0.51
1:a:359:LYS:HG2	1:a:412:MET:HE2	1.93	0.51
1:B:70:ILE:HB	1:B:352:THR:HG22	1.91	0.51
1:p:379:ASP:OD2	1:p:380:GLY:N	2.44	0.51
1:C:42:PHE:HE2	1:o:52:GLN:HA	1.74	0.51
1:S:414:ASP:OD1	1:S:414:ASP:N	2.43	0.50
1:B:409:LEU:HB3	1:B:410:PRO:HD3	1.93	0.50
1:D:409:LEU:HB3	1:D:410:PRO:HD3	1.93	0.50
1:g:18:THR:HG21	1:m:36:LEU:HD21	1.93	0.50
1:k:20:ILE:HG13	1:m:43:LEU:HD13	1.93	0.50
1:p:452:PRO:HD3	1:p:463:VAL:HG12	1.92	0.50
1:E:28:VAL:HG11	1:k:16:ILE:HG13	1.93	0.50
1:V:452:PRO:HD3	1:V:463:VAL:HG12	1.93	0.50
1:n:433:MET:HG2	1:n:449:ILE:HD12	1.94	0.50
1:C:409:LEU:HB3	1:C:410:PRO:HD3	1.93	0.50
1:e:375:THR:OG1	1:e:382:ASN:OD1	2.28	0.50
1:f:419:ARG:HH21	1:j:381:THR:HG23	1.76	0.50
1:k:404:ASP:OD2	1:k:404:ASP:N	2.41	0.50
1:e:414:ASP:OD1	1:e:414:ASP:N	2.43	0.50
1:l:359:LYS:HG3	1:l:412:MET:HE2	1.92	0.50
1:H:359:LYS:NZ	1:H:413:THR:O	2.44	0.50
1:I:392:THR:OG1	1:I:395:GLN:HB2	2.12	0.50
1:n:392:THR:HB	1:n:395:GLN:HB2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:375:THR:HB	1:S:433:MET:HE3	1.92	0.50
1:T:414:ASP:OD1	1:T:414:ASP:N	2.42	0.50
1:d:435:LEU:HB2	1:d:447:ILE:HB	1.93	0.50
1:H:14:VAL:O	1:H:18:THR:OG1	2.24	0.50
1:M:408:SER:HB2	1:M:411:VAL:HG22	1.92	0.50
1:W:382:ASN:OD1	1:W:382:ASN:N	2.45	0.50
1:N:414:ASP:OD1	1:N:414:ASP:N	2.44	0.50
1:L:22:PHE:HE1	1:P:16:ILE:HG13	1.77	0.49
1:O:414:ASP:OD1	1:O:414:ASP:N	2.44	0.49
1:d:62:ILE:HG22	1:d:366:ILE:HD13	1.94	0.49
1:i:396:THR:OG1	1:i:397:PHE:N	2.45	0.49
1:j:21:VAL:HG13	1:j:25:MET:HE3	1.93	0.49
1:j:25:MET:HE2	1:j:25:MET:N	2.27	0.49
1:L:15:GLY:HA3	1:T:28:VAL:HG12	1.92	0.49
1:a:45:SER:HB2	1:e:448:ARG:HH21	1.77	0.49
1:E:13:GLN:HB3	1:m:25:MET:HE1	1.93	0.49
1:j:23:ILE:HG21	1:B:59:THR:HG22	1.94	0.49
1:R:382:ASN:ND2	1:R:394:ASP:OD1	2.32	0.49
1:l:409:LEU:HB3	1:l:410:PRO:HD3	1.94	0.49
1:E:462:GLN:NE2	1:I:436:GLU:OE1	2.45	0.49
1:m:415:SER:O	1:m:415:SER:OG	2.23	0.49
1:K:14:VAL:O	1:K:18:THR:OG1	2.28	0.49
1:a:409:LEU:HD22	1:a:418:PHE:HE2	1.78	0.49
1:n:24:ALA:O	1:n:28:VAL:HG23	2.12	0.49
1:D:433:MET:HE3	1:D:435:LEU:HD21	1.94	0.49
1:T:388:ASP:OD1	1:T:389:ASP:N	2.45	0.49
1:E:409:LEU:HB3	1:E:410:PRO:HD3	1.94	0.49
1:k:414:ASP:OD2	1:k:414:ASP:N	2.46	0.49
1:m:406:ASP:OD1	1:m:406:ASP:N	2.46	0.49
1:f:409:LEU:HB3	1:f:410:PRO:HD3	1.94	0.49
1:i:412:MET:HE2	1:i:418:PHE:CD2	2.47	0.49
1:l:416:ASP:HB3	1:l:418:PHE:CE1	2.46	0.49
1:I:63:GLN:HG2	1:I:360:GLY:HA2	1.95	0.49
1:b:359:LYS:NZ	1:b:364:ASP:O	2.46	0.49
1:l:392:THR:HB	1:l:395:GLN:HB2	1.93	0.49
1:H:375:THR:OG1	1:H:382:ASN:OD1	2.31	0.48
1:L:40:ALA:HB1	1:P:31:ILE:HD11	1.94	0.48
1:L:414:ASP:OD1	1:L:414:ASP:N	2.45	0.48
1:R:21:VAL:O	1:R:25:MET:HG2	2.13	0.48
1:m:56:ASP:O	1:m:60:ASN:HB2	2.12	0.48
1:N:412:MET:HG2	1:N:418:PHE:CE2	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:375:THR:OG1	1:d:382:ASN:O	2.31	0.48
1:M:392:THR:OG1	1:M:395:GLN:HB2	2.14	0.48
1:V:68:VAL:HG11	1:Z:381:THR:HG21	1.95	0.48
1:B:433:MET:HB3	1:B:449:ILE:HB	1.95	0.48
1:H:414:ASP:N	1:H:414:ASP:OD1	2.44	0.48
1:P:379:ASP:OD1	1:P:380:GLY:N	2.45	0.48
1:B:406:ASP:OD1	1:B:406:ASP:N	2.46	0.48
1:U:61:GLN:HG3	1:U:443:ALA:HB1	1.95	0.48
1:d:14:VAL:O	1:d:18:THR:OG1	2.30	0.48
1:j:452:PRO:HD3	1:j:463:VAL:HG12	1.95	0.48
1:B:64:VAL:HG21	1:B:447:ILE:HD11	1.94	0.48
1:H:62:ILE:HD11	1:H:357:ALA:HB1	1.96	0.48
1:e:401:SER:HB2	1:e:409:LEU:HD23	1.94	0.48
1:n:409:LEU:HB3	1:n:410:PRO:HD3	1.96	0.48
1:B:58:VAL:HG13	1:B:59:THR:HG23	1.96	0.48
1:H:13:GLN:HA	1:H:13:GLN:OE1	2.14	0.48
1:N:382:ASN:ND2	1:N:394:ASP:OD2	2.47	0.48
1:W:441:SER:O	1:W:441:SER:OG	2.32	0.48
1:e:62:ILE:HG22	1:e:366:ILE:HD13	1.94	0.48
1:T:70:ILE:HB	1:T:352:THR:HG22	1.95	0.48
1:H:70:ILE:HB	1:H:352:THR:HG22	1.95	0.47
1:Y:359:LYS:HG2	1:Y:412:MET:HE2	1.96	0.47
1:k:70:ILE:HB	1:k:352:THR:HG22	1.96	0.47
1:A:21:VAL:O	1:A:25:MET:HG2	2.14	0.47
1:P:22:PHE:HE1	1:U:16:ILE:HG13	1.79	0.47
1:V:23:ILE:O	1:V:27:LEU:HD12	2.14	0.47
1:Z:402:ILE:HD11	1:Z:419:ARG:NH1	2.30	0.47
1:d:61:GLN:HG2	1:d:443:ALA:HB1	1.97	0.47
1:d:431:GLU:OE1	1:d:431:GLU:N	2.44	0.47
1:i:388:ASP:OD2	1:i:388:ASP:N	2.46	0.47
1:M:61:GLN:HG2	1:M:443:ALA:HB1	1.96	0.47
1:U:379:ASP:OD2	1:U:380:GLY:N	2.47	0.47
1:G:22:PHE:HZ	1:p:39:THR:HG21	1.79	0.47
1:W:68:VAL:HG11	1:a:381:THR:HG21	1.97	0.47
1:X:400:GLU:OE1	1:X:419:ARG:NH1	2.47	0.47
1:g:385:THR:O	1:g:396:THR:OG1	2.27	0.47
1:C:14:VAL:O	1:C:18:THR:OG1	2.27	0.47
1:I:376:ILE:HD13	1:I:381:THR:HB	1.96	0.47
1:e:416:ASP:HB3	1:e:418:PHE:HE2	1.79	0.47
1:m:70:ILE:HB	1:m:352:THR:HG22	1.95	0.47
1:C:364:ASP:OD2	1:C:364:ASP:N	2.46	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:n:57:GLN:OE1	1:B:63:GLN:NE2	2.47	0.47
1:n:401:SER:HA	1:n:418:PHE:HD2	1.79	0.47
1:E:22:PHE:HE1	1:I:16:ILE:HG13	1.79	0.47
1:G:409:LEU:HB3	1:G:410:PRO:HD3	1.96	0.47
1:I:406:ASP:OD1	1:I:406:ASP:N	2.48	0.47
1:O:452:PRO:HD3	1:O:463:VAL:HG12	1.95	0.47
1:P:14:VAL:O	1:P:18:THR:OG1	2.25	0.47
1:R:452:PRO:HD3	1:R:463:VAL:HG12	1.96	0.47
1:a:416:ASP:HB3	1:a:418:PHE:HE1	1.79	0.47
1:m:409:LEU:HB3	1:m:410:PRO:HD3	1.97	0.47
1:n:56:ASP:O	1:n:60:ASN:HB2	2.15	0.47
1:A:13:GLN:HB3	1:C:25:MET:HG3	1.96	0.47
1:I:375:THR:HB	1:I:433:MET:HE2	1.95	0.47
1:M:439:THR:O	1:M:439:THR:OG1	2.32	0.47
1:R:387:SER:OG	1:R:390:GLY:O	2.29	0.47
1:b:415:SER:O	1:b:415:SER:OG	2.24	0.47
1:g:36:LEU:HD13	1:k:28:VAL:HG21	1.97	0.47
1:i:27:LEU:O	1:i:31:ILE:HG12	2.15	0.47
1:H:409:LEU:HB3	1:H:410:PRO:HD3	1.96	0.47
1:P:382:ASN:ND2	1:P:394:ASP:OD1	2.48	0.47
1:T:14:VAL:O	1:T:18:THR:OG1	2.30	0.47
1:V:25:MET:HE2	1:Z:13:GLN:HB3	1.97	0.47
1:Z:378:PRO:HG3	1:Z:431:GLU:OE1	2.15	0.47
1:e:392:THR:OG1	1:e:395:GLN:HB2	2.15	0.47
1:K:409:LEU:HB3	1:K:410:PRO:HD3	1.97	0.47
1:U:382:ASN:OD1	1:U:382:ASN:N	2.47	0.47
1:W:409:LEU:HB3	1:W:410:PRO:HD3	1.97	0.47
1:n:396:THR:OG1	1:n:397:PHE:N	2.48	0.47
1:e:16:ILE:HD13	1:i:43:LEU:HD12	1.96	0.46
1:H:455:LEU:HD23	1:H:461:VAL:HG11	1.97	0.46
1:K:412:MET:HG2	1:K:418:PHE:CE2	2.50	0.46
1:M:15:GLY:HA3	1:U:28:VAL:HG12	1.96	0.46
1:P:414:ASP:N	1:P:414:ASP:OD1	2.44	0.46
1:R:392:THR:OG1	1:R:395:GLN:HB2	2.16	0.46
1:Z:392:THR:OG1	1:Z:396:THR:OG1	2.33	0.46
1:i:409:LEU:HB3	1:i:410:PRO:HD3	1.96	0.46
1:j:63:GLN:HE21	1:j:360:GLY:HA2	1.80	0.46
1:I:393:GLU:OE1	1:I:394:ASP:HB2	2.15	0.46
1:b:22:PHE:HE1	1:g:16:ILE:HG13	1.80	0.46
1:n:28:VAL:HG13	1:B:40:ALA:HB2	1.98	0.46
1:p:56:ASP:O	1:p:60:ASN:HB2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ILE:HD11	1:A:357:ALA:HB1	1.96	0.46
1:E:387:SER:HB2	1:E:396:THR:HB	1.98	0.46
1:E:389:ASP:OD1	1:E:389:ASP:N	2.48	0.46
1:G:428:GLU:N	1:G:431:GLU:OE1	2.34	0.46
1:J:13:GLN:HG2	1:R:25:MET:HE1	1.97	0.46
1:V:21:VAL:O	1:V:25:MET:HG2	2.16	0.46
1:f:26:VAL:HG11	1:B:54:SER:HB3	1.97	0.46
1:j:396:THR:OG1	1:j:397:PHE:N	2.47	0.46
1:j:409:LEU:HB3	1:j:410:PRO:HD3	1.97	0.46
1:O:409:LEU:HB3	1:O:410:PRO:HD3	1.98	0.46
1:U:392:THR:HB	1:U:395:GLN:HB2	1.98	0.46
1:d:409:LEU:HB3	1:d:410:PRO:HD3	1.96	0.46
1:f:439:THR:O	1:f:440:GLU:HG3	2.16	0.46
1:A:412:MET:HG2	1:A:418:PHE:CE2	2.51	0.46
1:H:406:ASP:OD1	1:H:406:ASP:N	2.49	0.46
1:S:387:SER:OG	1:S:390:GLY:O	2.31	0.46
1:S:409:LEU:HB3	1:S:410:PRO:HD3	1.98	0.46
1:T:409:LEU:HB3	1:T:410:PRO:HD3	1.98	0.46
1:Z:416:ASP:HB3	1:Z:418:PHE:HE1	1.81	0.46
1:a:409:LEU:HB3	1:a:410:PRO:HD3	1.97	0.46
1:n:25:MET:HE2	1:n:25:MET:HA	1.98	0.46
1:o:31:ILE:O	1:o:35:VAL:HG23	2.15	0.46
1:o:409:LEU:HB3	1:o:410:PRO:HD3	1.98	0.46
1:A:14:VAL:O	1:A:18:THR:OG1	2.29	0.46
1:k:27:LEU:O	1:k:31:ILE:HG12	2.15	0.46
1:n:414:ASP:OD1	1:n:414:ASP:N	2.47	0.46
1:G:387:SER:HB2	1:G:396:THR:HB	1.96	0.46
1:V:409:LEU:HB3	1:V:410:PRO:HD3	1.98	0.46
1:o:368:MET:HE3	1:o:368:MET:HB3	1.82	0.46
1:I:412:MET:HG2	1:I:416:ASP:HB2	1.98	0.46
1:N:423:ASP:OD1	1:N:423:ASP:O	2.34	0.46
1:S:68:VAL:HG11	1:W:381:THR:HG21	1.97	0.46
1:e:416:ASP:HB3	1:e:418:PHE:CE2	2.51	0.46
1:o:369:GLU:HB3	1:o:370:GLU:OE2	2.15	0.46
1:B:432:THR:O	1:B:433:MET:HE2	2.16	0.46
1:K:375:THR:OG1	1:K:382:ASN:OD1	2.30	0.46
1:L:375:THR:HB	1:L:433:MET:HE3	1.97	0.46
1:R:379:ASP:OD1	1:R:380:GLY:N	2.49	0.46
1:g:409:LEU:HB3	1:g:410:PRO:HD3	1.98	0.46
1:j:59:THR:HG22	1:k:23:ILE:HG21	1.97	0.46
1:K:15:GLY:HA3	1:S:28:VAL:HG12	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:406:ASP:OD1	1:Y:406:ASP:N	2.47	0.45
1:g:56:ASP:O	1:g:60:ASN:HB2	2.17	0.45
1:j:22:PHE:HE1	1:m:16:ILE:HG13	1.81	0.45
1:j:70:ILE:HB	1:j:352:THR:HG22	1.97	0.45
1:E:32:ALA:HA	1:k:19:LEU:HD21	1.97	0.45
1:P:21:VAL:O	1:P:25:MET:HG2	2.16	0.45
1:R:14:VAL:O	1:R:18:THR:OG1	2.33	0.45
1:C:25:MET:HE1	1:o:36:LEU:HD23	1.98	0.45
1:K:435:LEU:HD11	1:K:449:ILE:HD11	1.99	0.45
1:W:406:ASP:OD1	1:W:406:ASP:N	2.48	0.45
1:D:13:GLN:HG2	1:K:25:MET:HE1	1.97	0.45
1:G:24:ALA:O	1:G:28:VAL:HG23	2.16	0.45
1:O:22:PHE:HE1	1:T:16:ILE:HG13	1.81	0.45
1:f:373:ILE:HG12	1:f:437:VAL:HG12	1.98	0.45
1:n:14:VAL:O	1:n:18:THR:OG1	2.30	0.45
1:C:439:THR:O	1:C:440:GLU:HB3	2.16	0.45
1:R:409:LEU:HB3	1:R:410:PRO:HD3	1.99	0.45
1:X:428:GLU:OE1	1:X:428:GLU:N	2.49	0.45
1:k:409:LEU:HB3	1:k:410:PRO:HD3	1.97	0.45
1:l:14:VAL:O	1:l:18:THR:OG1	2.33	0.45
1:n:353:LEU:HD23	1:n:353:LEU:HA	1.76	0.45
1:p:409:LEU:HB3	1:p:410:PRO:HD3	1.99	0.45
1:C:439:THR:O	1:C:439:THR:HG23	2.16	0.45
1:K:461:VAL:HG23	1:K:463:VAL:HG13	1.99	0.45
1:L:70:ILE:HB	1:L:352:THR:HG23	1.98	0.45
1:S:14:VAL:O	1:S:18:THR:OG1	2.31	0.45
1:C:56:ASP:O	1:C:60:ASN:HB2	2.17	0.45
1:Y:392:THR:OG1	1:Y:395:GLN:HB2	2.15	0.45
1:m:370:GLU:HB2	1:m:440:GLU:HG3	1.99	0.45
1:B:18:THR:O	1:B:22:PHE:N	2.44	0.45
1:D:412:MET:HG2	1:D:418:PHE:CE2	2.52	0.45
1:I:455:LEU:HD23	1:I:461:VAL:HG11	1.99	0.45
1:S:387:SER:HB3	1:S:396:THR:HB	1.99	0.45
1:e:446:GLU:HG2	1:e:448:ARG:NH1	2.31	0.45
1:k:428:GLU:HB2	1:k:431:GLU:HG3	1.99	0.45
1:o:65:ALA:O	1:o:356:VAL:HG22	2.17	0.45
1:B:368:MET:N	1:B:410:PRO:O	2.32	0.45
1:L:409:LEU:HB3	1:L:410:PRO:HD3	1.99	0.45
1:b:409:LEU:HB3	1:b:410:PRO:HD3	1.99	0.45
1:I:409:LEU:HB3	1:I:410:PRO:HD3	1.98	0.44
1:i:66:SER:O	1:i:66:SER:OG	2.31	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:417:ARG:HH22	1:U:440:GLU:HA	1.82	0.44
1:S:412:MET:HG2	1:S:418:PHE:CE2	2.53	0.44
1:U:359:LYS:HG2	1:U:366:ILE:HD12	1.99	0.44
1:J:409:LEU:HB3	1:J:410:PRO:HD3	2.00	0.44
1:T:56:ASP:O	1:T:60:ASN:HB2	2.18	0.44
1:b:56:ASP:O	1:b:60:ASN:HB2	2.18	0.44
1:i:59:THR:HG22	1:B:23:ILE:HG21	1.99	0.44
1:A:429:THR:HG22	1:A:455:LEU:HD12	2.00	0.44
1:R:439:THR:O	1:R:439:THR:OG1	2.35	0.44
1:j:370:GLU:HB2	1:j:440:GLU:HG2	2.00	0.44
1:j:462:GLN:N	1:j:462:GLN:OE1	2.50	0.44
1:A:428:GLU:N	1:A:431:GLU:OE1	2.32	0.44
1:D:381:THR:HG21	1:n:68:VAL:HG11	2.00	0.44
1:L:370:GLU:HB2	1:L:440:GLU:HG3	2.00	0.44
1:L:455:LEU:HD23	1:L:461:VAL:HG11	2.00	0.44
1:N:392:THR:OG1	1:N:395:GLN:HB2	2.18	0.44
1:R:20:ILE:HG21	1:p:29:ALA:HB1	1.99	0.44
1:X:359:LYS:NZ	1:X:364:ASP:O	2.50	0.44
1:o:370:GLU:OE2	1:o:370:GLU:N	2.50	0.44
1:B:366:ILE:HB	1:B:412:MET:HB2	1.99	0.44
1:G:379:ASP:OD1	1:G:379:ASP:C	2.61	0.44
1:M:448:ARG:HB3	1:M:448:ARG:NH1	2.32	0.44
1:Z:416:ASP:HB3	1:Z:418:PHE:CE1	2.53	0.44
1:b:25:MET:SD	1:g:13:GLN:HB3	2.58	0.44
1:p:71:VAL:HA	1:p:350:VAL:HA	2.00	0.44
1:B:42:PHE:O	1:B:45:SER:OG	2.29	0.44
1:G:375:THR:OG1	1:G:382:ASN:OD1	2.23	0.44
1:J:22:PHE:HE1	1:N:16:ILE:HG13	1.83	0.44
1:N:409:LEU:HB3	1:N:410:PRO:HD3	2.00	0.44
1:T:412:MET:HG2	1:T:418:PHE:CE2	2.53	0.44
1:X:409:LEU:HB3	1:X:410:PRO:HD3	1.99	0.44
1:b:21:VAL:O	1:b:25:MET:HG3	2.18	0.44
1:P:409:LEU:HB3	1:P:410:PRO:HD3	2.00	0.44
1:Y:369:GLU:HB2	1:Y:370:GLU:OE2	2.17	0.44
1:g:401:SER:HB2	1:g:409:LEU:HD23	1.99	0.44
1:L:56:ASP:O	1:L:60:ASN:HB2	2.17	0.44
1:b:388:ASP:N	1:b:388:ASP:OD1	2.49	0.44
1:B:446:GLU:OE2	1:B:448:ARG:NH2	2.51	0.44
1:A:409:LEU:HB3	1:A:410:PRO:HD3	2.00	0.43
1:D:42:PHE:CD1	1:D:43:LEU:HD22	2.53	0.43
1:D:452:PRO:HD3	1:D:463:VAL:HG12	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:61:GLN:HG2	1:K:443:ALA:HB1	1.99	0.43
1:K:350:VAL:HG22	1:K:427:LEU:HB2	1.98	0.43
1:j:27:LEU:O	1:j:31:ILE:HG12	2.18	0.43
1:j:427:LEU:HD21	1:j:433:MET:HE2	2.00	0.43
1:B:374:THR:HG22	1:B:436:GLU:HB3	2.00	0.43
1:L:21:VAL:O	1:L:25:MET:HG2	2.18	0.43
1:P:406:ASP:OD1	1:P:406:ASP:N	2.51	0.43
1:Y:428:GLU:HB2	1:Y:431:GLU:HG3	2.00	0.43
1:a:59:THR:HG22	1:b:23:ILE:HG21	2.00	0.43
1:f:64:VAL:HG21	1:f:447:ILE:HG21	2.00	0.43
1:R:43:LEU:HD23	1:R:43:LEU:HA	1.85	0.43
1:V:359:LYS:HG2	1:V:366:ILE:HD12	2.00	0.43
1:k:392:THR:HG23	1:k:395:GLN:HB2	1.99	0.43
1:m:42:PHE:C	1:m:42:PHE:CD2	2.97	0.43
1:Y:453:ASN:OD1	1:Y:453:ASN:N	2.52	0.43
1:b:392:THR:HG22	1:b:395:GLN:HB2	2.00	0.43
1:B:25:MET:N	1:B:25:MET:SD	2.92	0.43
1:P:455:LEU:HD23	1:P:455:LEU:HA	1.87	0.43
1:T:68:VAL:HG11	1:X:381:THR:HG21	2.00	0.43
1:N:379:ASP:OD1	1:N:379:ASP:N	2.41	0.43
1:Y:62:ILE:HG13	1:Y:366:ILE:HD13	2.01	0.43
1:D:21:VAL:O	1:D:25:MET:HG2	2.19	0.43
1:P:359:LYS:HG2	1:P:366:ILE:HD12	2.01	0.43
1:e:409:LEU:HB3	1:e:410:PRO:HD3	2.00	0.43
1:f:21:VAL:O	1:f:25:MET:HG3	2.19	0.43
1:l:62:ILE:HD11	1:l:357:ALA:HB1	2.01	0.43
1:A:440:GLU:OE1	1:C:415:SER:OG	2.22	0.43
1:R:22:PHE:CE1	1:V:16:ILE:HG13	2.53	0.43
1:X:56:ASP:O	1:X:60:ASN:HB2	2.19	0.43
1:A:461:VAL:HG23	1:A:463:VAL:HG13	2.00	0.43
1:M:350:VAL:HG12	1:M:427:LEU:HB2	2.00	0.43
1:R:417:ARG:HE	1:V:438:THR:HG21	1.84	0.43
1:l:435:LEU:HD11	1:l:449:ILE:HD11	2.00	0.43
1:D:368:MET:HE3	1:D:368:MET:HB3	1.82	0.43
1:D:389:ASP:OD2	1:D:389:ASP:C	2.62	0.43
1:K:63:GLN:HA	1:K:63:GLN:OE1	2.19	0.43
1:Y:373:ILE:HG23	1:Y:437:VAL:HG22	2.01	0.43
1:g:28:VAL:HA	1:g:31:ILE:HG22	2.00	0.43
1:G:412:MET:HG2	1:G:418:PHE:CE2	2.54	0.42
1:J:462:GLN:NE2	1:N:436:GLU:OE2	2.52	0.42
1:M:379:ASP:OD1	1:M:379:ASP:N	2.41	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:382:ASN:OD1	1:R:382:ASN:N	2.51	0.42
1:d:370:GLU:OE2	1:d:370:GLU:N	2.50	0.42
1:B:439:THR:O	1:B:439:THR:OG1	2.27	0.42
1:K:368:MET:HE3	1:K:368:MET:HB3	1.93	0.42
1:L:461:VAL:HG23	1:L:463:VAL:HG13	2.01	0.42
1:e:26:VAL:HG11	1:i:54:SER:HB3	2.01	0.42
1:D:359:LYS:HG2	1:D:366:ILE:HD12	1.99	0.42
1:U:389:ASP:N	1:U:389:ASP:OD1	2.51	0.42
1:V:23:ILE:O	1:V:26:VAL:HG22	2.19	0.42
1:W:374:THR:O	1:W:436:GLU:N	2.50	0.42
1:l:412:MET:HE2	1:l:412:MET:HB3	1.83	0.42
1:n:16:ILE:HG13	1:B:22:PHE:HE1	1.84	0.42
1:d:392:THR:H	1:d:392:THR:HG1	1.55	0.42
1:I:62:ILE:HD11	1:I:357:ALA:HB1	2.01	0.42
1:T:415:SER:O	1:T:415:SER:OG	2.35	0.42
1:i:370:GLU:HB2	1:i:440:GLU:HG3	2.01	0.42
1:C:461:VAL:HG23	1:C:463:VAL:HG13	2.00	0.42
1:J:21:VAL:O	1:J:25:MET:HG2	2.20	0.42
1:K:455:LEU:HD23	1:K:461:VAL:HG11	2.02	0.42
1:a:441:SER:O	1:a:441:SER:OG	2.36	0.42
1:b:63:GLN:OE1	1:b:63:GLN:HA	2.20	0.42
1:l:428:GLU:CD	1:l:429:THR:H	2.28	0.42
1:m:401:SER:HB3	1:m:409:LEU:HD23	2.01	0.42
1:p:455:LEU:HD23	1:p:461:VAL:HG11	2.02	0.42
1:I:56:ASP:O	1:I:60:ASN:HB2	2.19	0.42
1:M:349:GLY:HA2	1:M:455:LEU:HD13	2.02	0.42
1:b:385:THR:O	1:b:396:THR:OG1	2.25	0.42
1:k:26:VAL:HG12	1:l:16:ILE:HG21	2.02	0.42
1:l:461:VAL:HG22	1:l:462:GLN:H	1.85	0.42
1:D:61:GLN:HG2	1:D:443:ALA:HB1	2.02	0.42
1:D:388:ASP:OD2	1:D:389:ASP:N	2.53	0.42
1:i:373:ILE:HD13	1:i:373:ILE:HA	1.85	0.42
1:k:364:ASP:OD1	1:k:364:ASP:C	2.62	0.42
1:n:62:ILE:HD12	1:n:368:MET:HE1	2.00	0.42
1:I:369:GLU:HG3	1:I:410:PRO:HB3	2.01	0.42
1:U:402:ILE:HD13	1:U:402:ILE:HA	1.94	0.42
1:V:38:ASN:OD1	1:V:38:ASN:N	2.52	0.42
1:W:435:LEU:HD11	1:W:449:ILE:HD11	2.02	0.42
1:X:19:LEU:HD21	1:f:32:ALA:HA	2.02	0.42
1:j:435:LEU:HD11	1:j:449:ILE:HD11	2.02	0.42
1:H:412:MET:HG2	1:H:418:PHE:CE2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:56:ASP:O	1:K:60:ASN:HB2	2.20	0.42
1:P:15:GLY:O	1:P:19:LEU:HG	2.19	0.42
1:f:56:ASP:O	1:f:60:ASN:HB2	2.20	0.42
1:m:376:ILE:HD13	1:m:376:ILE:HA	1.89	0.42
1:n:393:GLU:C	1:n:395:GLN:H	2.28	0.42
1:E:33:ALA:O	1:E:37:ILE:HD12	2.20	0.41
1:g:379:ASP:OD1	1:g:380:GLY:N	2.53	0.41
1:o:385:THR:O	1:o:396:THR:OG1	2.23	0.41
1:N:362:GLY:HA3	1:S:50:THR:HG22	2.00	0.41
1:R:13:GLN:HB3	1:p:25:MET:HE2	2.03	0.41
1:g:368:MET:O	1:g:368:MET:HG3	2.20	0.41
1:A:22:PHE:HE1	1:K:16:ILE:HG13	1.86	0.41
1:S:61:GLN:HG2	1:S:443:ALA:HB1	2.03	0.41
1:V:70:ILE:HB	1:V:352:THR:HG22	2.02	0.41
1:X:64:VAL:HG21	1:X:447:ILE:HD13	2.02	0.41
1:e:461:VAL:HG23	1:e:463:VAL:HG13	2.03	0.41
1:i:402:ILE:HD11	1:i:419:ARG:NH1	2.34	0.41
1:j:382:ASN:N	1:j:382:ASN:ND2	2.67	0.41
1:k:25:MET:N	1:k:25:MET:HE2	2.34	0.41
1:p:21:VAL:O	1:p:25:MET:HG2	2.20	0.41
1:G:39:THR:HG21	1:o:22:PHE:HZ	1.85	0.41
1:Y:399:VAL:HB	1:Y:420:VAL:HG12	2.02	0.41
1:Y:455:LEU:HD23	1:Y:461:VAL:HG11	2.02	0.41
1:d:16:ILE:H	1:d:16:ILE:HG12	1.72	0.41
1:E:370:GLU:OE2	1:E:440:GLU:HG3	2.21	0.41
1:N:406:ASP:N	1:N:406:ASP:OD1	2.46	0.41
1:k:56:ASP:O	1:k:60:ASN:HB2	2.20	0.41
1:H:461:VAL:HG23	1:H:463:VAL:HG13	2.01	0.41
1:J:379:ASP:OD1	1:J:379:ASP:C	2.63	0.41
1:S:429:THR:HG22	1:S:455:LEU:HD12	2.02	0.41
1:a:388:ASP:OD1	1:a:389:ASP:N	2.54	0.41
1:a:395:GLN:HA	1:a:395:GLN:OE1	2.21	0.41
1:e:361:SER:HB2	1:B:57:GLN:HG3	2.02	0.41
1:T:437:VAL:O	1:T:444:THR:HA	2.20	0.41
1:Y:359:LYS:NZ	1:Y:413:THR:O	2.54	0.41
1:j:428:GLU:OE1	1:j:428:GLU:HA	2.19	0.41
1:l:67:LYS:HG2	1:l:355:ILE:HD11	2.02	0.41
1:C:42:PHE:CD1	1:C:42:PHE:C	2.97	0.41
1:H:13:GLN:NE2	1:O:25:MET:HE1	2.36	0.41
1:J:350:VAL:HG23	1:J:427:LEU:HB2	2.02	0.41
1:M:56:ASP:O	1:M:60:ASN:HB2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:36:LEU:HA	1:W:36:LEU:HD23	1.82	0.41
1:X:22:PHE:HE1	1:b:16:ILE:HG13	1.86	0.41
1:Y:56:ASP:O	1:Y:60:ASN:HB2	2.21	0.41
1:Z:67:LYS:HZ3	1:Z:449:ILE:HG12	1.85	0.41
1:D:461:VAL:HG23	1:D:463:VAL:HG13	2.03	0.41
1:P:22:PHE:HZ	1:X:39:THR:HG21	1.86	0.41
1:P:27:LEU:O	1:P:31:ILE:HG23	2.21	0.41
1:P:461:VAL:HG23	1:P:463:VAL:HG13	2.02	0.41
1:R:22:PHE:HE1	1:V:16:ILE:HG13	1.86	0.41
1:U:379:ASP:OD2	1:U:379:ASP:C	2.64	0.41
1:V:15:GLY:HA3	1:d:28:VAL:HG12	2.03	0.41
1:Y:36:LEU:HD23	1:Y:36:LEU:HA	1.90	0.41
1:e:71:VAL:HB	1:e:459:SER:HA	2.03	0.41
1:B:23:ILE:O	1:B:27:LEU:HG	2.21	0.41
1:B:48:GLU:O	1:B:52:GLN:HG2	2.20	0.41
1:M:461:VAL:HG23	1:M:463:VAL:HG13	2.03	0.41
1:U:56:ASP:O	1:U:60:ASN:HB2	2.21	0.41
1:X:369:GLU:HB3	1:X:370:GLU:OE1	2.21	0.41
1:X:402:ILE:HD13	1:X:402:ILE:HA	1.88	0.41
1:d:422:ILE:HG23	1:d:424:PRO:HD3	2.03	0.41
1:g:29:ALA:HB2	1:k:21:VAL:HG22	2.03	0.41
1:l:379:ASP:OD1	1:l:379:ASP:C	2.63	0.41
1:B:21:VAL:HG13	1:B:25:MET:HE2	2.02	0.41
1:P:64:VAL:HG23	1:P:355:ILE:HG23	2.03	0.40
1:U:409:LEU:HB3	1:U:410:PRO:HD3	2.02	0.40
1:i:362:GLY:HA3	1:o:50:THR:HG22	2.02	0.40
1:j:385:THR:O	1:j:396:THR:OG1	2.31	0.40
1:n:394:ASP:OD1	1:n:394:ASP:O	2.39	0.40
1:H:387:SER:HB2	1:H:396:THR:HB	2.03	0.40
1:R:70:ILE:HB	1:R:352:THR:HG23	2.02	0.40
1:U:364:ASP:OD2	1:U:364:ASP:N	2.49	0.40
1:b:412:MET:HG2	1:b:418:PHE:HE1	1.85	0.40
1:d:23:ILE:H	1:d:23:ILE:HG13	1.66	0.40
1:e:402:ILE:HD11	1:e:419:ARG:HB2	2.04	0.40
1:j:48:GLU:O	1:j:52:GLN:HG2	2.21	0.40
1:l:409:LEU:HD22	1:l:418:PHE:HE2	1.85	0.40
1:C:412:MET:HG2	1:C:418:PHE:CE2	2.56	0.40
1:I:461:VAL:HG23	1:I:463:VAL:HG13	2.02	0.40
1:K:359:LYS:HG3	1:K:366:ILE:HD12	2.03	0.40
1:W:21:VAL:O	1:W:25:MET:HG2	2.22	0.40
1:f:415:SER:O	1:f:415:SER:OG	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:ILE:HG21	1:o:26:VAL:HG12	2.03	0.40
1:C:431:GLU:HA	1:C:431:GLU:OE2	2.20	0.40
1:D:424:PRO:HB3	1:D:433:MET:HE1	2.03	0.40
1:E:56:ASP:O	1:E:60:ASN:HB2	2.21	0.40
1:M:409:LEU:HB3	1:M:410:PRO:HD3	2.04	0.40
1:S:412:MET:HE3	1:S:412:MET:HB3	1.95	0.40
1:T:45:SER:HB2	1:W:448:ARG:CZ	2.51	0.40
1:g:18:THR:HA	1:k:13:GLN:HE22	1.86	0.40
1:n:401:SER:HA	1:n:418:PHE:CD2	2.56	0.40
1:A:402:ILE:HD11	1:A:419:ARG:HB2	2.03	0.40
1:C:454:THR:HG22	1:n:365:GLN:NE2	2.37	0.40
1:G:56:ASP:O	1:G:60:ASN:HB2	2.21	0.40
1:I:370:GLU:HB2	1:I:440:GLU:HG3	2.04	0.40
1:N:350:VAL:HG22	1:N:427:LEU:HB2	2.04	0.40
1:W:22:PHE:HE1	1:a:16:ILE:HG13	1.87	0.40
1:W:437:VAL:O	1:W:444:THR:HA	2.22	0.40
1:X:14:VAL:HB	1:j:21:VAL:HG21	2.03	0.40
1:Z:56:ASP:O	1:Z:60:ASN:HB2	2.22	0.40
1:a:387:SER:OG	1:a:389:ASP:O	2.39	0.40
1:j:385:THR:C	1:j:396:THR:HG1	2.24	0.40
1:l:355:ILE:HD12	1:l:355:ILE:HA	1.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	172/463 (37%)	160 (93%)	12 (7%)	0	100	100
1	B	172/463 (37%)	166 (96%)	6 (4%)	0	100	100
1	C	172/463 (37%)	164 (95%)	8 (5%)	0	100	100
1	D	172/463 (37%)	162 (94%)	10 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	172/463 (37%)	165 (96%)	7 (4%)	0	100	100
1	G	172/463 (37%)	162 (94%)	10 (6%)	0	100	100
1	H	172/463 (37%)	160 (93%)	12 (7%)	0	100	100
1	I	172/463 (37%)	164 (95%)	8 (5%)	0	100	100
1	J	172/463 (37%)	160 (93%)	12 (7%)	0	100	100
1	K	172/463 (37%)	162 (94%)	10 (6%)	0	100	100
1	L	172/463 (37%)	160 (93%)	12 (7%)	0	100	100
1	M	172/463 (37%)	162 (94%)	10 (6%)	0	100	100
1	N	172/463 (37%)	159 (92%)	13 (8%)	0	100	100
1	O	172/463 (37%)	163 (95%)	9 (5%)	0	100	100
1	P	172/463 (37%)	164 (95%)	8 (5%)	0	100	100
1	R	172/463 (37%)	164 (95%)	8 (5%)	0	100	100
1	S	172/463 (37%)	162 (94%)	10 (6%)	0	100	100
1	T	172/463 (37%)	162 (94%)	10 (6%)	0	100	100
1	U	172/463 (37%)	163 (95%)	9 (5%)	0	100	100
1	V	172/463 (37%)	160 (93%)	12 (7%)	0	100	100
1	W	172/463 (37%)	162 (94%)	10 (6%)	0	100	100
1	X	172/463 (37%)	160 (93%)	12 (7%)	0	100	100
1	Y	172/463 (37%)	160 (93%)	12 (7%)	0	100	100
1	Z	172/463 (37%)	164 (95%)	8 (5%)	0	100	100
1	a	172/463 (37%)	164 (95%)	8 (5%)	0	100	100
1	b	172/463 (37%)	158 (92%)	14 (8%)	0	100	100
1	d	172/463 (37%)	161 (94%)	11 (6%)	0	100	100
1	e	172/463 (37%)	165 (96%)	7 (4%)	0	100	100
1	f	172/463 (37%)	167 (97%)	5 (3%)	0	100	100
1	g	172/463 (37%)	166 (96%)	6 (4%)	0	100	100
1	i	171/463 (37%)	164 (96%)	7 (4%)	0	100	100
1	j	172/463 (37%)	166 (96%)	6 (4%)	0	100	100
1	k	172/463 (37%)	163 (95%)	9 (5%)	0	100	100
1	l	172/463 (37%)	161 (94%)	11 (6%)	0	100	100
1	m	172/463 (37%)	162 (94%)	10 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	n	172/463 (37%)	163 (95%)	9 (5%)	0	100	100
1	o	172/463 (37%)	162 (94%)	10 (6%)	0	100	100
1	p	172/463 (37%)	161 (94%)	11 (6%)	0	100	100
All	All	6535/17594 (37%)	6173 (94%)	362 (6%)	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	142/377 (38%)	141 (99%)	1 (1%)	76	79
1	B	142/377 (38%)	136 (96%)	6 (4%)	26	54
1	C	142/377 (38%)	141 (99%)	1 (1%)	76	79
1	D	142/377 (38%)	135 (95%)	7 (5%)	22	49
1	E	142/377 (38%)	137 (96%)	5 (4%)	32	58
1	G	142/377 (38%)	138 (97%)	4 (3%)	38	62
1	H	142/377 (38%)	139 (98%)	3 (2%)	47	67
1	I	142/377 (38%)	138 (97%)	4 (3%)	38	62
1	J	142/377 (38%)	138 (97%)	4 (3%)	38	62
1	K	142/377 (38%)	141 (99%)	1 (1%)	76	79
1	L	142/377 (38%)	138 (97%)	4 (3%)	38	62
1	M	142/377 (38%)	138 (97%)	4 (3%)	38	62
1	N	142/377 (38%)	139 (98%)	3 (2%)	47	67
1	O	142/377 (38%)	140 (99%)	2 (1%)	59	72
1	P	142/377 (38%)	137 (96%)	5 (4%)	32	58
1	R	142/377 (38%)	139 (98%)	3 (2%)	47	67
1	S	142/377 (38%)	137 (96%)	5 (4%)	32	58
1	T	142/377 (38%)	139 (98%)	3 (2%)	47	67

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	142/377 (38%)	141 (99%)	1 (1%)	76	79
1	V	142/377 (38%)	141 (99%)	1 (1%)	76	79
1	W	142/377 (38%)	138 (97%)	4 (3%)	38	62
1	X	142/377 (38%)	138 (97%)	4 (3%)	38	62
1	Y	142/377 (38%)	137 (96%)	5 (4%)	32	58
1	Z	142/377 (38%)	138 (97%)	4 (3%)	38	62
1	a	142/377 (38%)	137 (96%)	5 (4%)	32	58
1	b	142/377 (38%)	141 (99%)	1 (1%)	76	79
1	d	142/377 (38%)	137 (96%)	5 (4%)	32	58
1	e	142/377 (38%)	139 (98%)	3 (2%)	47	67
1	f	142/377 (38%)	137 (96%)	5 (4%)	32	58
1	g	142/377 (38%)	132 (93%)	10 (7%)	14	37
1	i	141/377 (37%)	136 (96%)	5 (4%)	32	58
1	j	142/377 (38%)	134 (94%)	8 (6%)	19	45
1	k	142/377 (38%)	138 (97%)	4 (3%)	38	62
1	l	142/377 (38%)	137 (96%)	5 (4%)	32	58
1	m	142/377 (38%)	136 (96%)	6 (4%)	26	54
1	n	142/377 (38%)	138 (97%)	4 (3%)	38	62
1	o	142/377 (38%)	140 (99%)	2 (1%)	59	72
1	p	142/377 (38%)	138 (97%)	4 (3%)	38	62
All	All	5395/14326 (38%)	5244 (97%)	151 (3%)	38	62

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	409	LEU
1	C	364	ASP
1	D	37	ILE
1	D	64	VAL
1	D	359	LYS
1	D	364	ASP
1	D	399	VAL
1	D	406	ASP
1	D	435	LEU
1	E	62	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	64	VAL
1	E	406	ASP
1	E	435	LEU
1	E	440	GLU
1	G	27	LEU
1	G	52	GLN
1	G	64	VAL
1	G	381	THR
1	H	45	SER
1	H	64	VAL
1	H	381	THR
1	I	64	VAL
1	I	384	LEU
1	I	399	VAL
1	I	434	THR
1	J	352	THR
1	J	364	ASP
1	J	406	ASP
1	J	409	LEU
1	K	432	THR
1	L	71	VAL
1	L	352	THR
1	L	381	THR
1	L	382	ASN
1	M	379	ASP
1	M	387	SER
1	M	389	ASP
1	M	411	VAL
1	N	45	SER
1	N	399	VAL
1	N	409	LEU
1	O	409	LEU
1	O	438	THR
1	P	66	SER
1	P	68	VAL
1	P	409	LEU
1	P	421	VAL
1	P	440	GLU
1	R	387	SER
1	R	399	VAL
1	R	406	ASP
1	S	379	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S	399	VAL
1	S	409	LEU
1	S	437	VAL
1	S	461	VAL
1	T	381	THR
1	T	382	ASN
1	T	409	LEU
1	U	353	LEU
1	V	370	GLU
1	W	379	ASP
1	W	406	ASP
1	W	409	LEU
1	W	458	GLU
1	X	364	ASP
1	X	405	ASP
1	X	406	ASP
1	X	438	THR
1	Y	45	SER
1	Y	64	VAL
1	Y	364	ASP
1	Y	404	ASP
1	Y	407	ASP
1	Z	14	VAL
1	Z	55	SER
1	Z	383	THR
1	Z	450	SER
1	a	48	GLU
1	a	374	THR
1	a	382	ASN
1	a	396	THR
1	a	406	ASP
1	b	461	VAL
1	d	383	THR
1	d	389	ASP
1	d	409	LEU
1	d	434	THR
1	d	461	VAL
1	e	35	VAL
1	e	388	ASP
1	e	409	LEU
1	f	372	THR
1	f	392	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	f	396	THR
1	f	421	VAL
1	f	426	THR
1	g	25	MET
1	g	36	LEU
1	g	46	SER
1	g	58	VAL
1	g	370	GLU
1	g	392	THR
1	g	396	THR
1	g	399	VAL
1	g	409	LEU
1	g	434	THR
1	i	64	VAL
1	i	352	THR
1	i	379	ASP
1	i	440	GLU
1	i	461	VAL
1	j	57	GLN
1	j	68	VAL
1	j	382	ASN
1	j	394	ASP
1	j	400	GLU
1	j	401	SER
1	j	439	THR
1	j	454	THR
1	k	28	VAL
1	k	406	ASP
1	k	414	ASP
1	k	434	THR
1	l	352	THR
1	l	370	GLU
1	l	405	ASP
1	l	437	VAL
1	l	440	GLU
1	m	62	ILE
1	m	369	GLU
1	m	371	THR
1	m	406	ASP
1	m	409	LEU
1	m	440	GLU
1	n	371	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	n	440	GLU
1	n	459	SER
1	n	461	VAL
1	o	352	THR
1	o	438	THR
1	p	27	LEU
1	p	406	ASP
1	p	409	LEU
1	p	440	GLU
1	B	389	ASP
1	B	406	ASP
1	B	439	THR
1	B	446	GLU
1	B	458	GLU
1	B	461	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	63	GLN
1	D	60	ASN
1	D	63	GLN
1	E	60	ASN
1	G	38	ASN
1	G	44	GLN
1	G	60	ASN
1	H	63	GLN
1	H	462	GLN
1	J	63	GLN
1	K	44	GLN
1	K	354	ASN
1	K	403	GLN
1	M	60	ASN
1	N	395	GLN
1	O	44	GLN
1	O	63	GLN
1	P	38	ASN
1	S	403	GLN
1	T	57	GLN
1	T	63	GLN
1	V	61	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	W	13	GLN
1	W	60	ASN
1	Y	60	ASN
1	Y	403	GLN
1	b	403	GLN
1	d	38	ASN
1	e	13	GLN
1	f	382	ASN
1	g	60	ASN
1	g	365	GLN
1	i	382	ASN
1	j	13	GLN
1	j	63	GLN
1	j	382	ASN
1	k	13	GLN
1	k	63	GLN
1	l	57	GLN
1	m	57	GLN
1	n	63	GLN
1	p	13	GLN
1	p	403	GLN
1	B	38	ASN
1	B	44	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 38 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

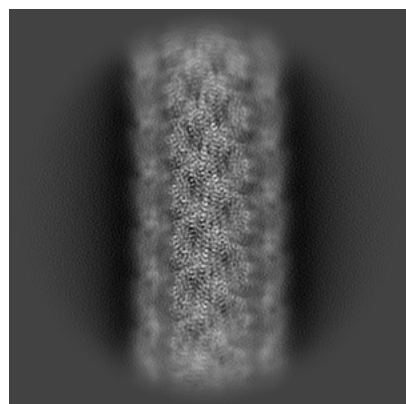
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64862. These allow visual inspection of the internal detail of the map and identification of artifacts.

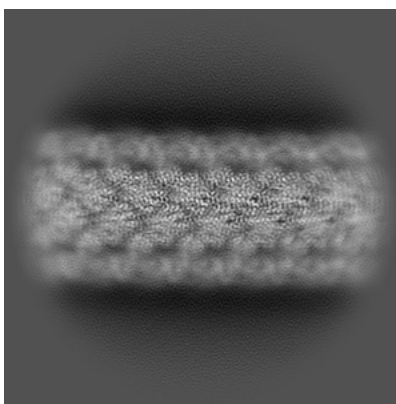
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

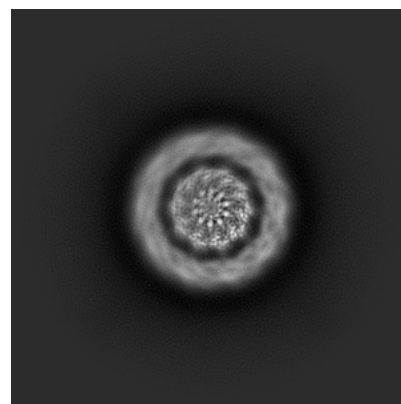
6.1.1 Primary map



X

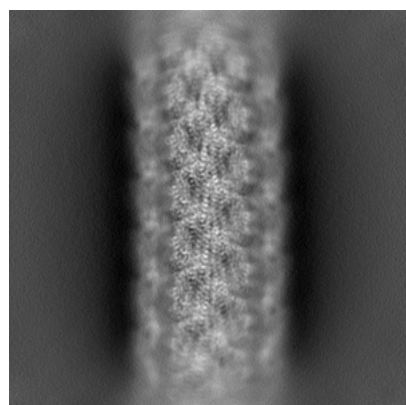


Y

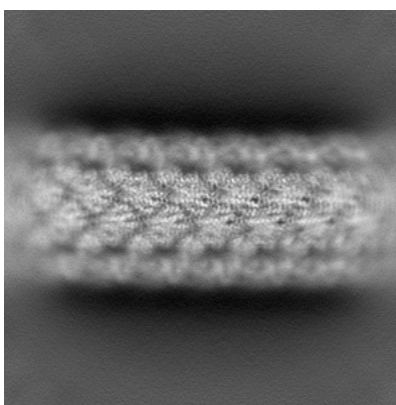


Z

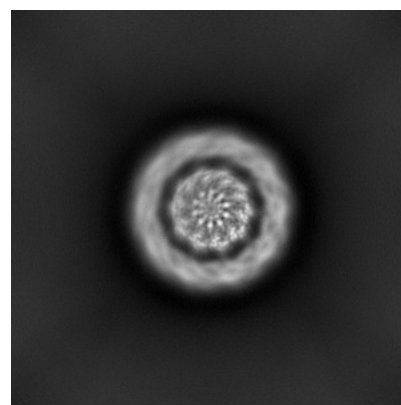
6.1.2 Raw map



X



Y

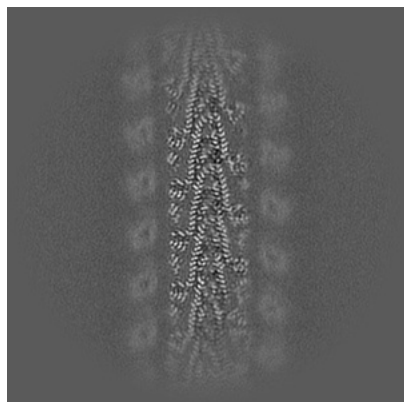


Z

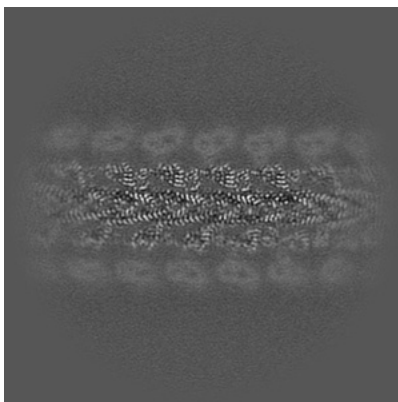
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

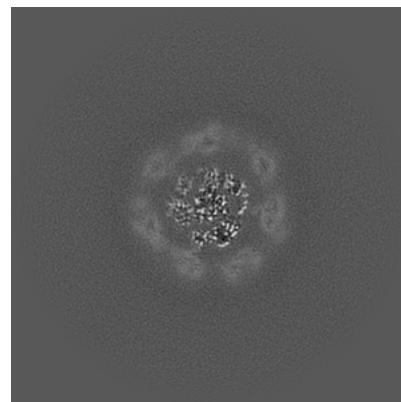
6.2.1 Primary map



X Index: 200

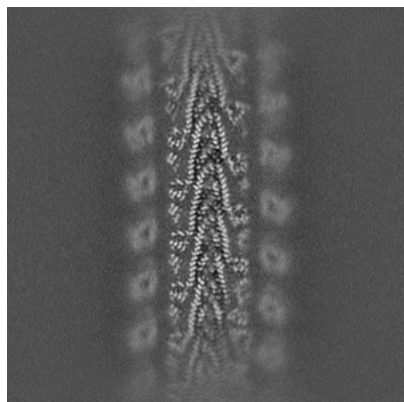


Y Index: 200

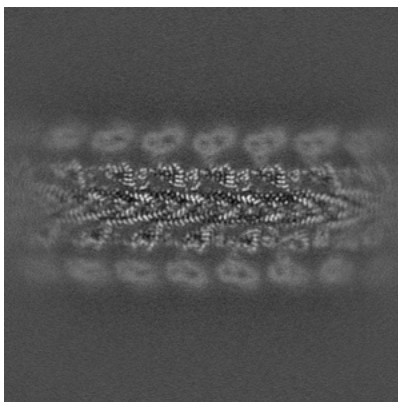


Z Index: 200

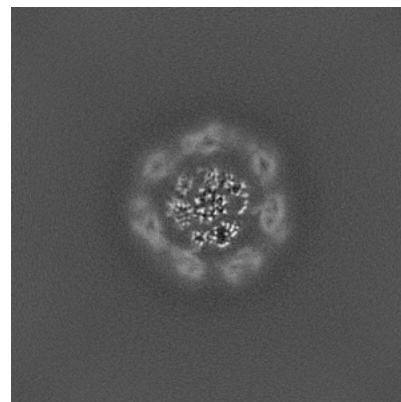
6.2.2 Raw map



X Index: 200



Y Index: 200

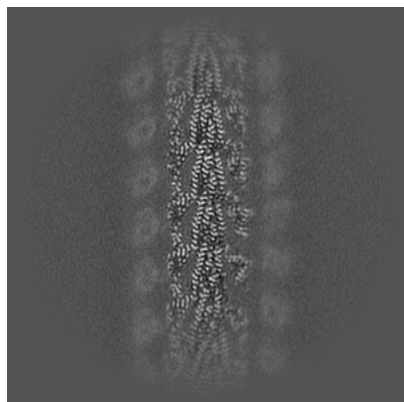


Z Index: 200

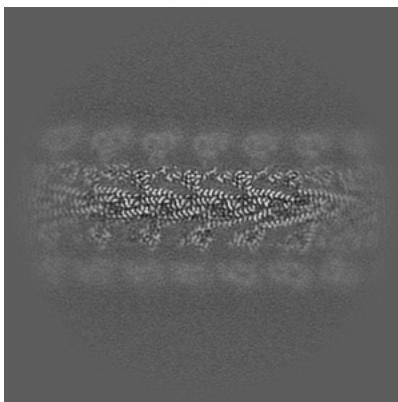
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

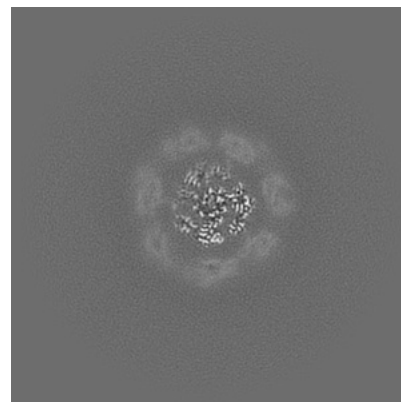
6.3.1 Primary map



X Index: 207

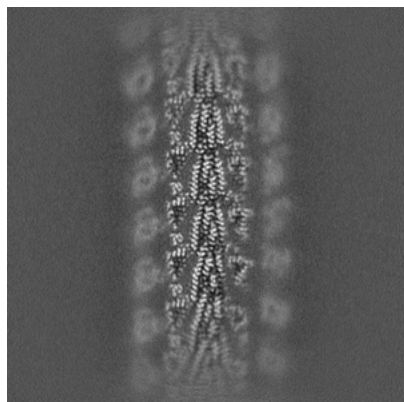


Y Index: 194

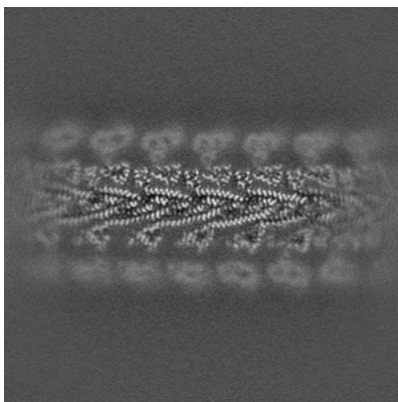


Z Index: 172

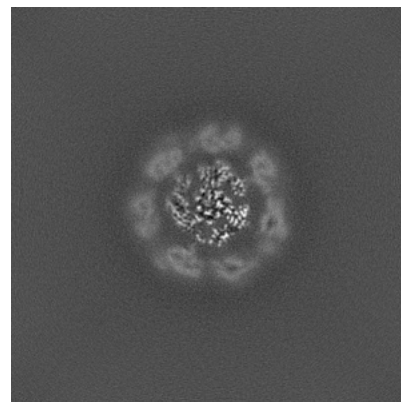
6.3.2 Raw map



X Index: 208



Y Index: 196

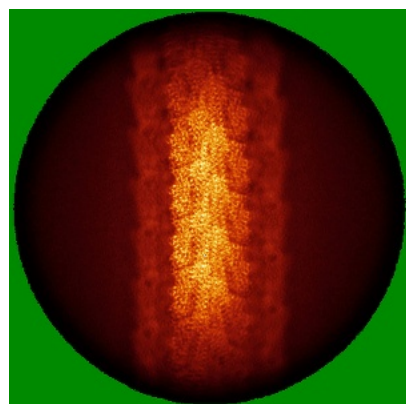


Z Index: 193

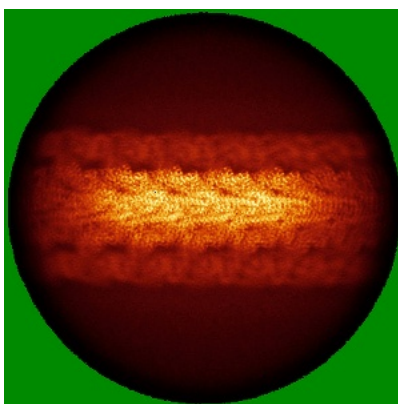
The images above show the largest variance slices of the map in three orthogonal directions.

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

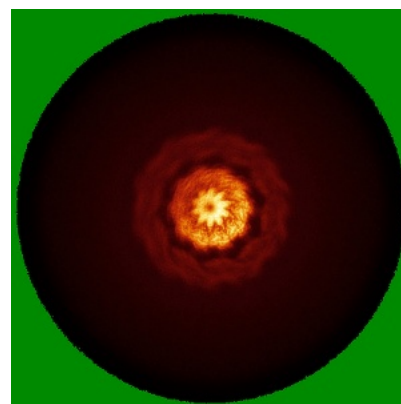
6.4.1 Primary map



X

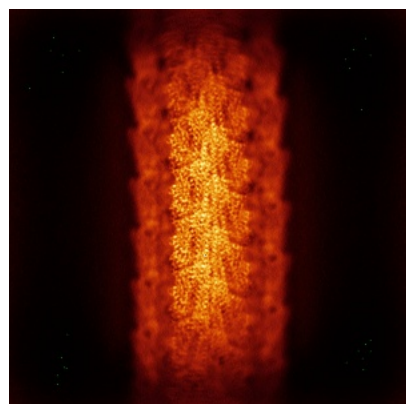


Y

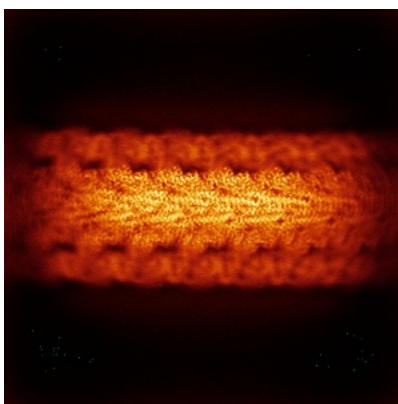


Z

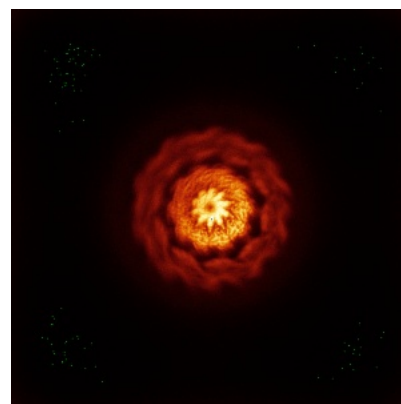
6.4.2 Raw map



X



Y

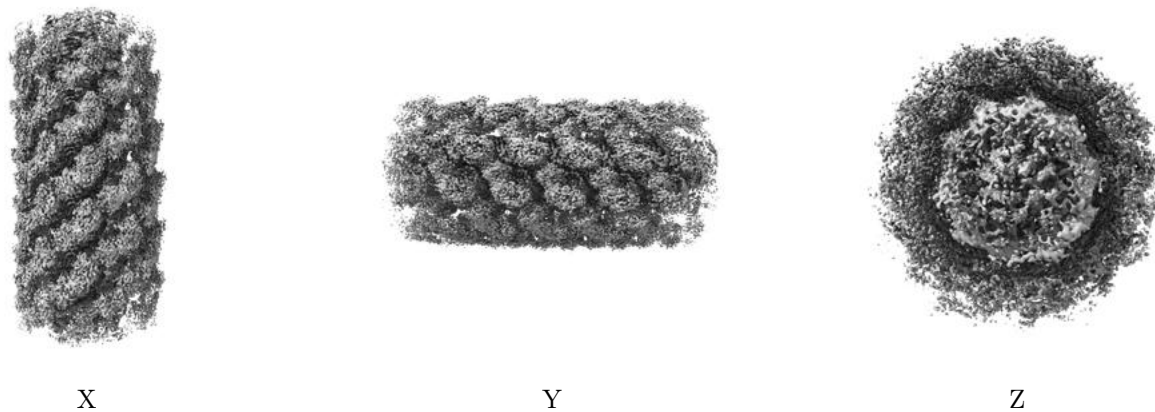


Z

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.

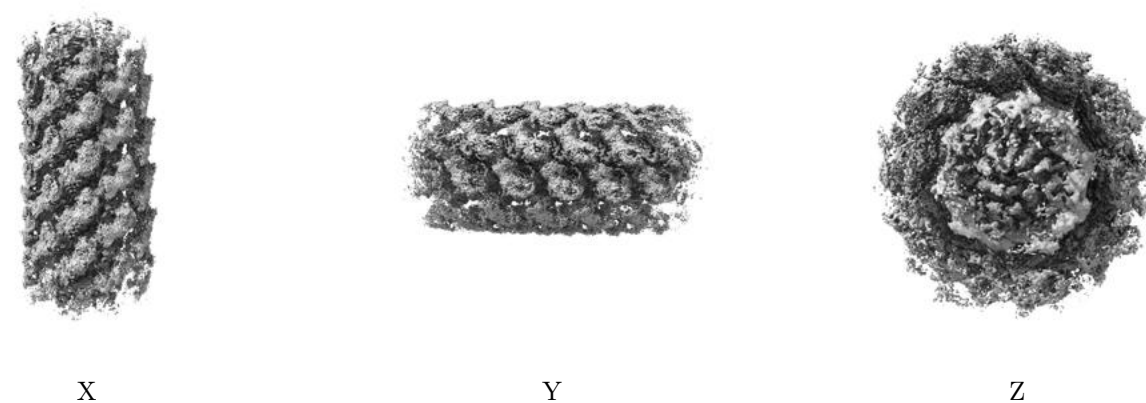
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

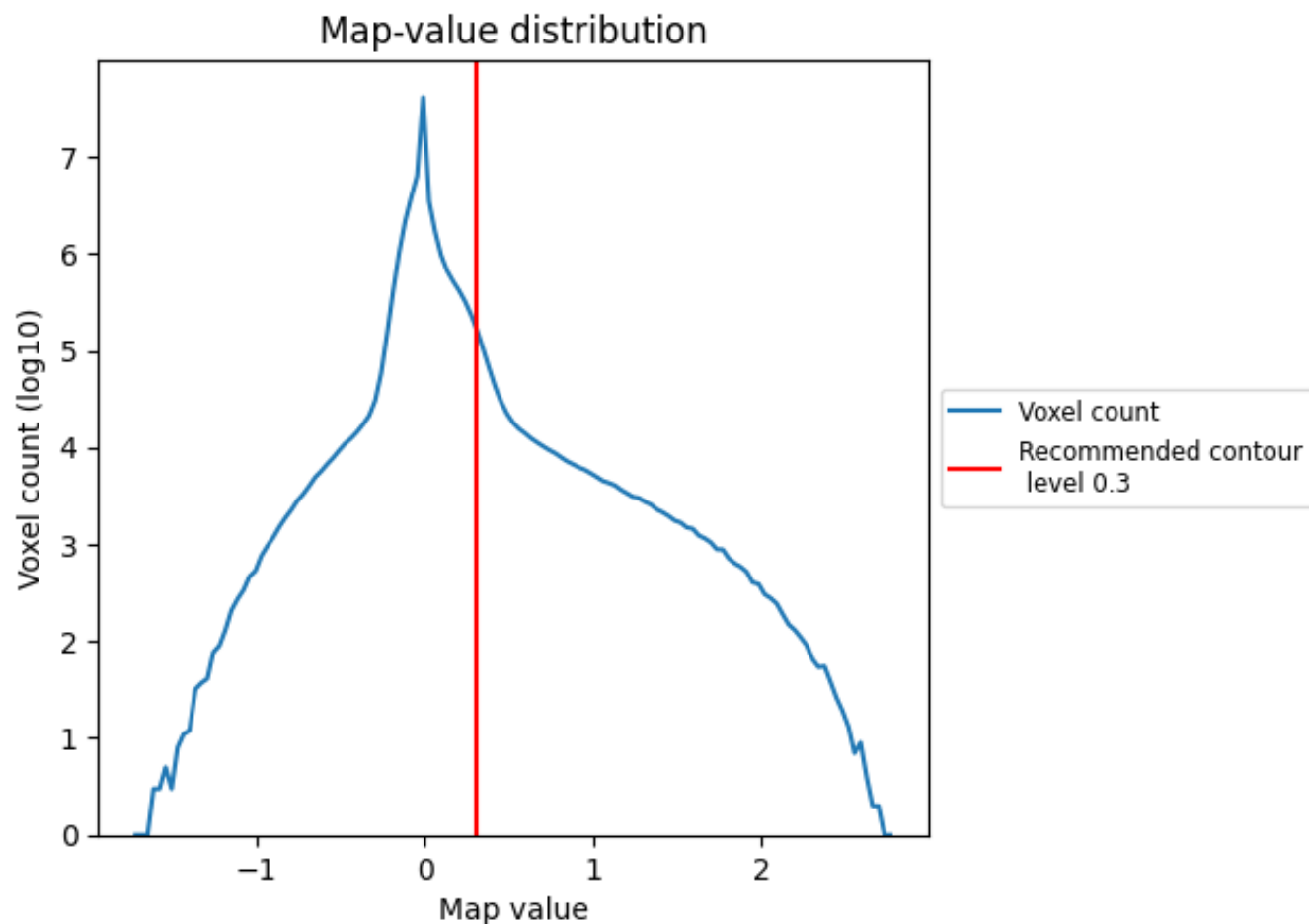
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

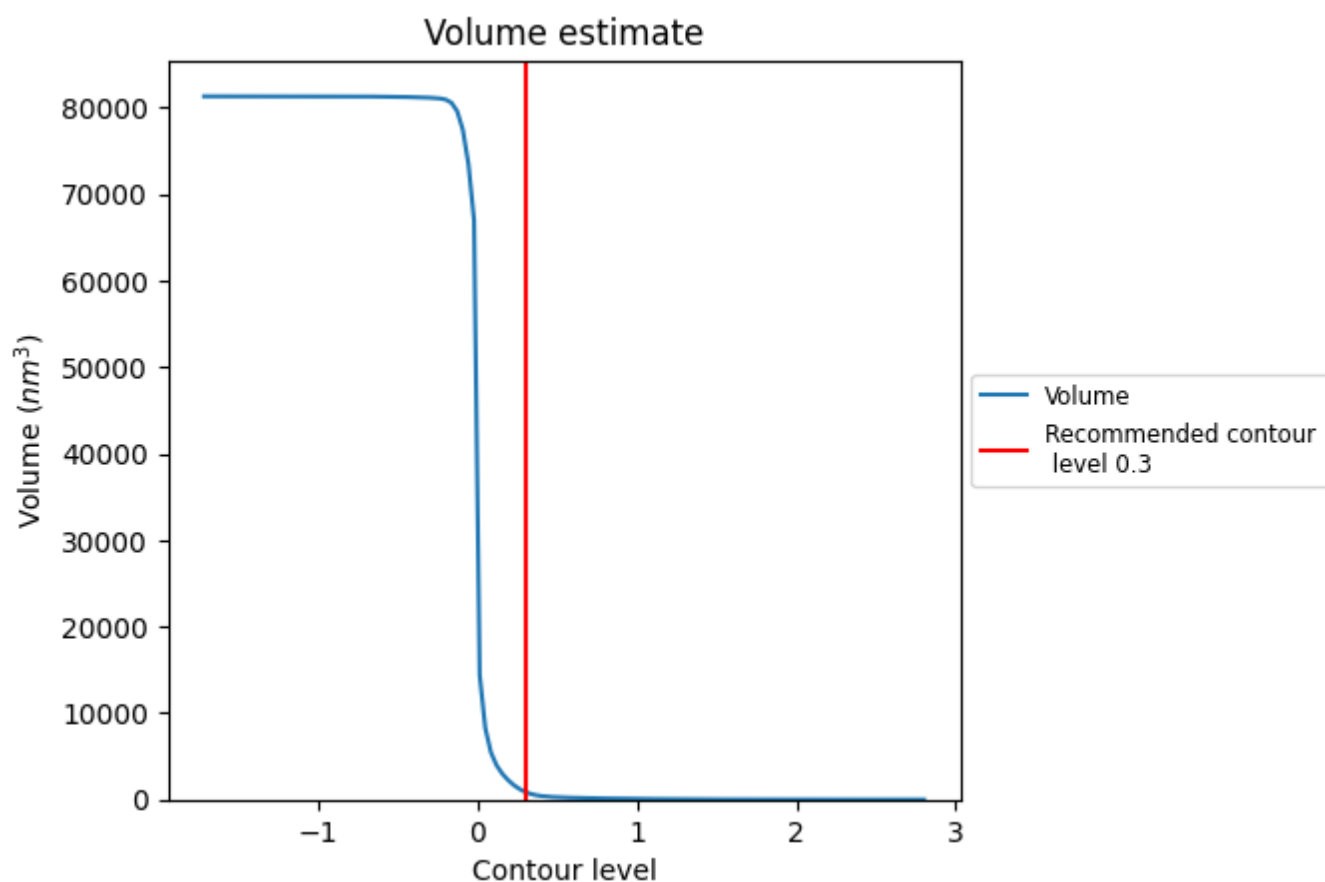
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

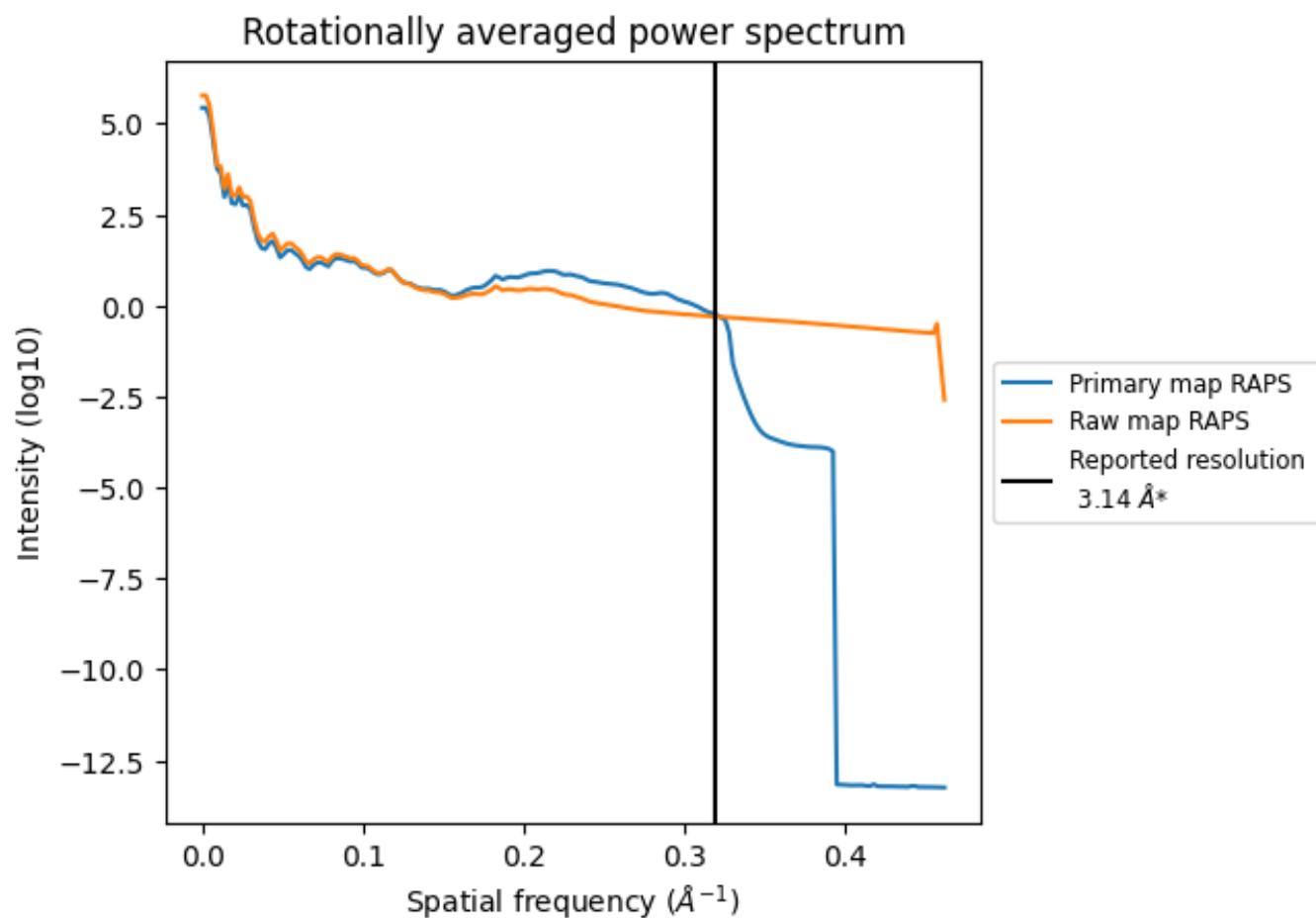
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 869 nm³; this corresponds to an approximate mass of 785 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

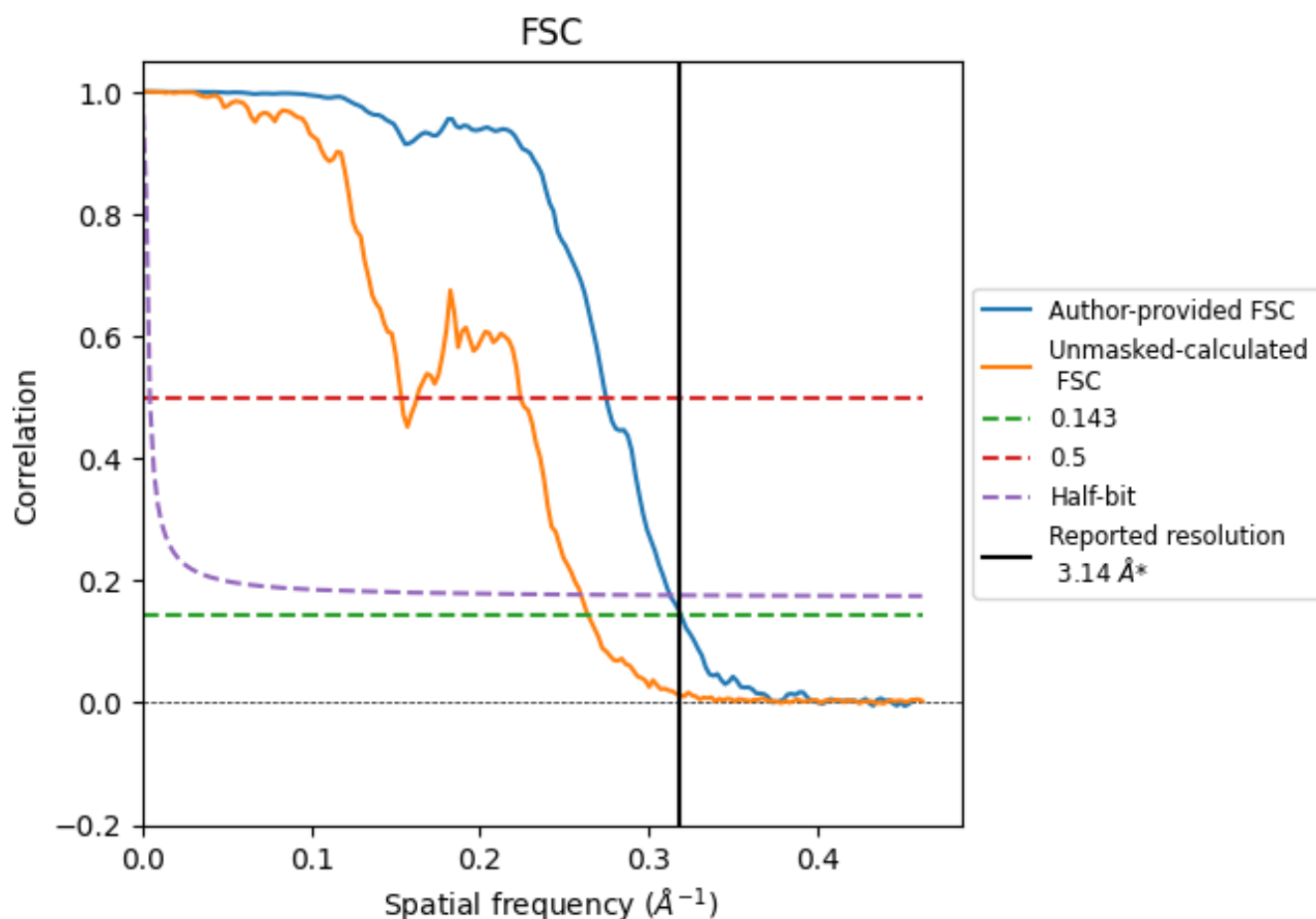


*Reported resolution corresponds to spatial frequency of 0.318 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.318 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

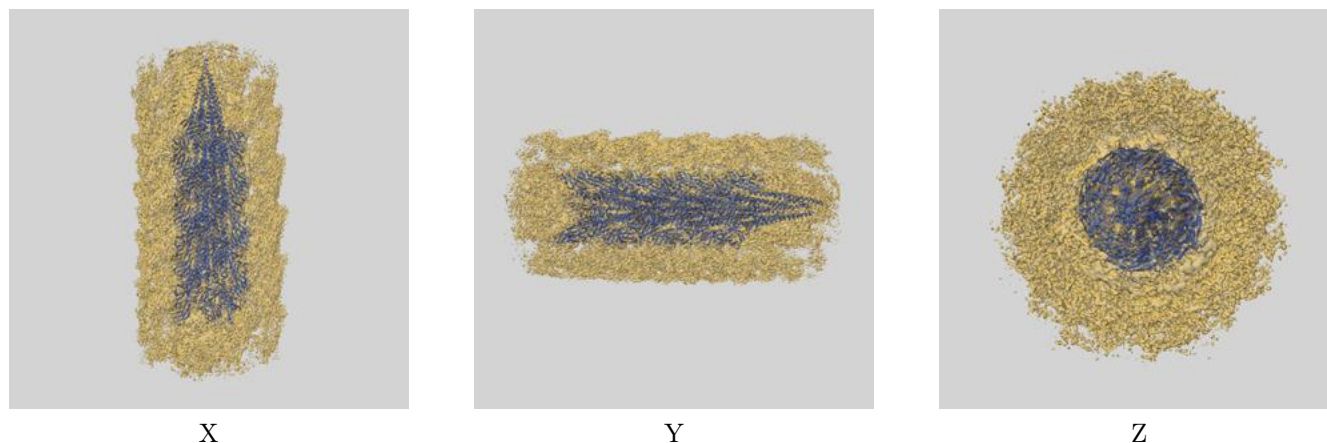
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.14	-	-
Author-provided FSC curve	3.14	3.64	3.20
Unmasked-calculated*	3.79	6.52	3.85

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.79 differs from the reported value 3.14 by more than 10 %

9 Map-model fit [i](#)

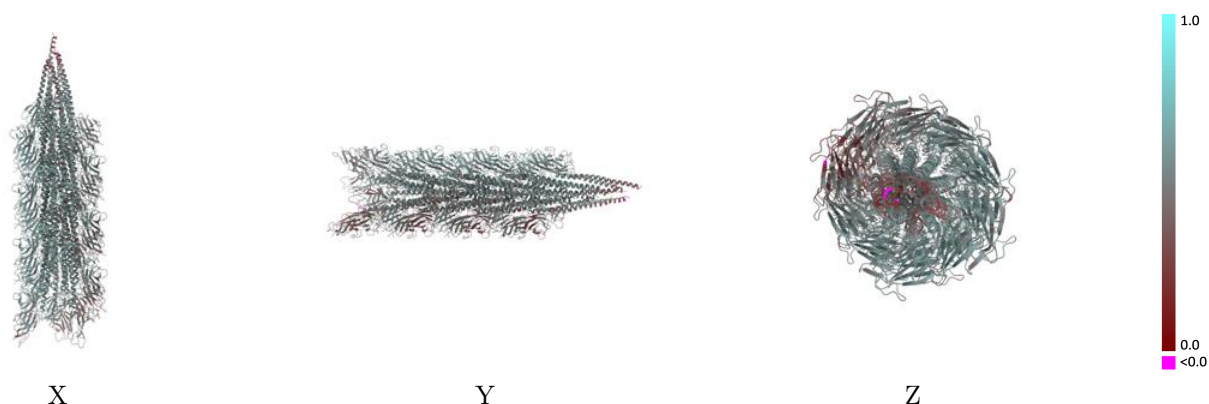
This section contains information regarding the fit between EMDB map EMD-64862 and PDB model 9V96. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



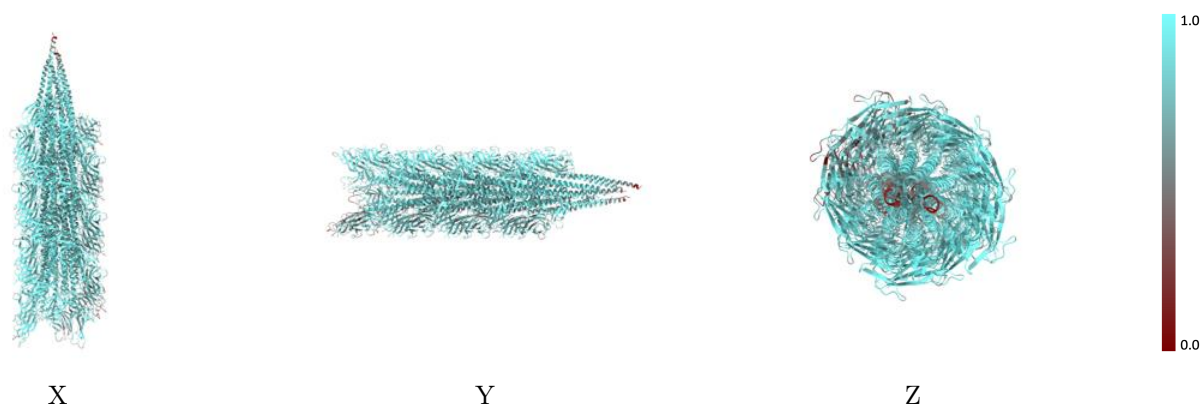
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



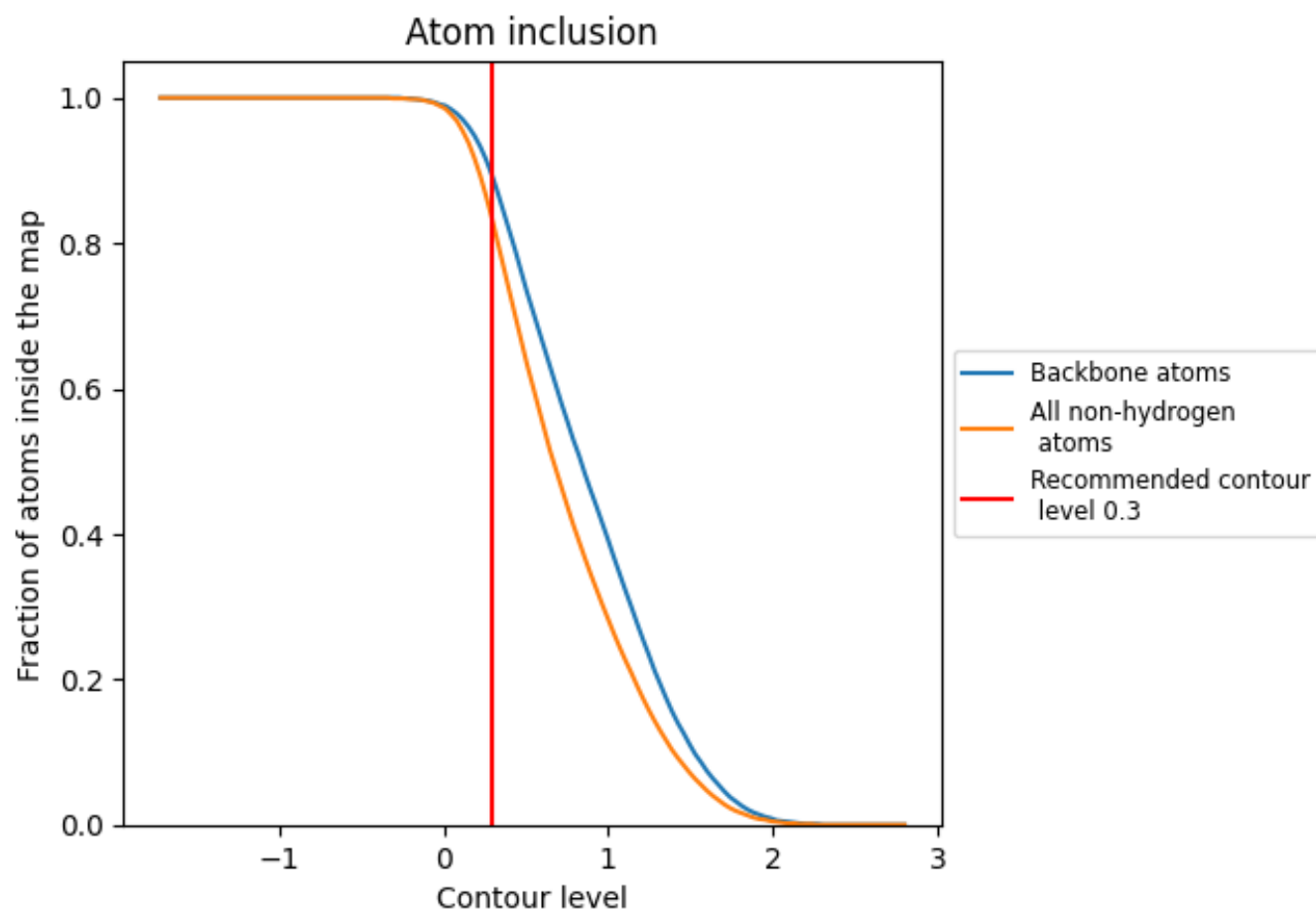
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion ⓘ



At the recommended contour level, 89% of all backbone atoms, 83% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8290	 0.5030
A	 0.9130	 0.5580
B	 0.6960	 0.3820
C	 0.8770	 0.5410
D	 0.8780	 0.5430
E	 0.8470	 0.5320
G	 0.8630	 0.5230
H	 0.9050	 0.5550
I	 0.8650	 0.5340
J	 0.9010	 0.5530
K	 0.9190	 0.5600
L	 0.9080	 0.5620
M	 0.8210	 0.5020
N	 0.9050	 0.5560
O	 0.9160	 0.5650
P	 0.8880	 0.5470
R	 0.8550	 0.5220
S	 0.9090	 0.5550
T	 0.9010	 0.5530
U	 0.8900	 0.5340
V	 0.8770	 0.5350
W	 0.8950	 0.5370
X	 0.8810	 0.5300
Y	 0.8120	 0.4940
Z	 0.8360	 0.5050
a	 0.8480	 0.4990
b	 0.8150	 0.4900
d	 0.7060	 0.4500
e	 0.7520	 0.4610
f	 0.7570	 0.4530
g	 0.6860	 0.4070
i	 0.6600	 0.3750
j	 0.6950	 0.3810
k	 0.6470	 0.3940
l	 0.7000	 0.4500



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
m	 0.8130	 0.4910
n	 0.8260	 0.4970
o	 0.8190	 0.4920
p	 0.8250	 0.5010