



## Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 02:19 AM EDT

PDB ID : 8FOP  
EMDB ID : EMD-29353  
Title : Structure of Agrobacterium tumefaciens bacteriophage Milano curved tail  
Authors : Sonani, R.R.; Leiman, P.G.; Wang, F.; Kreutzberger, M.A.B.; Sebastian, A.;  
Esteves, N.C.; Kelly, R.J.; Scharf, B.; Egelman, E.H.  
Deposited on : 2023-01-03  
Resolution : 3.20 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.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

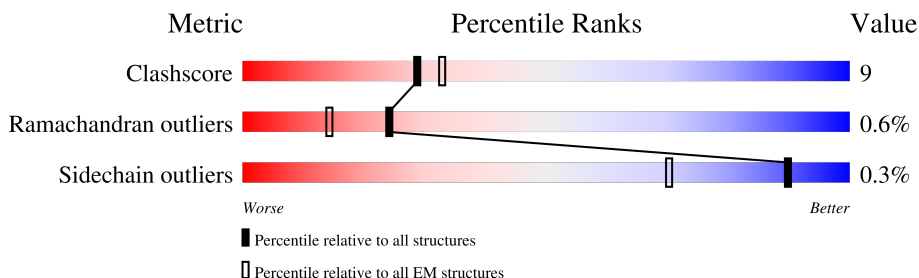
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 Å.

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









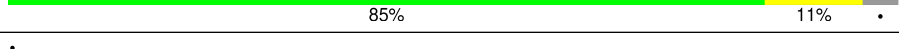
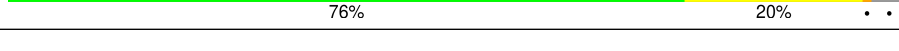
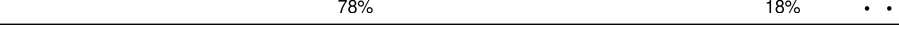
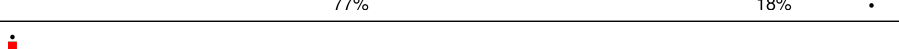
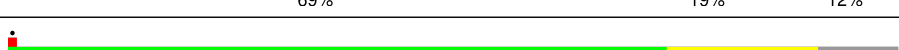

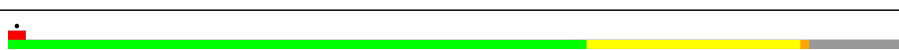
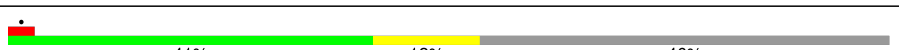
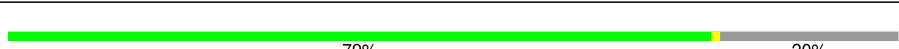





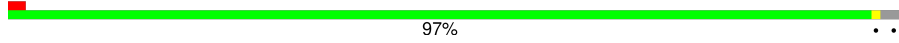

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	B	136	
1	C	136	
1	D	136	
1	E	136	
1	F	136	
1	G	136	
1	H	136	
1	I	136	

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Mol	Chain	Length	Quality of chain
1	J	136	
1	K	136	
1	L	136	
1	M	136	
1	N	136	
1	O	136	
1	P	136	
1	Q	136	
1	R	136	
1	S	136	
2	T	503	
2	U	503	
2	W	503	
2	X	503	
2	Z	503	
2	a	503	
2	c	503	
2	d	503	
2	f	503	
2	g	503	
2	i	503	
2	j	503	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 55484 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 Virion-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	130	Total	C	N	O	S	0	0
			989	614	164	205	6		
1	C	131	Total	C	N	O	S	0	0
			995	617	165	206	7		
1	D	130	Total	C	N	O	S	0	0
			989	614	164	205	6		
1	E	131	Total	C	N	O	S	0	0
			995	617	165	206	7		
1	F	130	Total	C	N	O	S	0	0
			989	614	164	205	6		
1	G	131	Total	C	N	O	S	0	0
			995	617	165	206	7		
1	H	131	Total	C	N	O	S	0	0
			995	617	165	206	7		
1	I	131	Total	C	N	O	S	0	0
			995	617	165	206	7		
1	J	131	Total	C	N	O	S	0	0
			995	617	165	206	7		
1	K	131	Total	C	N	O	S	0	0
			995	617	165	206	7		
1	L	131	Total	C	N	O	S	0	0
			995	617	165	206	7		
1	M	131	Total	C	N	O	S	0	0
			995	617	165	206	7		
1	N	131	Total	C	N	O	S	0	0
			995	617	165	206	7		
1	O	131	Total	C	N	O	S	0	0
			995	617	165	206	7		
1	P	131	Total	C	N	O	S	0	0
			995	617	165	206	7		
1	Q	131	Total	C	N	O	S	0	0
			995	617	165	206	7		
1	R	131	Total	C	N	O	S	0	0
			995	617	165	206	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	S	130	Total	C	N	O	S	0	0
			989	614	164	205	6		

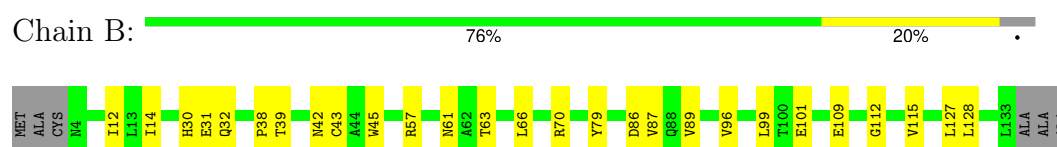
- Molecule 2 is a protein called Tail sheath protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	T	442	Total	C	N	O	S	0	0
			3369	2123	569	657	20		
2	U	460	Total	C	N	O	S	0	0
			3485	2191	591	683	20		
2	W	423	Total	C	N	O	S	0	0
			3216	2023	549	625	19		
2	X	449	Total	C	N	O	S	0	0
			3418	2150	578	670	20		
2	Z	271	Total	C	N	O	S	0	0
			2115	1326	367	410	12		
2	a	401	Total	C	N	O	S	0	0
			3076	1926	528	602	20		
2	c	408	Total	C	N	O	S	0	0
			3113	1952	535	607	19		
2	d	439	Total	C	N	O	S	0	0
			3331	2088	569	654	20		
2	f	397	Total	C	N	O	S	0	0
			3030	1900	522	590	18		
2	g	376	Total	C	N	O	S	0	0
			2890	1812	495	564	19		
2	i	373	Total	C	N	O	S	0	0
			2868	1802	488	560	18		
2	j	490	Total	C	N	O	S	0	0
			3687	2315	623	728	21		

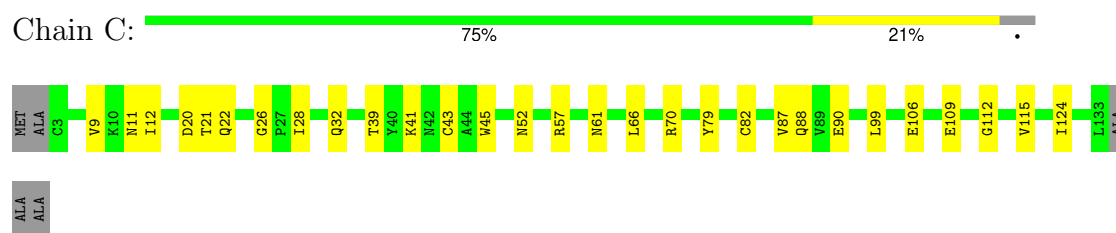
### 3 Residue-property plots

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

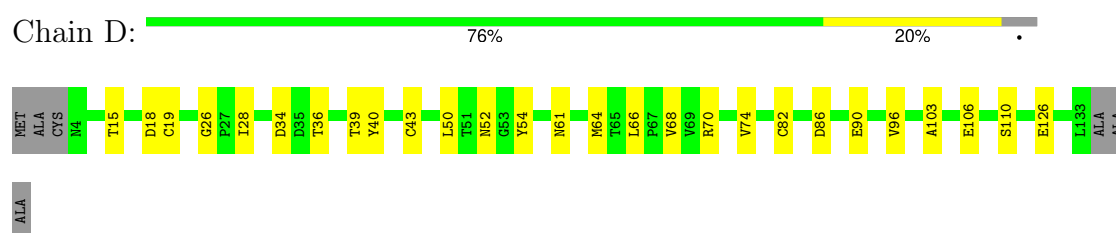
- Molecule 1: Virion-associated protein



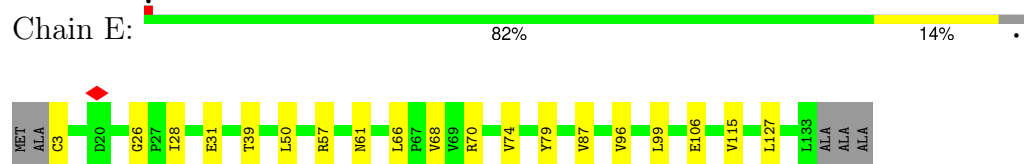
- Molecule 1: Virion-associated protein



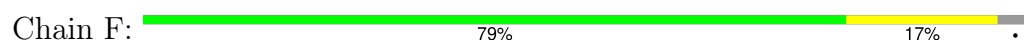
- Molecule 1: Virion-associated protein



- Molecule 1: Virion-associated protein

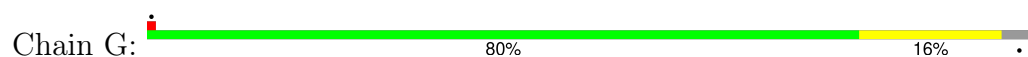


- Molecule 1: Virion-associated protein

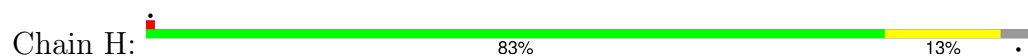




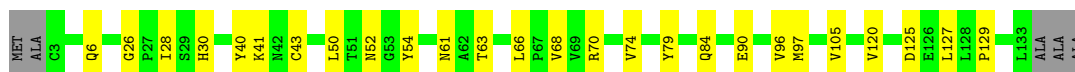
- Molecule 1: Virion-associated protein



- Molecule 1: Virion-associated protein



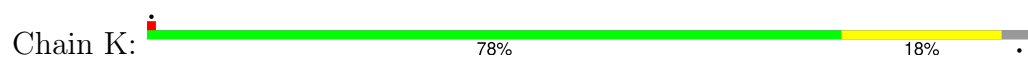
- Molecule 1: Virion-associated protein



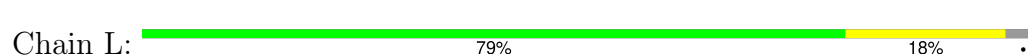
- Molecule 1: Virion-associated protein




- Molecule 1: Virion-associated protein



- Molecule 1: Virion-associated protein




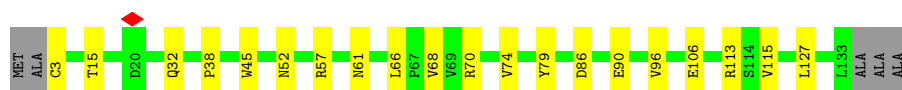
- Molecule 1: Virion-associated protein

Chain M:  81% 15%



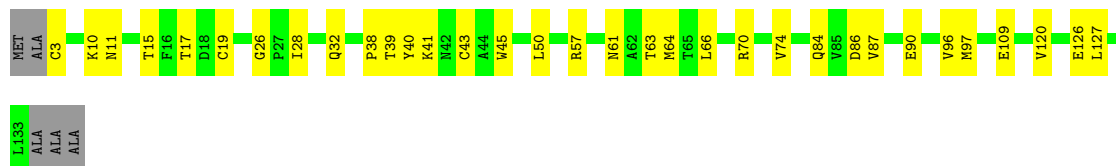
- Molecule 1: Virion-associated protein

Chain N:  82% 15%




- Molecule 1: Virion-associated protein

Chain O:  72% 24%




- Molecule 1: Virion-associated protein

Chain P:  85% 11%



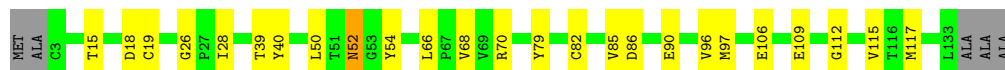
- Molecule 1: Virion-associated protein

Chain Q:  76% 20%



- Molecule 1: Virion-associated protein

Chain R:  78% 18%



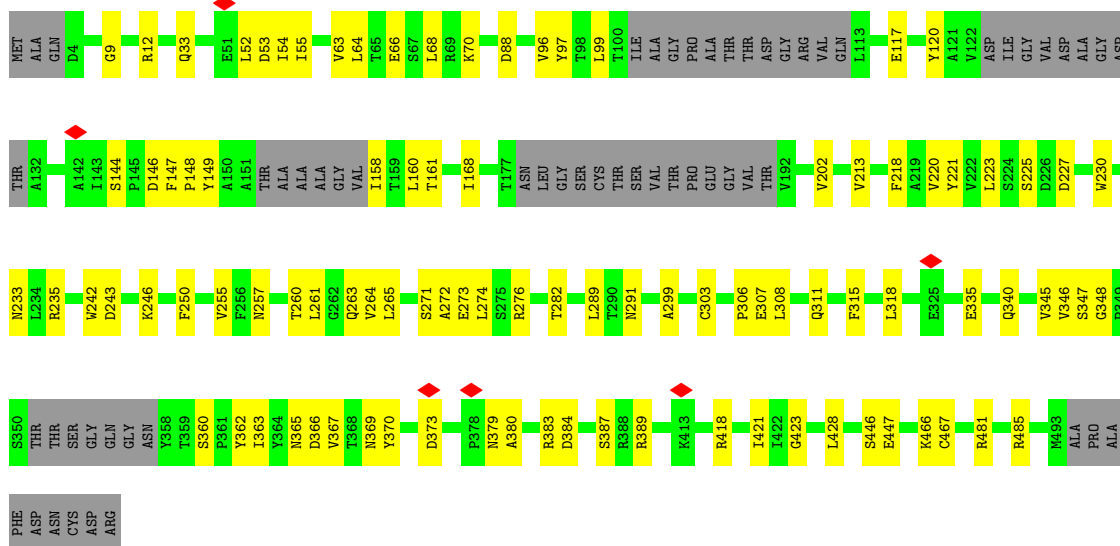
- Molecule 1: Virion-associated protein

Chain S:  77% 18%

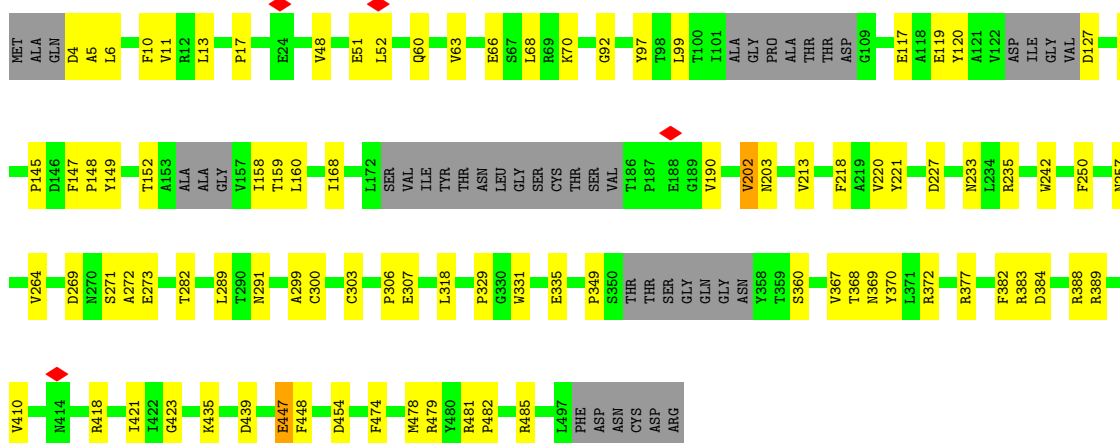




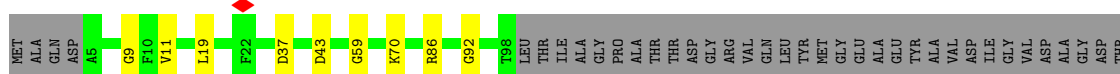
• Molecule 2: Tail sheath protein

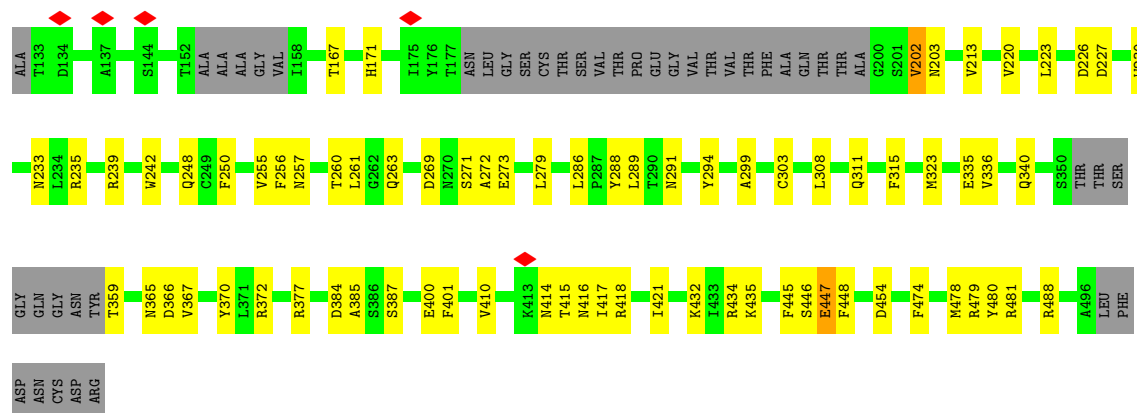


• Molecule 2: Tail sheath protein

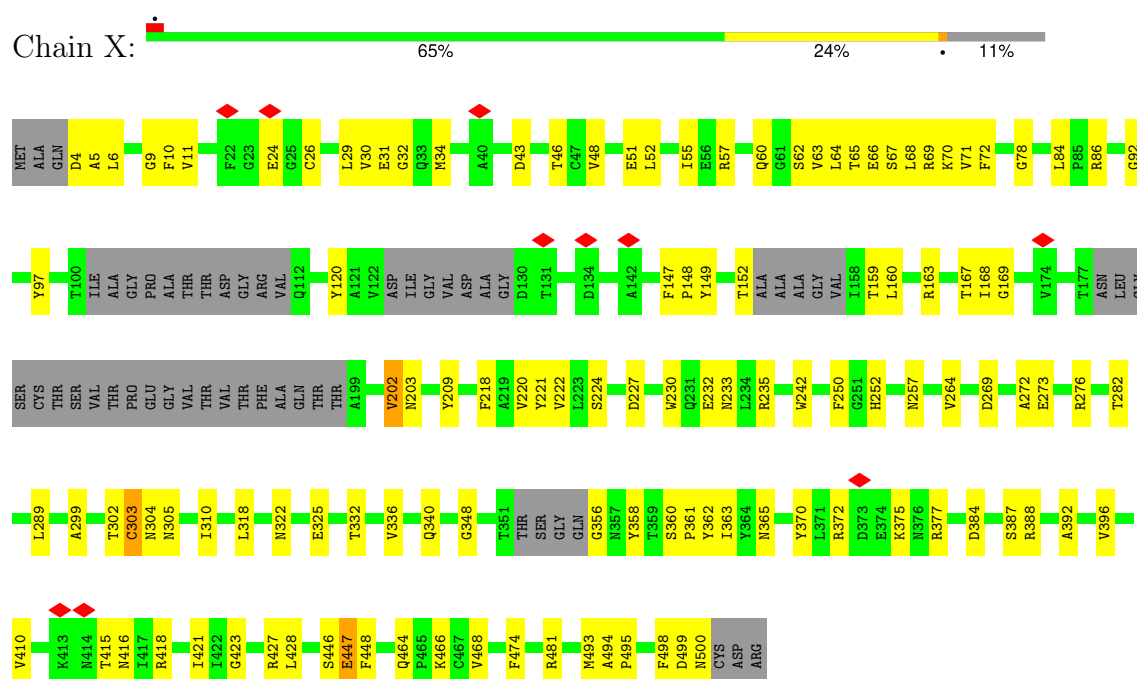


• Molecule 2: Tail sheath protein

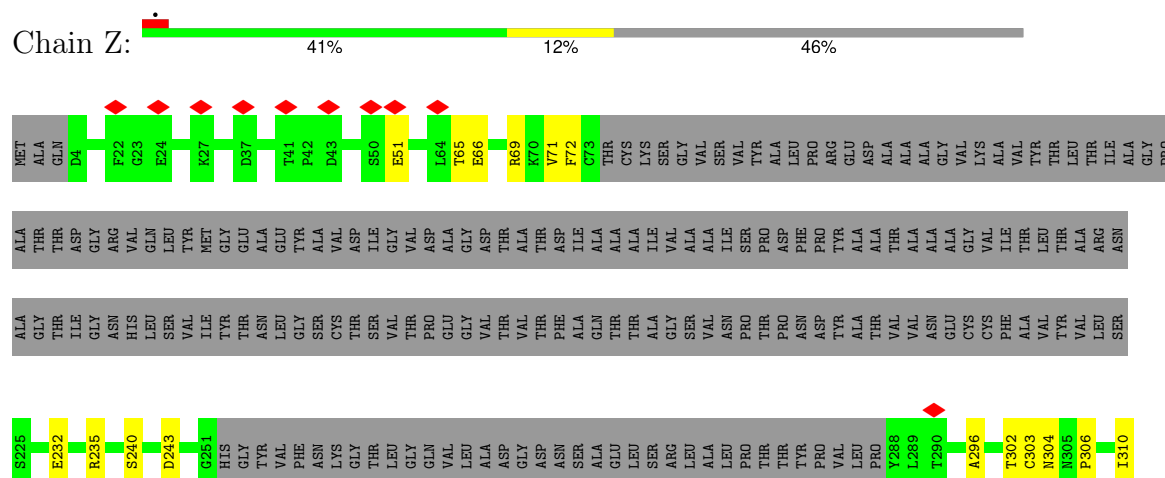




- Molecule 2: Tail sheath protein

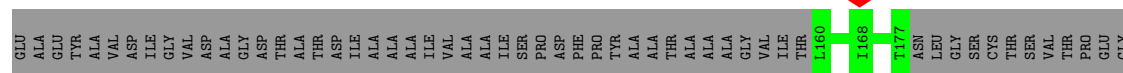


- Molecule 2: Tail sheath protein



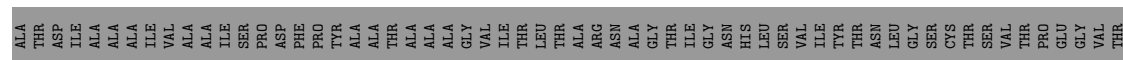


Frequency	Percentage
Often	78%
Not often	21%



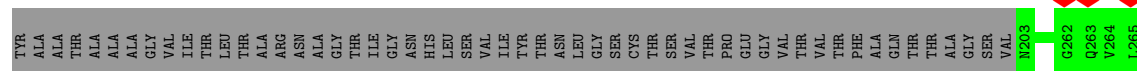
- Molecule 2: Tail sheath protein

Category	Percentage
Good job	73%
Not a good job	25%



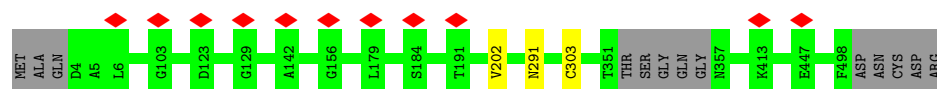
- Molecule 2: Tail sheath protein

Response	Percentage
Very bad	74%
Not very bad	26%



- Molecule 2: Tail sheath protein

Response	Percentage
Doing a good job	97%
Not doing a good job	3%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	228393	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)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.024	Depositor
Minimum map value	-0.595	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.048	Depositor
Recommended contour level	0.15	Depositor
Map size ( $\text{\AA}$ )	414.72003, 414.72003, 414.72003	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.08, 1.08, 1.08	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	B	0.26	0/1005	0.52	0/1374
1	C	0.26	0/1011	0.50	0/1382
1	D	0.27	0/1005	0.51	0/1374
1	E	0.26	0/1011	0.50	0/1382
1	F	0.25	0/1005	0.50	0/1374
1	G	0.26	0/1011	0.53	0/1382
1	H	0.26	0/1011	0.51	0/1382
1	I	0.25	0/1011	0.49	0/1382
1	J	0.26	0/1011	0.49	0/1382
1	K	0.27	0/1011	0.53	0/1382
1	L	0.25	0/1011	0.50	0/1382
1	M	0.25	0/1011	0.50	0/1382
1	N	0.26	0/1011	0.53	0/1382
1	O	0.26	0/1011	0.50	0/1382
1	P	0.25	0/1011	0.51	0/1382
1	Q	0.27	0/1011	0.56	1/1382 (0.1%)
1	R	0.26	0/1011	0.52	0/1382
1	S	0.26	0/1005	0.52	0/1374
2	T	0.25	0/3436	0.49	0/4681
2	U	0.26	0/3553	0.51	1/4843 (0.0%)
2	W	0.25	0/3281	0.51	0/4471
2	X	0.25	0/3486	0.50	0/4750
2	Z	0.25	0/2155	0.52	0/2919
2	a	0.26	0/3138	0.51	0/4269
2	c	0.25	0/3175	0.50	0/4324
2	d	0.26	0/3398	0.50	0/4635
2	f	0.25	0/3093	0.51	0/4212
2	g	0.25	0/2951	0.52	0/4018
2	i	0.26	0/2929	0.51	0/3988
2	j	0.25	0/3762	0.50	0/5138
All	All	0.26	0/56531	0.51	2/77092 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	U	0	1
2	W	0	1
2	X	0	1
2	d	0	1
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	300	CYS	CA-CB-SG	5.54	123.97	114.00
1	Q	3	CYS	C-N-CA	5.12	134.49	121.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	U	447	GLU	Peptide
2	W	447	GLU	Peptide
2	X	447	GLU	Peptide
2	d	447	GLU	Peptide

## 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	B	989	0	963	21	0
1	C	995	0	968	23	0
1	D	989	0	963	19	0
1	E	995	0	968	14	0
1	F	989	0	964	17	0
1	G	995	0	968	19	0
1	H	995	0	968	15	0
1	I	995	0	969	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	995	0	968	17	0
1	K	995	0	968	23	0
1	L	995	0	968	22	0
1	M	995	0	968	16	0
1	N	995	0	968	14	0
1	O	995	0	968	25	0
1	P	995	0	968	11	0
1	Q	995	0	968	21	0
1	R	995	0	968	17	0
1	S	989	0	963	18	0
2	T	3369	0	3258	60	0
2	U	3485	0	3372	56	0
2	W	3216	0	3118	61	0
2	X	3418	0	3296	92	0
2	Z	2115	0	2028	46	0
2	a	3076	0	2950	0	0
2	c	3113	0	3016	0	0
2	d	3331	0	3235	0	0
2	f	3030	0	2931	0	0
2	g	2890	0	2779	0	0
2	i	2868	0	2757	0	0
2	j	3687	0	3568	0	0
All	All	55484	0	53714	551	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 9.

All (551) 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:M:19:CYS:HG	1:O:3:CYS:N	1.53	1.05
1:L:19:CYS:HG	1:N:3:CYS:N	1.58	1.01
2:U:272:ALA:HB2	2:U:370:TYR:HB2	1.65	0.78
1:B:109:GLU:HG2	1:E:39:THR:HG22	1.64	0.77
2:X:415:THR:HG22	2:X:416:ASN:H	1.50	0.76
2:X:52:LEU:HD11	2:Z:377:ARG:H	1.50	0.76
1:D:15:THR:HB	1:D:86:ASP:HB2	1.68	0.76
2:X:372:ARG:HG2	2:X:377:ARG:HA	1.68	0.75
2:X:242:TRP:HE1	2:X:250:PHE:HA	1.52	0.74
1:M:100:THR:HG22	1:M:101:GLU:HG3	1.70	0.74
2:W:480:TYR:HE1	2:X:493:MET:HB3	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:235:ARG:NH1	2:U:269:ASP:OD2	2.21	0.73
1:L:15:THR:HB	1:L:86:ASP:HB2	1.70	0.73
2:T:53:ASP:O	2:T:55:ILE:N	2.22	0.73
2:W:415:THR:HG22	2:W:416:ASN:H	1.52	0.72
2:Z:447:GLU:HG3	2:Z:448:PHE:H	1.55	0.72
2:W:235:ARG:HG3	2:W:271:SER:HB2	1.71	0.72
2:T:12:ARG:HG3	2:W:488:ARG:HH21	1.53	0.72
1:H:113:ARG:HE	1:L:54:TYR:HD1	1.38	0.71
1:H:70:ARG:NH2	1:K:126:GLU:OE2	2.24	0.70
1:S:9:VAL:HG21	1:S:32:GLN:HE21	1.56	0.69
2:U:66:GLU:OE1	2:U:120:TYR:OH	2.08	0.69
1:J:70:ARG:NH2	1:M:126:GLU:OE2	2.26	0.69
1:N:113:ARG:HH21	1:R:54:TYR:HD2	1.41	0.69
1:L:109:GLU:HG2	1:O:41:LYS:HB2	1.76	0.68
1:I:41:LYS:NZ	1:I:43:CYS:O	2.27	0.68
1:H:32:GLN:HE21	1:H:33:PRO:HD2	1.59	0.67
2:W:481:ARG:HD3	2:X:498:PHE:H	1.58	0.67
2:X:31:GLU:HB3	2:X:84:LEU:HB3	1.77	0.67
2:X:303:CYS:SG	2:X:304:ASN:N	2.68	0.66
1:J:32:GLN:NE2	1:J:67:PRO:O	2.29	0.66
1:P:14:ILE:HG12	1:P:87:VAL:HG23	1.75	0.66
1:K:3:CYS:N	1:K:6:GLN:OE1	2.29	0.66
2:W:242:TRP:HE1	2:W:250:PHE:HA	1.61	0.66
2:T:271:SER:OG	2:T:273:GLU:OE1	2.13	0.66
2:W:70:LYS:HE2	2:W:289:LEU:HD23	1.76	0.65
1:M:19:CYS:SG	1:O:3:CYS:N	2.67	0.65
2:W:286:LEU:HB2	2:W:289:LEU:HD13	1.79	0.65
1:E:70:ARG:NH2	1:E:74:VAL:O	2.30	0.65
1:N:15:THR:HB	1:N:86:ASP:HB2	1.79	0.65
2:W:323:MET:O	2:W:359:THR:N	2.30	0.65
2:T:242:TRP:HE1	2:T:250:PHE:HA	1.60	0.65
2:W:261:LEU:HD22	2:W:335:GLU:HG3	1.78	0.65
2:W:446:SER:N	2:W:481:ARG:O	2.30	0.65
1:Q:66:LEU:HB3	1:Q:117:MET:HB2	1.77	0.64
2:Z:466:LYS:NZ	2:Z:467:CYS:SG	2.71	0.64
1:L:70:ARG:NH2	1:L:74:VAL:O	2.27	0.63
1:S:15:THR:HB	1:S:86:ASP:HB2	1.81	0.63
2:U:329:PRO:HB3	2:U:349:PRO:HD2	1.79	0.63
2:U:372:ARG:HG2	2:U:377:ARG:HA	1.79	0.63
2:T:97:TYR:HB2	2:T:160:LEU:HB2	1.81	0.63
2:U:48:VAL:HG11	2:U:68:LEU:HD21	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:261:LEU:HD22	2:T:335:GLU:HG2	1.80	0.63
1:I:70:ARG:NH2	1:I:74:VAL:O	2.28	0.63
2:U:203:ASN:HD22	2:U:227:ASP:HB2	1.63	0.62
1:G:88:GLN:HG2	2:X:428:LEU:HD22	1.80	0.62
1:L:90:GLU:HG3	1:L:96:VAL:HG22	1.80	0.62
1:H:40:TYR:OH	1:H:89:VAL:HG11	2.00	0.62
1:M:12:ILE:HG12	1:M:89:VAL:HG23	1.82	0.62
2:W:410:VAL:HG11	2:W:474:PHE:HZ	1.64	0.62
1:H:109:GLU:HB3	1:K:39:THR:HG22	1.81	0.61
2:U:410:VAL:HG11	2:U:474:PHE:HZ	1.65	0.61
2:Z:380:ALA:HA	2:Z:383:ARG:HG3	1.83	0.61
1:F:15:THR:HB	1:F:86:ASP:HB2	1.84	0.60
1:G:21:THR:OG1	1:G:23:GLU:OE1	2.19	0.60
1:S:90:GLU:HG3	1:S:96:VAL:HG22	1.84	0.60
2:X:257:ASN:HD21	2:X:276:ARG:HD2	1.66	0.60
1:K:4:ASN:OD1	1:K:5:LYS:N	2.34	0.60
2:X:235:ARG:NH1	2:X:269:ASP:OD2	2.34	0.60
1:K:26:GLY:HA2	1:K:28:ILE:HG13	1.84	0.59
1:R:40:TYR:CE2	1:R:97:MET:HG3	2.37	0.59
2:X:149:TYR:OH	2:X:169:GLY:O	2.20	0.59
2:Z:450:ASN:HB3	2:Z:453:GLU:HG2	1.84	0.59
1:E:87:VAL:HG12	1:E:99:LEU:HD22	1.84	0.59
2:U:269:ASP:O	2:U:369:ASN:ND2	2.35	0.59
2:U:17:PRO:HA	2:X:495:PRO:HD2	1.83	0.59
2:X:302:THR:O	2:X:305:ASN:N	2.29	0.59
1:C:39:THR:HG22	1:R:109:GLU:HB3	1.85	0.59
2:Z:401:PHE:HZ	2:Z:432:LYS:HG2	1.67	0.59
2:Z:470:GLN:HB2	2:Z:473:ILE:HD12	1.84	0.59
1:C:61:ASN:ND2	1:F:50:LEU:O	2.30	0.59
2:U:63:VAL:HG21	2:U:168:ILE:HD12	1.85	0.59
2:U:331:TRP:HE3	2:U:335:GLU:HG3	1.66	0.58
1:O:64:MET:HE1	1:O:87:VAL:HG11	1.85	0.58
1:B:45:TRP:CB	1:B:57:ARG:HE	2.17	0.58
2:U:52:LEU:H	2:W:377:ARG:NH1	2.01	0.58
2:U:318:LEU:O	2:U:360:SER:OG	2.22	0.58
1:G:50:LEU:HD11	1:G:56:GLN:HB2	1.86	0.57
1:L:66:LEU:HD22	1:L:87:VAL:HG11	1.86	0.57
2:Z:342:ASN:HA	2:Z:371:LEU:HD11	1.86	0.57
1:H:110:SER:O	1:K:40:TYR:N	2.33	0.57
2:X:499:ASP:OD1	2:X:500:ASN:N	2.33	0.57
2:X:232:GLU:OE2	2:X:235:ARG:NH2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:15:THR:HB	1:K:86:ASP:HB2	1.87	0.57
2:Z:418:ARG:HB3	2:Z:421:ILE:HD13	1.85	0.57
2:T:243:ASP:HB3	2:T:246:LYS:HG2	1.86	0.57
1:C:11:ASN:ND2	1:C:90:GLU:OE1	2.36	0.57
1:S:18:ASP:OD1	1:S:19:CYS:N	2.38	0.57
2:T:272:ALA:HB2	2:T:370:TYR:HB2	1.87	0.57
1:G:70:ARG:NH2	1:G:74:VAL:O	2.32	0.57
1:I:40:TYR:CE2	1:I:97:MET:HG3	2.40	0.57
2:Z:332:THR:OG1	2:Z:335:GLU:OE1	2.19	0.57
1:N:70:ARG:NH2	1:N:74:VAL:O	2.38	0.57
1:J:100:THR:HG22	1:J:101:GLU:HG3	1.85	0.56
1:R:90:GLU:HG3	1:R:96:VAL:HG22	1.86	0.56
2:T:223:LEU:HD23	2:T:225:SER:H	1.68	0.56
2:U:271:SER:OG	2:U:273:GLU:OE1	2.19	0.56
1:B:61:ASN:ND2	1:E:50:LEU:O	2.36	0.56
1:Q:96:VAL:HB	1:Q:127:LEU:HB2	1.88	0.56
2:T:346:VAL:HG23	2:T:365:ASN:HD21	1.69	0.56
2:X:46:THR:OG1	2:X:57:ARG:NH2	2.37	0.56
1:B:31:GLU:OE1	1:F:52:ASN:ND2	2.38	0.56
1:L:14:ILE:HG12	1:L:87:VAL:HG22	1.88	0.56
2:T:9:GLY:HA2	2:T:12:ARG:HH12	1.70	0.56
2:Z:372:ARG:HD3	2:Z:377:ARG:HE	1.71	0.56
1:N:90:GLU:HG3	1:N:96:VAL:HG22	1.88	0.56
1:B:63:THR:OG1	1:Q:109:GLU:OE2	2.24	0.56
1:M:14:ILE:HG12	1:M:87:VAL:HG22	1.87	0.56
2:X:43:ASP:OD1	2:X:86:ARG:NH1	2.39	0.56
1:M:15:THR:HB	1:M:86:ASP:HB2	1.87	0.56
1:B:42:ASN:HD22	1:Q:76:LEU:HD22	1.71	0.55
1:D:61:ASN:ND2	1:G:50:LEU:O	2.29	0.55
2:Z:384:ASP:O	2:Z:387:SER:OG	2.21	0.55
1:J:109:GLU:HB3	1:M:39:THR:HG22	1.87	0.55
2:Z:396:VAL:O	2:Z:400:GLU:HG2	2.06	0.55
2:X:318:LEU:HB2	2:X:361:PRO:HG2	1.89	0.55
2:U:481:ARG:HD2	2:U:482:PRO:HD2	1.87	0.55
2:X:52:LEU:HD13	2:Z:377:ARG:HD3	1.88	0.55
1:K:5:LYS:HD2	1:L:54:TYR:HE2	1.71	0.55
2:U:435:LYS:NZ	2:U:439:ASP:OD2	2.38	0.55
1:J:19:CYS:HG	1:L:3:CYS:N	2.04	0.54
2:U:367:VAL:HA	2:U:384:ASP:HA	1.88	0.54
1:L:32:GLN:NE2	1:L:38:PRO:HD3	2.22	0.54
1:O:17:THR:HB	1:O:84:GLN:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:70:ARG:HH21	1:J:76:LEU:N	2.05	0.54
1:Q:18:ASP:OD2	1:Q:19:CYS:N	2.40	0.54
2:X:32:GLY:H	2:X:64:LEU:HD12	1.72	0.54
1:C:109:GLU:HB3	1:F:39:THR:HG22	1.89	0.54
2:U:13:LEU:O	2:W:248:GLN:NE2	2.39	0.54
1:K:3:CYS:SG	1:K:4:ASN:N	2.80	0.54
1:L:61:ASN:ND2	1:O:50:LEU:O	2.33	0.54
1:M:90:GLU:HG3	1:M:96:VAL:HG22	1.89	0.54
1:B:32:GLN:HE22	1:B:38:PRO:HD3	1.73	0.54
1:B:39:THR:HB	1:Q:109:GLU:HB3	1.90	0.54
1:C:99:LEU:HD12	1:C:124:ILE:HG12	1.89	0.54
1:H:96:VAL:HB	1:H:127:LEU:HB2	1.90	0.54
2:Z:65:THR:HG22	2:Z:69:ARG:NH1	2.22	0.54
1:K:40:TYR:CE2	1:K:97:MET:HG3	2.44	0.53
1:S:70:ARG:HD2	1:S:76:LEU:HD13	1.88	0.53
2:T:466:LYS:HD2	2:T:467:CYS:N	2.23	0.53
2:X:415:THR:HG22	2:X:416:ASN:N	2.20	0.53
1:I:26:GLY:HA2	1:I:28:ILE:HG13	1.91	0.53
1:I:90:GLU:HG3	1:I:96:VAL:HG22	1.89	0.53
2:U:99:LEU:HB3	2:U:158:ILE:HB	1.90	0.53
2:T:117:GLU:H	2:T:120:TYR:HD2	1.57	0.53
2:U:117:GLU:HG3	2:U:119:GLU:H	1.73	0.53
2:X:325:GLU:OE1	2:X:356:GLY:N	2.41	0.53
1:I:84:GLN:NE2	1:K:3:CYS:SG	2.81	0.53
1:N:61:ASN:ND2	1:Q:50:LEU:O	2.34	0.53
2:X:392:ALA:O	2:X:396:VAL:HG23	2.08	0.53
2:Z:336:VAL:O	2:Z:340:GLN:HG2	2.08	0.53
1:K:40:TYR:OH	1:K:89:VAL:HG11	2.09	0.53
2:Z:384:ASP:OD1	2:Z:385:ALA:N	2.42	0.53
1:B:45:TRP:HB3	1:B:57:ARG:HE	1.73	0.53
1:D:39:THR:HG22	1:S:109:GLU:HB3	1.90	0.53
2:X:446:SER:N	2:X:481:ARG:O	2.41	0.53
1:B:79:TYR:HB3	1:B:115:VAL:HG11	1.91	0.53
2:U:220:VAL:HG21	2:U:299:ALA:HB2	1.90	0.53
1:F:63:THR:HG22	1:F:120:VAL:HG22	1.91	0.53
1:N:79:TYR:HB3	1:N:115:VAL:HG11	1.89	0.53
1:Q:40:TYR:CZ	1:Q:97:MET:HG3	2.44	0.53
2:U:127:ASP:N	2:U:130:ASP:OD2	2.41	0.53
2:U:152:THR:OG1	2:U:159:THR:O	2.26	0.53
2:W:415:THR:HG22	2:W:416:ASN:N	2.22	0.53
2:Z:375:LYS:O	2:Z:375:LYS:HD3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:66:LEU:HD22	1:G:87:VAL:HG21	1.90	0.53
2:U:97:TYR:HB2	2:U:160:LEU:HB2	1.90	0.53
2:X:167:THR:OG1	2:X:203:ASN:ND2	2.36	0.53
1:C:41:LYS:HB2	1:R:109:GLU:HG2	1.91	0.52
1:K:12:ILE:HG12	1:K:89:VAL:HG23	1.90	0.52
2:W:92:GLY:HA2	2:W:202:VAL:HB	1.90	0.52
1:R:26:GLY:HA2	1:R:28:ILE:HG13	1.90	0.52
2:X:66:GLU:HB3	2:X:289:LEU:HD21	1.91	0.52
2:X:152:THR:OG1	2:X:159:THR:O	2.24	0.52
1:C:9:VAL:HG22	1:C:32:GLN:HE21	1.74	0.52
1:E:61:ASN:ND2	1:H:50:LEU:O	2.38	0.52
2:T:318:LEU:O	2:T:360:SER:OG	2.26	0.52
1:O:15:THR:HB	1:O:86:ASP:HB2	1.92	0.52
2:U:368:THR:N	2:U:383:ARG:O	2.36	0.52
2:W:294:TYR:OH	2:W:366:ASP:OD1	2.26	0.52
2:X:63:VAL:HG21	2:X:168:ILE:HD12	1.92	0.52
1:G:40:TYR:OH	1:G:89:VAL:HG11	2.09	0.52
1:H:60:SER:OG	1:H:61:ASN:N	2.42	0.52
2:T:144:SER:OG	2:T:146:ASP:OD1	2.22	0.52
2:T:264:VAL:HG13	2:T:265:LEU:HD12	1.92	0.52
1:N:96:VAL:HB	1:N:127:LEU:HB2	1.92	0.52
2:X:92:GLY:HA2	2:X:202:VAL:HB	1.92	0.52
1:H:32:GLN:NE2	1:H:67:PRO:O	2.43	0.52
2:X:66:GLU:OE1	2:X:120:TYR:OH	2.28	0.52
2:X:242:TRP:CZ3	2:X:273:GLU:HG3	2.44	0.52
2:T:384:ASP:O	2:T:387:SER:OG	2.25	0.52
2:X:318:LEU:O	2:X:360:SER:OG	2.28	0.52
1:F:110:SER:O	1:I:40:TYR:N	2.36	0.51
1:C:87:VAL:HG12	1:C:99:LEU:HD22	1.93	0.51
1:G:26:GLY:HA2	1:G:28:ILE:HG13	1.92	0.51
1:S:14:ILE:HG12	1:S:87:VAL:HG22	1.92	0.51
2:Z:331:TRP:HE3	2:Z:335:GLU:HB3	1.76	0.51
1:D:18:ASP:OD1	1:D:19:CYS:N	2.43	0.51
1:Q:32:GLN:NE2	1:Q:67:PRO:O	2.43	0.51
1:C:26:GLY:HA2	1:C:28:ILE:HG13	1.92	0.51
1:L:109:GLU:HB3	1:O:39:THR:HG22	1.93	0.51
2:T:220:VAL:HG21	2:T:299:ALA:HB2	1.93	0.51
1:P:84:GLN:HE21	1:P:101:GLU:HA	1.76	0.51
2:U:331:TRP:CE3	2:U:335:GLU:HG3	2.45	0.51
2:W:480:TYR:CE1	2:X:493:MET:HB3	2.40	0.51
2:Z:65:THR:O	2:Z:69:ARG:NH1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:70:LYS:NZ	2:T:117:GLU:OE2	2.37	0.51
2:T:99:LEU:HB3	2:T:158:ILE:HB	1.93	0.51
1:J:12:ILE:HG12	1:J:89:VAL:HG22	1.92	0.51
1:M:105:VAL:HG23	1:M:106:GLU:HG2	1.93	0.50
1:D:26:GLY:HA2	1:D:28:ILE:HG13	1.93	0.50
2:W:414:ASN:HB3	2:X:447:GLU:OE1	2.11	0.50
2:Z:232:GLU:HG2	2:Z:235:ARG:HH21	1.76	0.50
1:O:109:GLU:HB3	1:R:39:THR:HB	1.93	0.50
2:Z:66:GLU:HA	2:Z:69:ARG:CZ	2.41	0.50
1:E:66:LEU:HD22	1:E:87:VAL:HG21	1.93	0.50
2:U:92:GLY:HA2	2:U:202:VAL:HB	1.93	0.50
2:X:9:GLY:O	2:X:11:VAL:N	2.43	0.50
2:X:410:VAL:HG11	2:X:474:PHE:HZ	1.77	0.50
1:D:52:ASN:N	1:S:61:ASN:OD1	2.45	0.50
1:F:70:ARG:NH2	1:F:74:VAL:O	2.34	0.50
2:X:322:ASN:HB3	2:X:358:TYR:HB3	1.93	0.50
1:S:40:TYR:CE2	1:S:97:MET:HG3	2.46	0.50
1:C:52:ASN:ND2	1:Q:31:GLU:OE2	2.45	0.50
1:P:17:THR:HB	1:P:84:GLN:HB3	1.93	0.50
2:W:9:GLY:O	2:W:11:VAL:N	2.45	0.50
1:K:5:LYS:HD2	1:L:54:TYR:CE2	2.46	0.50
1:Q:14:ILE:HG12	1:Q:87:VAL:HG23	1.93	0.50
2:U:418:ARG:HB2	2:U:421:ILE:HD13	1.94	0.50
2:X:6:LEU:HD11	2:Z:403:GLN:HG3	1.94	0.50
2:X:257:ASN:ND2	2:X:276:ARG:HD2	2.26	0.49
2:X:418:ARG:HB2	2:X:421:ILE:HD13	1.93	0.49
1:S:64:MET:HB3	1:S:119:ILE:HB	1.94	0.49
2:T:260:THR:HG22	2:T:263:GLN:HG2	1.95	0.49
2:W:43:ASP:OD1	2:W:86:ARG:NH1	2.38	0.49
1:D:40:TYR:HD1	1:D:64:MET:HG3	1.78	0.49
2:X:242:TRP:CH2	2:X:388:ARG:HD3	2.48	0.49
2:X:273:GLU:N	2:X:273:GLU:OE1	2.45	0.49
2:Z:446:SER:N	2:Z:481:ARG:O	2.45	0.49
1:D:103:ALA:HB3	1:G:55:VAL:HG21	1.94	0.49
1:J:87:VAL:HG21	1:J:119:ILE:HD13	1.95	0.49
2:Z:425:ASN:OD1	2:Z:428:LEU:HG	2.12	0.49
1:H:105:VAL:HG23	1:H:106:GLU:H	1.78	0.49
2:T:66:GLU:OE1	2:T:120:TYR:OH	2.31	0.49
1:J:30:HIS:NE2	1:J:79:TYR:OH	2.27	0.49
1:O:45:TRP:HB2	1:O:57:ARG:HH21	1.76	0.49
1:P:105:VAL:HA	1:S:47:ASN:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:TYR:HB3	1:C:115:VAL:HG11	1.95	0.49
1:R:79:TYR:HB3	1:R:115:VAL:HG11	1.94	0.49
2:T:63:VAL:HG11	2:T:168:ILE:HG21	1.95	0.49
2:T:307:GLU:OE1	2:T:485:ARG:NH2	2.46	0.49
2:W:340:GLN:OE1	2:W:365:ASN:ND2	2.46	0.49
1:C:66:LEU:HD22	1:C:87:VAL:HG21	1.94	0.49
1:H:109:GLU:HG2	1:K:41:LYS:HB2	1.95	0.48
2:U:70:LYS:NZ	2:U:117:GLU:OE2	2.30	0.48
2:X:68:LEU:HD11	2:X:72:PHE:CZ	2.49	0.48
1:F:125:ASP:HB2	2:W:435:LYS:HD3	1.95	0.48
2:T:347:SER:HA	2:T:363:ILE:HA	1.95	0.48
2:U:257:ASN:HB2	2:U:264:VAL:HG23	1.96	0.48
2:U:421:ILE:HG22	2:U:423:GLY:H	1.78	0.48
2:X:272:ALA:HB2	2:X:370:TYR:HB2	1.94	0.48
2:W:171:HIS:NE2	2:W:226:ASP:OD2	2.40	0.48
2:X:302:THR:OG1	2:X:303:CYS:N	2.46	0.48
1:R:85:VAL:HG11	1:R:117:MET:HE1	1.95	0.48
2:U:479:ARG:NE	2:U:479:ARG:HA	2.28	0.48
2:W:167:THR:OG1	2:W:203:ASN:ND2	2.41	0.48
1:G:40:TYR:CE2	1:G:97:MET:HG3	2.48	0.48
1:D:34:ASP:OD1	1:D:36:THR:OG1	2.27	0.48
1:O:63:THR:HG22	1:O:120:VAL:HG22	1.95	0.48
2:X:48:VAL:HG11	2:X:68:LEU:HD21	1.95	0.48
1:G:109:GLU:HB3	1:J:39:THR:HB	1.94	0.48
2:U:51:GLU:HB2	2:W:377:ARG:HH22	1.79	0.47
2:U:52:LEU:H	2:W:377:ARG:HH12	1.62	0.47
2:W:415:THR:CG2	2:W:416:ASN:H	2.25	0.47
1:O:32:GLN:HE22	1:O:38:PRO:HD3	1.78	0.47
2:U:447:GLU:O	2:U:448:PHE:CD2	2.67	0.47
1:E:66:LEU:HG	1:E:68:VAL:HG13	1.95	0.47
2:Z:447:GLU:CG	2:Z:448:PHE:H	2.25	0.47
1:C:88:GLN:HG2	2:T:428:LEU:HD22	1.97	0.47
1:F:26:GLY:HA2	1:F:28:ILE:HG13	1.96	0.47
1:R:15:THR:HB	1:R:86:ASP:HB2	1.96	0.47
1:O:90:GLU:HB2	1:O:96:VAL:HG22	1.95	0.47
2:U:307:GLU:OE1	2:U:485:ARG:NH2	2.47	0.47
1:B:96:VAL:HB	1:B:127:LEU:HB2	1.96	0.47
1:O:32:GLN:NE2	1:O:38:PRO:HD3	2.28	0.47
1:C:22:GLN:NE2	1:E:3:CYS:SG	2.79	0.47
1:G:66:LEU:HG	1:G:68:VAL:HG13	1.96	0.47
2:U:282:THR:HG22	2:U:282:THR:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:272:ALA:HB2	2:W:370:TYR:HD1	1.79	0.47
2:X:4:ASP:OD1	2:X:5:ALA:N	2.47	0.47
1:S:34:ASP:OD2	1:S:36:THR:HG22	2.15	0.47
1:M:4:ASN:OD1	1:M:5:LYS:N	2.47	0.47
2:T:242:TRP:CZ3	2:T:273:GLU:HG3	2.50	0.47
1:B:87:VAL:HG12	1:B:99:LEU:HD22	1.96	0.46
2:X:221:TYR:N	2:X:252:HIS:O	2.48	0.46
2:X:227:ASP:OD1	2:X:230:TRP:N	2.39	0.46
2:Z:240:SER:O	2:Z:243:ASP:HB2	2.15	0.46
1:S:32:GLN:HE22	1:S:38:PRO:HD3	1.79	0.46
2:T:96:VAL:HG22	2:T:161:THR:HG23	1.97	0.46
2:X:70:LYS:HA	2:X:70:LYS:HD3	1.59	0.46
1:B:128:LEU:HD21	1:Q:75:PRO:HA	1.97	0.46
2:U:242:TRP:HE1	2:U:250:PHE:HA	1.79	0.46
2:U:306:PRO:HB2	2:U:389:ARG:HB3	1.97	0.46
1:L:19:CYS:SG	1:N:3:CYS:N	2.75	0.46
1:L:48:THR:OG1	1:L:56:GLN:HB3	2.16	0.46
1:O:70:ARG:NH2	1:O:74:VAL:O	2.48	0.46
2:Z:51:GLU:HG3	2:Z:72:PHE:HD2	1.81	0.46
2:W:480:TYR:OH	2:X:495:PRO:HG3	2.15	0.46
1:C:45:TRP:HB2	1:C:57:ARG:HH21	1.79	0.46
1:Q:12:ILE:HG12	1:Q:89:VAL:HG23	1.98	0.46
2:X:415:THR:CG2	2:X:416:ASN:H	2.25	0.46
1:S:66:LEU:HD22	1:S:87:VAL:HG11	1.98	0.46
2:W:242:TRP:CZ3	2:W:273:GLU:HG3	2.51	0.46
1:F:11:ASN:HD21	2:W:417:ILE:H	1.64	0.46
2:W:454:ASP:O	2:W:478:MET:HA	2.16	0.46
2:Z:421:ILE:HG22	2:Z:423:GLY:H	1.81	0.46
2:T:380:ALA:HB1	2:T:383:ARG:HH21	1.80	0.45
2:U:66:GLU:HB3	2:U:289:LEU:HD21	1.98	0.45
2:W:260:THR:HG22	2:W:263:GLN:HG2	1.97	0.45
1:D:126:GLU:OE2	1:S:70:ARG:NH2	2.49	0.45
2:X:34:MET:HA	2:X:62:SER:HB2	1.99	0.45
2:X:447:GLU:O	2:X:448:PHE:CD2	2.70	0.45
1:C:106:GLU:OE1	1:C:106:GLU:HA	2.17	0.45
1:F:11:ASN:HD21	2:W:416:ASN:HB2	1.82	0.45
2:U:454:ASP:O	2:U:478:MET:HA	2.17	0.45
2:X:32:GLY:HA3	2:X:224:SER:HB2	1.96	0.45
2:X:464:GLN:HB3	2:X:468:VAL:HB	1.97	0.45
1:I:61:ASN:ND2	1:L:50:LEU:O	2.42	0.45
1:D:106:GLU:OE1	1:D:106:GLU:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:340:GLN:CD	2:T:365:ASN:HD22	2.20	0.45
2:W:37:ASP:HB3	2:W:59:GLY:HA2	1.98	0.45
2:W:336:VAL:O	2:W:340:GLN:HG2	2.16	0.45
2:Z:394:THR:HG21	2:Z:480:TYR:CE1	2.51	0.45
1:D:110:SER:O	1:G:40:TYR:N	2.39	0.45
1:G:15:THR:HB	1:G:86:ASP:HB2	1.97	0.45
2:T:70:LYS:HG3	2:T:289:LEU:HD22	1.98	0.45
2:X:52:LEU:CD1	2:Z:377:ARG:H	2.24	0.45
1:B:86:ASP:OD1	1:B:101:GLU:N	2.43	0.45
1:G:10:LYS:HG3	2:X:416:ASN:HD22	1.81	0.45
2:W:213:VAL:HG13	2:W:213:VAL:O	2.17	0.45
2:X:209:TYR:OH	2:X:230:TRP:NE1	2.49	0.45
1:E:26:GLY:HA2	1:E:28:ILE:HG13	1.98	0.45
1:H:14:ILE:HG13	1:H:87:VAL:HG23	1.98	0.45
1:Q:26:GLY:HA2	1:Q:28:ILE:HG13	1.99	0.45
2:T:418:ARG:HB3	2:T:421:ILE:HD13	1.97	0.45
2:Z:310:ILE:HG22	2:Z:363:ILE:HD11	1.98	0.45
1:O:19:CYS:HG	1:Q:3:CYS:N	2.14	0.45
1:O:97:MET:SD	1:O:126:GLU:HG3	2.56	0.45
1:R:106:GLU:OE1	1:R:106:GLU:HA	2.16	0.45
2:T:306:PRO:HB2	2:T:389:ARG:HB3	1.99	0.45
1:O:26:GLY:HA2	1:O:28:ILE:HG13	1.99	0.45
2:U:52:LEU:HB2	2:W:377:ARG:CZ	2.47	0.45
2:W:220:VAL:HG21	2:W:299:ALA:HB2	1.99	0.45
2:W:308:LEU:HD21	2:W:315:PHE:HB3	1.99	0.45
2:X:32:GLY:N	2:X:64:LEU:HD12	2.32	0.45
2:X:52:LEU:HD22	2:Z:377:ARG:HD3	1.99	0.45
2:Z:306:PRO:HB2	2:Z:389:ARG:HB3	1.98	0.44
1:C:9:VAL:HG22	1:C:32:GLN:NE2	2.31	0.44
1:M:128:LEU:HD12	1:M:128:LEU:HA	1.85	0.44
1:P:106:GLU:OE1	1:P:106:GLU:HA	2.16	0.44
2:X:29:LEU:HB2	2:X:218:PHE:CD2	2.53	0.44
2:X:282:THR:HG22	2:X:282:THR:O	2.18	0.44
2:W:227:ASP:OD1	2:W:230:TRP:N	2.41	0.44
2:X:147:PHE:O	2:X:163:ARG:NE	2.51	0.44
2:T:52:LEU:HD23	2:T:52:LEU:HA	1.81	0.44
2:U:213:VAL:O	2:U:213:VAL:HG13	2.18	0.44
2:W:372:ARG:HG2	2:W:377:ARG:HG2	1.98	0.44
1:B:43:CYS:SG	1:Q:82:CYS:N	2.91	0.44
1:E:106:GLU:HA	1:E:106:GLU:OE1	2.16	0.44
1:Q:70:ARG:NH1	1:Q:76:LEU:HB2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:ILE:HD13	1:C:66:LEU:HD11	1.98	0.44
1:D:70:ARG:NH2	1:D:74:VAL:O	2.50	0.44
2:T:64:LEU:O	2:T:68:LEU:HD23	2.18	0.44
2:U:4:ASP:OD1	2:U:5:ALA:N	2.51	0.44
2:U:242:TRP:CH2	2:U:388:ARG:HD2	2.53	0.44
2:W:311:GLN:HE21	2:W:366:ASP:H	1.66	0.44
2:W:447:GLU:O	2:W:448:PHE:CD2	2.71	0.44
2:X:147:PHE:CE2	2:X:149:TYR:HB2	2.53	0.44
1:C:70:ARG:HD3	1:C:112:GLY:O	2.17	0.44
1:C:82:CYS:N	1:F:43:CYS:SG	2.91	0.44
1:O:61:ASN:ND2	1:R:50:LEU:O	2.40	0.44
2:T:255:VAL:HA	2:T:291:ASN:HD21	1.83	0.44
1:N:106:GLU:OE2	1:N:106:GLU:HA	2.18	0.44
2:X:384:ASP:O	2:X:387:SER:OG	2.35	0.44
1:B:42:ASN:ND2	1:Q:76:LEU:HD22	2.33	0.44
2:T:168:ILE:HD12	2:T:168:ILE:H	1.83	0.44
1:D:39:THR:CG2	1:S:109:GLU:HB3	2.48	0.43
1:G:129:PRO:HA	2:X:427:ARG:NH2	2.33	0.43
1:K:61:ASN:OD1	1:N:52:ASN:N	2.50	0.43
2:T:213:VAL:O	2:T:213:VAL:HG13	2.18	0.43
2:U:60:GLN:NE2	2:U:145:PRO:HB2	2.33	0.43
2:W:235:ARG:HD3	2:W:239:ARG:HH21	1.83	0.43
2:Z:394:THR:HG21	2:Z:480:TYR:HE1	1.83	0.43
1:B:12:ILE:HG12	1:B:89:VAL:HG23	2.00	0.43
1:B:14:ILE:HD12	1:B:30:HIS:ND1	2.33	0.43
1:F:87:VAL:HG21	1:F:119:ILE:HD13	1.98	0.43
1:N:32:GLN:NE2	1:N:38:PRO:HD3	2.34	0.43
1:P:66:LEU:HD22	1:P:87:VAL:HG21	1.99	0.43
2:X:257:ASN:HB2	2:X:264:VAL:HG23	1.99	0.43
2:Z:340:GLN:HB3	2:Z:365:ASN:HD22	1.83	0.43
1:C:20:ASP:OD1	1:C:21:THR:N	2.52	0.43
1:D:43:CYS:SG	1:S:82:CYS:N	2.91	0.43
1:D:90:GLU:HB2	1:D:96:VAL:HG22	2.00	0.43
1:I:30:HIS:NE2	1:I:79:TYR:OH	2.37	0.43
2:T:345:VAL:HA	2:T:365:ASN:OD1	2.18	0.43
2:W:384:ASP:O	2:W:387:SER:OG	2.35	0.43
1:L:128:LEU:HD23	1:L:128:LEU:HA	1.84	0.43
2:T:308:LEU:HD11	2:T:315:PHE:HD2	1.84	0.43
1:I:63:THR:HG22	1:I:120:VAL:HG22	1.99	0.43
1:I:105:VAL:HA	1:L:47:ASN:HB2	2.01	0.43
2:W:479:ARG:HD2	2:X:494:ALA:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:66:LEU:HG	1:R:68:VAL:HG13	2.01	0.43
2:T:276:ARG:HG3	2:T:369:ASN:HD22	1.82	0.43
2:U:218:PHE:HB2	2:U:221:TYR:CZ	2.53	0.43
2:Z:336:VAL:HG22	2:Z:346:VAL:HG11	2.01	0.43
1:J:61:ASN:HB3	1:J:120:VAL:HG13	2.01	0.43
1:K:66:LEU:HG	1:K:68:VAL:HG13	2.00	0.43
2:W:256:PHE:O	2:W:257:ASN:ND2	2.52	0.43
2:X:55:ILE:HG23	2:X:60:GLN:HB3	2.01	0.43
2:X:147:PHE:HA	2:X:148:PRO:HD3	1.91	0.43
1:B:32:GLN:NE2	1:B:38:PRO:HD3	2.34	0.43
1:I:61:ASN:OD1	1:L:52:ASN:N	2.52	0.43
1:I:90:GLU:HB2	2:Z:428:LEU:HD21	2.01	0.43
1:K:79:TYR:HB3	1:K:115:VAL:HG11	2.01	0.43
2:T:272:ALA:HB2	2:T:370:TYR:CD2	2.54	0.43
2:X:51:GLU:OE2	2:X:69:ARG:HG3	2.19	0.43
2:X:220:VAL:HG21	2:X:299:ALA:HB2	2.01	0.43
1:P:96:VAL:HB	1:P:127:LEU:HB2	2.01	0.42
2:W:19:LEU:HD23	2:W:19:LEU:HA	1.89	0.42
2:X:302:THR:HG23	2:X:310:ILE:HD11	2.00	0.42
1:I:66:LEU:HG	1:I:68:VAL:HG13	2.01	0.42
2:U:6:LEU:HD21	2:W:400:GLU:N	2.34	0.42
1:D:66:LEU:HG	1:D:68:VAL:HG13	2.02	0.42
1:I:125:ASP:OD2	2:Z:434:ARG:NH1	2.52	0.42
2:Z:390:LEU:HD23	2:Z:390:LEU:HA	1.89	0.42
1:O:10:LYS:HG2	1:O:11:ASN:OD1	2.20	0.42
1:R:52:ASN:O	1:R:52:ASN:ND2	2.41	0.42
2:T:235:ARG:HH11	2:T:271:SER:HB2	1.84	0.42
2:U:368:THR:OG1	2:U:382:PHE:O	2.38	0.42
2:Z:379:ASN:ND2	2:Z:381:THR:HG23	2.34	0.42
1:F:128:LEU:HD23	1:F:128:LEU:HA	1.82	0.42
2:T:348:GLY:O	2:T:362:TYR:N	2.53	0.42
2:X:55:ILE:HD13	2:X:65:THR:HG21	2.00	0.42
2:X:466:LYS:HA	2:X:466:LYS:HD2	1.73	0.42
1:B:66:LEU:HD22	1:B:87:VAL:HG21	2.01	0.42
1:R:70:ARG:HD3	1:R:112:GLY:O	2.19	0.42
2:T:447:GLU:OE1	2:T:447:GLU:N	2.44	0.42
2:Z:342:ASN:C	2:Z:371:LEU:HD21	2.40	0.42
1:N:45:TRP:HB2	1:N:57:ARG:HH21	1.84	0.42
1:Q:117:MET:HB3	1:Q:119:ILE:HG13	2.01	0.42
2:T:311:GLN:HE21	2:T:366:ASP:HB2	1.83	0.42
2:T:365:ASN:O	2:T:367:VAL:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:310:ILE:HG22	2:X:363:ILE:HD11	2.02	0.42
1:D:82:CYS:N	1:G:43:CYS:SG	2.92	0.42
1:K:128:LEU:HD23	1:K:128:LEU:HA	1.90	0.42
1:N:66:LEU:HG	1:N:68:VAL:HG13	2.01	0.42
2:T:273:GLU:C	2:T:274:LEU:HD12	2.39	0.42
2:U:273:GLU:OE1	2:U:273:GLU:N	2.50	0.42
1:I:129:PRO:HA	2:Z:427:ARG:NH2	2.35	0.42
1:J:3:CYS:O	1:J:5:LYS:N	2.52	0.42
2:W:445:PHE:CE1	2:W:478:MET:HE1	2.55	0.42
2:X:209:TYR:HH	2:X:230:TRP:HE1	1.62	0.42
1:P:82:CYS:N	1:S:43:CYS:SG	2.93	0.42
2:T:147:PHE:CE2	2:T:149:TYR:HB2	2.54	0.42
2:T:273:GLU:OE1	2:T:273:GLU:N	2.49	0.42
2:X:299:ALA:O	2:X:303:CYS:HB3	2.19	0.42
1:M:61:ASN:OD1	1:P:52:ASN:N	2.53	0.41
2:W:365:ASN:O	2:W:367:VAL:N	2.53	0.41
2:X:269:ASP:OD1	2:X:269:ASP:N	2.52	0.41
1:H:105:VAL:HA	1:K:47:ASN:HB2	2.01	0.41
1:O:61:ASN:HB3	1:O:120:VAL:HG13	2.02	0.41
1:P:70:ARG:HD3	1:P:112:GLY:O	2.20	0.41
1:Q:128:LEU:HD23	1:Q:128:LEU:HA	1.90	0.41
2:T:282:THR:O	2:T:282:THR:HG22	2.20	0.41
2:X:97:TYR:O	2:X:160:LEU:N	2.38	0.41
1:M:105:VAL:HG23	1:M:106:GLU:N	2.34	0.41
2:T:257:ASN:OD1	2:T:276:ARG:HD2	2.20	0.41
2:U:147:PHE:HA	2:U:148:PRO:HD3	1.92	0.41
2:W:288:TYR:CD1	2:W:289:LEU:HD12	2.54	0.41
1:G:88:GLN:NE2	2:X:428:LEU:O	2.53	0.41
1:G:89:VAL:CG1	1:G:97:MET:HB2	2.51	0.41
1:O:40:TYR:CZ	1:O:97:MET:HG3	2.56	0.41
1:P:128:LEU:HD23	1:P:128:LEU:HA	1.81	0.41
2:U:235:ARG:HH11	2:U:271:SER:HB2	1.84	0.41
2:X:218:PHE:HB2	2:X:221:TYR:CZ	2.56	0.41
1:H:70:ARG:HH22	1:K:126:GLU:CD	2.23	0.41
2:T:33:GLN:NE2	2:T:88:ASP:OD1	2.53	0.41
2:T:421:ILE:HG22	2:T:423:GLY:H	1.84	0.41
2:U:147:PHE:CE2	2:U:149:TYR:HB2	2.55	0.41
2:W:269:ASP:OD1	2:W:269:ASP:N	2.52	0.41
2:W:384:ASP:OD1	2:W:385:ALA:N	2.53	0.41
1:E:57:ARG:HE	1:E:57:ARG:HB3	1.72	0.41
1:F:125:ASP:OD1	1:F:126:GLU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:70:ARG:NH1	1:K:76:LEU:HB2	2.36	0.41
1:R:18:ASP:OD2	1:R:19:CYS:N	2.53	0.41
2:U:10:PHE:HB3	2:U:11:VAL:H	1.72	0.41
2:Z:394:THR:HG22	2:Z:444:LEU:HD13	2.03	0.41
1:B:70:ARG:HD3	1:B:112:GLY:O	2.21	0.41
1:L:66:LEU:HG	1:L:68:VAL:HG13	2.02	0.41
1:Q:99:LEU:HD11	1:Q:121:ALA:CB	2.50	0.41
2:T:227:ASP:OD1	2:T:230:TRP:N	2.44	0.41
2:T:446:SER:N	2:T:481:ARG:O	2.50	0.41
2:X:332:THR:O	2:X:336:VAL:HG23	2.21	0.41
2:X:340:GLN:HE22	2:X:365:ASN:HB2	1.85	0.41
1:C:90:GLU:HB2	2:T:428:LEU:HD21	2.02	0.41
1:F:66:LEU:HG	1:F:68:VAL:HG13	2.03	0.41
1:J:48:THR:HB	1:J:56:GLN:HB3	2.02	0.41
1:I:96:VAL:HB	1:I:127:LEU:HB2	2.03	0.41
1:J:90:GLU:HG3	1:J:96:VAL:HG22	2.03	0.41
2:T:218:PHE:HB2	2:T:221:TYR:CZ	2.56	0.41
2:X:67:SER:O	2:X:71:VAL:HG23	2.21	0.41
2:X:348:GLY:O	2:X:362:TYR:N	2.48	0.41
2:Z:302:THR:O	2:Z:304:ASN:N	2.53	0.41
1:O:66:LEU:HD22	1:O:87:VAL:HG21	2.02	0.41
2:W:279:LEU:HD23	2:W:279:LEU:HA	1.90	0.41
2:X:421:ILE:HG22	2:X:423:GLY:H	1.86	0.41
1:E:79:TYR:HB3	1:E:115:VAL:HG11	2.03	0.40
1:E:96:VAL:HB	1:E:127:LEU:HB2	2.03	0.40
1:I:6:GLN:HB3	1:J:57:ARG:HG3	2.03	0.40
2:W:223:LEU:HB3	2:W:255:VAL:HG12	2.03	0.40
1:C:43:CYS:SG	1:R:82:CYS:N	2.95	0.40
1:F:34:ASP:OD1	1:F:36:THR:OG1	2.24	0.40
2:T:147:PHE:HA	2:T:148:PRO:HD3	1.98	0.40
2:X:30:VAL:HA	2:X:222:VAL:HB	2.03	0.40
2:Z:71:VAL:HG22	2:Z:296:ALA:HB2	2.03	0.40
1:K:23:GLU:N	1:K:23:GLU:OE2	2.54	0.40
1:L:82:CYS:N	1:O:43:CYS:SG	2.94	0.40
1:M:70:ARG:HD3	1:M:112:GLY:O	2.22	0.40
1:O:127:LEU:HD12	1:O:127:LEU:HA	1.89	0.40
2:U:447:GLU:H	2:U:447:GLU:HG3	1.62	0.40
2:W:401:PHE:HZ	2:W:432:LYS:HG2	1.87	0.40
1:D:50:LEU:HB2	1:D:54:TYR:O	2.22	0.40
1:E:31:GLU:OE1	1:I:52:ASN:ND2	2.52	0.40
1:I:50:LEU:HB2	1:I:54:TYR:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:40:TYR:CZ	1:J:97:MET:HG3	2.57	0.40
1:J:109:GLU:HB3	1:M:39:THR:CG2	2.51	0.40
2:T:373:ASP:HB2	2:T:379:ASN:OD1	2.21	0.40
2:W:418:ARG:HB2	2:W:421:ILE:HD13	2.03	0.40
2:W:434:ARG:HE	2:W:434:ARG:HB3	1.70	0.40
2:X:26:CYS:HB2	2:X:78:GLY:O	2.22	0.40
2:X:34:MET:HG3	2:X:86:ARG:O	2.21	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	B	128/136 (94%)	120 (94%)	8 (6%)	0	100	100
1	C	129/136 (95%)	122 (95%)	7 (5%)	0	100	100
1	D	128/136 (94%)	119 (93%)	9 (7%)	0	100	100
1	E	129/136 (95%)	123 (95%)	6 (5%)	0	100	100
1	F	128/136 (94%)	125 (98%)	3 (2%)	0	100	100
1	G	129/136 (95%)	121 (94%)	8 (6%)	0	100	100
1	H	129/136 (95%)	123 (95%)	6 (5%)	0	100	100
1	I	129/136 (95%)	125 (97%)	4 (3%)	0	100	100
1	J	129/136 (95%)	123 (95%)	6 (5%)	0	100	100
1	K	129/136 (95%)	122 (95%)	7 (5%)	0	100	100
1	L	129/136 (95%)	126 (98%)	3 (2%)	0	100	100
1	M	129/136 (95%)	123 (95%)	6 (5%)	0	100	100
1	N	129/136 (95%)	124 (96%)	5 (4%)	0	100	100
1	O	129/136 (95%)	125 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	129/136 (95%)	125 (97%)	4 (3%)	0	100	100
1	Q	129/136 (95%)	125 (97%)	4 (3%)	0	100	100
1	R	129/136 (95%)	122 (95%)	7 (5%)	0	100	100
1	S	128/136 (94%)	123 (96%)	5 (4%)	0	100	100
2	T	430/503 (86%)	392 (91%)	35 (8%)	3 (1%)	19	54
2	U	448/503 (89%)	409 (91%)	36 (8%)	3 (1%)	19	54
2	W	413/503 (82%)	381 (92%)	30 (7%)	2 (0%)	25	60
2	X	437/503 (87%)	399 (91%)	34 (8%)	4 (1%)	14	49
2	Z	261/503 (52%)	232 (89%)	28 (11%)	1 (0%)	30	64
2	a	391/503 (78%)	360 (92%)	26 (7%)	5 (1%)	10	41
2	c	400/503 (80%)	365 (91%)	29 (7%)	6 (2%)	8	38
2	d	435/503 (86%)	396 (91%)	35 (8%)	4 (1%)	14	49
2	f	391/503 (78%)	350 (90%)	36 (9%)	5 (1%)	10	41
2	g	370/503 (74%)	319 (86%)	45 (12%)	6 (2%)	8	37
2	i	367/503 (73%)	330 (90%)	37 (10%)	0	100	100
2	j	486/503 (97%)	447 (92%)	37 (8%)	2 (0%)	30	64
All	All	7147/8484 (84%)	6596 (92%)	510 (7%)	41 (1%)	24	57

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	X	303	CYS
2	Z	303	CYS
2	a	375	LYS
2	a	414	ASN
2	c	448	PHE
2	f	468	VAL
2	g	55	ILE
2	g	81	VAL
2	T	54	ILE
2	T	303	CYS
2	U	303	CYS
2	W	303	CYS
2	c	414	ASN
2	d	182	CYS
2	f	319	SER

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Mol	Chain	Res	Type
2	f	448	PHE
2	g	303	CYS
2	j	303	CYS
2	X	10	PHE
2	c	303	CYS
2	f	414	ASN
2	T	202	VAL
2	W	202	VAL
2	a	377	ARG
2	c	11	VAL
2	j	202	VAL
2	U	202	VAL
2	X	202	VAL
2	a	202	VAL
2	a	413	LYS
2	c	202	VAL
2	c	413	LYS
2	d	202	VAL
2	f	202	VAL
2	g	318	LEU
2	g	333	PHE
2	g	358	TYR
2	X	24	GLU
2	d	303	CYS
2	U	190	VAL
2	d	190	VAL

### 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	B	114/116 (98%)	114 (100%)	0	100	100
1	C	115/116 (99%)	115 (100%)	0	100	100
1	D	114/116 (98%)	114 (100%)	0	100	100
1	E	115/116 (99%)	115 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	114/116 (98%)	114 (100%)	0	100	100
1	G	115/116 (99%)	115 (100%)	0	100	100
1	H	115/116 (99%)	115 (100%)	0	100	100
1	I	115/116 (99%)	115 (100%)	0	100	100
1	J	115/116 (99%)	115 (100%)	0	100	100
1	K	115/116 (99%)	115 (100%)	0	100	100
1	L	115/116 (99%)	115 (100%)	0	100	100
1	M	115/116 (99%)	115 (100%)	0	100	100
1	N	115/116 (99%)	115 (100%)	0	100	100
1	O	115/116 (99%)	115 (100%)	0	100	100
1	P	115/116 (99%)	115 (100%)	0	100	100
1	Q	115/116 (99%)	115 (100%)	0	100	100
1	R	115/116 (99%)	114 (99%)	1 (1%)	75	89
1	S	114/116 (98%)	114 (100%)	0	100	100
2	T	365/408 (90%)	364 (100%)	1 (0%)	91	96
2	U	376/408 (92%)	374 (100%)	2 (0%)	86	93
2	W	350/408 (86%)	348 (99%)	2 (1%)	84	92
2	X	370/408 (91%)	368 (100%)	2 (0%)	86	93
2	Z	230/408 (56%)	229 (100%)	1 (0%)	89	94
2	a	336/408 (82%)	335 (100%)	1 (0%)	91	96
2	c	341/408 (84%)	340 (100%)	1 (0%)	91	96
2	d	367/408 (90%)	365 (100%)	2 (0%)	86	93
2	f	331/408 (81%)	331 (100%)	0	100	100
2	g	318/408 (78%)	317 (100%)	1 (0%)	91	96
2	i	315/408 (77%)	314 (100%)	1 (0%)	91	96
2	j	398/408 (98%)	397 (100%)	1 (0%)	91	96
All	All	6163/6984 (88%)	6147 (100%)	16 (0%)	90	96

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	52	ASN
2	T	233	ASN

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Mol	Chain	Res	Type
2	U	233	ASN
2	U	291	ASN
2	W	233	ASN
2	W	291	ASN
2	X	233	ASN
2	X	375	LYS
2	Z	379	ASN
2	a	291	ASN
2	c	291	ASN
2	d	60	GLN
2	d	291	ASN
2	g	305	ASN
2	i	377	ARG
2	j	291	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	32	GLN
1	F	11	ASN
1	H	32	GLN
1	I	84	GLN
1	M	32	GLN
1	O	11	ASN
1	O	32	GLN
1	P	84	GLN
1	S	32	GLN
1	S	88	GLN
2	W	291	ASN
2	a	20	ASN
2	a	369	ASN
2	c	252	HIS
2	c	257	ASN
2	c	416	ASN
2	c	440	ASN
2	d	379	ASN
2	f	340	GLN
2	g	365	ASN
2	i	438	GLN
2	j	291	ASN
2	j	365	ASN
2	j	490	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

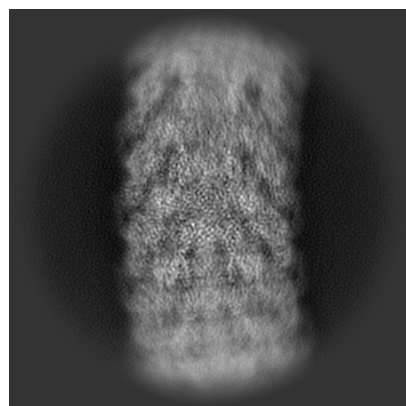
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29353. These allow visual inspection of the internal detail of the map and identification of artifacts.

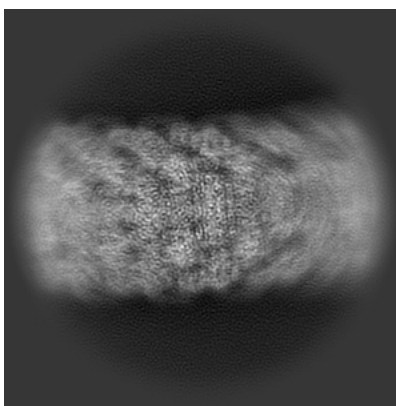
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

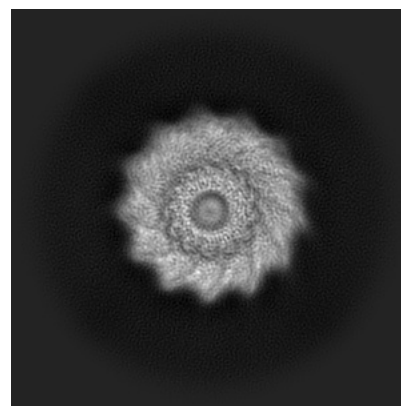
#### 6.1.1 Primary map



X

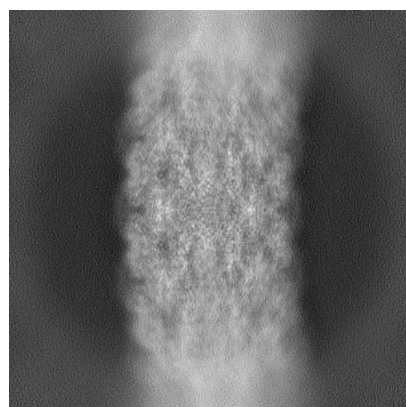


Y

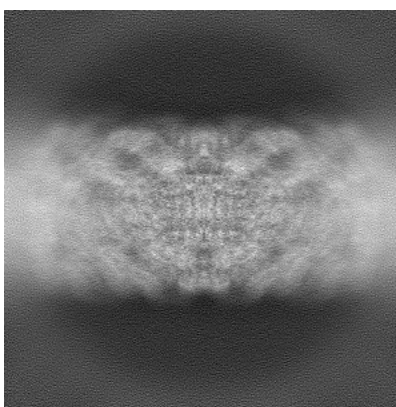


Z

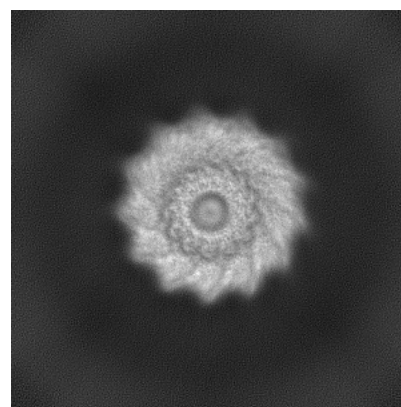
#### 6.1.2 Raw map



X



Y

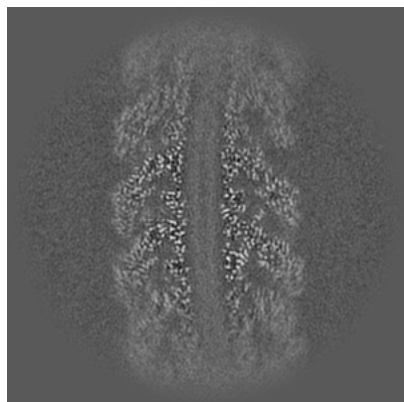


Z

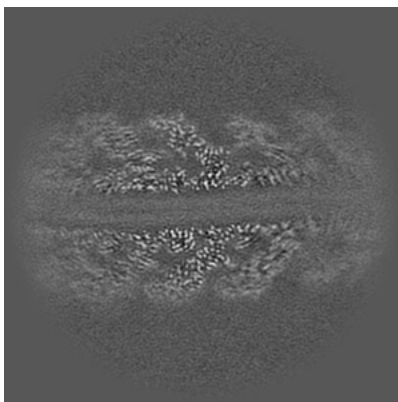
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

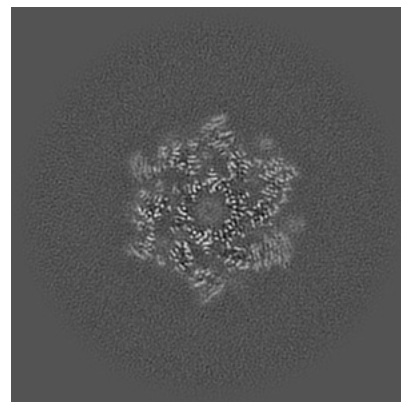
### 6.2.1 Primary map



X Index: 192

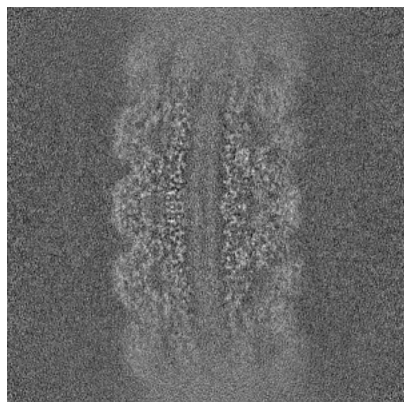


Y Index: 192

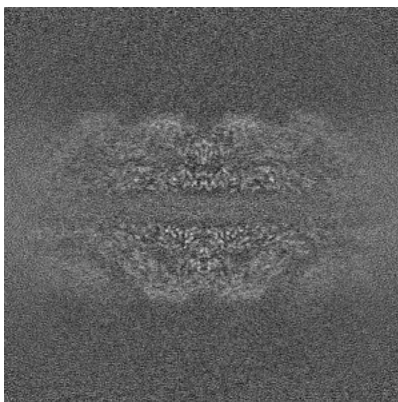


Z Index: 192

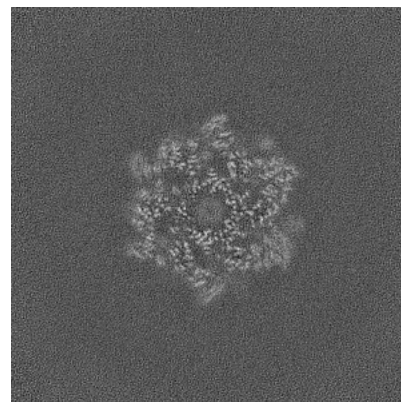
### 6.2.2 Raw map



X Index: 192



Y Index: 192



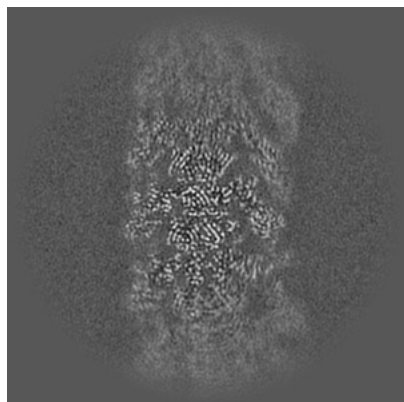
Z Index: 192

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

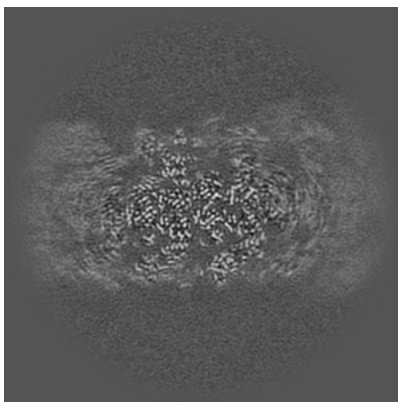


## 6.3 Largest variance slices [i](#)

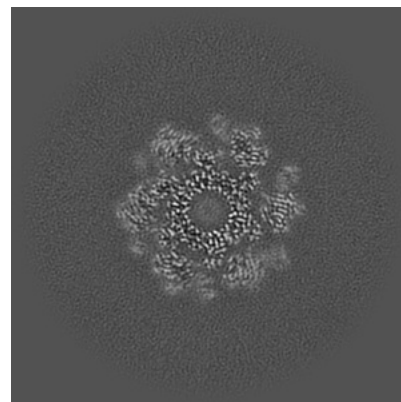
### 6.3.1 Primary map



X Index: 168

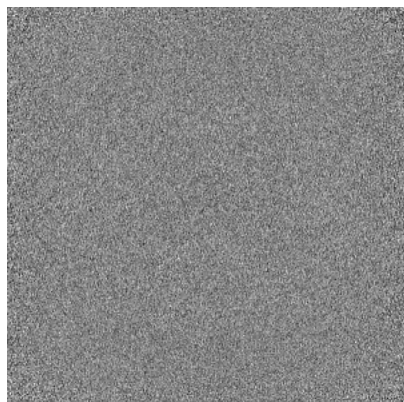


Y Index: 168

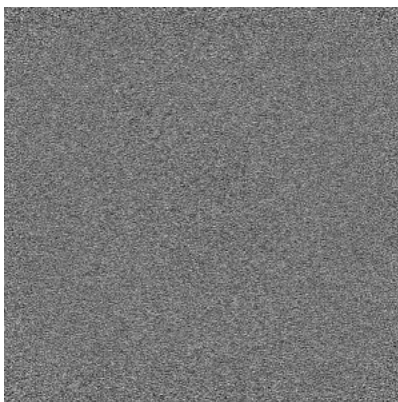


Z Index: 171

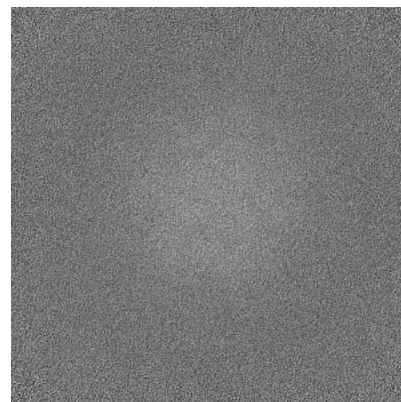
### 6.3.2 Raw map



X Index: 0



Y Index: 0

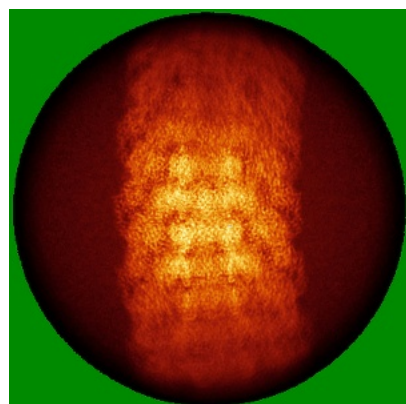


Z Index: 0

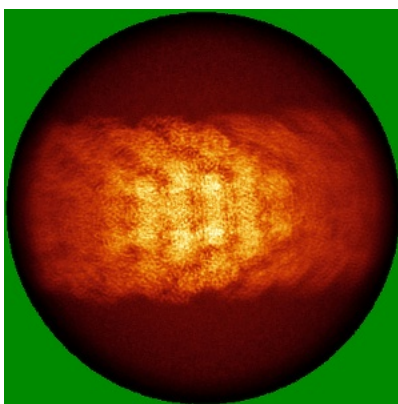
The images above show the largest variance slices of the map in three orthogonal directions.

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

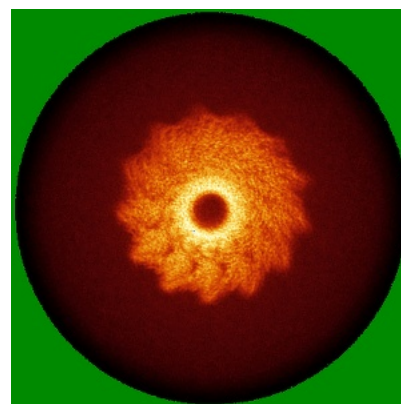
### 6.4.1 Primary map



X

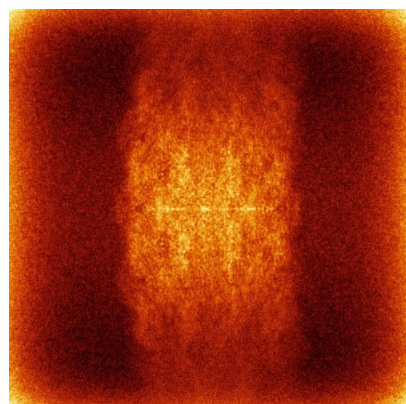


Y

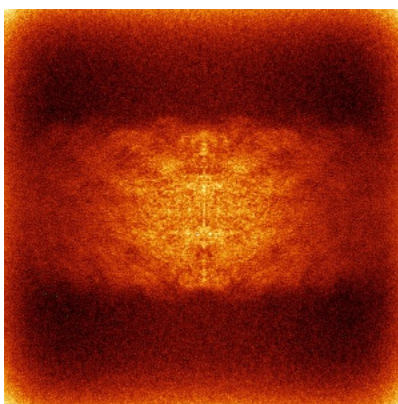


Z

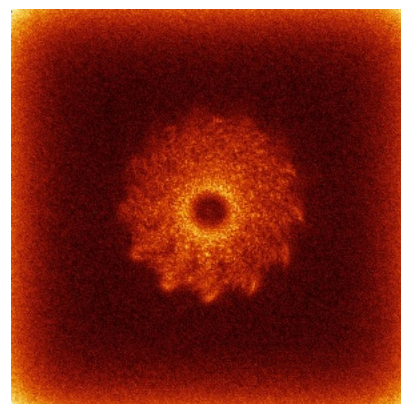
### 6.4.2 Raw map



X



Y

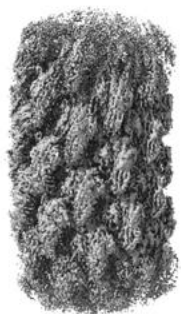


Z

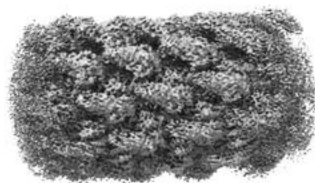
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

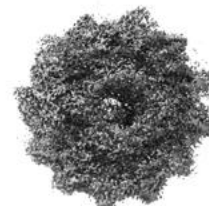
### 6.5.1 Primary map



X



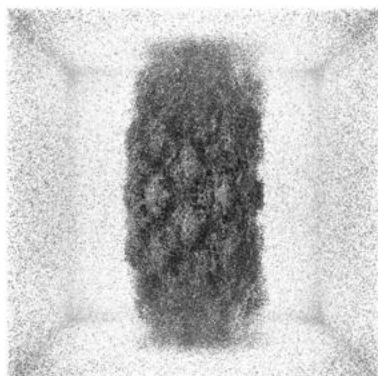
Y



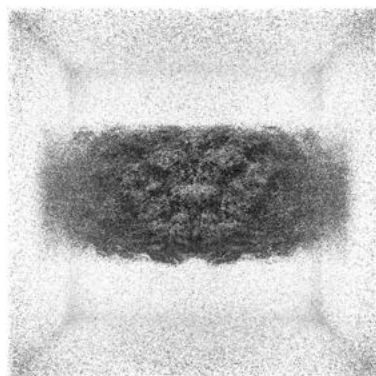
Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

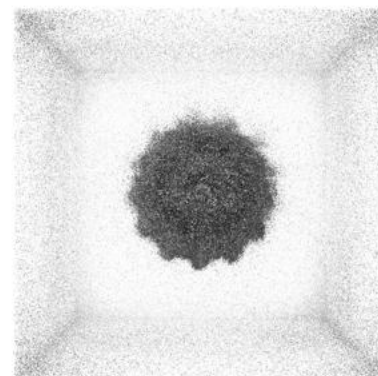
### 6.5.2 Raw map



X



Y



Z

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

## 6.6 Mask visualisation [i](#)

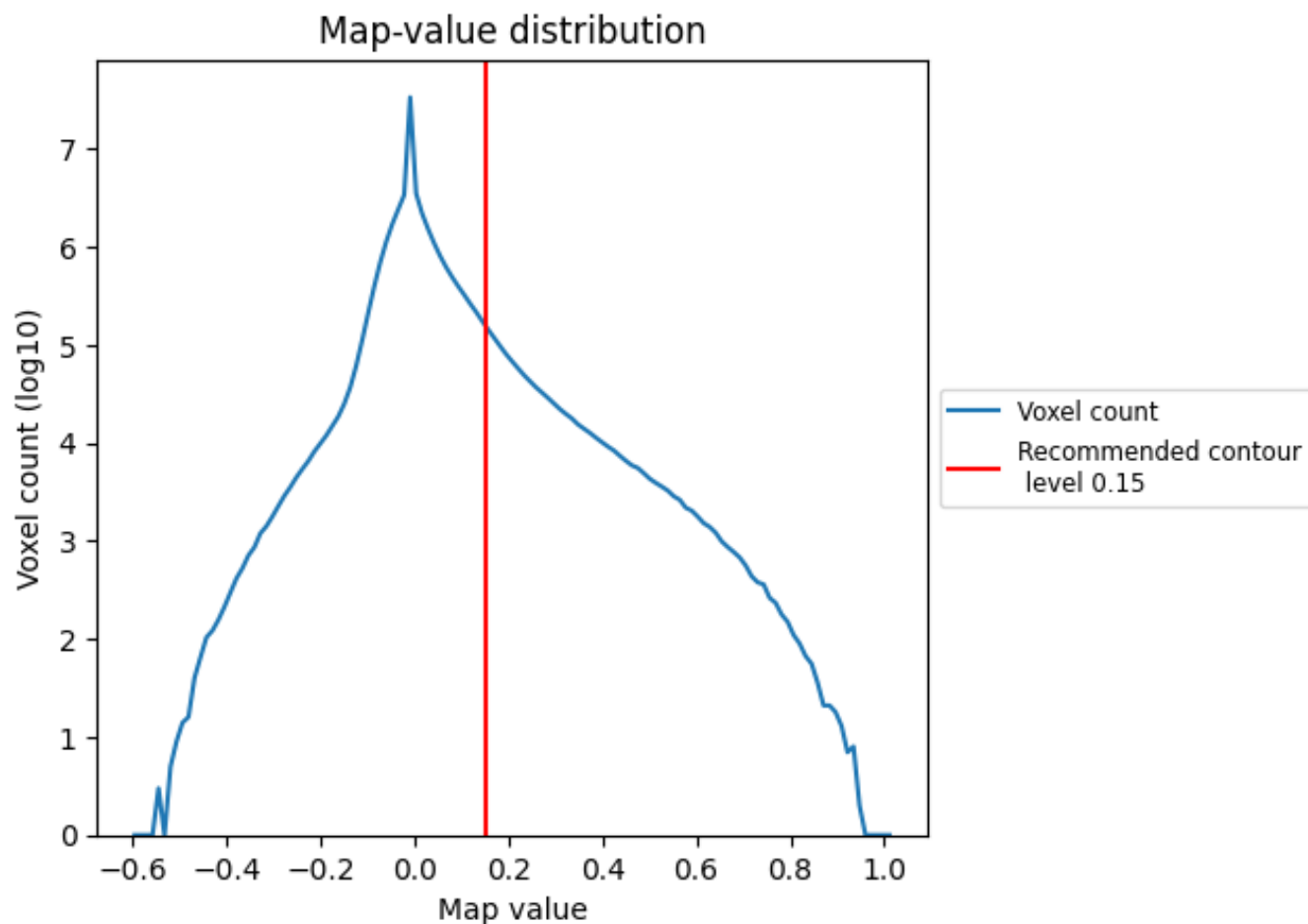
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

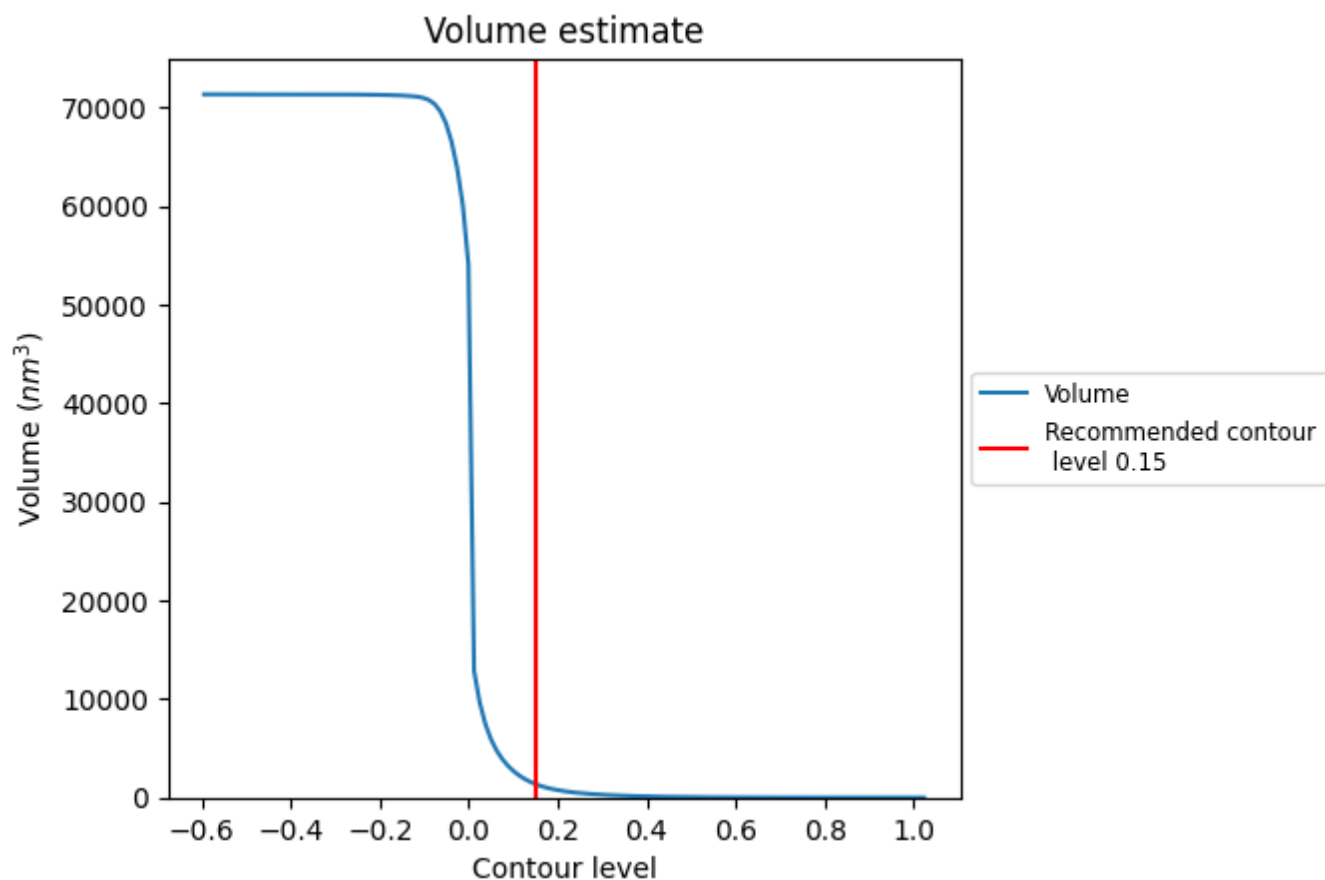
This section contains the results of statistical analysis of the map.

### 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.

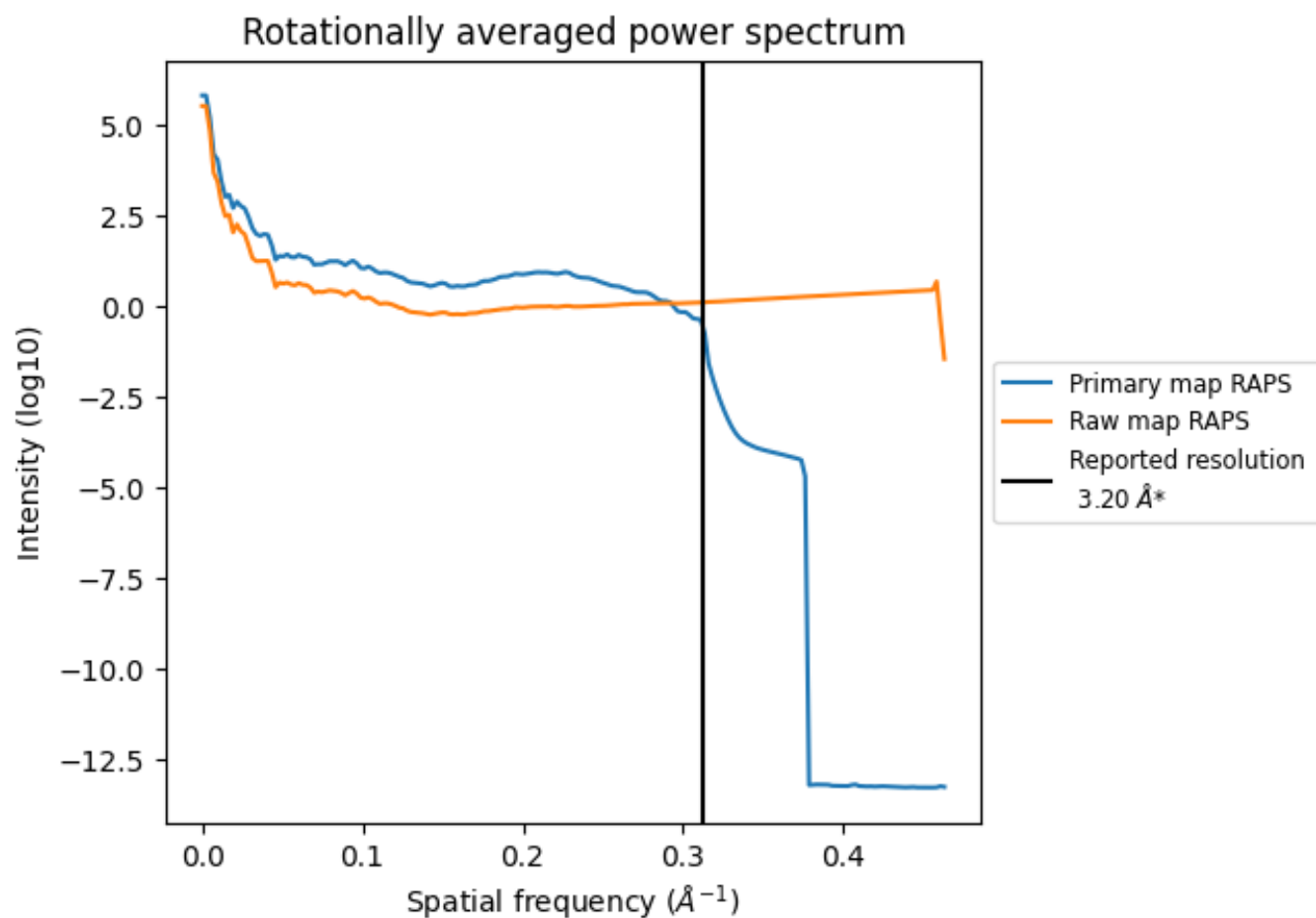
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1369 nm<sup>3</sup>; this corresponds to an approximate mass of 1237 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 ⓘ

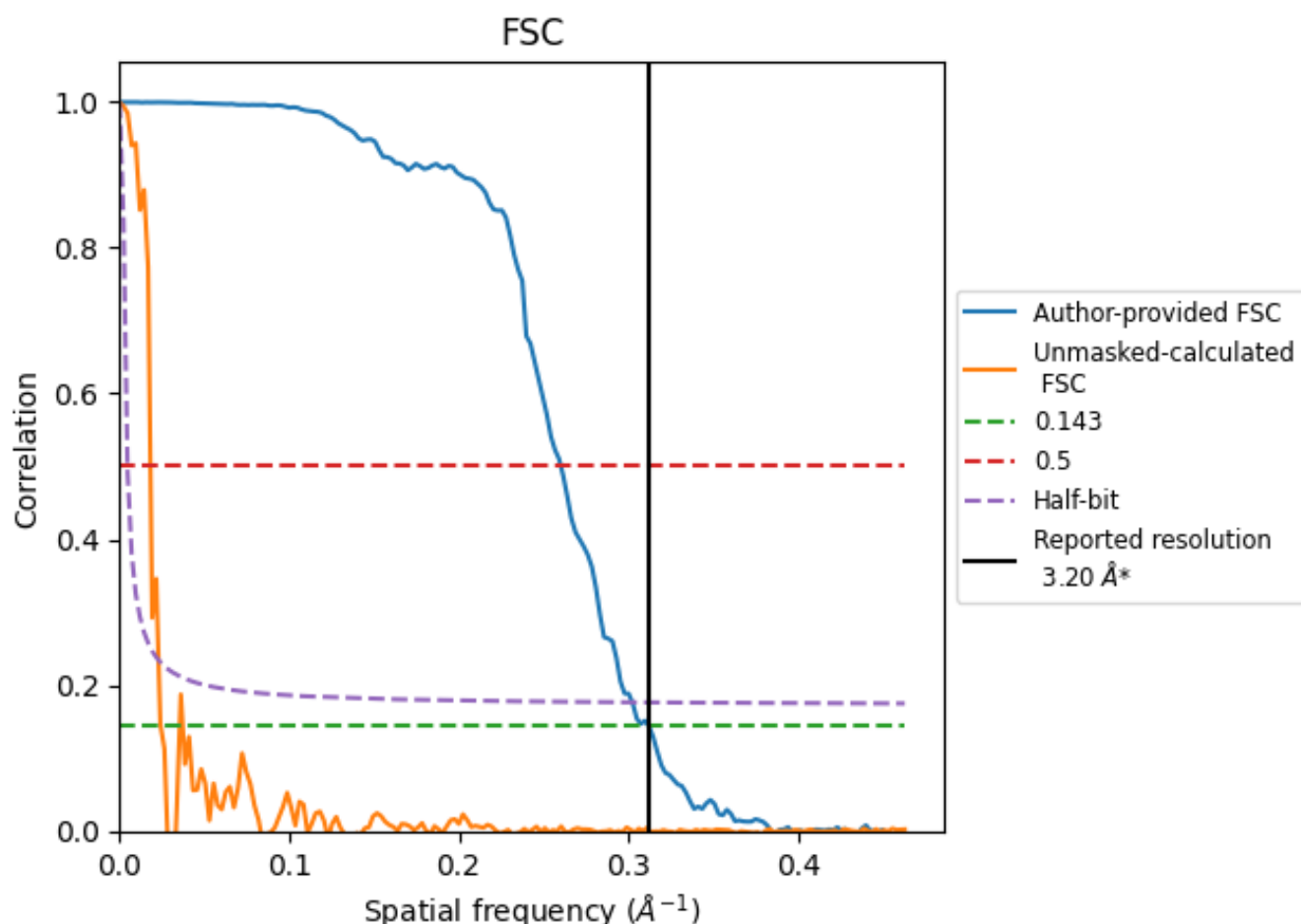


\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 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 0.312 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

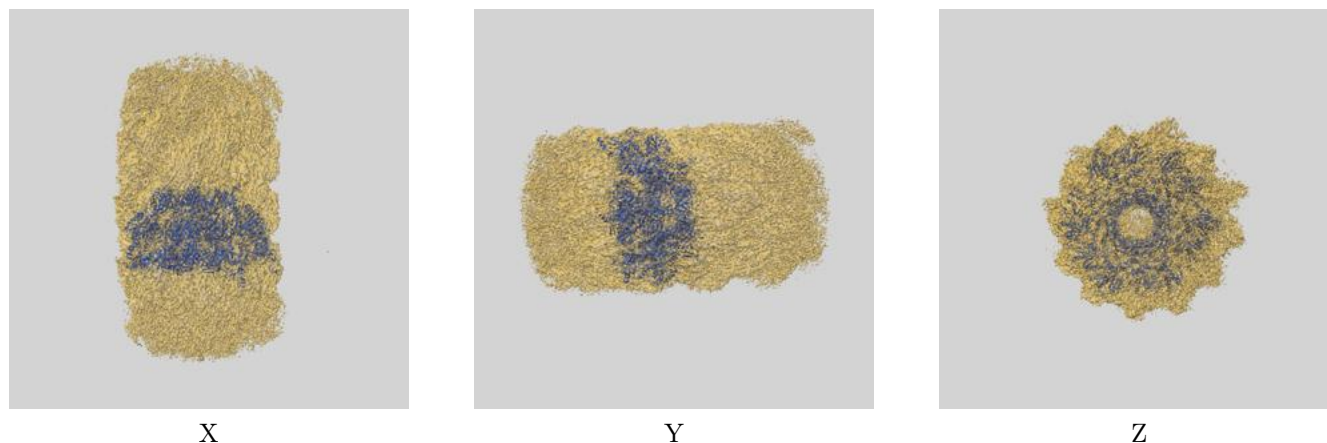
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.20	3.84	3.31
Unmasked-calculated*	41.15	54.64	43.48

\*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 41.15 differs from the reported value 3.2 by more than 10 %

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

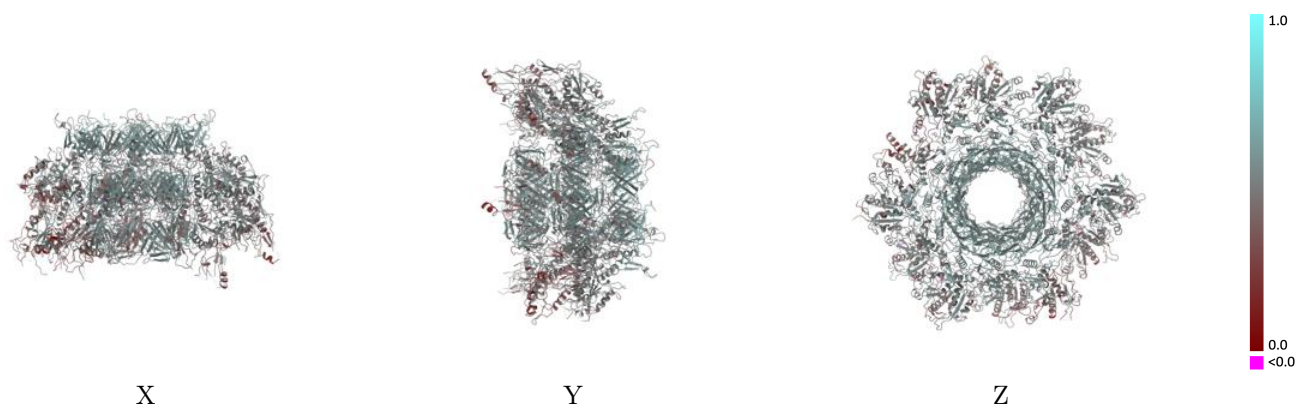
This section contains information regarding the fit between EMDB map EMD-29353 and PDB model 8FOP. Per-residue inclusion information can be found in section 3 on page 6.

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



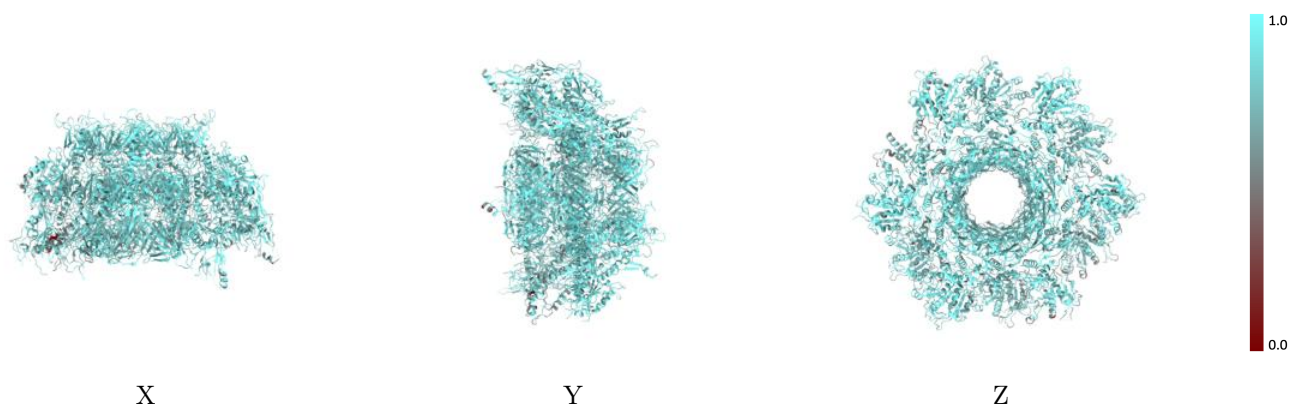
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



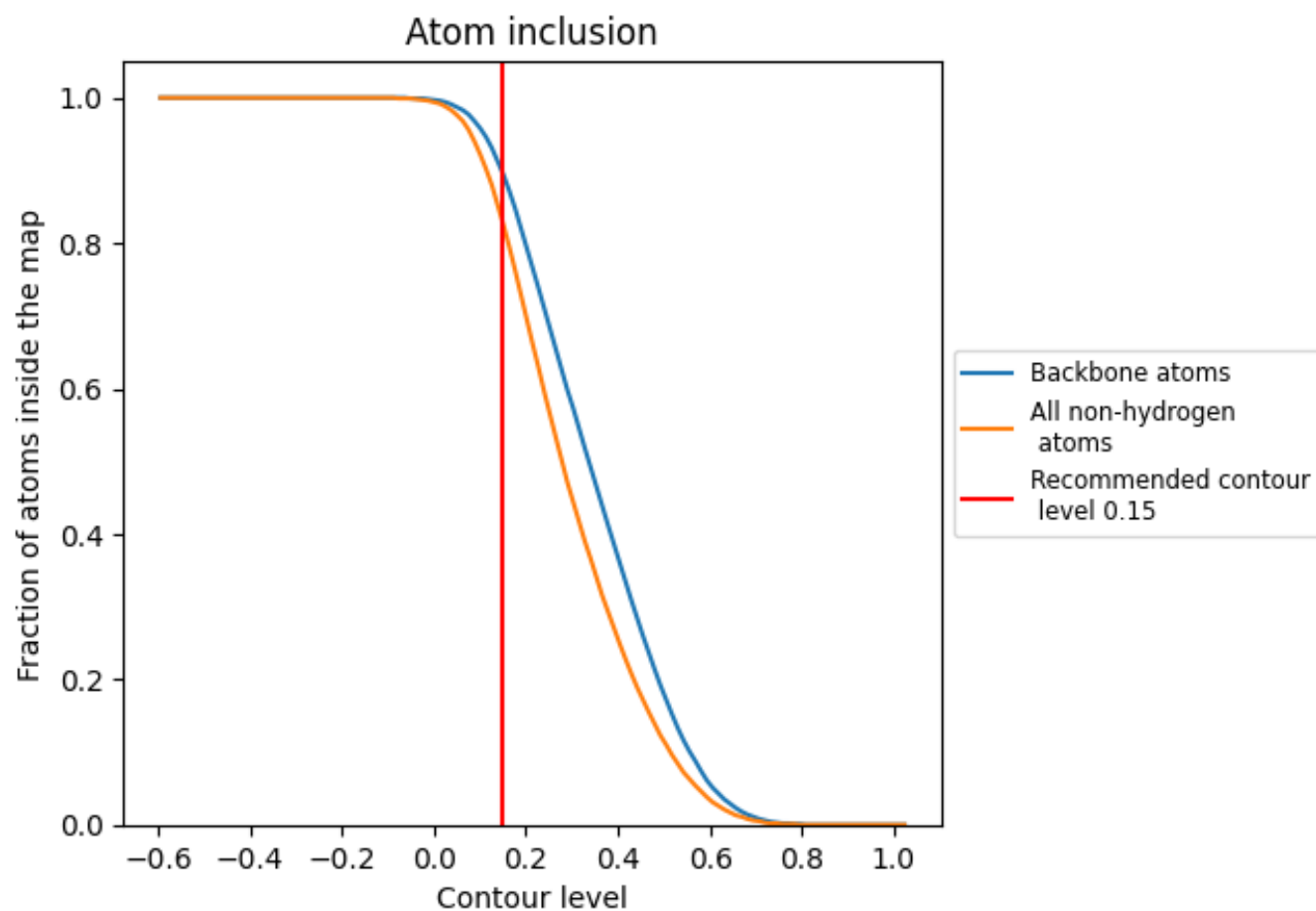
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

## 9.4 Atom inclusion [i](#)

































































At the recommended contour level, 90% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8270	 0.4890
B	 0.8490	 0.5280
C	 0.8570	 0.5450
D	 0.8580	 0.5570
E	 0.8510	 0.5460
F	 0.8710	 0.5550
G	 0.8490	 0.5410
H	 0.8350	 0.5250
I	 0.8650	 0.5520
J	 0.8570	 0.5450
K	 0.8400	 0.5300
L	 0.8700	 0.5520
M	 0.8760	 0.5510
N	 0.8530	 0.5480
O	 0.8630	 0.5510
P	 0.8510	 0.5470
Q	 0.8250	 0.5240
R	 0.8570	 0.5480
S	 0.8640	 0.5490
T	 0.8160	 0.4690
U	 0.8580	 0.4940
W	 0.8260	 0.4740
X	 0.8150	 0.4540
Z	 0.7490	 0.4040
a	 0.8460	 0.4870
c	 0.8170	 0.4710
d	 0.8240	 0.4680
f	 0.7930	 0.4530
g	 0.7910	 0.4340
i	 0.7680	 0.4410
j	 0.8310	 0.4810

