



## Full wwPDB EM Validation Report ⓘ

Jul 21, 2025 – 05:19 PM EDT

PDB ID : 9OUU / pdb\_00009ouu  
EMDB ID : EMD-70882  
Title : SPOP double donut locally refined MATH domains  
Authors : Cuneo, M.J.  
Deposited on : 2025-05-29  
Resolution : 4.30 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.dev118  
MolProbity : 4-5-2 with Phenix2.0rc1  
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) : 2.44

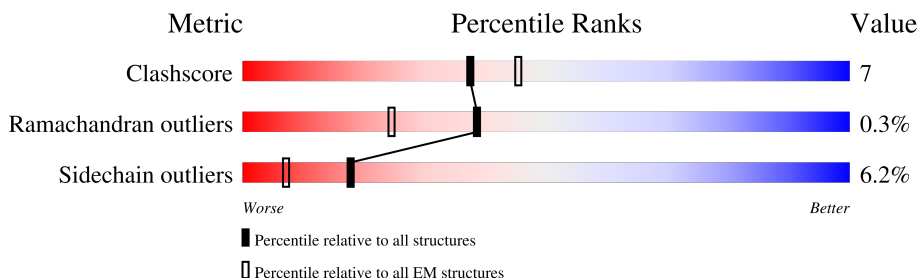
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.30 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.








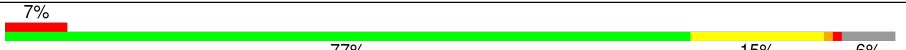
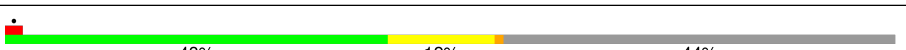
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	A	373	
1	B	373	
1	C	373	
1	D	373	
1	E	373	
1	F	373	
1	G	373	
1	H	373	

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Mol	Chain	Length	Quality of chain
1	I	373	
1	J	373	
1	K	373	
1	L	373	
1	M	373	
1	N	373	
1	P	373	

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 35456 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.

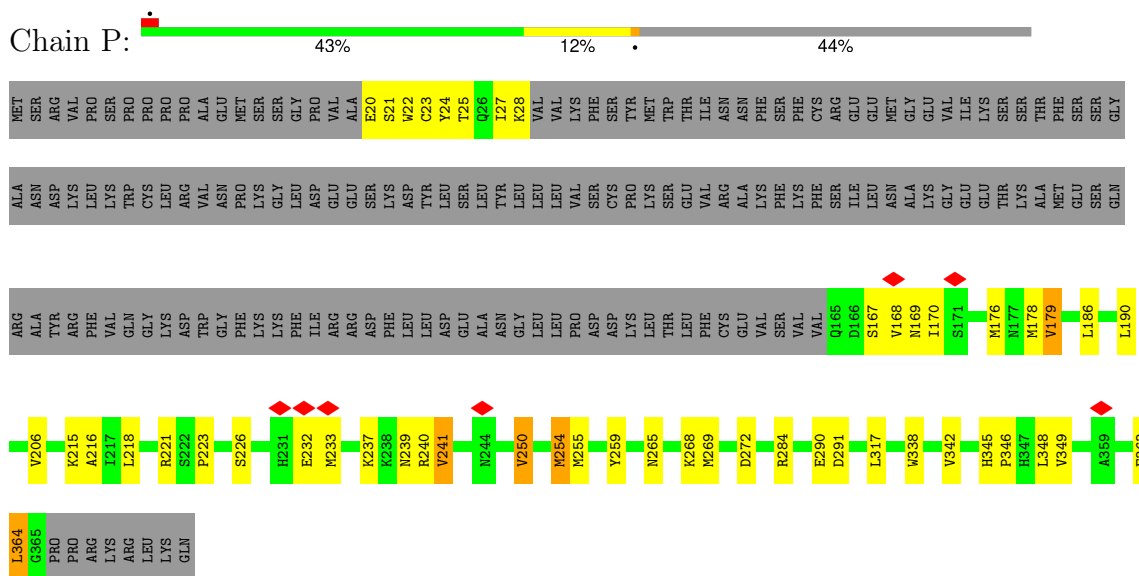
- Molecule 1 is a protein called Speckle-type POZ protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	P	210	Total	C	N	O	S	0	0
			1634	1024	273	319	18		
1	B	349	Total	C	N	O	S	1	0
			2760	1751	459	525	25		
1	D	348	Total	C	N	O	S	1	0
			2752	1745	458	524	25		
1	A	348	Total	C	N	O	S	1	0
			2752	1745	458	524	25		
1	C	349	Total	C	N	O	S	1	0
			2760	1751	459	525	25		
1	F	349	Total	C	N	O	S	1	0
			2760	1751	459	525	25		
1	I	135	Total	C	N	O	S	1	0
			1100	709	182	202	7		
1	J	346	Total	C	N	O	S	1	0
			2734	1731	456	522	25		
1	E	135	Total	C	N	O	S	1	0
			1100	709	182	202	7		
1	G	160	Total	C	N	O	S	1	0
			1290	826	214	242	8		
1	H	352	Total	C	N	O	S	1	0
			2778	1763	462	528	25		
1	K	346	Total	C	N	O	S	1	0
			2734	1731	456	522	25		
1	M	349	Total	C	N	O	S	1	0
			2760	1751	459	525	25		
1	L	352	Total	C	N	O	S	1	0
			2778	1763	462	528	25		
1	N	350	Total	C	N	O	S	1	0
			2764	1753	460	526	25		

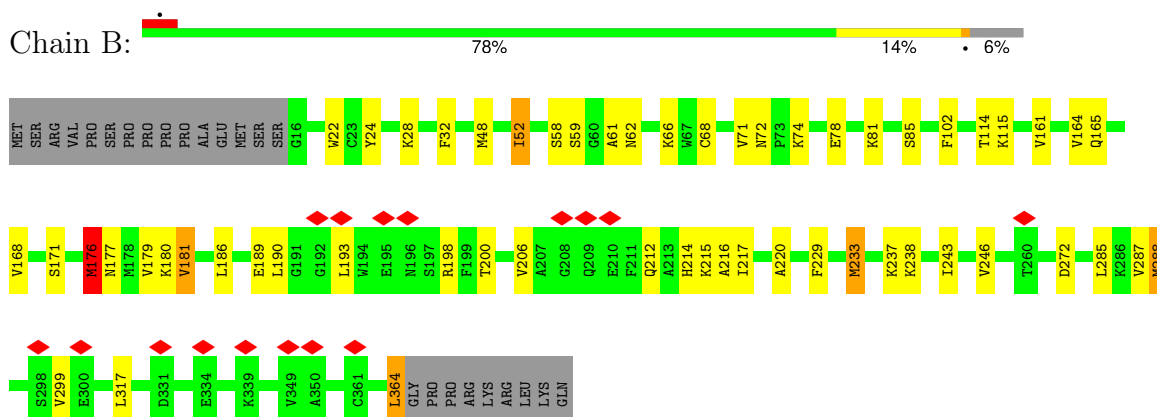
### 3 Residue-property plots

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: Speckle-type POZ protein



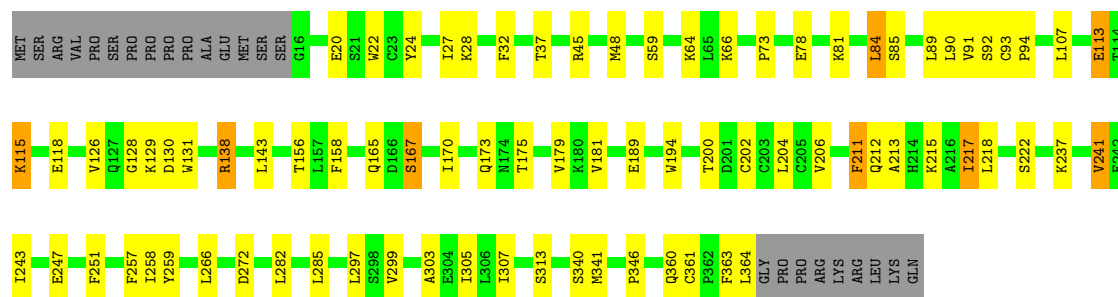
#### • Molecule 1: Speckle-type POZ protein



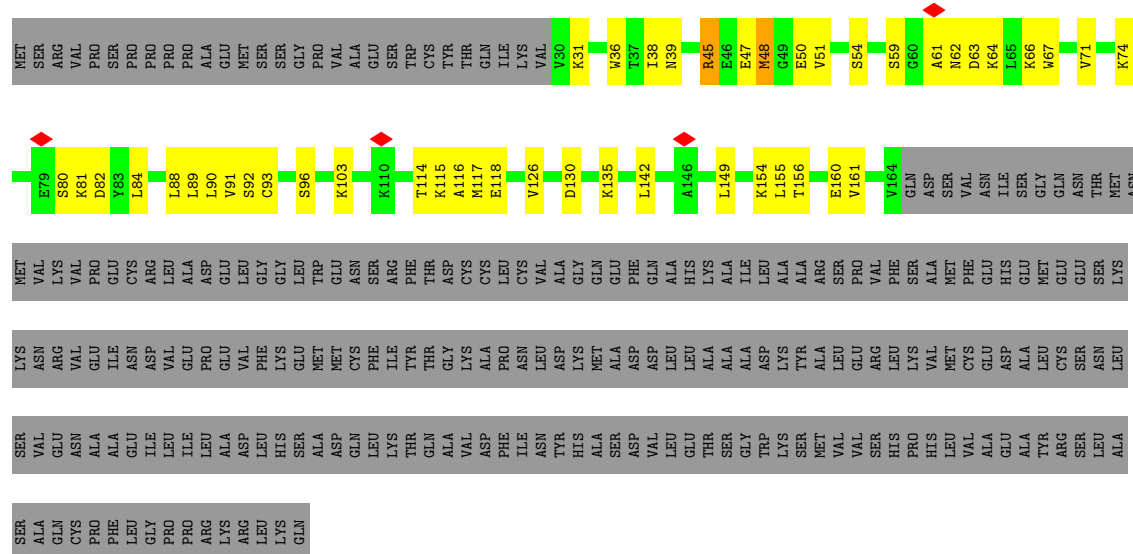
#### • Molecule 1: Speckle-type POZ protein



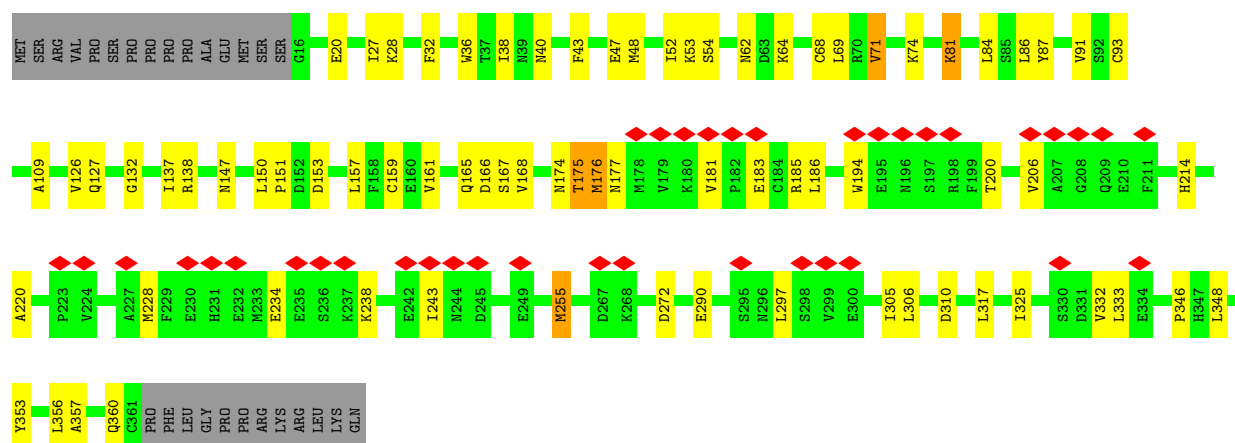




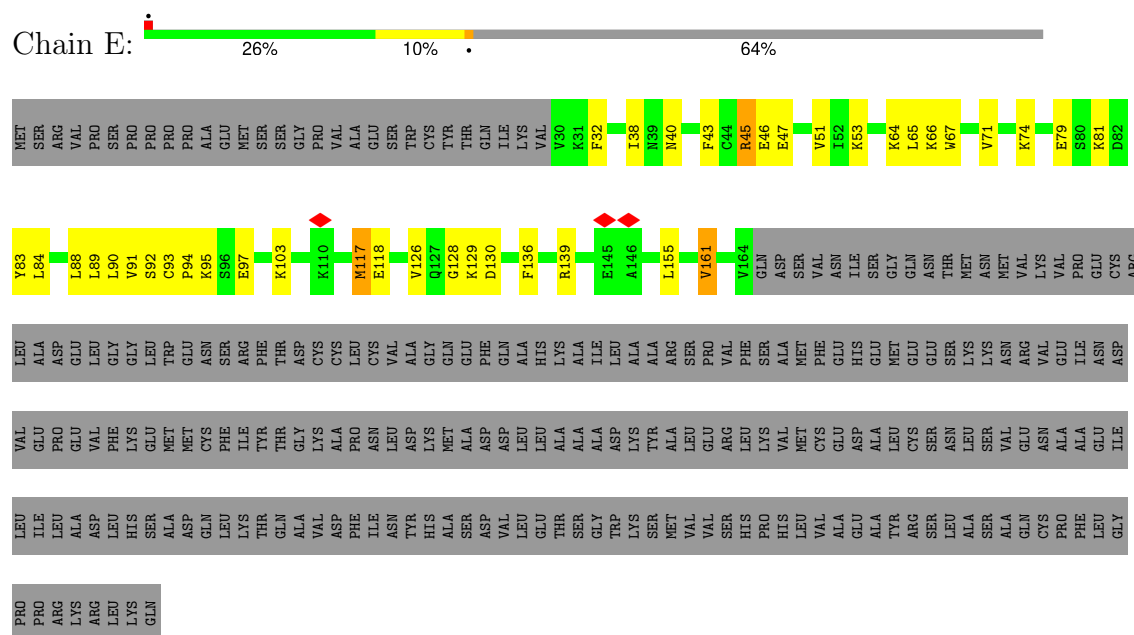
• Molecule 1: Speckle-type POZ protein



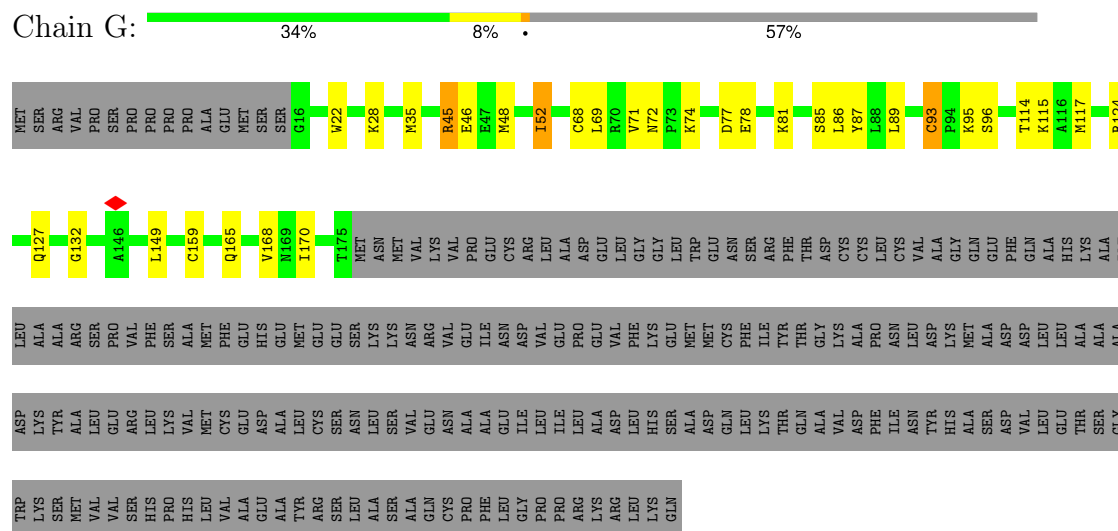
• Molecule 1: Speckle-type POZ protein



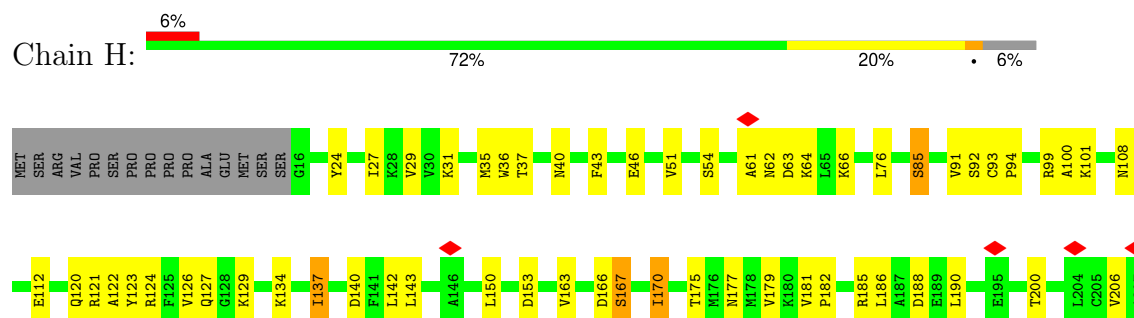
• Molecule 1: Speckle-type POZ protein



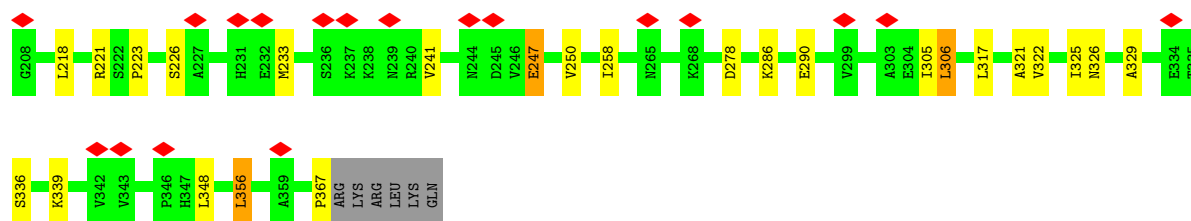
- Molecule 1: Speckle-type POZ protein



- Molecule 1: Speckle-type POZ protein

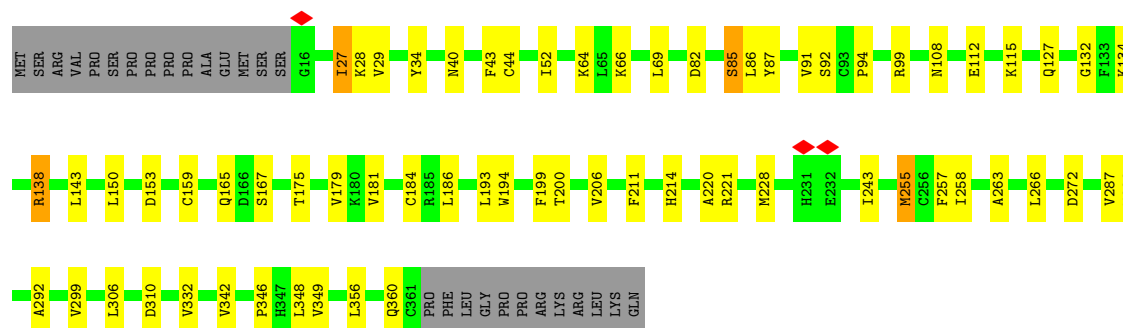






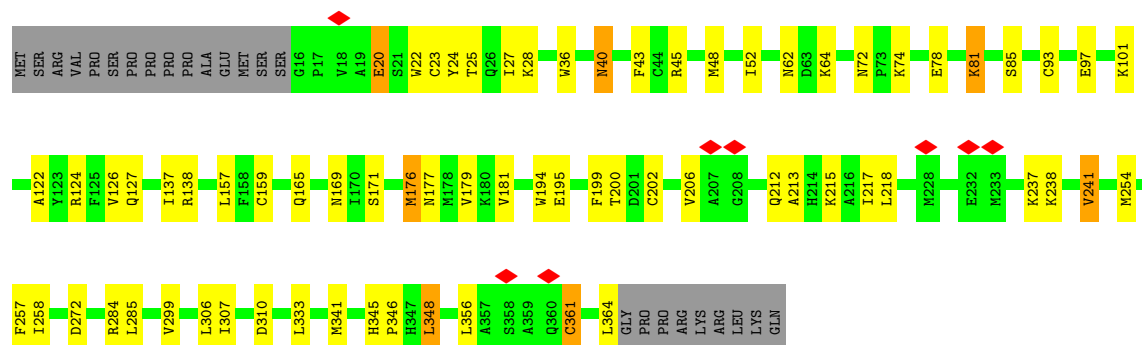
• Molecule 1: Speckle-type POZ protein

Chain K: 75% 17% 7%



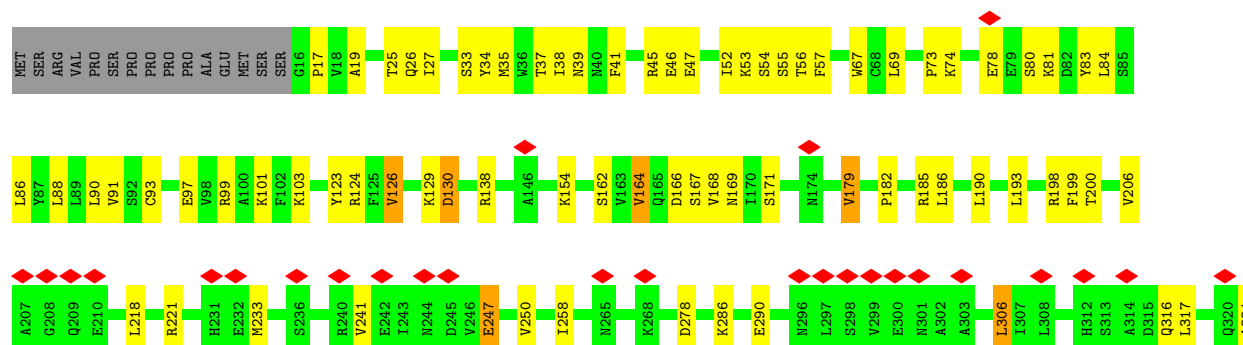
• Molecule 1: Speckle-type POZ protein

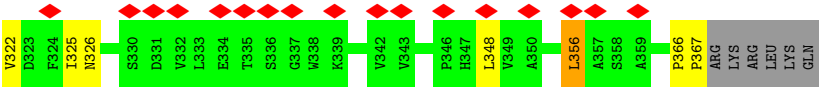
Chain M: 75% 17% 6%



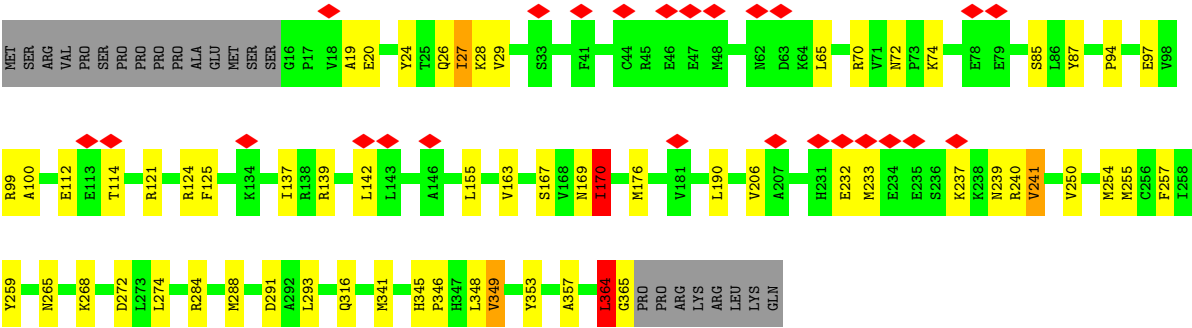
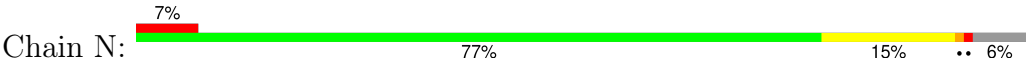
• Molecule 1: Speckle-type POZ protein

Chain L: 12% 72% 21% 6%





● Molecule 1: Speckle-type POZ protein



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	510000	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 ( $e^-/\text{\AA}^2$ )	1.0	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.406	Depositor
Minimum map value	-0.985	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.179	Depositor
Map size ( $\text{\AA}$ )	549.64, 549.64, 549.64	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.057, 1.057, 1.057	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	A	0.30	0/2806	0.55	1/3783 (0.0%)
1	B	0.24	0/2815	0.49	0/3797
1	C	0.23	0/2815	0.47	0/3797
1	D	0.26	1/2807 (0.0%)	0.50	0/3786
1	E	0.21	0/1123	0.48	0/1505
1	F	0.30	0/2815	0.52	2/3797 (0.1%)
1	G	0.27	0/1317	0.50	0/1771
1	H	0.23	0/2835	0.48	0/3826
1	I	0.31	0/1123	0.56	1/1505 (0.1%)
1	J	0.25	0/2787	0.50	2/3758 (0.1%)
1	K	0.24	0/2787	0.47	0/3758
1	L	0.22	0/2835	0.47	0/3826
1	M	0.26	0/2814	0.49	0/3794
1	N	0.24	0/2819	0.54	3/3802 (0.1%)
1	P	0.21	0/1662	0.50	0/2244
All	All	0.25	1/36160 (0.0%)	0.50	9/48749 (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
1	I	0	1
1	J	0	1
1	K	0	1
1	L	0	1
1	M	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	181	VAL	CA-C	5.01	1.56	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	20	GLU	N-CA-C	5.97	120.28	111.87
1	J	174	ASN	CA-C-N	5.60	132.24	121.54
1	J	174	ASN	C-N-CA	5.60	132.24	121.54
1	I	45	ARG	N-CA-CB	-5.55	107.84	114.17
1	N	169	ASN	CA-C-N	5.47	131.82	121.97
1	N	169	ASN	C-N-CA	5.47	131.82	121.97
1	A	198	ARG	N-CA-C	5.33	118.55	111.30
1	F	360	GLN	CA-C-N	5.01	134.02	121.80
1	F	360	GLN	C-N-CA	5.01	134.02	121.80

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	63	ASP	Peptide
1	J	175	THR	Peptide
1	K	175	THR	Peptide
1	L	166	ASP	Peptide
1	M	177	ASN	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2752	0	2706	31	0
1	B	2760	0	2718	37	0
1	C	2760	0	2718	33	0
1	D	2752	0	2707	47	0
1	E	1100	0	1101	31	0
1	F	2760	0	2717	48	0
1	G	1290	0	1280	21	0
1	H	2778	0	2735	67	0
1	I	1100	0	1101	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	2734	0	2690	40	0
1	K	2734	0	2690	41	0
1	L	2778	0	2734	75	0
1	M	2760	0	2716	42	0
1	N	2764	0	2721	45	0
1	P	1634	0	1583	48	0
All	All	35456	0	34917	515	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 7.

All (515) 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:P:25:THR:HG21	1:L:53:LYS:O	1.18	1.28
1:P:23:CYS:HB2	1:L:55:SER:OG	1.11	1.26
1:P:23:CYS:CB	1:L:55:SER:OG	1.85	1.24
1:E:45:ARG:HH22	1:H:124:ARG:NH1	1.48	1.11
1:E:128:GLY:O	1:H:51:VAL:HG21	1.49	1.11
1:H:186:LEU:HD21	1:N:190:LEU:HD12	1.42	0.99
1:P:25:THR:CG2	1:L:53:LYS:O	2.12	0.98
1:P:21:SER:OG	1:L:57:PHE:HB2	1.64	0.97
1:E:45:ARG:NH2	1:H:124:ARG:NH1	2.15	0.94
1:P:20:GLU:HG2	1:L:33:SER:O	1.68	0.93
1:F:27:ILE:HG13	1:F:167:SER:HB3	1.52	0.92
1:C:193:LEU:HD13	1:J:220:ALA:HA	1.53	0.91
1:P:23:CYS:HB2	1:L:55:SER:HG	1.09	0.90
1:P:179:VAL:HG13	1:L:316:GLN:HG3	1.55	0.89
1:J:48:MET:SD	1:J:81:LYS:NZ	2.48	0.86
1:H:40:ASN:HD21	1:N:27:ILE:HG23	1.40	0.85
1:A:53:LYS:HE3	1:A:68:CYS:SG	2.18	0.84
1:L:38:ILE:HD11	1:L:41:PHE:CD1	2.14	0.83
1:C:327:TYR:CE1	1:I:62:ASN:HB3	2.14	0.82
1:H:182:PRO:HD2	1:N:284:ARG:HG3	1.59	0.81
1:B:186:LEU:HD12	1:K:221:ARG:HH12	1.46	0.81
1:E:45:ARG:HH22	1:H:124:ARG:HH11	1.26	0.80
1:L:38:ILE:CD1	1:L:41:PHE:HD1	1.95	0.79
1:C:327:TYR:CD1	1:I:62:ASN:HB3	2.17	0.79
1:H:27:ILE:CG1	1:H:167:SER:HB3	2.12	0.79
1:E:45:ARG:NH2	1:H:124:ARG:HH12	1.80	0.78
1:I:64:LYS:HG3	1:I:64:LYS:O	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:346:PRO:HB3	1:M:346:PRO:HB3	1.66	0.76
1:P:25:THR:CG2	1:L:54:SER:HA	2.16	0.75
1:L:99:ARG:HA	1:L:123:TYR:O	1.87	0.74
1:E:45:ARG:HH22	1:H:124:ARG:HH12	1.31	0.74
1:D:72:ASN:HB2	1:D:85:SER:OG	1.87	0.74
1:F:237:LYS:O	1:F:241:VAL:HB	1.88	0.73
1:C:287:VAL:HG11	1:J:181:VAL:HG22	1.69	0.72
1:P:25:THR:HG23	1:L:54:SER:HA	1.72	0.72
1:H:29:VAL:HG12	1:H:31:LYS:HZ2	1.56	0.70
1:H:27:ILE:HG13	1:H:167:SER:HB3	1.74	0.70
1:B:364:LEU:HB2	1:G:22:TRP:HZ2	1.55	0.70
1:H:40:ASN:ND2	1:N:27:ILE:HG23	2.06	0.70
1:M:93:CYS:H	1:M:127:GLN:HE21	1.39	0.70
1:K:69:LEU:HD23	1:K:86:LEU:HD11	1.75	0.69
1:P:24:TYR:CE1	1:L:37:THR:O	2.45	0.69
1:A:233:MET:HE1	1:A:241:VAL:HB	1.74	0.69
1:F:158:PHE:HE2	1:L:19:ALA:HB2	1.57	0.69
1:E:128:GLY:C	1:H:51:VAL:HG21	2.17	0.69
1:F:27:ILE:HG13	1:F:167:SER:CB	2.23	0.68
1:L:38:ILE:CD1	1:L:41:PHE:CD1	2.75	0.68
1:F:346:PRO:HB3	1:K:346:PRO:HB3	1.74	0.68
1:H:27:ILE:HG12	1:H:167:SER:HB3	1.76	0.68
1:P:21:SER:OG	1:L:57:PHE:CB	2.41	0.68
1:D:346:PRO:HB3	1:N:346:PRO:HB3	1.76	0.67
1:J:360:GLN:HE21	1:M:364:LEU:HB3	1.59	0.67
1:C:69:LEU:HD22	1:C:86:LEU:HD11	1.74	0.67
1:D:27:ILE:HG23	1:D:167:SER:HB3	1.77	0.67
1:H:336:SER:HA	1:H:339:LYS:HD3	1.77	0.67
1:E:126:VAL:HG22	1:E:129:LYS:HB2	1.76	0.66
1:D:233:MET:HE1	1:D:241:VAL:HB	1.76	0.66
1:H:177:ASN:OD1	1:N:291:ASP:OD1	2.14	0.66
1:N:24:TYR:HB3	1:N:170:ILE:HD11	1.77	0.66
1:C:66:LYS:HB2	1:C:92:SER:HB3	1.79	0.65
1:H:35:MET:HB2	1:N:19:ALA:HB3	1.78	0.65
1:H:120:GLN:HG2	1:H:121:ARG:HG3	1.79	0.65
1:K:200:THR:HG22	1:K:214:HIS:HD1	1.62	0.64
1:K:64:LYS:HD3	1:K:94:PRO:HB3	1.79	0.64
1:L:38:ILE:HD12	1:L:41:PHE:HD1	1.62	0.64
1:J:48:MET:HA	1:J:74:LYS:HB3	1.79	0.64
1:K:108:ASN:HD21	1:K:112:GLU:HB2	1.63	0.64
1:F:64:LYS:HD3	1:F:94:PRO:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:177:ASN:ND2	1:N:291:ASP:OD2	2.30	0.63
1:G:96:SER:HB2	1:H:166:ASP:HB2	1.81	0.63
1:N:72:ASN:HB2	1:N:85:SER:HB2	1.81	0.63
1:H:27:ILE:HG12	1:H:167:SER:CB	2.29	0.63
1:K:257:PHE:HB2	1:K:263:ALA:HB2	1.81	0.62
1:N:65:LEU:HD22	1:N:94:PRO:HB3	1.82	0.62
1:L:67:TRP:HE1	1:L:90:LEU:HD12	1.65	0.62
1:E:89:LEU:HD12	1:E:130:ASP:HB3	1.81	0.62
1:B:186:LEU:HD12	1:K:221:ARG:NH1	2.16	0.61
1:C:324:PHE:O	1:C:328:HIS:HB2	2.00	0.61
1:H:290:GLU:HG2	1:H:317:LEU:HB2	1.83	0.61
1:L:27:ILE:HG23	1:L:27:ILE:O	2.01	0.61
1:G:45:ARG:NH2	1:K:99:ARG:HD3	2.16	0.60
1:A:53:LYS:HG2	1:A:54:SER:N	2.16	0.60
1:D:356:LEU:HD21	1:N:357:ALA:HB2	1.83	0.60
1:E:67:TRP:HB3	1:E:88:LEU:HD11	1.83	0.60
1:N:100:ALA:HB3	1:N:125:PHE:HE2	1.67	0.60
1:A:205:CYS:HB3	1:A:242:GLU:HG2	1.84	0.59
1:E:45:ARG:CZ	1:H:124:ARG:HH12	2.15	0.59
1:N:257:PHE:HE1	1:N:284:ARG:HH11	1.50	0.59
1:P:190:LEU:HD12	1:L:186:LEU:HD21	1.84	0.59
1:H:36:TRP:CE2	1:H:54:SER:HB3	2.38	0.59
1:L:78:GLU:HA	1:L:81:LYS:HE2	1.85	0.59
1:F:200:THR:HG21	1:F:212:GLN:HB2	1.84	0.58
1:M:200:THR:HG21	1:M:212:GLN:HB2	1.84	0.58
1:H:101:LYS:HD3	1:M:43:PHE:HE1	1.68	0.58
1:K:206:VAL:HG12	1:K:243:ILE:HB	1.85	0.58
1:L:73:PRO:HA	1:L:84:LEU:HD12	1.85	0.58
1:N:265:ASN:HB3	1:N:268:LYS:HE2	1.86	0.58
1:L:290:GLU:HG2	1:L:317:LEU:HB2	1.85	0.58
1:G:52:ILE:HG23	1:G:71:VAL:HG13	1.83	0.58
1:M:48:MET:SD	1:M:81:LYS:NZ	2.76	0.58
1:P:23:CYS:CB	1:L:55:SER:CB	2.81	0.58
1:P:364:LEU:CD1	1:F:24:TYR:HD2	2.16	0.58
1:C:37:THR:HG22	1:C:156:THR:HG23	1.86	0.57
1:I:59:SER:OG	1:I:61:ALA:O	2.17	0.57
1:J:93:CYS:H	1:J:127:GLN:HE21	1.53	0.57
1:G:45:ARG:CZ	1:K:99:ARG:HD3	2.35	0.57
1:D:36:TRP:HE3	1:D:157:LEU:HD12	1.70	0.57
1:H:233:MET:HE1	1:H:241:VAL:HG12	1.86	0.57
1:F:89:LEU:HD13	1:F:130:ASP:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:32:PHE:HB2	1:J:161:VAL:HB	1.86	0.56
1:F:113:GLU:HG2	1:L:17:PRO:HD3	1.86	0.56
1:F:303:ALA:HB1	1:F:341:MET:HG3	1.87	0.56
1:J:357:ALA:HB2	1:M:356:LEU:HD21	1.87	0.56
1:M:62:ASN:HB2	1:M:64:LYS:HD2	1.87	0.56
1:I:81:LYS:HG2	1:I:82:ASP:N	2.21	0.56
1:I:64:LYS:O	1:I:64:LYS:CG	2.52	0.56
1:D:230:GLU:HB3	1:M:199:PHE:HZ	1.70	0.56
1:A:190:LEU:HD13	1:A:193:LEU:HD23	1.86	0.56
1:H:367:PRO:HD3	1:N:26:GLN:HE21	1.71	0.56
1:M:20:GLU:HB2	1:M:176:MET:HE1	1.87	0.56
1:L:56:THR:HG22	1:L:91:VAL:HG21	1.87	0.56
1:P:21:SER:HG	1:L:57:PHE:HB2	1.71	0.56
1:P:23:CYS:SG	1:L:55:SER:OG	2.63	0.56
1:A:48:MET:HA	1:A:74:LYS:HB2	1.88	0.56
1:P:345:HIS:HB3	1:P:348:LEU:HD23	1.88	0.55
1:H:305:ILE:HD11	1:H:317:LEU:HD11	1.88	0.55
1:N:341:MET:HE3	1:N:349:VAL:HG22	1.88	0.55
1:I:81:LYS:HG2	1:I:82:ASP:H	1.71	0.55
1:E:66:LYS:HB2	1:E:92:SER:HB3	1.88	0.55
1:D:150:LEU:HG	1:D:153:ASP:HA	1.88	0.55
1:E:74:LYS:HA	1:E:139:ARG:HD2	1.89	0.55
1:M:40:ASN:HB2	1:M:43:PHE:HD2	1.70	0.55
1:N:97:GLU:HG3	1:N:124:ARG:HH21	1.70	0.55
1:B:78:GLU:HA	1:B:81:LYS:HE3	1.88	0.55
1:D:108:ASN:HD21	1:D:112:GLU:HB2	1.72	0.55
1:F:22:TRP:H	1:F:173:GLN:HA	1.72	0.55
1:D:205:CYS:HB3	1:D:242:GLU:HG2	1.88	0.55
1:D:336:SER:HA	1:D:339:LYS:HD2	1.88	0.55
1:J:206:VAL:HG12	1:J:243:ILE:HB	1.88	0.55
1:H:126:VAL:HG12	1:H:129:LYS:HB2	1.88	0.55
1:D:218:LEU:O	1:D:222:SER:HB3	2.07	0.55
1:H:29:VAL:CG1	1:H:31:LYS:HZ2	2.19	0.54
1:H:85:SER:HB3	1:H:134:LYS:HA	1.88	0.54
1:B:216:ALA:HB2	1:K:199:PHE:HB2	1.88	0.54
1:J:310:ASP:HB2	1:J:348:LEU:HD21	1.89	0.54
1:P:364:LEU:HD21	1:A:37:THR:OG1	2.08	0.54
1:B:215:LYS:HE3	1:B:238:LYS:HE3	1.90	0.54
1:A:24:TYR:HB3	1:A:170:ILE:HG12	1.89	0.54
1:L:193:LEU:HD12	1:L:198:ARG:HG3	1.87	0.54
1:C:306:LEU:HD23	1:C:341:MET:HE1	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:345:HIS:HB3	1:M:348:LEU:HD23	1.89	0.54
1:H:64:LYS:HG3	1:H:94:PRO:HG3	1.89	0.54
1:K:28:LYS:HB3	1:K:165:GLN:HE21	1.73	0.54
1:H:367:PRO:HD3	1:N:26:GLN:NE2	2.23	0.53
1:M:48:MET:HA	1:M:74:LYS:HB3	1.88	0.53
1:B:22:TRP:HH2	1:F:364:LEU:HG	1.72	0.53
1:F:218:LEU:HD23	1:F:258:ILE:HG21	1.91	0.53
1:M:218:LEU:HD23	1:M:258:ILE:HG21	1.91	0.53
1:A:69:LEU:HD23	1:A:86:LEU:HD11	1.90	0.53
1:A:52:ILE:HG23	1:A:71:VAL:HG13	1.91	0.53
1:F:66:LYS:HB2	1:F:92:SER:HB3	1.89	0.53
1:F:73:PRO:HA	1:F:84:LEU:HD12	1.89	0.53
1:N:27:ILE:HG13	1:N:167:SER:HB3	1.90	0.53
1:L:101:LYS:HB3	1:L:162:SER:HB2	1.91	0.53
1:I:36:TRP:CE2	1:I:54:SER:HB3	2.44	0.53
1:I:59:SER:HB3	1:J:20:GLU:OE2	2.09	0.53
1:H:66:LYS:HB2	1:H:92:SER:HB3	1.91	0.53
1:P:291:ASP:HB2	1:L:179:VAL:HG21	1.90	0.52
1:D:346:PRO:HB3	1:N:346:PRO:CB	2.39	0.52
1:P:23:CYS:CA	1:L:55:SER:OG	2.53	0.52
1:H:150:LEU:HG	1:H:153:ASP:HA	1.91	0.52
1:N:345:HIS:HB3	1:N:348:LEU:HD23	1.91	0.52
1:H:181:VAL:HG12	1:N:288:MET:HA	1.92	0.52
1:K:66:LYS:HB2	1:K:92:SER:HB3	1.91	0.52
1:P:27:ILE:HD12	1:P:167:SER:HB3	1.90	0.52
1:I:84:LEU:HD11	1:I:142:LEU:HD22	1.92	0.52
1:M:24:TYR:CG	1:N:364:LEU:HD23	2.45	0.52
1:A:194:TRP:HB2	1:A:259:TYR:CD2	2.45	0.52
1:H:108:ASN:HD21	1:H:112:GLU:HB2	1.74	0.52
1:H:182:PRO:CD	1:N:284:ARG:HG3	2.35	0.52
1:P:364:LEU:HD11	1:F:24:TYR:HD2	1.75	0.51
1:D:21:SER:HB3	1:D:173:GLN:HG2	1.92	0.51
1:K:64:LYS:HB3	1:K:94:PRO:HD3	1.92	0.51
1:B:52:ILE:HG23	1:B:71:VAL:HG13	1.91	0.51
1:I:66:LYS:HB2	1:I:92:SER:HB3	1.92	0.51
1:P:186:LEU:HD13	1:L:221:ARG:HH11	1.76	0.51
1:D:66:LYS:HB2	1:D:92:SER:HB3	1.91	0.51
1:E:45:ARG:NH1	1:H:124:ARG:HH12	2.08	0.51
1:K:34:TYR:HB3	1:K:159:CYS:HB3	1.93	0.51
1:L:233:MET:HE1	1:L:241:VAL:HG12	1.92	0.51
1:J:200:THR:HA	1:J:214:HIS:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:38:ILE:HD12	1:E:155:LEU:HD11	1.92	0.51
1:K:27:ILE:HG23	1:K:167:SER:HB3	1.91	0.51
1:M:22:TRP:CZ2	1:N:365:GLY:HA3	2.46	0.51
1:E:65:LEU:HB3	1:E:67:TRP:HE1	1.76	0.51
1:D:250:VAL:HG22	1:D:273:LEU:HD13	1.93	0.50
1:A:250:VAL:HG22	1:A:273:LEU:HD13	1.92	0.50
1:D:182:PRO:HD2	1:M:284:ARG:HG3	1.93	0.50
1:H:326:ASN:HD22	1:H:356:LEU:HD12	1.76	0.50
1:D:341:MET:HE3	1:D:349:VAL:HG22	1.93	0.50
1:F:222:SER:HB2	1:F:282:LEU:HD21	1.93	0.50
1:P:22:TRP:CZ2	1:L:35:MET:HG3	2.47	0.50
1:P:363:PHE:HZ	1:F:170:ILE:CD1	2.25	0.50
1:J:52:ILE:HB	1:J:71:VAL:HG13	1.93	0.50
1:D:87:TYR:HA	1:D:132:GLY:HA3	1.94	0.49
1:F:45:ARG:HD3	1:L:27:ILE:HD11	1.94	0.49
1:I:67:TRP:HB3	1:I:88:LEU:HD11	1.93	0.49
1:A:190:LEU:HA	1:A:193:LEU:HD23	1.94	0.49
1:F:90:LEU:HD21	1:F:93:CYS:HB3	1.94	0.49
1:B:181:VAL:HA	1:K:287:VAL:HG21	1.93	0.49
1:F:194:TRP:HZ3	1:F:213:ALA:HB2	1.78	0.49
1:A:274:LEU:HB2	1:A:289:CYS:HB3	1.95	0.49
1:D:90:LEU:HD21	1:D:93:CYS:HB3	1.94	0.49
1:C:287:VAL:CG1	1:J:181:VAL:HG22	2.39	0.49
1:J:27:ILE:HG12	1:J:167:SER:HB3	1.94	0.49
1:D:69:LEU:HD22	1:D:86:LEU:HD11	1.93	0.49
1:D:51:VAL:HG23	1:D:51:VAL:O	2.12	0.49
1:B:193:LEU:HD13	1:K:220:ALA:HA	1.95	0.48
1:C:193:LEU:HD22	1:J:220:ALA:CB	2.42	0.48
1:I:39:ASN:HA	1:I:154:LYS:HG2	1.95	0.48
1:E:45:ARG:NH2	1:H:124:ARG:HH11	1.97	0.48
1:L:45:ARG:HD3	1:L:74:LYS:HE3	1.95	0.48
1:K:299:VAL:HG13	1:K:332:VAL:HG12	1.96	0.48
1:B:200:THR:HG22	1:B:212:GLN:HG3	1.95	0.48
1:D:79:GLU:HB3	1:D:135:LYS:HZ1	1.79	0.48
1:E:40:ASN:HB2	1:E:43:PHE:HD1	1.78	0.48
1:A:100:ALA:O	1:A:122:ALA:HA	2.14	0.48
1:C:327:TYR:CE2	1:I:64:LYS:HB3	2.48	0.48
1:G:45:ARG:HG2	1:G:46:GLU:HG2	1.96	0.48
1:G:87:TYR:HA	1:G:132:GLY:HA3	1.95	0.48
1:P:239:ASN:HD22	1:P:240:ARG:HE	1.61	0.48
1:J:183:GLU:HB2	1:J:185:ARG:HH21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:23:CYS:CB	1:L:55:SER:HG	1.98	0.48
1:P:265:ASN:HB3	1:P:268:LYS:HE2	1.95	0.48
1:A:35:MET:HB3	1:F:22:TRP:HA	1.96	0.48
1:J:40:ASN:HB2	1:J:43:PHE:HD2	1.79	0.48
1:K:228:MET:HE3	1:K:228:MET:HB3	1.75	0.48
1:I:31:LYS:HA	1:I:161:VAL:O	2.14	0.48
1:J:62:ASN:HB2	1:J:64:LYS:HD2	1.95	0.48
1:M:36:TRP:HD1	1:M:157:LEU:HD12	1.78	0.48
1:B:32:PHE:HB2	1:B:161:VAL:HG12	1.95	0.48
1:D:255:MET:HE2	1:D:255:MET:HB3	1.77	0.48
1:H:322:VAL:HA	1:H:325:ILE:HG22	1.95	0.48
1:K:310:ASP:HB2	1:K:348:LEU:HD21	1.95	0.48
1:L:322:VAL:HA	1:L:325:ILE:HG22	1.95	0.47
1:J:332:VAL:HG23	1:J:333:LEU:HD12	1.94	0.47
1:L:88:LEU:O	1:L:130:ASP:HA	2.14	0.47
1:L:247:GLU:HG3	1:L:250:VAL:HG12	1.96	0.47
1:B:24:TYR:CZ	1:F:363:PHE:HB2	2.49	0.47
1:L:47:GLU:HA	1:L:74:LYS:HB2	1.96	0.47
1:A:246:VAL:HG11	1:A:276:ALA:HB2	1.96	0.47
1:F:64:LYS:HB3	1:F:94:PRO:HD3	1.96	0.47
1:M:101:LYS:HZ3	1:M:122:ALA:N	2.13	0.47
1:D:126:VAL:HG12	1:D:129:LYS:HB2	1.97	0.47
1:J:297:LEU:HD23	1:J:305:ILE:HD13	1.96	0.47
1:D:32:PHE:HE1	1:D:59:SER:H	1.62	0.47
1:J:28:LYS:HB2	1:J:165:GLN:HB2	1.97	0.47
1:K:150:LEU:HG	1:K:153:ASP:HA	1.97	0.47
1:N:237:LYS:HZ2	1:N:241:VAL:HA	1.80	0.47
1:E:97:GLU:OE2	1:H:46:GLU:OE2	2.32	0.47
1:H:278:ASP:HA	1:H:286:LYS:HD2	1.96	0.47
1:L:326:ASN:HA	1:L:356:LEU:HD12	1.95	0.47
1:D:182:PRO:HG2	1:M:284:ARG:HA	1.97	0.47
1:H:137:ILE:HD13	1:H:142:LEU:HB2	1.97	0.47
1:L:25:THR:HA	1:L:169:ASN:HA	1.97	0.47
1:D:257:PHE:CE2	1:D:285:LEU:HB2	2.50	0.46
1:C:22:TRP:CD1	1:C:174:ASN:HD22	2.33	0.46
1:P:237:LYS:HZ2	1:P:241:VAL:HA	1.80	0.46
1:A:78:GLU:HA	1:A:81:LYS:HE3	1.97	0.46
1:C:190:LEU:HD11	1:J:186:LEU:HD21	1.97	0.46
1:D:36:TRP:HD1	1:M:23:CYS:HB3	1.79	0.46
1:H:61:ALA:HA	1:H:62:ASN:HA	1.64	0.46
1:M:307:ILE:HD11	1:M:341:MET:HG2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:LYS:HB2	1:B:165:GLN:HB2	1.97	0.46
1:B:58:SER:HB2	1:B:66:LYS:HD3	1.97	0.46
1:B:214:HIS:HB2	1:B:217:ILE:HG22	1.97	0.46
1:D:64:LYS:HG3	1:D:94:PRO:HG3	1.96	0.46
1:J:150:LEU:HG	1:J:153:ASP:HA	1.97	0.46
1:N:99:ARG:HH22	1:N:121:ARG:CZ	2.29	0.46
1:L:80:SER:HB2	1:L:83:TYR:HB2	1.96	0.46
1:P:218:LEU:HD21	1:P:255:MET:HE1	1.96	0.46
1:A:33:SER:HG	1:F:20:GLU:H	1.63	0.46
1:J:228:MET:HE3	1:J:228:MET:HB3	1.88	0.46
1:G:68:CYS:SG	1:G:89:LEU:HB3	2.56	0.46
1:H:218:LEU:HD23	1:H:258:ILE:HG21	1.97	0.46
1:H:247:GLU:HG3	1:H:250:VAL:HG12	1.97	0.46
1:B:48:MET:HA	1:B:74:LYS:HB2	1.97	0.46
1:D:356:LEU:CD2	1:N:357:ALA:HB2	2.46	0.46
1:A:53:LYS:HG2	1:A:54:SER:O	2.16	0.46
1:L:34:TYR:HE2	1:L:69:LEU:HG	1.81	0.46
1:A:53:LYS:CG	1:A:54:SER:N	2.78	0.46
1:C:79:GLU:HB3	1:C:135:LYS:HZ1	1.79	0.46
1:M:23:CYS:SG	1:M:169:ASN:HB3	2.55	0.46
1:M:97:GLU:HB3	1:M:124:ARG:HH21	1.81	0.46
1:B:229:PHE:HE1	1:B:237:LYS:HB3	1.81	0.46
1:C:126:VAL:HG12	1:C:129:LYS:HB2	1.98	0.46
1:K:40:ASN:HB3	1:K:43:PHE:HD2	1.81	0.46
1:B:102:PHE:HB3	1:B:161:VAL:HG23	1.97	0.45
1:D:83:TYR:HE1	1:D:138:ARG:HG2	1.81	0.45
1:I:117:MET:HE3	1:I:117:MET:HB2	1.84	0.45
1:J:353:TYR:CE1	1:M:356:LEU:HD22	2.51	0.45
1:F:364:LEU:HD13	1:K:360:GLN:HG3	1.98	0.45
1:J:325:ILE:HG23	1:J:332:VAL:HG21	1.98	0.45
1:B:186:LEU:HD21	1:K:186:LEU:HB3	1.98	0.45
1:D:36:TRP:CD1	1:M:23:CYS:HB3	2.50	0.45
1:F:28:LYS:HB3	1:F:165:GLN:HE21	1.81	0.45
1:B:176:MET:HB2	1:B:177:ASN:H	1.53	0.45
1:C:138:ARG:HB2	1:C:141:PHE:HB3	1.99	0.45
1:N:239:ASN:HD22	1:N:240:ARG:HE	1.64	0.45
1:D:22:TRP:NE1	1:D:174:ASN:HB3	2.31	0.45
1:C:76:LEU:HD23	1:C:134:LYS:HD3	1.98	0.45
1:C:85:SER:HB3	1:C:134:LYS:HA	1.97	0.45
1:F:45:ARG:HH11	1:L:164:VAL:HB	1.82	0.45
1:P:168:VAL:HG13	1:P:169:ASN:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:128:GLY:O	1:I:51:VAL:HG21	2.17	0.45
1:I:38:ILE:HD12	1:I:155:LEU:HD11	1.98	0.45
1:M:176:MET:HE3	1:M:176:MET:HB3	1.71	0.45
1:M:310:ASP:HB2	1:M:348:LEU:HD11	1.98	0.45
1:L:83:TYR:HD1	1:L:138:ARG:HA	1.82	0.45
1:N:70[A]:ARG:HH12	1:N:87:TYR:HB3	1.81	0.45
1:C:65:LEU:HD23	1:C:65:LEU:HA	1.85	0.45
1:C:81:LYS:HB2	1:C:81:LYS:HE2	1.64	0.45
1:F:48:MET:HE3	1:F:48:MET:HB2	1.88	0.45
1:F:257:PHE:CE2	1:F:285:LEU:HB2	2.52	0.45
1:J:47:GLU:HA	1:J:74:LYS:NZ	2.32	0.45
1:E:32:PHE:HB2	1:E:161:VAL:HG13	1.98	0.45
1:E:103:LYS:HA	1:E:118:GLU:HA	1.98	0.45
1:P:24:TYR:OH	1:L:39:ASN:ND2	2.50	0.45
1:D:222:SER:HB3	1:D:225:PHE:HB2	1.98	0.45
1:A:245:ASP:HB2	1:A:279:LYS:HE2	1.98	0.45
1:E:84:LEU:O	1:E:136:PHE:HB3	2.17	0.45
1:K:87:TYR:HA	1:K:132:GLY:HA3	1.99	0.45
1:M:48:MET:HE1	1:M:78:GLU:OE2	2.17	0.45
1:I:80:SER:HB3	1:I:135:LYS:HE2	1.99	0.44
1:E:90:LEU:HD21	1:E:93:CYS:HB3	2.00	0.44
1:M:72:ASN:HB2	1:M:85:SER:OG	2.16	0.44
1:L:34:TYR:CE2	1:L:69:LEU:CD1	3.01	0.44
1:M:28:LYS:HB2	1:M:165:GLN:HB2	1.98	0.44
1:L:218:LEU:HD23	1:L:258:ILE:HG21	1.98	0.44
1:C:233:MET:HE2	1:C:233:MET:HB2	1.81	0.44
1:F:115:LYS:HA	1:F:115:LYS:HD2	1.76	0.44
1:F:297:LEU:HD21	1:F:305:ILE:HG21	1.99	0.44
1:L:233:MET:HE2	1:L:233:MET:HB2	1.81	0.44
1:P:290:GLU:HG2	1:P:317:LEU:HB2	2.00	0.44
1:A:175:THR:HB	1:A:178:MET:HE3	1.99	0.44
1:C:61:ALA:HA	1:C:62:ASN:HA	1.62	0.44
1:A:53:LYS:HG2	1:A:54:SER:H	1.83	0.44
1:K:194:TRP:HH2	1:K:211:PHE:HB3	1.83	0.44
1:P:255:MET:HE3	1:P:259:TYR:HE2	1.82	0.44
1:A:35:MET:HE1	1:A:107:LEU:HD11	2.00	0.44
1:A:229:PHE:CE1	1:A:233:MET:HE2	2.52	0.44
1:P:24:TYR:OH	1:L:39:ASN:CG	2.61	0.44
1:P:179:VAL:HG13	1:L:316:GLN:CG	2.38	0.44
1:F:32:PHE:HE1	1:F:59:SER:H	1.65	0.44
1:H:179:VAL:HG22	1:N:316:GLN:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:28:LYS:HE3	1:N:28:LYS:HB3	1.76	0.44
1:D:353:TYR:HA	1:N:353:TYR:HD1	1.83	0.44
1:L:39:ASN:HA	1:L:154:LYS:HG2	2.00	0.44
1:L:90:LEU:HD11	1:L:93:CYS:HB3	2.00	0.43
1:P:338:TRP:CH2	1:P:349:VAL:HG13	2.53	0.43
1:C:229:PHE:HE1	1:C:237:LYS:HB3	1.84	0.43
1:F:78:GLU:HA	1:F:81:LYS:HG3	2.00	0.43
1:F:211:PHE:HD1	1:F:211:PHE:HA	1.71	0.43
1:G:28:LYS:HB2	1:G:165:GLN:HB2	1.99	0.43
1:P:215:LYS:HE3	1:L:199:PHE:HD1	1.82	0.43
1:C:108:ASN:HD21	1:C:112:GLU:HB2	1.83	0.43
1:F:138:ARG:H	1:F:138:ARG:HG2	1.51	0.43
1:H:93:CYS:SG	1:H:127:GLN:HG2	2.59	0.43
1:H:223:PRO:HA	1:H:226:SER:HB3	2.00	0.43
1:N:274:LEU:HD13	1:N:293:LEU:HD12	1.99	0.43
1:B:61:ALA:HA	1:B:62:ASN:HA	1.82	0.43
1:D:48:MET:HA	1:D:74:LYS:HB2	2.00	0.43
1:F:204:LEU:HD22	1:F:243:ILE:HD12	2.01	0.43
1:K:85:SER:HB3	1:K:134:LYS:HA	1.99	0.43
1:L:190:LEU:HD12	1:L:190:LEU:HA	1.89	0.43
1:C:64:LYS:HG3	1:C:94:PRO:HG3	2.01	0.43
1:C:206:VAL:HG11	1:C:243:ILE:HB	2.01	0.43
1:E:64:LYS:HG3	1:E:94:PRO:HD3	2.00	0.43
1:M:194:TRP:HZ3	1:M:213:ALA:HB2	1.83	0.43
1:M:306:LEU:HD23	1:M:341:MET:HE1	1.99	0.43
1:B:220:ALA:HB2	1:K:193:LEU:HD22	2.01	0.43
1:D:102:PHE:HB3	1:D:161:VAL:HG12	2.01	0.43
1:A:115:LYS:HA	1:A:115:LYS:HD3	1.78	0.43
1:I:90:LEU:HD21	1:I:93:CYS:HB3	2.01	0.43
1:H:40:ASN:HB2	1:H:43:PHE:HD1	1.82	0.43
1:J:93:CYS:H	1:J:127:GLN:NE2	2.14	0.43
1:J:175:THR:N	1:J:176:MET:HG2	2.34	0.43
1:K:200:THR:HA	1:K:214:HIS:HB3	2.00	0.43
1:L:34:TYR:CE2	1:L:69:LEU:HG	2.54	0.43
1:P:28:LYS:HB3	1:P:28:LYS:HE3	1.74	0.43
1:B:72:ASN:HB2	1:B:85:SER:OG	2.18	0.43
1:C:193:LEU:HD22	1:J:220:ALA:HB2	2.01	0.43
1:J:54:SER:HB3	1:J:69:LEU:HB2	2.00	0.43
1:E:65:LEU:HB3	1:E:67:TRP:NE1	2.33	0.43
1:E:97:GLU:H	1:N:97:GLU:HG2	1.83	0.43
1:E:117:MET:HE2	1:E:117:MET:HB2	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:194:TRP:CD2	1:J:255:MET:HE2	2.54	0.43
1:J:290:GLU:HG3	1:J:317:LEU:HB2	2.00	0.43
1:L:278:ASP:HA	1:L:286:LYS:HD2	2.00	0.43
1:P:364:LEU:HG	1:F:24:TYR:CD2	2.53	0.43
1:N:74:LYS:HE2	1:N:139:ARG:HG2	2.01	0.43
1:L:39:ASN:OD1	1:L:154:LYS:HD3	2.19	0.42
1:B:186:LEU:HA	1:K:221:ARG:NH2	2.34	0.42
1:I:81:LYS:CG	1:I:82:ASP:H	2.32	0.42
1:H:325:ILE:O	1:H:329:ALA:HB2	2.19	0.42
1:L:97:GLU:HG3	1:L:124:ARG:HB3	2.01	0.42
1:D:61:ALA:HA	1:D:62:ASN:HA	1.67	0.42
1:D:103:LYS:HB2	1:D:118:GLU:HG2	2.00	0.42
1:C:32:PHE:HB2	1:C:161:VAL:HG23	2.02	0.42
1:C:51:VAL:HG23	1:C:51:VAL:O	2.19	0.42
1:A:200:THR:OG1	1:A:212:GLN:HB2	2.19	0.42
1:L:46:GLU:HB2	1:L:73:PRO:HD2	2.01	0.42
1:B:233:MET:HE2	1:B:233:MET:HB2	1.82	0.42
1:C:327:TYR:CE2	1:I:64:LYS:CB	3.03	0.42
1:F:217:ILE:HG12	1:F:259:TYR:CE1	2.55	0.42
1:F:237:LYS:O	1:F:241:VAL:CB	2.64	0.42
1:I:103:LYS:HE3	1:I:116:ALA:HB1	2.01	0.42
1:M:215:LYS:HG3	1:M:238:LYS:HE2	2.02	0.42
1:N:137:ILE:HD13	1:N:142:LEU:HD13	2.01	0.42
1:B:189:GLU:HB3	1:K:221:ARG:HG2	2.00	0.42
1:D:46:GLU:HB2	1:D:50:GLU:CD	2.44	0.42
1:F:307:ILE:HD11	1:F:341:MET:HG2	2.01	0.42
1:G:149:LEU:HD23	1:G:149:LEU:HA	1.92	0.42
1:M:257:PHE:CE2	1:M:285:LEU:HB2	2.54	0.42
1:L:366:PRO:HA	1:L:367:PRO:HD3	1.95	0.42
1:P:216:ALA:HB1	1:L:193:LEU:CD1	2.49	0.42
1:B:32:PHE:HE2	1:B:59:SER:H	1.67	0.42
1:B:115:LYS:HA	1:B:115:LYS:HD3	1.81	0.42
1:D:38:ILE:HA	1:M:25:THR:HB	2.01	0.42
1:D:230:GLU:HB3	1:M:199:PHE:CZ	2.54	0.42
1:G:93:CYS:N	1:G:127:GLN:HE22	2.18	0.42
1:G:95:LYS:HE2	1:G:95:LYS:HB2	1.84	0.42
1:H:76:LEU:HD23	1:H:134:LYS:HD3	2.02	0.42
1:M:237:LYS:O	1:M:241:VAL:HB	2.20	0.42
1:J:109:ALA:HA	1:J:151:PRO:HG3	2.00	0.42
1:H:24:TYR:HB3	1:H:170:ILE:HB	2.01	0.42
1:G:69:LEU:HD23	1:G:86:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:348:LEU:HD13	1:M:348:LEU:HA	1.84	0.42
1:L:126:VAL:HG23	1:L:129:LYS:HB2	2.02	0.42
1:B:114:THR:HG22	1:B:115:LYS:HG2	2.01	0.42
1:F:37:THR:HG22	1:F:156:THR:HG22	2.02	0.42
1:I:48:MET:HE2	1:I:48:MET:HB2	1.87	0.42
1:H:233:MET:HE2	1:H:233:MET:HB2	1.84	0.42
1:M:254:MET:HE3	1:M:254:MET:HB3	1.83	0.42
1:F:129:LYS:HE3	1:F:131:TRP:CZ2	2.55	0.41
1:G:115:LYS:HA	1:G:115:LYS:HD3	1.77	0.41
1:B:190:LEU:HD23	1:B:190:LEU:HA	1.85	0.41
1:J:234:GLU:HA	1:J:238:LYS:HB2	2.01	0.41
1:E:95:LYS:HB3	1:N:97:GLU:OE2	2.20	0.41
1:P:223:PRO:HA	1:P:226:SER:HB3	2.02	0.41
1:P:250:VAL:HA	1:P:269:MET:HE1	2.03	0.41
1:B:186:LEU:HA	1:K:221:ARG:HH22	1.85	0.41
1:D:193:LEU:HD13	1:D:198:ARG:HB3	2.02	0.41
1:L:129:LYS:HD2	1:L:129:LYS:HA	1.78	0.41
1:P:254:MET:HE3	1:P:254:MET:HB3	1.85	0.41
1:B:317:LEU:HD12	1:B:317:LEU:HA	1.92	0.41
1:B:364:LEU:HB2	1:G:22:TRP:CZ2	2.45	0.41
1:F:204:LEU:HD13	1:F:251:PHE:HZ	1.86	0.41
1:E:79:GLU:H	1:E:79:GLU:HG3	1.71	0.41
1:K:266:LEU:HD21	1:K:292:ALA:HB2	2.02	0.41
1:L:38:ILE:HG13	1:L:38:ILE:O	2.19	0.41
1:I:149:LEU:HD12	1:I:149:LEU:HA	1.95	0.41
1:H:40:ASN:OD1	1:N:27:ILE:HD13	2.20	0.41
1:L:306:LEU:HD13	1:L:306:LEU:HA	1.92	0.41
1:I:74:LYS:HA	1:I:74:LYS:HD3	1.93	0.41
1:J:36:TRP:CD1	1:J:157:LEU:HD12	2.54	0.41
1:G:72:ASN:HB2	1:G:85:SER:OG	2.20	0.41
1:H:177:ASN:CG	1:N:291:ASP:OD1	2.64	0.41
1:K:255:MET:HA	1:K:258:ILE:HD12	2.02	0.41
1:B:285:LEU:HA	1:B:288:MET:HG3	2.02	0.41
1:K:342:VAL:HA	1:K:349:VAL:HG21	2.03	0.41
1:F:126:VAL:HG12	1:F:129:LYS:HB2	2.03	0.41
1:E:45:ARG:HH12	1:H:124:ARG:HH12	1.67	0.41
1:G:35:MET:HE3	1:G:35:MET:HB2	1.90	0.41
1:H:100:ALA:O	1:H:122:ALA:HA	2.21	0.41
1:H:306:LEU:HD22	1:H:321:ALA:HB1	2.02	0.41
1:K:82:ASP:HB3	1:K:138:ARG:HH12	1.86	0.41
1:D:30:VAL:HB	1:D:163:VAL:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:38:ILE:O	1:I:154:LYS:HA	2.21	0.41
1:J:68:CYS:SG	1:J:91:VAL:CG1	3.09	0.41
1:G:48:MET:HA	1:G:74:LYS:HB2	2.02	0.41
1:L:103:LYS:HE2	1:L:103:LYS:HB2	1.86	0.41
1:N:27:ILE:HA	1:N:167:SER:HA	2.03	0.41
1:P:221:ARG:HH21	1:L:185:ARG:HH21	1.68	0.40
1:P:284:ARG:HG3	1:L:182:PRO:HD2	2.02	0.40
1:A:293:LEU:HD23	1:A:293:LEU:HA	1.86	0.40
1:C:64:LYS:HE2	1:C:94:PRO:HG3	2.04	0.40
1:H:306:LEU:HD13	1:H:306:LEU:HA	1.93	0.40
1:H:326:ASN:HA	1:H:356:LEU:HD12	2.03	0.40
1:K:194:TRP:CG	1:K:255:MET:HE2	2.56	0.40
1:L:306:LEU:HD22	1:L:321:ALA:HB1	2.04	0.40
1:N:255:MET:HE3	1:N:259:TYR:HE2	1.86	0.40
1:D:341:MET:HE2	1:D:341:MET:HB3	1.97	0.40
1:E:74:LYS:HE3	1:E:74:LYS:HB2	1.88	0.40
1:G:114:THR:HB	1:G:149:LEU:HD21	2.02	0.40
1:M:74:LYS:HB2	1:M:74:LYS:HE3	1.89	0.40
1:A:308:LEU:HD12	1:A:308:LEU:HA	1.92	0.40
1:F:204:LEU:HD13	1:F:251:PHE:CZ	2.56	0.40
1:I:47:GLU:H	1:I:47:GLU:HG3	1.74	0.40
1:J:87:TYR:HA	1:J:132:GLY:HA3	2.03	0.40
1:H:99:ARG:HA	1:H:123:TYR:O	2.20	0.40
1:L:26:GLN:HE21	1:L:27:ILE:N	2.18	0.40
1:B:206:VAL:HG11	1:B:243:ILE:HB	2.03	0.40
1:G:124:ARG:HH21	1:M:45:ARG:HH21	1.68	0.40
1:H:185:ARG:HA	1:H:188:ASP:OD2	2.21	0.40
1:P:346:PRO:HB3	1:A:346:PRO:HB3	2.04	0.40
1:B:180:LYS:HE2	1:B:180:LYS:HB2	1.77	0.40
1:D:83:TYR:CE1	1:D:138:ARG:HG2	2.56	0.40
1:C:198:ARG:HG3	1:C:199:PHE:HD1	1.87	0.40
1:I:115:LYS:HD3	1:I:115:LYS:HA	1.93	0.40
1:G:78:GLU:HA	1:G:81:LYS:HE3	2.04	0.40
1:H:37:THR:HB	1:N:24:TYR:HA	2.04	0.40
1:K:115:LYS:HD2	1:K:115:LYS:HA	1.85	0.40
1:K:266:LEU:HD13	1:K:288:MET:SD	2.61	0.40
1:N:288:MET:HE3	1:N:288:MET:HB2	1.88	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	344/373 (92%)	328 (95%)	16 (5%)	0	100	100
1	B	347/373 (93%)	330 (95%)	16 (5%)	1 (0%)	37	72
1	C	347/373 (93%)	329 (95%)	17 (5%)	1 (0%)	37	72
1	D	346/373 (93%)	329 (95%)	17 (5%)	0	100	100
1	E	133/373 (36%)	126 (95%)	6 (4%)	1 (1%)	16	53
1	F	347/373 (93%)	328 (94%)	18 (5%)	1 (0%)	37	72
1	G	158/373 (42%)	154 (98%)	4 (2%)	0	100	100
1	H	350/373 (94%)	333 (95%)	17 (5%)	0	100	100
1	I	133/373 (36%)	126 (95%)	7 (5%)	0	100	100
1	J	344/373 (92%)	328 (95%)	14 (4%)	2 (1%)	22	59
1	K	344/373 (92%)	329 (96%)	15 (4%)	0	100	100
1	L	350/373 (94%)	323 (92%)	26 (7%)	1 (0%)	37	72
1	M	345/373 (92%)	325 (94%)	18 (5%)	2 (1%)	22	59
1	N	348/373 (93%)	319 (92%)	27 (8%)	2 (1%)	22	59
1	P	204/373 (55%)	185 (91%)	18 (9%)	1 (0%)	25	63
All	All	4440/5595 (79%)	4192 (94%)	236 (5%)	12 (0%)	38	72

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	176	MET
1	F	361	CYS
1	J	176	MET
1	E	81	LYS
1	M	361	CYS
1	N	170	ILE
1	P	364	LEU
1	J	81	LYS

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Mol	Chain	Res	Type
1	M	81	LYS
1	N	364	LEU
1	L	167	SER
1	C	176	MET

### 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	303/326 (93%)	284 (94%)	19 (6%)	15	37
1	B	304/326 (93%)	288 (95%)	16 (5%)	19	42
1	C	304/326 (93%)	291 (96%)	13 (4%)	25	48
1	D	303/326 (93%)	283 (93%)	20 (7%)	14	35
1	E	122/326 (37%)	112 (92%)	10 (8%)	9	29
1	F	304/326 (93%)	278 (91%)	26 (9%)	8	27
1	G	144/326 (44%)	136 (94%)	8 (6%)	17	40
1	H	306/326 (94%)	288 (94%)	18 (6%)	16	39
1	I	122/326 (37%)	109 (89%)	13 (11%)	5	20
1	J	301/326 (92%)	284 (94%)	17 (6%)	17	40
1	K	301/326 (92%)	285 (95%)	16 (5%)	19	42
1	L	306/326 (94%)	292 (95%)	14 (5%)	23	46
1	M	304/326 (93%)	282 (93%)	22 (7%)	12	32
1	N	304/326 (93%)	287 (94%)	17 (6%)	17	40
1	P	179/326 (55%)	167 (93%)	12 (7%)	13	35
All	All	3907/4890 (80%)	3666 (94%)	241 (6%)	18	37

All (241) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	170	ILE
1	P	176	MET

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Mol	Chain	Res	Type
1	P	178	MET
1	P	179	VAL
1	P	206	VAL
1	P	232	GLU
1	P	233	MET
1	P	241	VAL
1	P	250	VAL
1	P	254	MET
1	P	272	ASP
1	P	342	VAL
1	B	52	ILE
1	B	68	CYS
1	B	164	VAL
1	B	168	VAL
1	B	171	SER
1	B	176	MET
1	B	179	VAL
1	B	181	VAL
1	B	198	ARG
1	B	233	MET
1	B	246	VAL
1	B	272	ASP
1	B	287	VAL
1	B	288	MET
1	B	299	VAL
1	B	364	LEU
1	D	21	SER
1	D	27	ILE
1	D	53	LYS
1	D	91	VAL
1	D	140	ASP
1	D	143	LEU
1	D	163	VAL
1	D	170	ILE
1	D	175	THR
1	D	179	VAL
1	D	181	VAL
1	D	190	LEU
1	D	198	ARG
1	D	204	LEU
1	D	232	GLU
1	D	233	MET

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Mol	Chain	Res	Type
1	D	246	VAL
1	D	250	VAL
1	D	255	MET
1	D	260	THR
1	A	77	ASP
1	A	85	SER
1	A	97	GLU
1	A	159	CYS
1	A	171	SER
1	A	178	MET
1	A	179	VAL
1	A	181	VAL
1	A	184	CYS
1	A	193	LEU
1	A	198	ARG
1	A	217	ILE
1	A	225	PHE
1	A	232	GLU
1	A	246	VAL
1	A	255	MET
1	A	260	THR
1	A	266	LEU
1	A	282	LEU
1	C	25	THR
1	C	80	SER
1	C	85	SER
1	C	91	VAL
1	C	140	ASP
1	C	143	LEU
1	C	163	VAL
1	C	188	ASP
1	C	233	MET
1	C	272	ASP
1	C	299	VAL
1	C	332	VAL
1	C	364	LEU
1	F	84	LEU
1	F	85	SER
1	F	91	VAL
1	F	107	LEU
1	F	113	GLU
1	F	115	LYS

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Mol	Chain	Res	Type
1	F	118	GLU
1	F	138	ARG
1	F	143	LEU
1	F	167	SER
1	F	175	THR
1	F	179	VAL
1	F	181	VAL
1	F	189	GLU
1	F	202	CYS
1	F	206	VAL
1	F	211	PHE
1	F	215	LYS
1	F	217	ILE
1	F	241	VAL
1	F	247	GLU
1	F	266	LEU
1	F	272	ASP
1	F	299	VAL
1	F	313	SER
1	F	340	SER
1	I	45	ARG
1	I	48	MET
1	I	50	GLU
1	I	71	VAL
1	I	89	LEU
1	I	91	VAL
1	I	96	SER
1	I	114	THR
1	I	118	GLU
1	I	126	VAL
1	I	130	ASP
1	I	156	THR
1	I	160	GLU
1	J	38	ILE
1	J	53	LYS
1	J	71	VAL
1	J	84	LEU
1	J	86	LEU
1	J	126	VAL
1	J	137	ILE
1	J	138	ARG
1	J	147	ASN

*Continued on next page...*

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Mol	Chain	Res	Type
1	J	159	CYS
1	J	166	ASP
1	J	168	VAL
1	J	177	ASN
1	J	255	MET
1	J	272	ASP
1	J	306	LEU
1	J	356	LEU
1	E	45	ARG
1	E	46	GLU
1	E	47	GLU
1	E	51	VAL
1	E	53	LYS
1	E	71	VAL
1	E	83	TYR
1	E	91	VAL
1	E	117	MET
1	E	161	VAL
1	G	45	ARG
1	G	52	ILE
1	G	77	ASP
1	G	93	CYS
1	G	117	MET
1	G	159	CYS
1	G	168	VAL
1	G	170	ILE
1	H	63	ASP
1	H	85	SER
1	H	91	VAL
1	H	137	ILE
1	H	140	ASP
1	H	143	LEU
1	H	163	VAL
1	H	167	SER
1	H	170	ILE
1	H	175	THR
1	H	190	LEU
1	H	200	THR
1	H	206	VAL
1	H	221	ARG
1	H	247	GLU
1	H	306	LEU

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Mol	Chain	Res	Type
1	H	348	LEU
1	H	356	LEU
1	K	27	ILE
1	K	29	VAL
1	K	44	CYS
1	K	52	ILE
1	K	85	SER
1	K	91	VAL
1	K	127	GLN
1	K	138	ARG
1	K	143	LEU
1	K	179	VAL
1	K	181	VAL
1	K	184	CYS
1	K	255	MET
1	K	272	ASP
1	K	306	LEU
1	K	356	LEU
1	M	20	GLU
1	M	27	ILE
1	M	40	ASN
1	M	52	ILE
1	M	126	VAL
1	M	137	ILE
1	M	138	ARG
1	M	159	CYS
1	M	171	SER
1	M	176	MET
1	M	179	VAL
1	M	181	VAL
1	M	195	GLU
1	M	202	CYS
1	M	206	VAL
1	M	217	ILE
1	M	241	VAL
1	M	272	ASP
1	M	299	VAL
1	M	333	LEU
1	M	348	LEU
1	M	361	CYS
1	L	52	ILE
1	L	86	LEU

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Mol	Chain	Res	Type
1	L	126	VAL
1	L	130	ASP
1	L	164	VAL
1	L	168	VAL
1	L	171	SER
1	L	179	VAL
1	L	200	THR
1	L	206	VAL
1	L	247	GLU
1	L	306	LEU
1	L	348	LEU
1	L	356	LEU
1	N	27	ILE
1	N	29	VAL
1	N	112	GLU
1	N	114	THR
1	N	155	LEU
1	N	163	VAL
1	N	170	ILE
1	N	176	MET
1	N	206	VAL
1	N	232	GLU
1	N	233	MET
1	N	241	VAL
1	N	250	VAL
1	N	254	MET
1	N	272	ASP
1	N	349	VAL
1	N	364	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	196	ASN
1	P	239	ASN
1	B	169	ASN
1	D	169	ASN
1	A	39	ASN
1	A	40	ASN
1	A	169	ASN
1	A	214	HIS
1	A	360	GLN

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Mol	Chain	Res	Type
1	C	127	GLN
1	F	39	ASN
1	F	165	GLN
1	J	26	GLN
1	J	127	GLN
1	J	360	GLN
1	G	26	GLN
1	H	212	GLN
1	H	326	ASN
1	K	165	GLN
1	K	169	ASN
1	K	320	GLN
1	K	326	ASN
1	K	360	GLN
1	M	127	GLN
1	M	347	HIS
1	L	26	GLN
1	L	196	ASN
1	L	212	GLN
1	L	231	HIS
1	N	26	GLN
1	N	108	ASN
1	N	196	ASN
1	N	214	HIS
1	N	239	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	M	1
1	A	1
1	P	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	175:THR	C	176:MET	N	6.80
1	A	175:THR	C	176:MET	N	4.66
1	P	170:ILE	C	171:SER	N	3.29

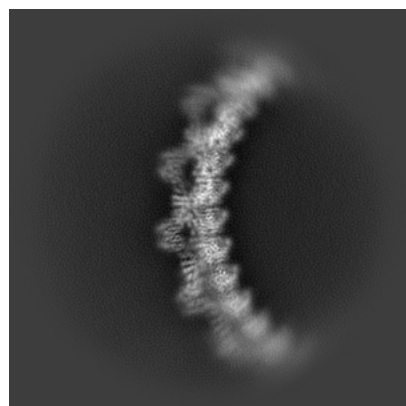
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70882. These allow visual inspection of the internal detail of the map and identification of artifacts.

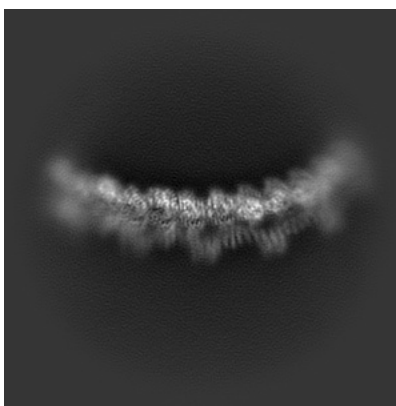
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

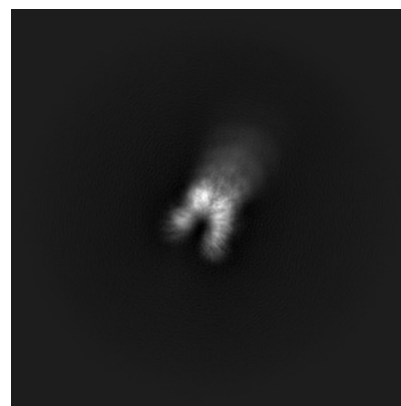
#### 6.1.1 Primary map



X

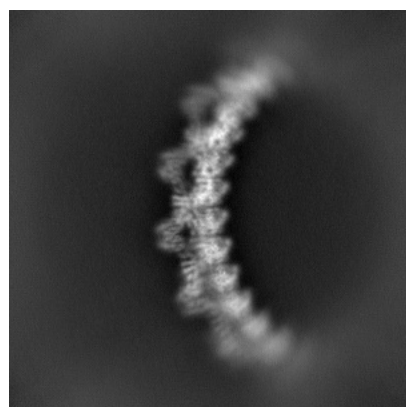


Y

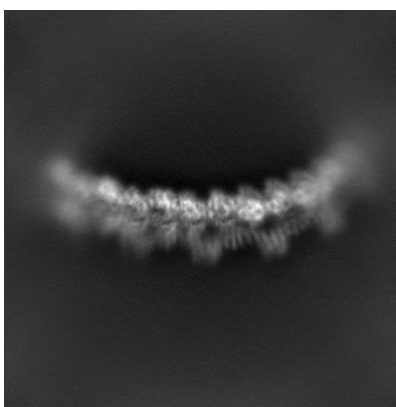


Z

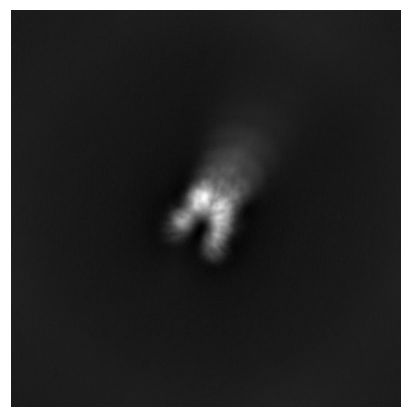
#### 6.1.2 Raw map



X



Y

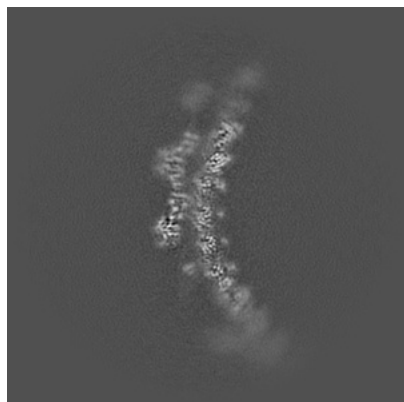


Z

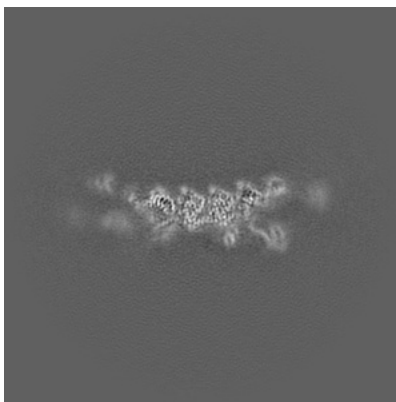
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

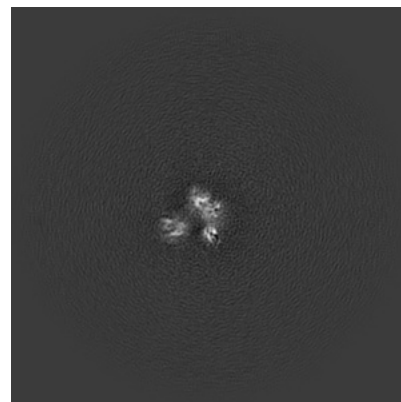
### 6.2.1 Primary map



X Index: 260

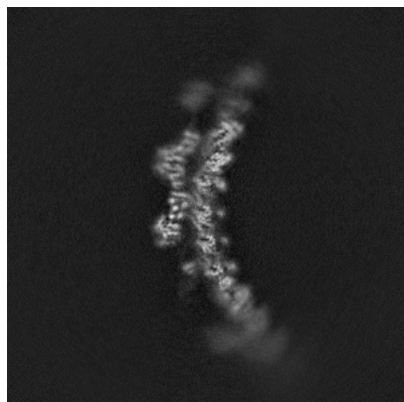


Y Index: 260

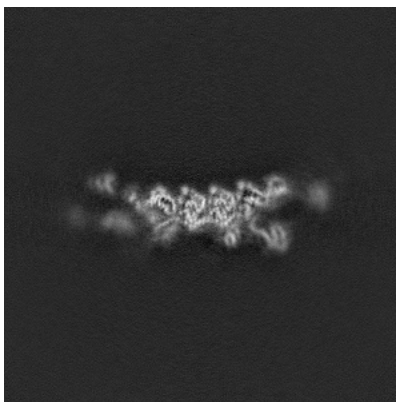


Z Index: 260

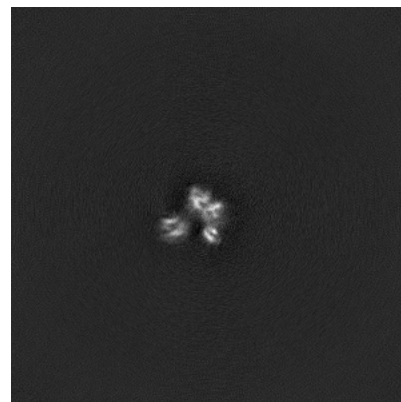
### 6.2.2 Raw map



X Index: 260



Y Index: 260

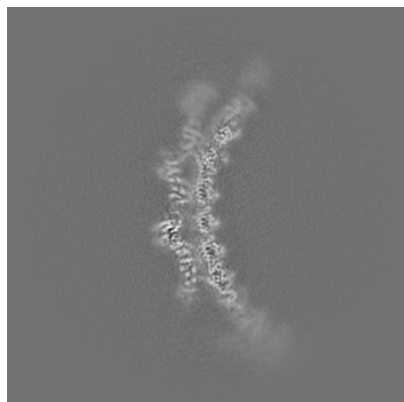


Z Index: 260

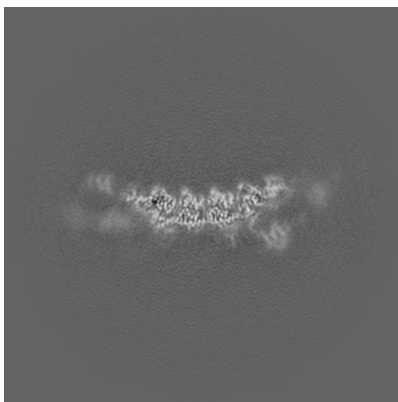
The images above show central slices of the map in three orthogonal directions.

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

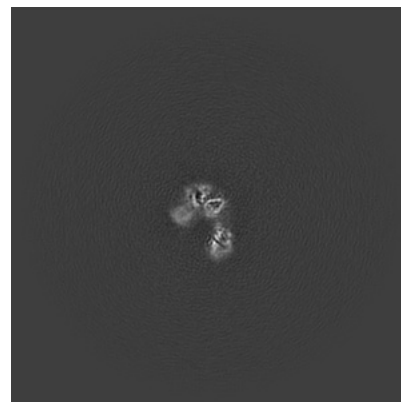
### 6.3.1 Primary map



X Index: 270

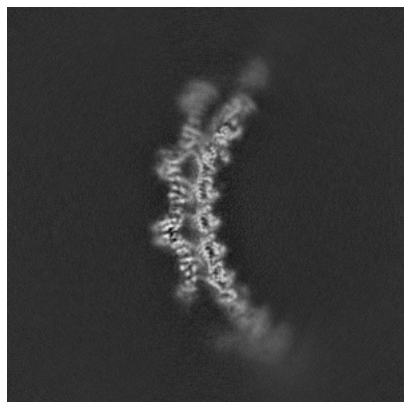


Y Index: 263

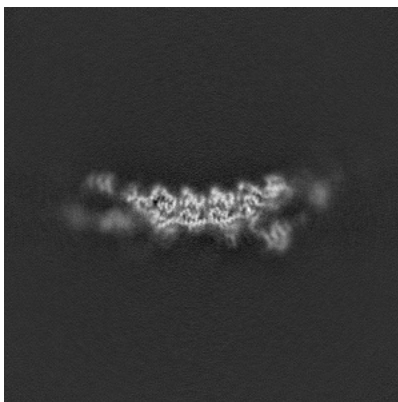


Z Index: 212

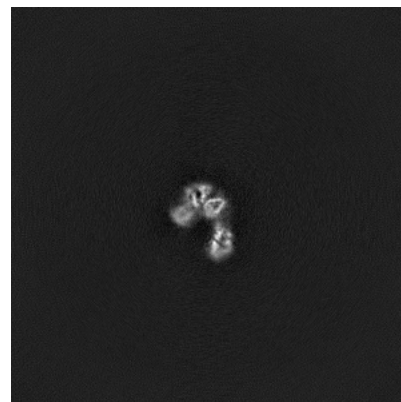
### 6.3.2 Raw map



X Index: 269



Y Index: 263



Z Index: 213

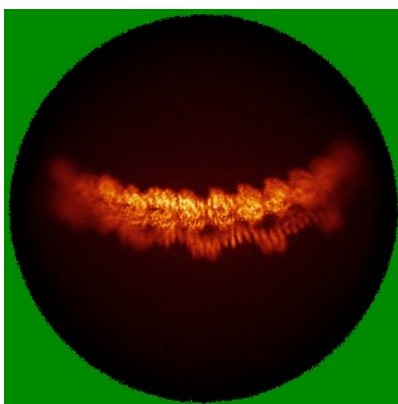
The images above show the largest variance slices of the map in three orthogonal directions.

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

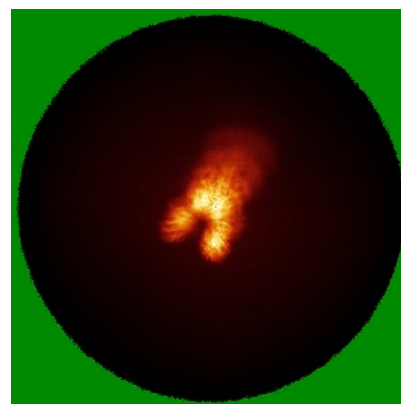
### 6.4.1 Primary map



X



Y

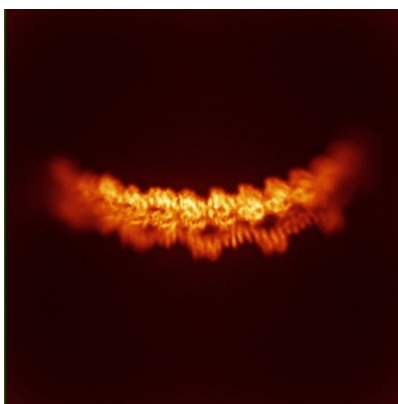


Z

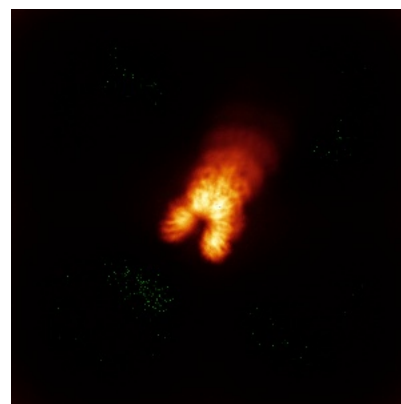
### 6.4.2 Raw map



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.



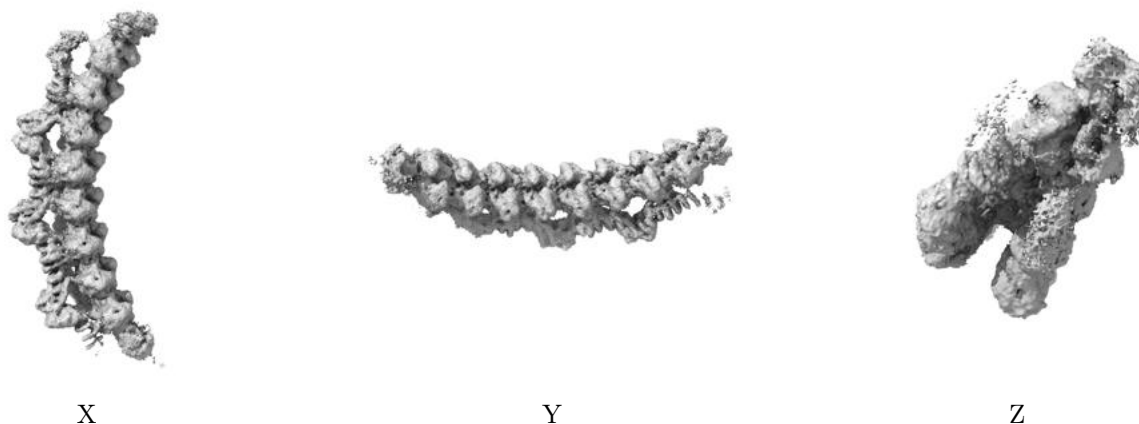
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.179. 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.

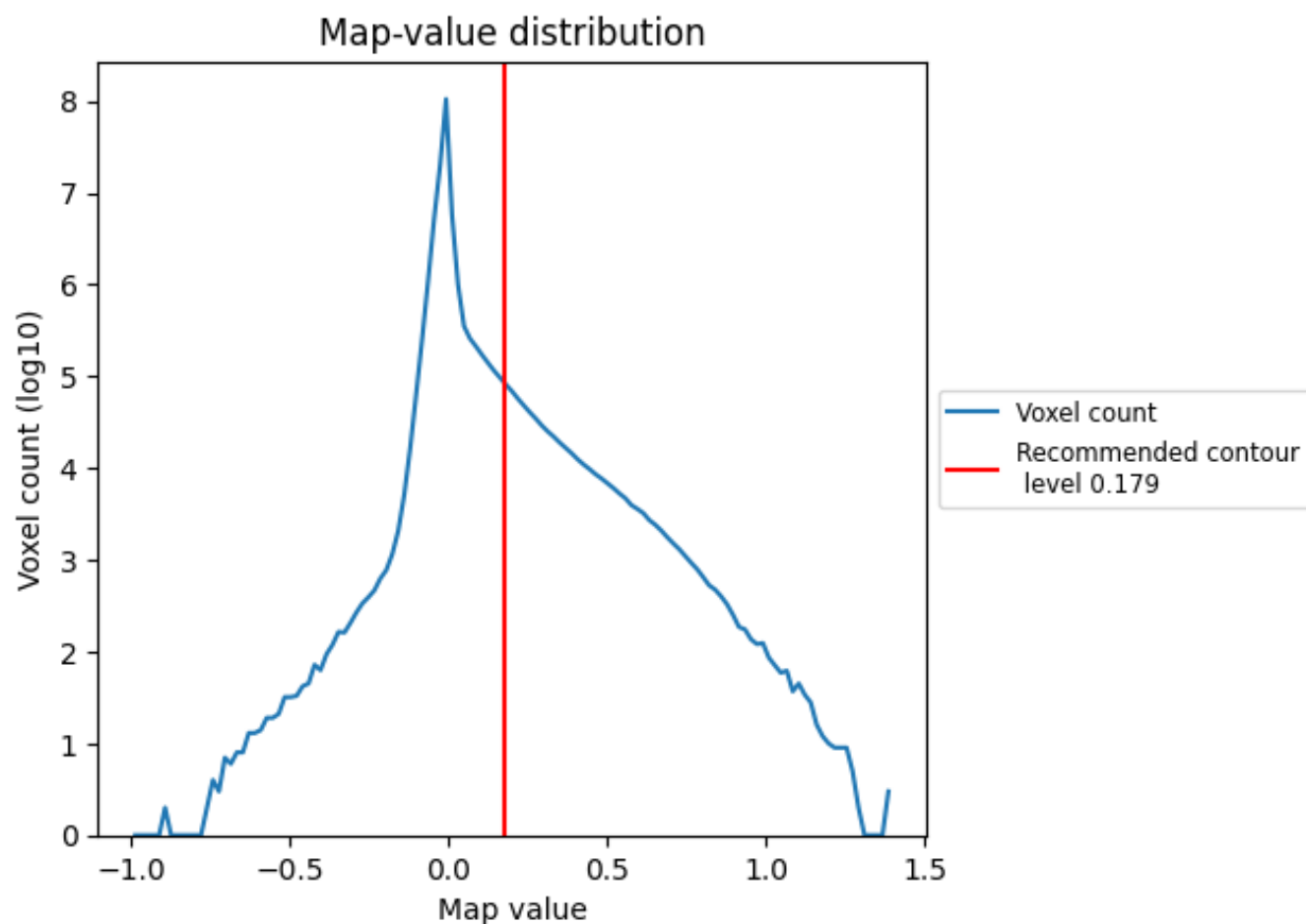
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

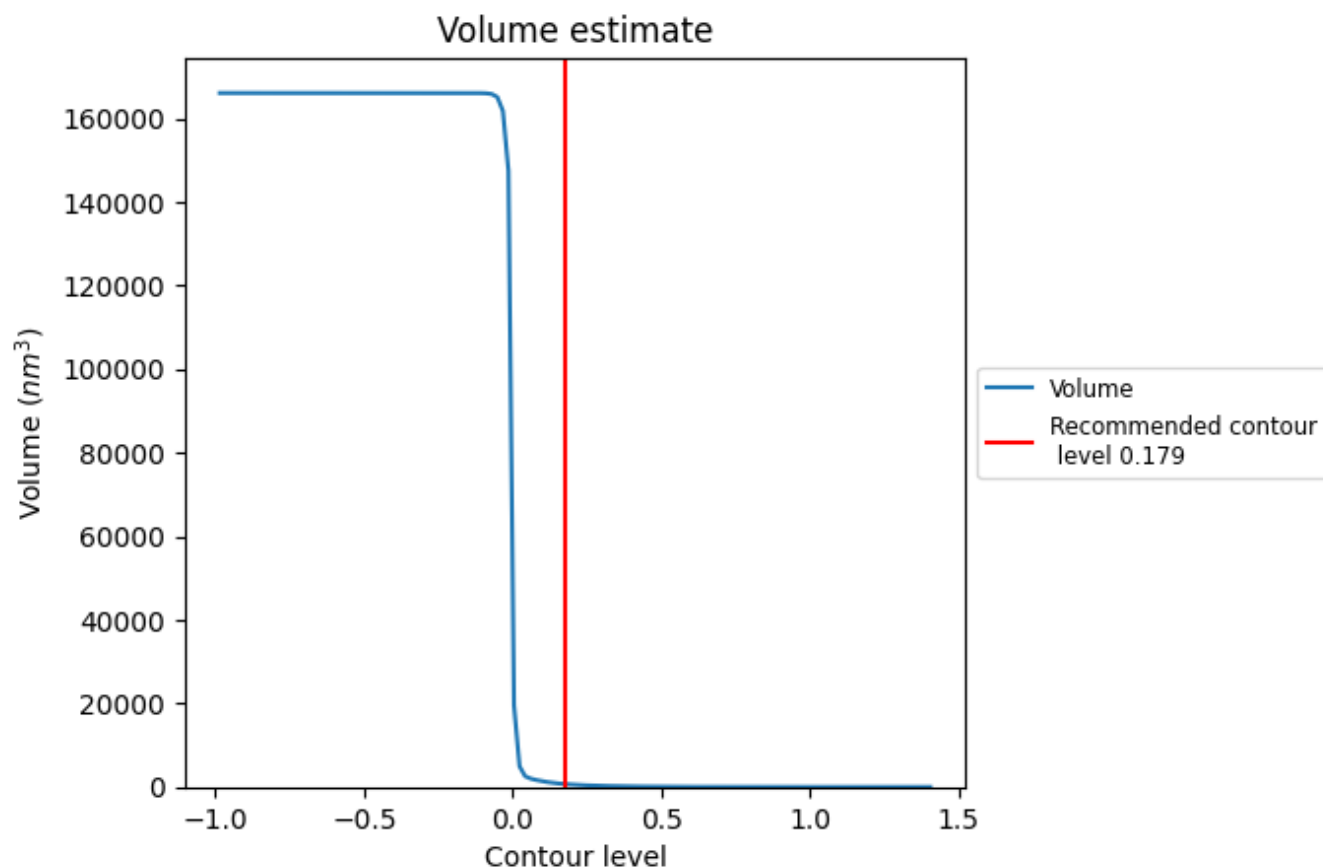
This section contains the results of statistical analysis of the map.

### 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.

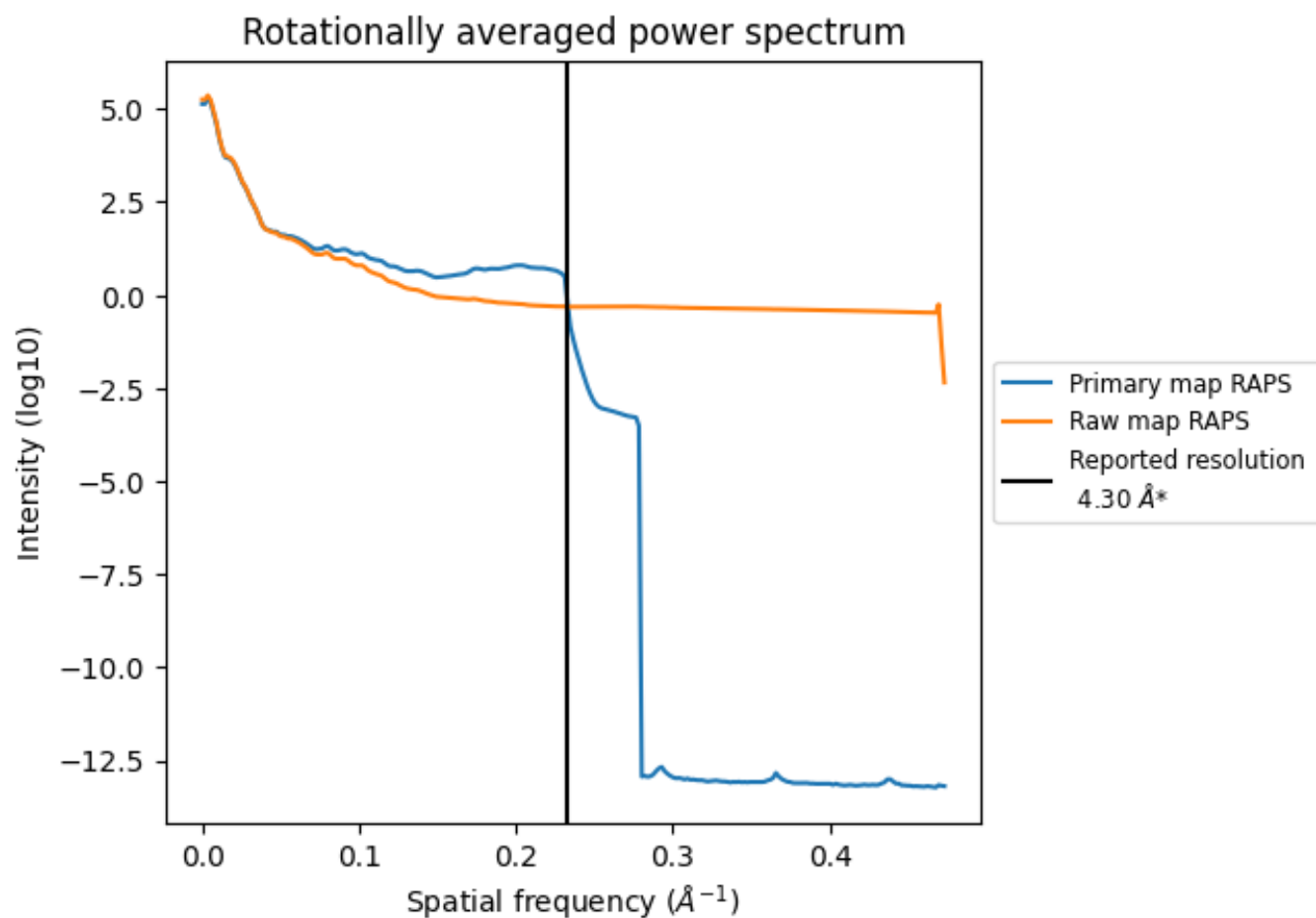
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 681 nm<sup>3</sup>; this corresponds to an approximate mass of 616 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 ⓘ

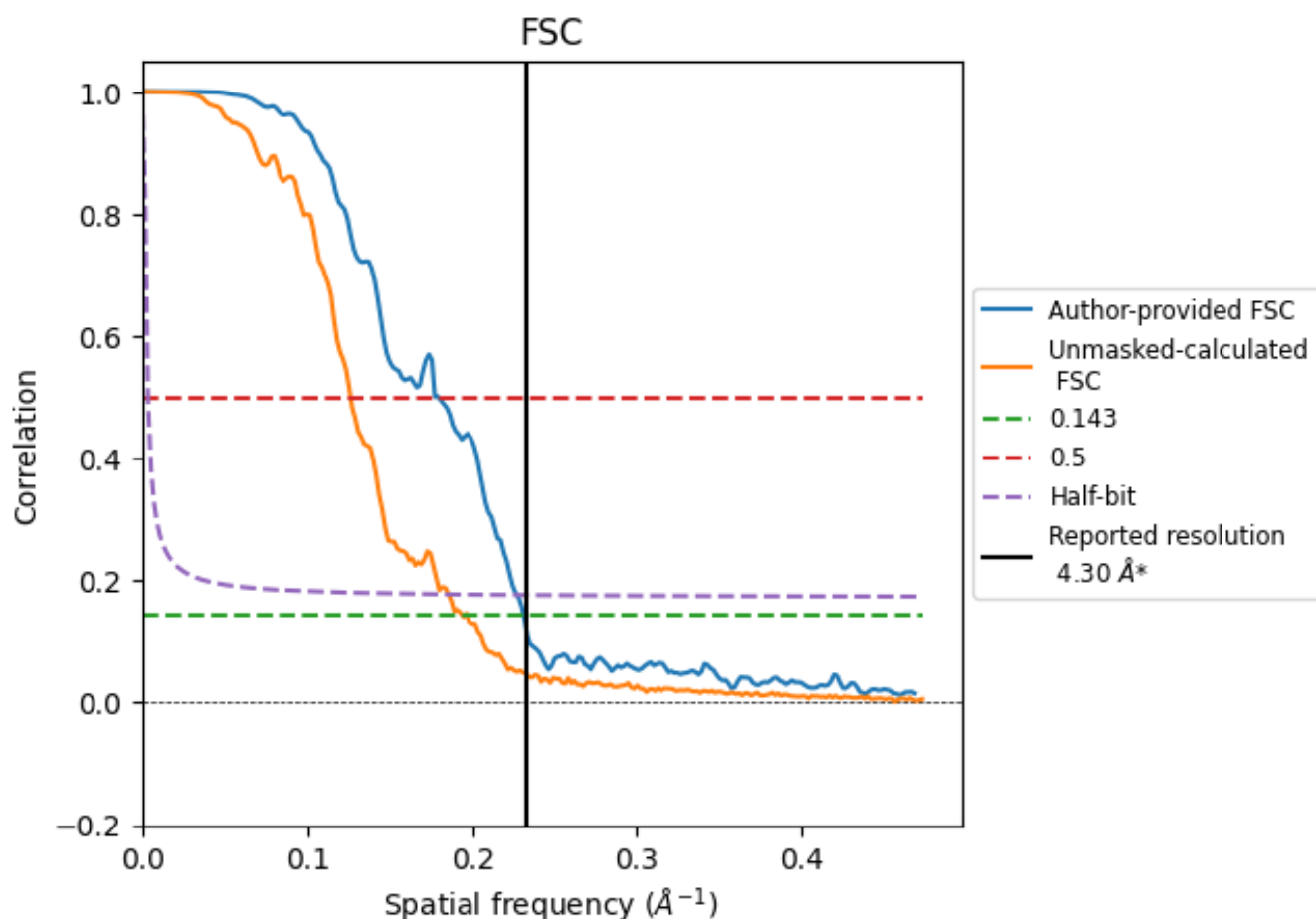


\*Reported resolution corresponds to spatial frequency of 0.233 Å<sup>-1</sup>

## 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  $0.233 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

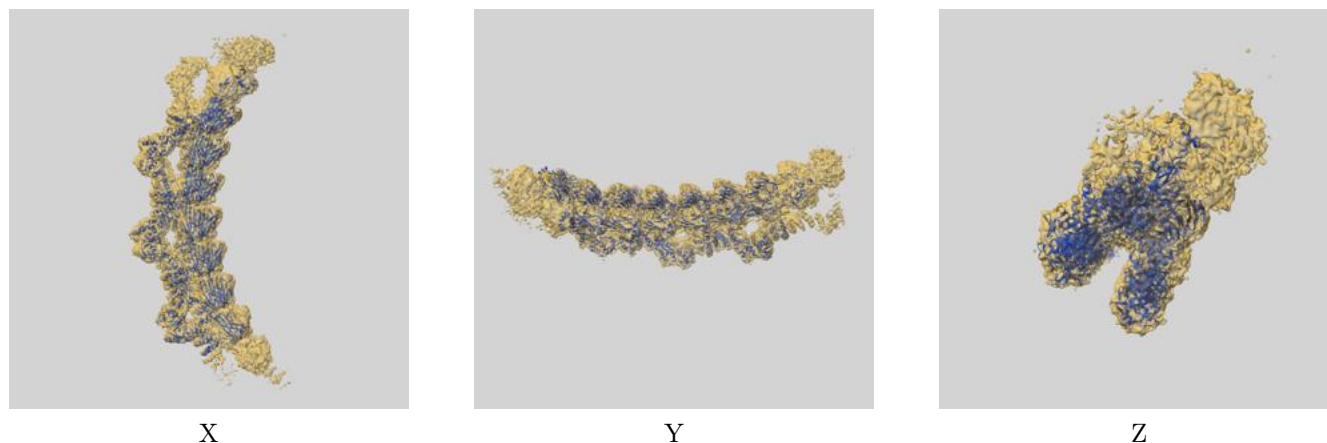
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.32	5.57	4.40
Unmasked-calculated*	5.16	7.91	5.39

\*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 5.16 differs from the reported value 4.3 by more than 10 %

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

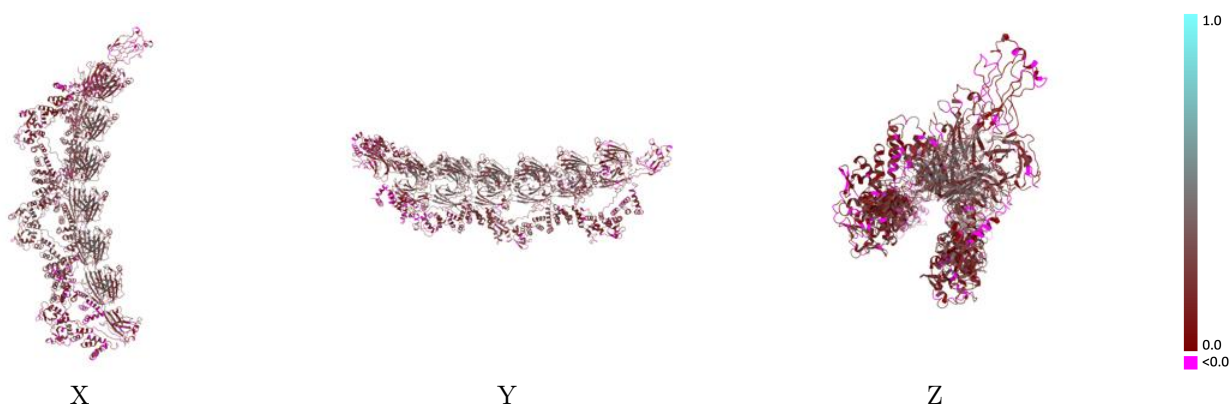
This section contains information regarding the fit between EMDB map EMD-70882 and PDB model 9OUU. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

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



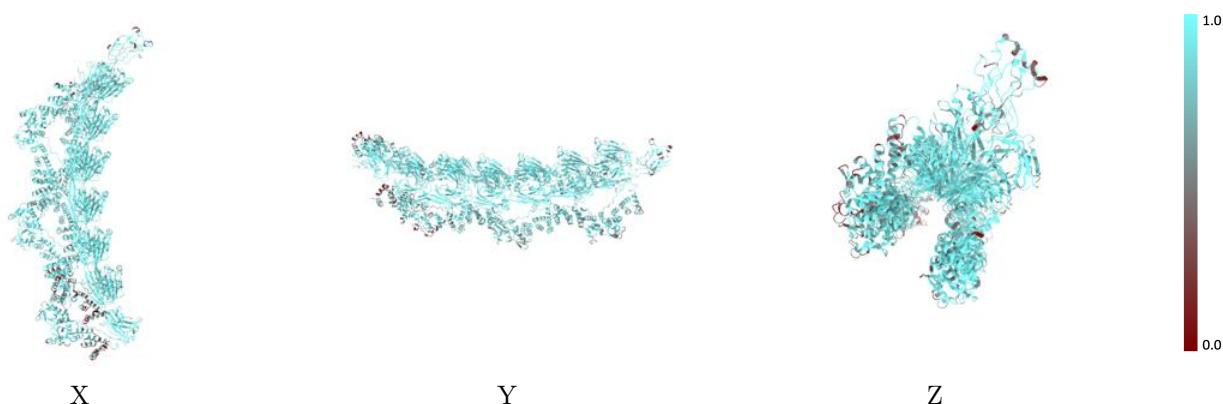
The images above show the 3D surface view of the map at the recommended contour level 0.179 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

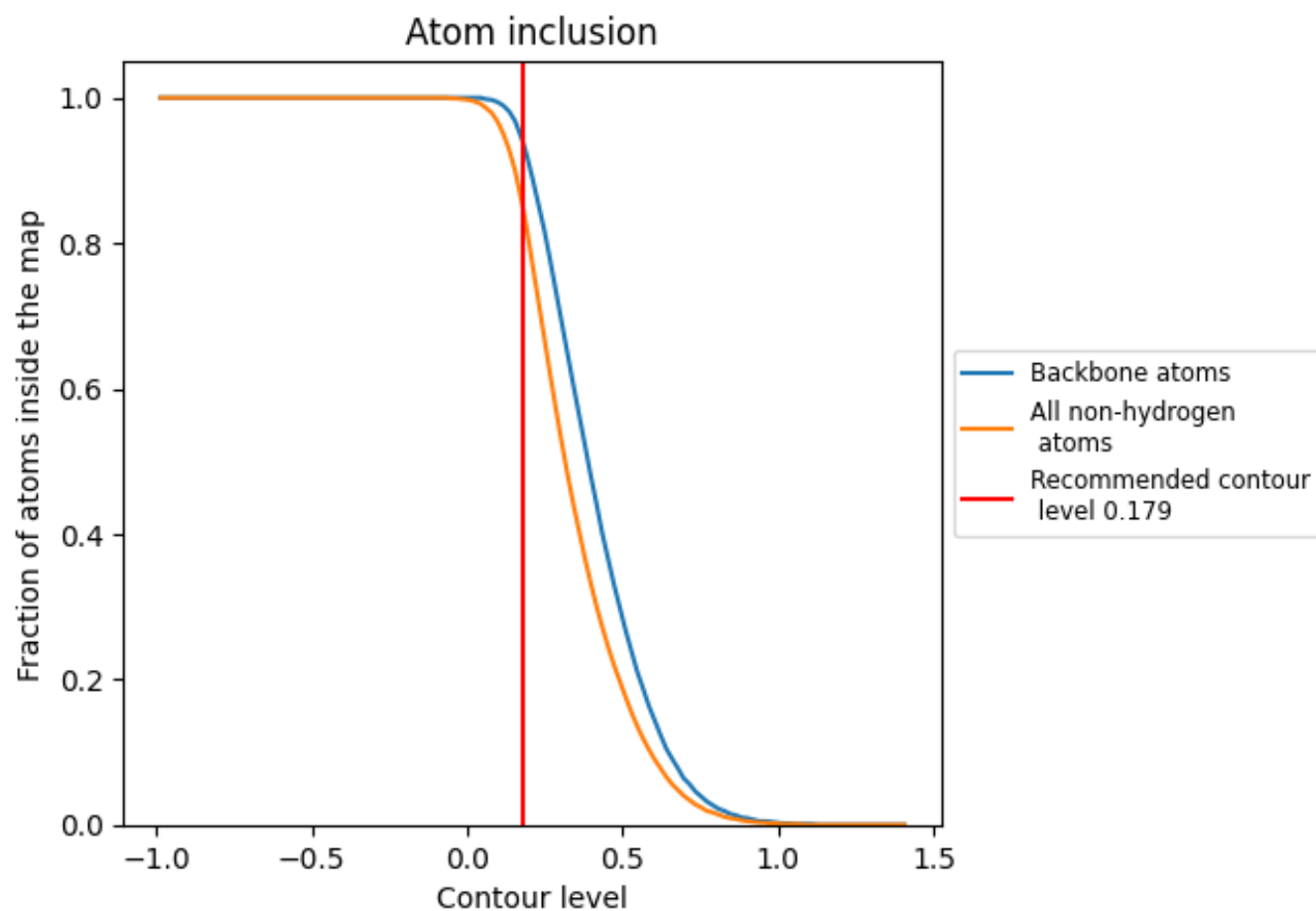
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.179).



































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 85% 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 (0.179) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8500	 0.2170
A	 0.9140	 0.3020
B	 0.8830	 0.2150
C	 0.7320	 0.1690
D	 0.8620	 0.2460
E	 0.8790	 0.2030
F	 0.9140	 0.2950
G	 0.9040	 0.2630
H	 0.8100	 0.1800
I	 0.8860	 0.2500
J	 0.8110	 0.2060
K	 0.9120	 0.2450
L	 0.7770	 0.1550
M	 0.8870	 0.2280
N	 0.8020	 0.1330
P	 0.8420	 0.1870

