



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 06:10 AM UTC

PDB ID : 7OM8 / pdb_00007om8
EMDB ID : EMD-12984
Title : Beta2 appendage domain of AP2 bound to terminal domains beneath the hub
of the 28 triskelia mini clathrin coat complex, class 15
Authors : Smith, S.M.; Smith, C.J.
Deposited on : 2021-05-21
Resolution : 10.50 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

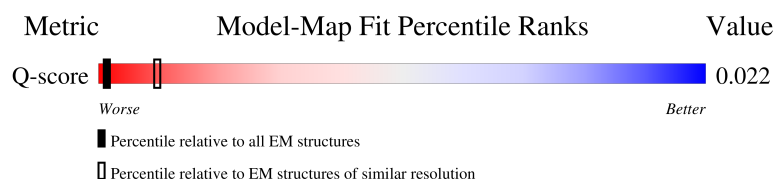
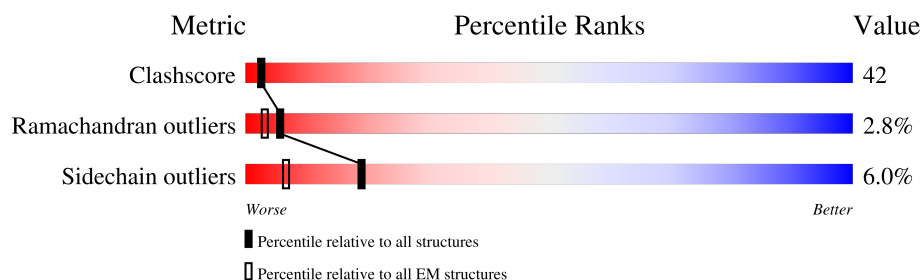
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 10.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	126 (10.00 - 11.00)

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

Mol	Chain	Length	Quality of chain
1	Y	299	
1	Z	299	
2	B	233	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8456 atoms, of which 4202 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 Clathrin heavy chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	Y	157	Total	C	H	N	O	S	0	0
			2430	785	1198	212	228	7		
1	Z	149	Total	C	H	N	O	S	0	0
			2296	738	1132	203	216	7		

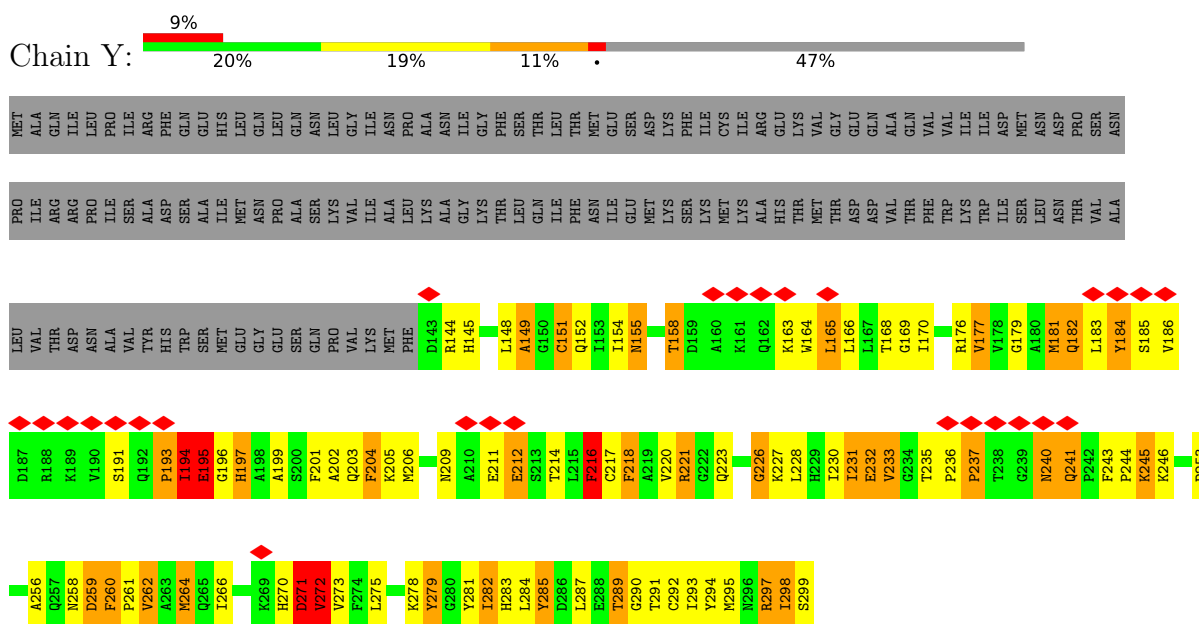
- Molecule 2 is a protein called AP-2 complex subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	233	Total	C	H	N	O	S	0	0
			3730	1194	1872	312	341	11		

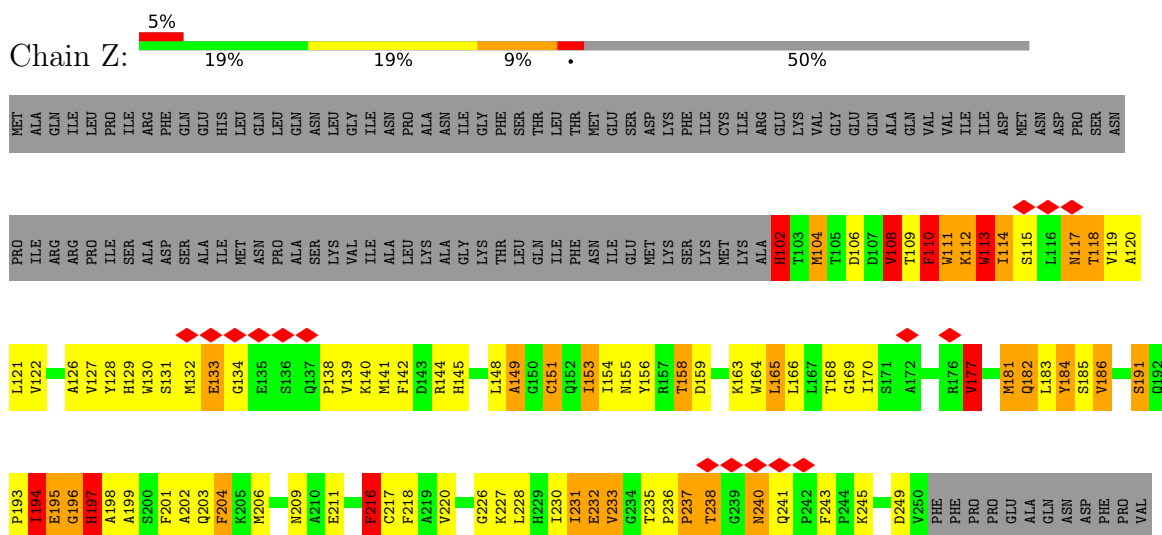
3 Residue-property plots

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: Clathrin heavy chain

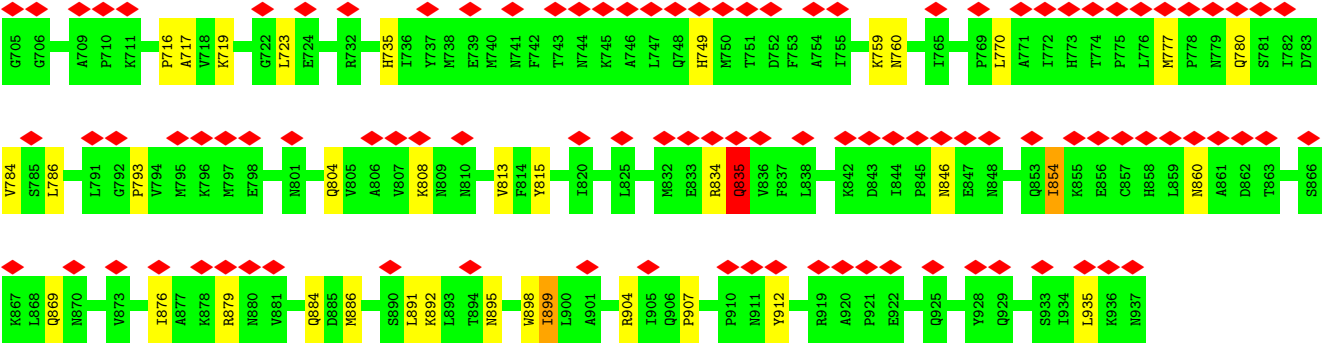
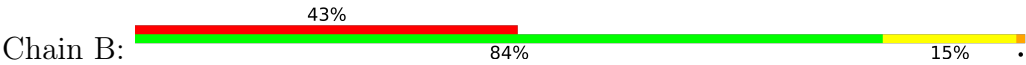


• Molecule 1: Clathrin heavy chain



ALA	MEI	GLN	ILE	SER	GLU	LYS	HIS	ASP	VAL	VAL	PHE	LEU	ILE	THR	LYS	TYR	GLY	TYR	ILE	HIS	LEU	TYR	ASP	LEU	GLU	THR	GLY	THR	CYS	ILE	TYR	MEI	ASN	ARG	ILE	SER
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● Molecule 2: AP-2 complex subunit beta



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	11676	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	64	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.123	Depositor
Minimum map value	-0.054	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0149	Depositor
Map size (Å)	973.0, 973.0, 973.0	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.78, 2.78, 2.78	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	Y	1.37	7/1261 (0.6%)	2.02	37/1705 (2.2%)
1	Z	1.41	10/1192 (0.8%)	2.27	63/1616 (3.9%)
2	B	0.80	0/1901	1.38	12/2583 (0.5%)
All	All	1.17	17/4354 (0.4%)	1.85	112/5904 (1.9%)

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	Y	0	8
1	Z	0	8
2	B	0	1
All	All	0	17

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Y	194	ILE	CA-C	16.00	1.73	1.52
1	Y	195	GLU	N-CA	14.72	1.64	1.46
1	Y	195	GLU	CA-C	12.19	1.65	1.52
1	Z	112	LYS	CA-C	10.48	1.65	1.52
1	Y	194	ILE	C-N	10.14	1.47	1.33
1	Z	113	TRP	N-CA	9.82	1.58	1.46
1	Z	195	GLU	CA-C	9.37	1.65	1.52
1	Y	194	ILE	N-CA	9.11	1.57	1.46
1	Z	110	PHE	CA-C	-7.94	1.42	1.52
1	Z	111	TRP	N-CA	-6.61	1.38	1.46
1	Z	195	GLU	N-CA	6.04	1.53	1.46
1	Y	193	PRO	CA-C	5.61	1.60	1.52
1	Z	111	TRP	NE1-CE2	-5.56	1.31	1.37
1	Z	113	TRP	NE1-CE2	-5.49	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Y	193	PRO	C-N	5.28	1.40	1.33
1	Z	194	ILE	C-N	5.26	1.41	1.34
1	Z	102	HIS	CD2-NE2	-5.14	1.32	1.37

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Z	195	GLU	N-CA-C	15.55	131.66	111.75
1	Y	195	GLU	O-C-N	-14.38	104.26	123.24
1	Y	194	ILE	CA-C-N	11.86	139.68	121.76
1	Y	194	ILE	C-N-CA	11.86	139.68	121.76
1	Y	195	GLU	N-CA-C	11.62	127.83	107.61
1	Z	194	ILE	O-C-N	11.33	136.74	122.57
1	Z	194	ILE	CA-C-O	-11.29	106.67	120.78
1	Z	111	TRP	N-CA-CB	-10.99	91.25	111.13
1	Z	216	PHE	CA-CB-CG	10.86	124.66	113.80
1	Z	102	HIS	CE1-NE2-CD2	-10.03	98.97	109.00
1	Z	194	ILE	CA-C-N	9.94	134.89	120.38
1	Z	194	ILE	C-N-CA	9.94	134.89	120.38
2	B	835	GLN	OE1-CD-NE2	-9.65	112.95	122.60
1	Z	110	PHE	CA-CB-CG	9.58	123.38	113.80
1	Y	216	PHE	CA-CB-CG	9.23	123.03	113.80
1	Z	102	HIS	CB-CG-CD2	-9.08	119.40	131.20
1	Z	153	ILE	CB-CA-C	8.34	123.34	111.08
1	Y	272	VAL	CA-CB-CG1	8.13	124.22	110.40
1	Z	186	VAL	CB-CA-C	8.12	122.56	111.92
1	Z	249	ASP	CA-CB-CG	7.76	120.36	112.60
1	Z	117	ASN	CA-CB-CG	-7.73	104.87	112.60
1	Z	102	HIS	ND1-CE1-NE2	7.71	116.11	108.40
1	Z	195	GLU	O-C-N	-7.67	113.45	122.20
1	Z	238	THR	N-CA-C	7.67	119.28	111.07
1	Y	195	GLU	N-CA-CB	-7.60	99.09	110.71
1	Y	194	ILE	CA-C-O	-7.49	111.42	120.78
1	Z	235	THR	CA-C-N	7.47	125.12	119.66
1	Z	235	THR	C-N-CA	7.47	125.12	119.66
1	Z	112	LYS	N-CA-CB	-7.41	98.36	110.81
1	Z	237	PRO	CB-CA-C	7.36	120.61	111.12
1	Z	158	THR	CA-CB-OG1	-7.29	98.66	109.60
1	Y	203	GLN	CB-CA-C	7.21	122.13	110.16
1	Z	198	ALA	N-CA-CB	7.20	121.61	109.87
1	Z	112	LYS	CA-C-N	7.15	135.19	121.54
1	Z	112	LYS	C-N-CA	7.15	135.19	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Z	195	GLU	CB-CA-C	-7.01	96.87	110.46
1	Y	158	THR	CA-CB-OG1	-6.98	99.13	109.60
1	Z	232	GLU	CB-CA-C	-6.97	97.74	109.65
1	Z	102	HIS	CG-CD2-NE2	6.96	114.16	107.20
1	Z	112	LYS	N-CA-C	6.85	120.82	108.69
2	B	760	ASN	CA-CB-CG	6.80	119.40	112.60
1	Z	236	PRO	N-CA-CB	6.79	106.99	103.19
1	Z	111	TRP	CB-CA-C	6.73	123.01	109.68
1	Z	194	ILE	N-CA-CB	6.70	122.29	111.23
1	Z	108	VAL	N-CA-CB	6.57	119.74	111.46
1	Z	153	ILE	CA-CB-CG1	6.52	121.48	110.40
1	Z	177	VAL	O-C-N	-6.50	114.44	122.57
1	Z	194	ILE	N-CA-C	6.48	122.83	109.34
2	B	907	PRO	CB-CA-C	6.43	119.75	111.46
2	B	780	GLN	OE1-CD-NE2	-6.41	116.19	122.60
1	Z	197	HIS	CB-CG-CD2	-6.24	123.09	131.20
1	Y	193	PRO	CA-C-N	6.19	133.11	121.97
1	Y	193	PRO	C-N-CA	6.19	133.11	121.97
1	Y	182	GLN	OE1-CD-NE2	-6.13	116.47	122.60
1	Z	151	CYS	N-CA-CB	-6.11	100.99	109.97
1	Y	151	CYS	N-CA-CB	-6.10	101.02	110.29
1	Z	104	MET	CA-CB-CG	-6.05	102.00	114.10
1	Y	240	ASN	CA-CB-CG	-5.97	106.63	112.60
1	Y	240	ASN	OD1-CG-ND2	-5.88	116.72	122.60
1	Y	241	GLN	N-CA-C	-5.84	102.29	109.65
1	Z	104	MET	N-CA-CB	5.80	118.55	110.26
1	Z	112	LYS	CB-CA-C	5.78	119.77	109.65
1	Y	194	ILE	N-CA-C	5.78	121.36	109.34
2	B	786	LEU	N-CA-CB	-5.77	102.84	110.17
1	Z	106	ASP	CA-CB-CG	5.76	118.36	112.60
1	Y	221	ARG	CA-C-O	5.73	126.62	120.32
1	Z	196	GLY	CA-C-N	5.72	132.47	121.54
1	Z	196	GLY	C-N-CA	5.72	132.47	121.54
1	Z	231	ILE	CA-CB-CG2	5.72	120.23	110.50
1	Z	191	SER	N-CA-C	5.66	117.63	108.34
1	Y	271	ASP	CA-CB-CG	5.66	118.26	112.60
1	Y	270	HIS	CA-C-O	-5.63	114.25	120.33
1	Z	165	LEU	CD1-CG-CD2	-5.62	98.43	110.80
2	B	786	LEU	N-CA-C	5.61	118.52	108.47
1	Z	240	ASN	OD1-CG-ND2	-5.61	116.99	122.60
1	Z	112	LYS	CA-CB-CG	-5.58	102.95	114.10
1	Z	240	ASN	CA-CB-CG	-5.58	107.03	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Z	115	SER	N-CA-C	5.57	115.63	108.34
1	Y	195	GLU	CB-CG-CD	5.51	121.97	112.60
2	B	834	ARG	CA-C-N	5.51	128.45	120.79
2	B	834	ARG	C-N-CA	5.51	128.45	120.79
1	Y	237	PRO	CB-CA-C	5.50	118.22	111.12
1	Z	196	GLY	CA-C-O	-5.50	110.99	120.57
1	Z	193	PRO	N-CA-CB	5.47	108.43	103.34
1	Y	245	LYS	CG-CD-CE	5.45	123.84	111.30
1	Z	114	ILE	CB-CG1-CD1	-5.42	102.41	113.80
1	Y	214	THR	CA-CB-OG1	5.40	117.71	109.60
1	Z	110	PHE	N-CA-CB	-5.38	103.38	111.56
1	Z	131	SER	N-CA-C	5.38	119.68	113.18
2	B	884	GLN	OE1-CD-NE2	-5.37	117.23	122.60
2	B	860	ASN	CA-CB-CG	5.36	117.96	112.60
2	B	895	ASN	CA-CB-CG	5.33	117.93	112.60
1	Y	259	ASP	N-CA-C	5.29	122.07	110.80
1	Y	231	ILE	CB-CG1-CD1	5.27	124.88	113.80
1	Y	165	LEU	CD1-CG-CD2	-5.25	99.25	110.80
1	Z	193	PRO	N-CA-C	-5.19	103.05	111.19
1	Y	297	ARG	CB-CA-C	-5.17	101.42	109.84
1	Z	191	SER	N-CA-CB	-5.15	102.69	110.77
1	Y	212	GLU	N-CA-C	5.14	117.07	108.23
1	Y	264	MET	CA-C-N	5.13	130.97	121.94
1	Y	264	MET	C-N-CA	5.13	130.97	121.94
1	Y	282	ILE	CA-CB-CG1	-5.13	101.69	110.40
2	B	735	HIS	CB-CG-CD2	-5.12	124.55	131.20
1	Y	299	SER	CA-CB-OG	5.12	121.33	111.10
1	Y	232	GLU	CB-CA-C	-5.09	100.50	109.62
1	Z	195	GLU	N-CA-CB	-5.07	102.12	110.14
1	Z	182	GLN	OE1-CD-NE2	-5.06	117.54	122.60
1	Z	197	HIS	CA-C-N	-5.05	114.40	121.72
1	Z	197	HIS	C-N-CA	-5.05	114.40	121.72
1	Y	258	ASN	CB-CA-C	5.04	119.17	110.86
1	Y	298	ILE	CA-CB-CG2	-5.02	101.97	110.50
1	Z	203	GLN	CB-CA-C	5.00	118.01	109.75

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	879	ARG	Sidechain
1	Y	184	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	Y	195	GLU	Peptide
1	Y	196	GLY	Peptide
1	Y	197	HIS	Sidechain
1	Y	204	PHE	Sidechain
1	Y	218	PHE	Sidechain
1	Y	279	TYR	Sidechain
1	Y	285	TYR	Sidechain
1	Z	102	HIS	Sidechain
1	Z	110	PHE	Sidechain
1	Z	177	VAL	Mainchain
1	Z	184	TYR	Sidechain
1	Z	194	ILE	Peptide
1	Z	195	GLU	Peptide
1	Z	204	PHE	Sidechain
1	Z	216	PHE	Sidechain

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	Y	1232	1198	1213	170	0
1	Z	1164	1132	1140	176	0
2	B	1858	1872	1868	23	0
All	All	4254	4202	4221	359	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 42.

All (359) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:260:PHE:CD2	1:Y:261:PRO:HD2	1.40	1.53
1:Z:181:MET:HB3	1:Z:194:ILE:CG1	1.39	1.52
1:Z:194:ILE:HG21	1:Z:197:HIS:CD2	1.51	1.44
1:Z:194:ILE:HG21	1:Z:197:HIS:NE2	1.21	1.40
1:Z:194:ILE:CG2	1:Z:197:HIS:NE2	1.82	1.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:194:ILE:CD1	1:Z:197:HIS:CD2	1.82	1.35
1:Z:181:MET:CB	1:Z:194:ILE:HG13	1.59	1.33
1:Z:194:ILE:CG1	1:Z:197:HIS:HD2	1.42	1.32
1:Y:260:PHE:CD2	1:Y:261:PRO:CD	2.14	1.28
1:Y:283:HIS:ND1	1:Y:285:TYR:CE2	2.03	1.26
1:Z:194:ILE:HD12	1:Z:197:HIS:CD2	1.19	1.25
1:Y:283:HIS:CE1	1:Y:285:TYR:CZ	2.23	1.25
1:Z:194:ILE:CG2	1:Z:197:HIS:CD2	2.15	1.21
1:Y:273:VAL:HG23	1:Y:287:LEU:CD2	1.74	1.18
1:Z:108:VAL:CG1	1:Z:121:LEU:HD11	1.74	1.18
1:Z:108:VAL:HG21	1:Z:121:LEU:CD1	1.72	1.18
1:Z:194:ILE:CB	1:Z:197:HIS:CD2	2.28	1.16
1:Z:194:ILE:CD1	1:Z:197:HIS:HD2	1.30	1.15
1:Y:283:HIS:CE1	1:Y:285:TYR:CE1	2.38	1.11
1:Y:272:VAL:HG13	1:Y:284:LEU:HD11	1.18	1.10
1:Z:108:VAL:HG21	1:Z:121:LEU:HD12	1.24	1.08
1:Y:273:VAL:HG23	1:Y:287:LEU:HD23	1.14	1.08
1:Y:272:VAL:CG1	1:Y:284:LEU:HD11	1.85	1.06
1:Z:108:VAL:HG11	1:Z:121:LEU:HD11	1.05	1.05
1:Z:194:ILE:HG22	1:Z:194:ILE:O	1.56	1.04
1:Y:202:ALA:HB2	1:Y:266:ILE:CD1	1.89	1.02
1:Z:194:ILE:HG21	1:Z:197:HIS:CE1	1.94	1.02
1:Y:260:PHE:CE2	1:Y:261:PRO:HD2	1.95	1.00
1:Y:285:TYR:HE1	1:Y:292:CYS:HG	1.01	0.98
1:Z:194:ILE:CG1	1:Z:197:HIS:CD2	2.29	0.98
1:Z:181:MET:HB3	1:Z:194:ILE:CD1	1.93	0.98
1:Z:108:VAL:HG11	1:Z:121:LEU:CD1	1.95	0.96
1:Y:283:HIS:ND1	1:Y:285:TYR:CZ	2.30	0.96
1:Z:117:ASN:O	1:Z:118:THR:HG23	1.66	0.95
1:Y:260:PHE:HD2	1:Y:261:PRO:N	1.61	0.95
1:Z:194:ILE:CG2	1:Z:194:ILE:O	2.15	0.93
1:Y:273:VAL:CG2	1:Y:287:LEU:CD2	2.47	0.92
1:Y:264:MET:HE2	1:Y:275:LEU:HD21	1.54	0.89
1:Y:260:PHE:CD2	1:Y:261:PRO:N	2.38	0.89
1:Z:108:VAL:CG2	1:Z:121:LEU:CD1	2.51	0.88
1:Y:283:HIS:HE1	1:Y:285:TYR:CD1	1.94	0.86
1:Z:170:ILE:HG21	1:Z:177:VAL:HG12	1.55	0.86
1:Y:283:HIS:CE1	1:Y:285:TYR:CD1	2.63	0.85
1:Y:193:PRO:C	1:Y:194:ILE:HG13	2.01	0.84
1:Y:283:HIS:ND1	1:Y:285:TYR:CD2	2.45	0.83
1:Y:264:MET:CE	1:Y:275:LEU:HD21	2.09	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:166:LEU:CD2	1:Z:183:LEU:HD23	2.09	0.82
1:Y:272:VAL:HG13	1:Y:284:LEU:CD1	2.08	0.82
1:Z:194:ILE:CB	1:Z:197:HIS:NE2	2.36	0.82
1:Y:283:HIS:CE1	1:Y:285:TYR:CE2	2.62	0.81
1:Z:181:MET:CB	1:Z:194:ILE:CG1	2.35	0.81
1:Y:166:LEU:CD2	1:Y:183:LEU:HD23	2.11	0.80
1:Y:260:PHE:CG	1:Y:261:PRO:HD2	2.14	0.79
1:Z:170:ILE:HG21	1:Z:177:VAL:CG1	2.11	0.79
1:Z:231:ILE:HD12	1:Z:245:LYS:HZ3	1.48	0.79
1:Z:231:ILE:HD12	1:Z:245:LYS:NZ	2.00	0.77
1:Z:194:ILE:HD13	1:Z:197:HIS:CD2	2.14	0.77
1:Y:170:ILE:HG21	1:Y:177:VAL:HG12	1.67	0.77
1:Z:108:VAL:CB	1:Z:121:LEU:HD11	2.15	0.77
1:Z:102:HIS:HD2	1:Z:130:TRP:CZ2	2.04	0.75
1:Z:111:TRP:CD1	1:Z:120:ALA:O	2.39	0.75
1:Z:181:MET:HE3	1:Z:197:HIS:O	1.86	0.75
1:Z:129:HIS:HD1	1:Z:141:MET:HG3	1.49	0.75
1:Z:194:ILE:HG21	1:Z:197:HIS:CG	2.20	0.74
1:Z:142:PHE:CE2	1:Z:165:LEU:HD12	2.22	0.74
2:B:759:LYS:HG3	2:B:793:PRO:HB2	1.69	0.73
1:Z:181:MET:HB3	1:Z:194:ILE:HG13	0.76	0.73
1:Y:202:ALA:HB2	1:Y:266:ILE:HD12	1.70	0.72
1:Z:158:THR:HG22	1:Z:165:LEU:HD23	1.71	0.72
1:Z:108:VAL:CG2	1:Z:121:LEU:HD11	2.19	0.72
1:Z:102:HIS:CE1	1:Z:138:PRO:HG2	2.25	0.71
1:Y:293:ILE:O	1:Y:294:TYR:CG	2.43	0.71
1:Y:283:HIS:CG	1:Y:285:TYR:CE2	2.80	0.70
1:Z:113:TRP:HE3	1:Z:113:TRP:N	1.89	0.70
1:Z:181:MET:CA	1:Z:194:ILE:HG13	2.21	0.70
1:Z:202:ALA:HB1	1:Z:204:PHE:CE1	2.26	0.70
1:Z:181:MET:CB	1:Z:194:ILE:CD1	2.70	0.68
1:Y:231:ILE:HD12	1:Y:245:LYS:HZ3	1.58	0.68
1:Z:114:ILE:HD11	1:Z:158:THR:HG21	1.75	0.68
1:Z:122:VAL:HG11	1:Z:153:ILE:HD13	1.75	0.67
1:Z:194:ILE:HB	1:Z:197:HIS:NE2	2.08	0.67
1:Y:184:TYR:CD1	1:Y:191:SER:HB3	2.29	0.67
1:Y:283:HIS:CE1	1:Y:285:TYR:CG	2.83	0.67
1:Y:283:HIS:CG	1:Y:285:TYR:CZ	2.82	0.67
1:Z:194:ILE:HB	1:Z:197:HIS:CD2	2.29	0.67
1:Z:102:HIS:CE1	1:Z:104:MET:SD	2.88	0.67
1:Y:202:ALA:HB2	1:Y:266:ILE:HD11	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:170:ILE:HG21	1:Y:177:VAL:CG1	2.25	0.66
1:Z:127:VAL:HG11	1:Z:156:TYR:CE1	2.30	0.66
1:Z:170:ILE:CG2	1:Z:177:VAL:HG12	2.24	0.66
1:Z:151:CYS:SG	1:Z:169:GLY:HA3	2.35	0.66
1:Z:114:ILE:HD11	1:Z:158:THR:CG2	2.27	0.65
1:Z:217:CYS:SG	1:Z:228:LEU:HD11	2.36	0.65
1:Y:193:PRO:O	1:Y:194:ILE:HG13	1.97	0.64
1:Y:170:ILE:CG2	1:Y:177:VAL:HG12	2.29	0.63
1:Y:177:VAL:HG21	1:Y:260:PHE:CB	2.28	0.63
1:Y:151:CYS:SG	1:Y:169:GLY:C	2.81	0.63
1:Z:177:VAL:HG12	1:Z:177:VAL:O	1.98	0.63
1:Y:204:PHE:CZ	1:Y:287:LEU:HD12	2.34	0.63
1:Y:217:CYS:SG	1:Y:228:LEU:HD11	2.38	0.63
1:Z:206:MET:H	1:Z:209:ASN:HD21	1.45	0.63
1:Y:231:ILE:HD12	1:Y:245:LYS:NZ	2.12	0.63
1:Y:177:VAL:HG21	1:Y:260:PHE:CG	2.34	0.63
1:Z:113:TRP:N	1:Z:113:TRP:CE3	2.67	0.62
1:Z:166:LEU:HB3	1:Z:181:MET:HE2	1.82	0.62
1:Z:142:PHE:HE2	1:Z:165:LEU:HD12	1.64	0.62
1:Y:281:TYR:CD1	1:Y:297:ARG:HG2	2.35	0.61
1:Y:199:ALA:HB2	1:Y:218:PHE:HB3	1.82	0.61
1:Y:284:LEU:HG	1:Y:293:ILE:HD11	1.82	0.61
1:Z:184:TYR:CD1	1:Z:191:SER:HB3	2.36	0.61
1:Y:271:ASP:C	1:Y:287:LEU:HG	2.26	0.60
1:Z:181:MET:SD	1:Z:194:ILE:HG12	2.41	0.60
1:Z:104:MET:HE2	1:Z:121:LEU:CD2	2.31	0.60
1:Y:236:PRO:HD3	2:B:815:TYR:CB	2.32	0.60
1:Y:170:ILE:HD11	1:Y:197:HIS:CG	2.35	0.60
1:Z:216:PHE:HB2	1:Z:233:VAL:HG21	1.84	0.59
1:Y:158:THR:HG22	1:Y:165:LEU:HD23	1.85	0.59
1:Y:272:VAL:CG2	1:Y:284:LEU:HG	2.31	0.59
1:Y:281:TYR:CE1	1:Y:297:ARG:HG2	2.36	0.59
1:Y:283:HIS:CE1	1:Y:285:TYR:CD2	2.88	0.59
1:Y:279:TYR:CZ	1:Y:297:ARG:NH1	2.70	0.59
1:Y:283:HIS:CG	1:Y:285:TYR:OH	2.54	0.59
1:Z:201:PHE:HE1	1:Z:216:PHE:CD2	2.20	0.59
1:Z:142:PHE:CE2	1:Z:165:LEU:CD1	2.86	0.59
1:Y:201:PHE:HE1	1:Y:216:PHE:CD2	2.21	0.58
1:Z:237:PRO:C	1:Z:240:ASN:HD22	2.10	0.58
1:Z:163:LYS:HA	1:Z:186:VAL:CG2	2.33	0.58
1:Z:114:ILE:CD1	1:Z:158:THR:HG21	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:272:VAL:HG22	1:Y:284:LEU:HG	1.85	0.58
1:Y:236:PRO:HD3	2:B:815:TYR:HB2	1.86	0.58
1:Z:142:PHE:HE2	1:Z:165:LEU:CD1	2.15	0.58
1:Z:133:GLU:HG3	1:Z:134:GLY:H	1.67	0.57
1:Y:283:HIS:HD2	1:Y:295:MET:HB2	1.69	0.57
1:Z:148:LEU:O	1:Z:151:CYS:HB3	2.05	0.57
1:Y:206:MET:H	1:Y:209:ASN:HD21	1.53	0.57
1:Y:216:PHE:HB2	1:Y:233:VAL:HG21	1.87	0.56
1:Y:155:ASN:HD21	1:Y:168:THR:CG2	2.19	0.56
1:Y:204:PHE:CZ	1:Y:287:LEU:CD1	2.88	0.56
1:Y:237:PRO:C	1:Y:240:ASN:HD22	2.13	0.56
1:Z:142:PHE:CD1	1:Z:184:TYR:CE2	2.93	0.56
1:Z:158:THR:HG22	1:Z:165:LEU:CD2	2.35	0.56
1:Y:163:LYS:HA	1:Y:186:VAL:CG2	2.36	0.56
1:Z:148:LEU:HD11	1:Z:182:GLN:HG2	1.87	0.56
1:Y:170:ILE:CD1	1:Y:197:HIS:CG	2.89	0.55
1:Y:164:TRP:CZ2	2:B:793:PRO:HB3	2.41	0.55
1:Y:293:ILE:O	1:Y:294:TYR:CD2	2.60	0.55
1:Z:126:ALA:HB3	1:Z:128:TYR:CZ	2.42	0.55
1:Z:206:MET:HB2	1:Z:209:ASN:ND2	2.22	0.55
2:B:854:ILE:HD13	2:B:935:LEU:HD12	1.87	0.55
1:Y:283:HIS:CD2	1:Y:285:TYR:OH	2.60	0.55
1:Y:246:LYS:HE3	1:Y:289:THR:HA	1.88	0.55
1:Z:102:HIS:CE1	1:Z:104:MET:CG	2.90	0.55
1:Z:102:HIS:HD2	1:Z:130:TRP:CE2	2.24	0.55
1:Y:206:MET:HB2	1:Y:209:ASN:ND2	2.21	0.55
1:Y:262:VAL:HG21	1:Y:278:LYS:HA	1.89	0.55
1:Y:285:TYR:CD1	1:Y:292:CYS:HA	2.42	0.55
1:Z:113:TRP:CE3	1:Z:113:TRP:C	2.85	0.54
1:Y:231:ILE:HB	1:Y:245:LYS:HD3	1.90	0.54
1:Z:102:HIS:HD2	1:Z:130:TRP:CH2	2.26	0.54
1:Z:164:TRP:CZ3	1:Z:185:SER:HB2	2.43	0.54
1:Z:148:LEU:HD11	1:Z:182:GLN:CG	2.38	0.53
1:Y:177:VAL:HG21	1:Y:260:PHE:HB3	1.90	0.53
1:Y:260:PHE:CD2	1:Y:260:PHE:C	2.87	0.53
1:Z:142:PHE:CD2	1:Z:165:LEU:HD12	2.43	0.53
1:Z:151:CYS:SG	1:Z:169:GLY:C	2.91	0.53
1:Y:155:ASN:HD21	1:Y:168:THR:HG23	1.73	0.53
1:Y:148:LEU:HD11	1:Y:182:GLN:HG2	1.89	0.53
1:Y:284:LEU:CD2	1:Y:293:ILE:HD11	2.38	0.53
2:B:898:TRP:C	2:B:899:ILE:HD12	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:155:ASN:HD21	1:Z:168:THR:CG2	2.22	0.53
1:Z:206:MET:N	1:Z:209:ASN:HD21	2.06	0.53
1:Z:184:TYR:CD1	1:Z:191:SER:CB	2.91	0.53
1:Y:236:PRO:CD	2:B:815:TYR:HB2	2.39	0.53
1:Z:102:HIS:CD2	1:Z:130:TRP:CH2	2.96	0.53
1:Y:285:TYR:CE1	1:Y:292:CYS:SG	3.00	0.53
1:Z:104:MET:CE	1:Z:121:LEU:HD23	2.39	0.53
1:Z:194:ILE:HG22	1:Z:197:HIS:NE2	2.10	0.53
1:Y:164:TRP:CZ3	1:Y:185:SER:HB2	2.45	0.52
2:B:892:LYS:HE3	2:B:898:TRP:CZ2	2.44	0.52
1:Y:220:VAL:HA	1:Y:260:PHE:CZ	2.44	0.52
1:Y:282:ILE:HD11	1:Y:298:ILE:HD11	1.92	0.52
1:Y:199:ALA:CB	1:Y:218:PHE:HB3	2.39	0.52
1:Y:206:MET:N	1:Y:209:ASN:HD21	2.08	0.52
1:Y:266:ILE:HG22	1:Y:273:VAL:HG22	1.91	0.52
1:Y:145:HIS:HB3	1:Y:182:GLN:CD	2.35	0.52
1:Z:117:ASN:O	1:Z:118:THR:CG2	2.51	0.52
2:B:759:LYS:HE3	2:B:793:PRO:HG2	1.91	0.52
1:Y:166:LEU:HD21	1:Y:183:LEU:HD23	1.90	0.51
1:Y:177:VAL:HG12	1:Y:177:VAL:O	2.10	0.51
1:Y:231:ILE:HB	1:Y:245:LYS:CE	2.40	0.51
1:Z:199:ALA:HB2	1:Z:218:PHE:HB3	1.92	0.51
1:Y:221:ARG:HB3	1:Y:260:PHE:CD1	2.45	0.51
1:Z:181:MET:HG2	1:Z:182:GLN:N	2.26	0.51
1:Y:158:THR:HG22	1:Y:165:LEU:CD2	2.41	0.51
1:Y:184:TYR:CD1	1:Y:191:SER:CB	2.94	0.50
1:Z:166:LEU:HD21	1:Z:183:LEU:HD23	1.92	0.50
1:Z:230:ILE:O	1:Z:245:LYS:HD2	2.12	0.50
1:Z:111:TRP:HA	1:Z:120:ALA:O	2.10	0.50
1:Z:145:HIS:HB3	1:Z:182:GLN:CD	2.36	0.50
1:Y:199:ALA:HB2	1:Y:218:PHE:CB	2.42	0.50
1:Z:142:PHE:CE1	1:Z:184:TYR:CE2	2.99	0.50
1:Z:153:ILE:HG23	1:Z:168:THR:O	2.11	0.50
1:Y:194:ILE:HG22	1:Y:195:GLU:H	1.77	0.50
1:Y:217:CYS:SG	1:Y:230:ILE:HG12	2.52	0.50
1:Y:232:GLU:CD	1:Y:243:PHE:HB3	2.37	0.50
1:Y:148:LEU:O	1:Y:151:CYS:HB2	2.11	0.50
1:Y:230:ILE:O	1:Y:245:LYS:HD2	2.12	0.50
1:Z:108:VAL:HG21	1:Z:121:LEU:CG	2.38	0.50
1:Z:113:TRP:CE3	1:Z:113:TRP:CA	2.94	0.50
1:Z:181:MET:CB	1:Z:194:ILE:HD11	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:154:ILE:HD13	1:Y:170:ILE:CD1	2.42	0.49
1:Y:283:HIS:CE1	1:Y:284:LEU:O	2.65	0.49
1:Z:108:VAL:CB	1:Z:121:LEU:CD1	2.83	0.49
1:Z:109:THR:O	1:Z:110:PHE:HB2	2.11	0.49
1:Z:170:ILE:CG2	1:Z:177:VAL:CG1	2.84	0.49
1:Z:201:PHE:CE1	1:Z:216:PHE:CD2	3.00	0.49
2:B:717:ALA:HA	2:B:723:LEU:O	2.12	0.49
2:B:854:ILE:HG23	2:B:912:TYR:HB2	1.93	0.49
1:Y:228:LEU:CD1	1:Y:264:MET:HE1	2.43	0.49
1:Y:272:VAL:C	1:Y:287:LEU:HD21	2.37	0.49
1:Z:196:GLY:HA3	1:Z:218:PHE:HB2	1.94	0.49
1:Y:221:ARG:HG3	1:Y:226:GLY:H	1.78	0.49
1:Y:144:ARG:HE	1:Y:148:LEU:HB3	1.77	0.49
1:Y:177:VAL:HG21	1:Y:260:PHE:CD1	2.48	0.49
1:Y:260:PHE:CE2	1:Y:261:PRO:CD	2.75	0.49
1:Z:102:HIS:HE1	1:Z:104:MET:SD	2.34	0.49
1:Y:211:GLU:HG3	1:Y:237:PRO:HB2	1.95	0.49
1:Z:111:TRP:HE1	1:Z:119:VAL:CA	2.23	0.49
1:Y:202:ALA:HB1	1:Y:204:PHE:CE1	2.47	0.48
1:Z:216:PHE:HB2	1:Z:233:VAL:CG2	2.43	0.48
1:Y:177:VAL:O	1:Y:197:HIS:CE1	2.66	0.48
1:Y:206:MET:HE2	1:Y:243:PHE:CD1	2.48	0.48
1:Z:127:VAL:HG11	1:Z:156:TYR:CZ	2.48	0.48
1:Z:151:CYS:SG	1:Z:169:GLY:CA	3.01	0.48
1:Y:170:ILE:HD11	1:Y:197:HIS:CB	2.44	0.48
1:Z:166:LEU:CD2	1:Z:183:LEU:CD2	2.85	0.48
1:Y:206:MET:HE2	1:Y:243:PHE:HD1	1.79	0.48
1:Z:114:ILE:HD11	1:Z:158:THR:CB	2.44	0.48
1:Z:144:ARG:HE	1:Z:148:LEU:HB3	1.79	0.48
1:Z:155:ASN:HD21	1:Z:168:THR:HG23	1.78	0.48
1:Y:177:VAL:CG2	1:Y:260:PHE:CD1	2.97	0.48
1:Y:201:PHE:CE1	1:Y:216:PHE:CD2	3.02	0.48
1:Z:181:MET:SD	1:Z:194:ILE:CG1	3.02	0.48
1:Z:202:ALA:CB	1:Z:204:PHE:CE1	2.95	0.48
1:Z:108:VAL:HG11	1:Z:121:LEU:HD21	1.95	0.47
1:Y:283:HIS:HE1	1:Y:285:TYR:CG	2.23	0.47
1:Y:151:CYS:SG	1:Y:170:ILE:N	2.87	0.47
1:Z:114:ILE:CD1	1:Z:158:THR:CG2	2.90	0.47
1:Z:217:CYS:SG	1:Z:230:ILE:HG12	2.55	0.47
1:Z:181:MET:HB3	1:Z:194:ILE:HD11	1.92	0.47
1:Y:260:PHE:HD2	1:Y:260:PHE:C	2.20	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:108:VAL:CG2	1:Z:121:LEU:HD12	2.16	0.47
1:Z:139:VAL:HG12	2:B:846:ASN:HB2	1.95	0.47
1:Y:166:LEU:CD2	1:Y:183:LEU:CD2	2.88	0.47
1:Z:211:GLU:HG3	1:Z:237:PRO:HB2	1.97	0.47
1:Y:170:ILE:HD11	1:Y:197:HIS:HB3	1.96	0.46
2:B:716:PRO:HG2	2:B:719:LYS:HD2	1.97	0.46
1:Y:273:VAL:CG2	1:Y:287:LEU:HD22	2.40	0.46
1:Z:104:MET:HE2	1:Z:121:LEU:HD23	1.97	0.46
1:Z:144:ARG:HG2	1:Z:148:LEU:HD12	1.98	0.46
1:Y:164:TRP:CZ2	2:B:793:PRO:HG3	2.50	0.46
1:Z:184:TYR:CE1	1:Z:191:SER:HB2	2.51	0.46
1:Y:260:PHE:HD2	1:Y:261:PRO:CA	2.26	0.46
1:Z:148:LEU:CG	1:Z:182:GLN:HG2	2.45	0.46
1:Z:112:LYS:HG2	1:Z:113:TRP:CZ3	2.50	0.46
1:Z:142:PHE:CE1	1:Z:184:TYR:CD2	3.03	0.46
2:B:808:LYS:HG3	2:B:813:VAL:HG22	1.98	0.46
1:Y:182:GLN:HA	1:Y:182:GLN:NE2	2.31	0.46
1:Y:283:HIS:CD2	1:Y:295:MET:HE3	2.51	0.46
1:Z:111:TRP:HD1	1:Z:120:ALA:O	1.97	0.46
1:Z:117:ASN:OD1	1:Z:132:MET:CB	2.64	0.46
1:Z:104:MET:CE	1:Z:121:LEU:CD2	2.93	0.45
1:Z:184:TYR:CE1	1:Z:191:SER:CB	2.99	0.45
1:Y:231:ILE:CG1	1:Y:245:LYS:HD3	2.47	0.45
1:Z:117:ASN:OD1	1:Z:132:MET:HB3	2.17	0.45
1:Z:206:MET:HE3	1:Z:206:MET:HB3	1.92	0.45
1:Y:144:ARG:HE	1:Y:148:LEU:CB	2.29	0.45
1:Y:262:VAL:HG21	1:Y:278:LYS:CA	2.46	0.45
1:Z:232:GLU:HG2	1:Z:243:PHE:HB3	1.99	0.45
1:Y:184:TYR:CE1	1:Y:191:SER:CB	2.99	0.45
1:Z:144:ARG:HE	1:Z:148:LEU:CB	2.29	0.45
1:Z:158:THR:CG2	1:Z:165:LEU:HD23	2.43	0.45
1:Z:102:HIS:CE1	1:Z:104:MET:HG2	2.51	0.45
1:Z:128:TYR:CD2	1:Z:140:LYS:HA	2.51	0.45
1:Y:193:PRO:C	1:Y:194:ILE:CG1	2.84	0.44
1:Y:235:THR:HA	2:B:815:TYR:HB3	1.99	0.44
1:Z:231:ILE:HB	1:Z:245:LYS:HD3	2.00	0.44
1:Y:279:TYR:HB3	1:Y:281:TYR:CE2	2.52	0.44
1:Z:206:MET:SD	1:Z:243:PHE:HD1	2.41	0.44
1:Y:163:LYS:C	1:Y:186:VAL:HG22	2.42	0.44
1:Z:114:ILE:HD11	1:Z:158:THR:OG1	2.18	0.44
1:Z:127:VAL:CG2	1:Z:142:PHE:CE1	3.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:148:LEU:O	1:Z:151:CYS:CB	2.65	0.44
1:Y:289:THR:C	1:Y:291:THR:H	2.25	0.44
1:Z:113:TRP:CE3	1:Z:113:TRP:O	2.71	0.44
1:Y:231:ILE:HB	1:Y:245:LYS:CD	2.48	0.44
1:Y:148:LEU:O	1:Y:151:CYS:CB	2.66	0.44
1:Y:231:ILE:CB	1:Y:245:LYS:HD3	2.47	0.44
1:Z:154:ILE:HD13	1:Z:170:ILE:CD1	2.48	0.44
1:Z:182:GLN:HA	1:Z:182:GLN:NE2	2.33	0.44
1:Z:206:MET:HB2	1:Z:209:ASN:HD22	1.83	0.44
1:Y:216:PHE:HB2	1:Y:233:VAL:CG2	2.48	0.43
2:B:854:ILE:HD13	2:B:935:LEU:CD1	2.48	0.43
1:Y:193:PRO:O	1:Y:194:ILE:CG1	2.65	0.43
1:Y:293:ILE:C	1:Y:294:TYR:CG	2.96	0.43
1:Z:102:HIS:CD2	1:Z:130:TRP:CE2	3.05	0.43
1:Z:127:VAL:HG21	1:Z:142:PHE:CE1	2.53	0.43
1:Z:122:VAL:CG1	1:Z:153:ILE:HD13	2.46	0.43
1:Z:140:LYS:O	2:B:846:ASN:HB3	2.19	0.43
1:Z:148:LEU:O	1:Z:149:ALA:C	2.62	0.43
1:Z:148:LEU:HD21	1:Z:182:GLN:HG2	2.00	0.43
2:B:886:MET:HE1	2:B:904:ARG:CZ	2.49	0.43
1:Y:148:LEU:CG	1:Y:182:GLN:HG2	2.49	0.43
1:Y:266:ILE:HG22	1:Y:273:VAL:HA	2.01	0.43
1:Y:283:HIS:NE2	1:Y:285:TYR:CZ	2.78	0.43
1:Y:202:ALA:CB	1:Y:204:PHE:CE1	3.02	0.43
1:Y:205:LYS:HD3	1:Y:212:GLU:CB	2.48	0.43
2:B:835:GLN:CD	2:B:835:GLN:H	2.27	0.43
1:Y:272:VAL:CG2	1:Y:284:LEU:CG	2.98	0.42
1:Y:148:LEU:O	1:Y:149:ALA:C	2.61	0.42
1:Y:293:ILE:O	1:Y:294:TYR:CD1	2.72	0.42
1:Z:104:MET:HE2	1:Z:121:LEU:HD22	1.98	0.42
1:Y:148:LEU:HD11	1:Y:182:GLN:CG	2.48	0.42
1:Y:243:PHE:CE2	1:Y:244:PRO:O	2.73	0.42
1:Y:283:HIS:CD2	1:Y:285:TYR:HH	2.37	0.42
1:Z:113:TRP:HE3	1:Z:113:TRP:CA	2.31	0.42
1:Z:128:TYR:HE2	1:Z:140:LYS:HD3	1.85	0.42
1:Z:142:PHE:CD1	1:Z:184:TYR:CD2	3.08	0.42
1:Y:176:ARG:NH1	1:Y:223:GLN:HG3	2.35	0.42
1:Y:179:GLY:HA3	1:Y:197:HIS:NE2	2.34	0.42
1:Y:221:ARG:HA	1:Y:226:GLY:HA2	2.02	0.42
1:Z:145:HIS:CD2	1:Z:182:GLN:HE22	2.37	0.42
1:Y:235:THR:HA	1:Y:236:PRO:HD3	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:260:PHE:H	1:Y:278:LYS:HG2	1.84	0.42
1:Y:272:VAL:HG21	1:Y:284:LEU:HG	2.01	0.42
1:Y:152:GLN:O	1:Y:169:GLY:HA2	2.19	0.42
1:Z:102:HIS:HE1	1:Z:104:MET:CG	2.32	0.42
1:Y:216:PHE:CD1	1:Y:218:PHE:CD1	3.07	0.42
1:Z:231:ILE:HB	1:Z:245:LYS:CE	2.50	0.42
1:Y:216:PHE:CE1	1:Y:218:PHE:CD1	3.08	0.41
1:Y:253:PRO:O	1:Y:256:ALA:HB3	2.20	0.41
1:Z:144:ARG:HH21	1:Z:148:LEU:HB3	1.85	0.41
1:Z:102:HIS:ND1	1:Z:104:MET:HG2	2.35	0.41
1:Y:179:GLY:HA3	1:Y:197:HIS:CD2	2.56	0.41
1:Z:159:ASP:OD1	1:Z:201:PHE:CE2	2.74	0.41
1:Y:271:ASP:HA	1:Y:287:LEU:HD12	2.02	0.41
1:Y:166:LEU:HD22	1:Y:181:MET:HE2	2.03	0.41
1:Z:112:LYS:HG2	1:Z:113:TRP:CE3	2.56	0.41
1:Y:206:MET:CE	1:Y:243:PHE:HD1	2.34	0.41
1:Z:163:LYS:C	1:Z:186:VAL:HG22	2.45	0.41
1:Z:220:VAL:O	1:Z:226:GLY:HA2	2.19	0.41
1:Y:235:THR:HG23	2:B:804:GLN:HB3	2.03	0.40
1:Z:144:ARG:NH2	1:Z:153:ILE:HG12	2.36	0.40
1:Z:119:VAL:HB	1:Z:130:TRP:HB3	2.03	0.40
1:Y:164:TRP:CH2	2:B:793:PRO:HG3	2.56	0.40
2:B:770:LEU:HD11	2:B:784:VAL:HG11	2.03	0.40
1:Y:282:ILE:HD11	1:Y:298:ILE:CD1	2.51	0.40
1:Z:114:ILE:CG2	1:Z:118:THR:OG1	2.69	0.40
1:Z:128:TYR:HD2	1:Z:140:LYS:HA	1.87	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	Y	155/299 (52%)	134 (86%)	13 (8%)	8 (5%)	1	15
1	Z	147/299 (49%)	123 (84%)	17 (12%)	7 (5%)	2	16
2	B	231/233 (99%)	228 (99%)	3 (1%)	0	100	100
All	All	533/831 (64%)	485 (91%)	33 (6%)	15 (3%)	6	24

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Y	259	ASP
1	Z	133	GLU
1	Z	194	ILE
1	Y	177	VAL
1	Y	194	ILE
1	Y	271	ASP
1	Y	290	GLY
1	Z	118	THR
1	Z	149	ALA
1	Y	149	ALA
1	Y	262	VAL
1	Z	177	VAL
1	Z	113	TRP
1	Z	197	HIS
1	Y	226	GLY

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	Y	132/258 (51%)	121 (92%)	11 (8%)	10	30
1	Z	125/258 (48%)	116 (93%)	9 (7%)	13	35
2	B	209/209 (100%)	201 (96%)	8 (4%)	29	50
All	All	466/725 (64%)	438 (94%)	28 (6%)	19	39

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Y	155	ASN
1	Y	181	MET
1	Y	195	GLU
1	Y	216	PHE
1	Y	227	LYS
1	Y	233	VAL
1	Y	241	GLN
1	Y	260	PHE
1	Y	271	ASP
1	Y	272	VAL
1	Y	289	THR
1	Z	108	VAL
1	Z	113	TRP
1	Z	181	MET
1	Z	194	ILE
1	Z	216	PHE
1	Z	227	LYS
1	Z	233	VAL
1	Z	238	THR
1	Z	241	GLN
2	B	749	HIS
2	B	777	MET
2	B	835	GLN
2	B	854	ILE
2	B	869	GLN
2	B	876	ILE
2	B	891	LEU
2	B	899	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	Y	145	HIS
1	Y	155	ASN
1	Y	162	GLN
1	Y	174	GLN
1	Y	175	ASN
1	Y	209	ASN
1	Y	283	HIS
1	Z	102	HIS
1	Z	155	ASN
1	Z	174	GLN
1	Z	182	GLN

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Mol	Chain	Res	Type
1	Z	197	HIS
1	Z	209	ASN
2	B	804	GLN
2	B	846	ASN
2	B	853	GLN
2	B	869	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

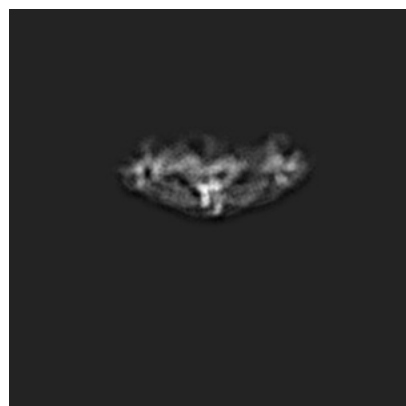
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12984. These allow visual inspection of the internal detail of the map and identification of artifacts.

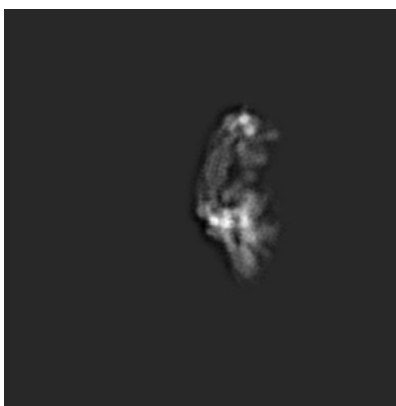
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

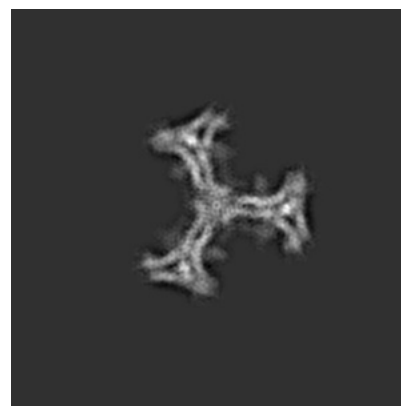
6.1.1 Primary map



X



Y

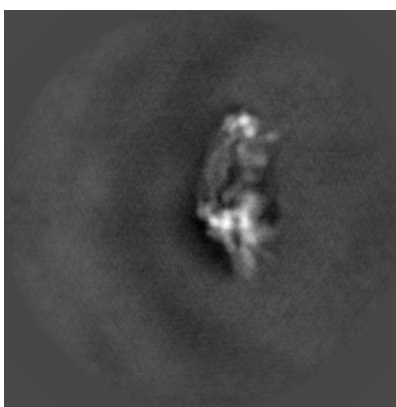


Z

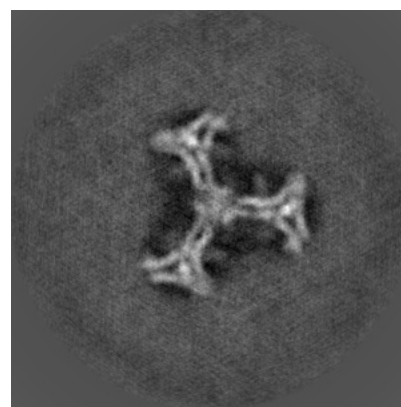
6.1.2 Raw map



X



Y

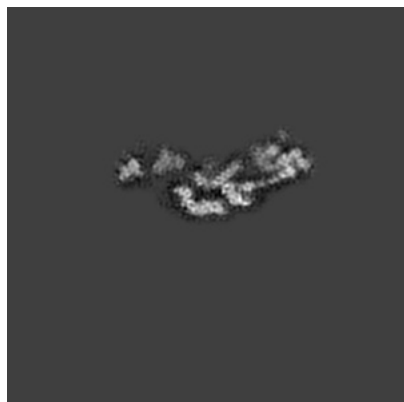


Z

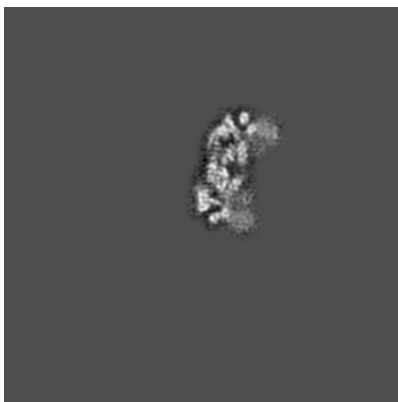
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 175

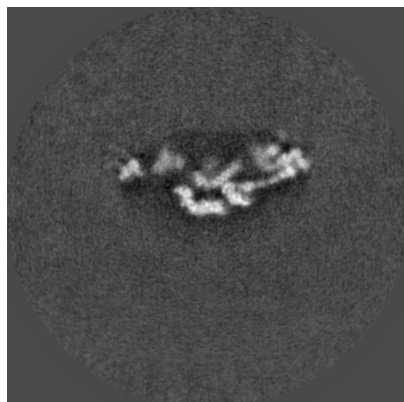


Y Index: 175

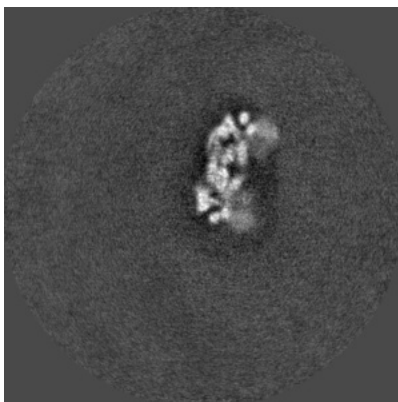


Z Index: 175

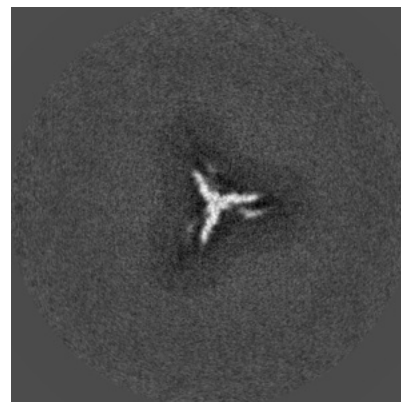
6.2.2 Raw map



X Index: 175



Y Index: 175

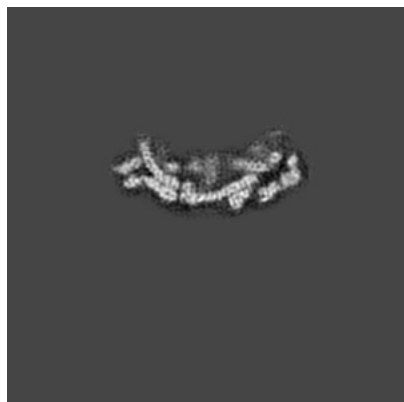


Z Index: 175

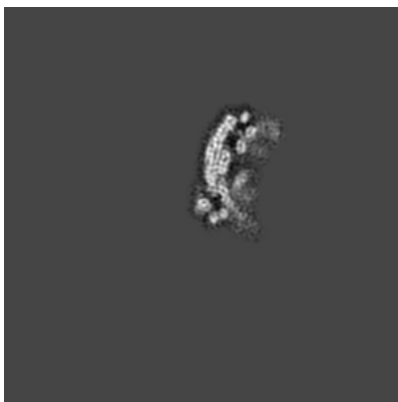
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

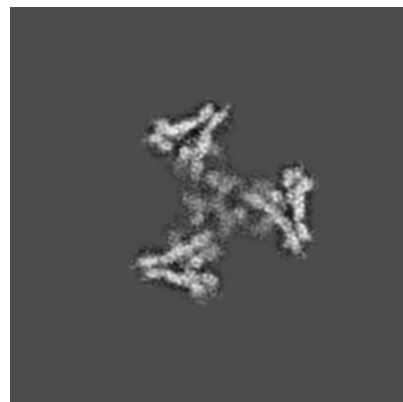
6.3.1 Primary map



X Index: 163

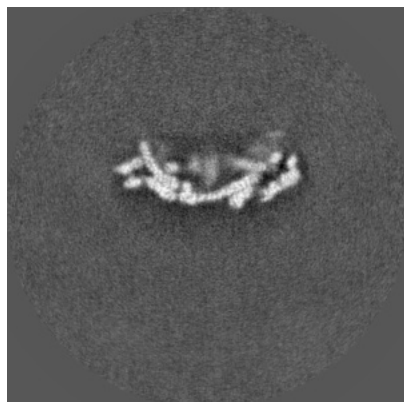


Y Index: 171

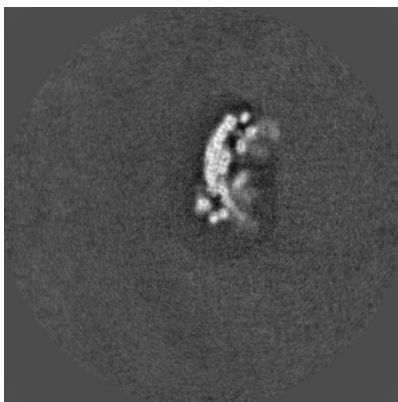


Z Index: 210

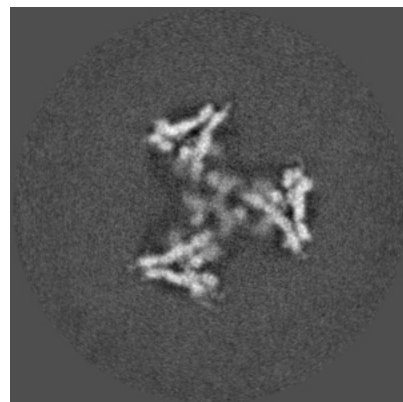
6.3.2 Raw map



X Index: 162



Y Index: 171

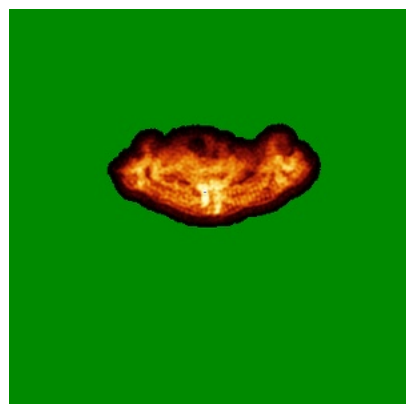


Z Index: 210

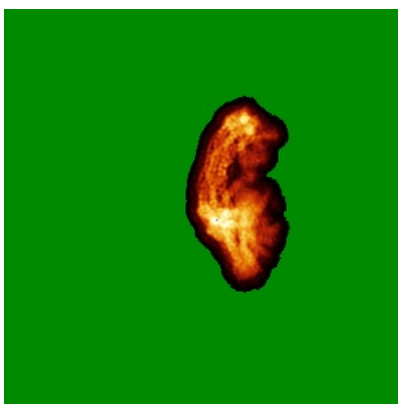
The images above show the largest variance slices of the map in three orthogonal directions.

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

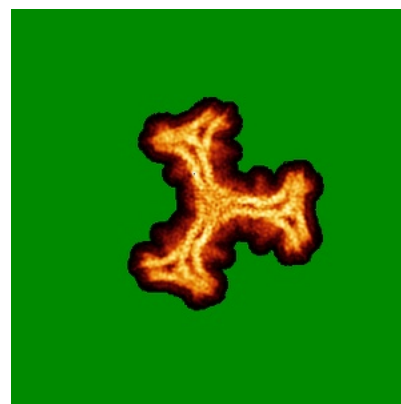
6.4.1 Primary map



X

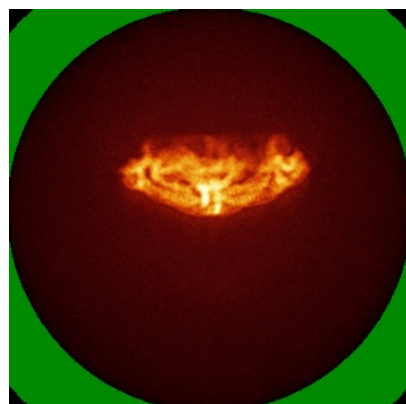


Y



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.

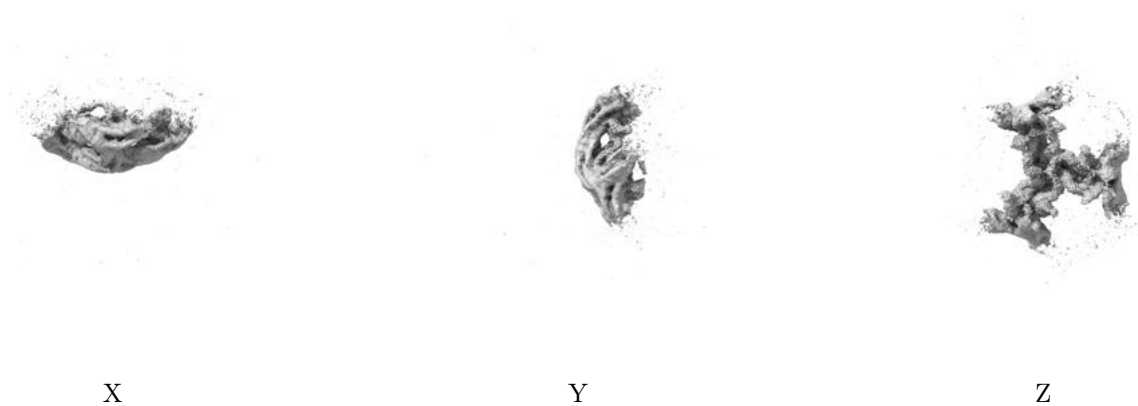
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0149. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

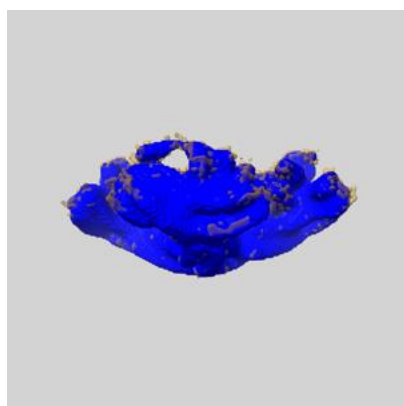
6.6 Mask visualisation [i](#)

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

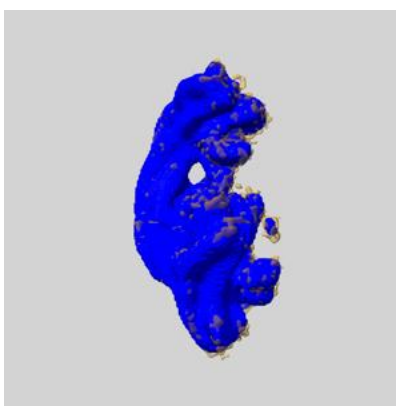
A mask typically either:

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

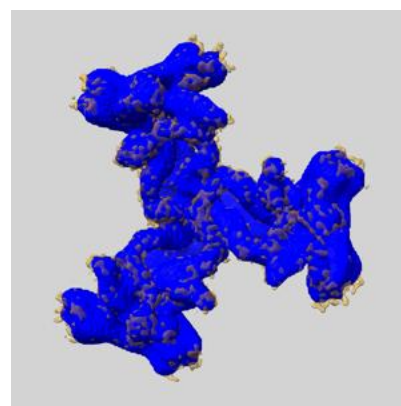
6.6.1 emd_12984_msk_1.map [i](#)



X



Y

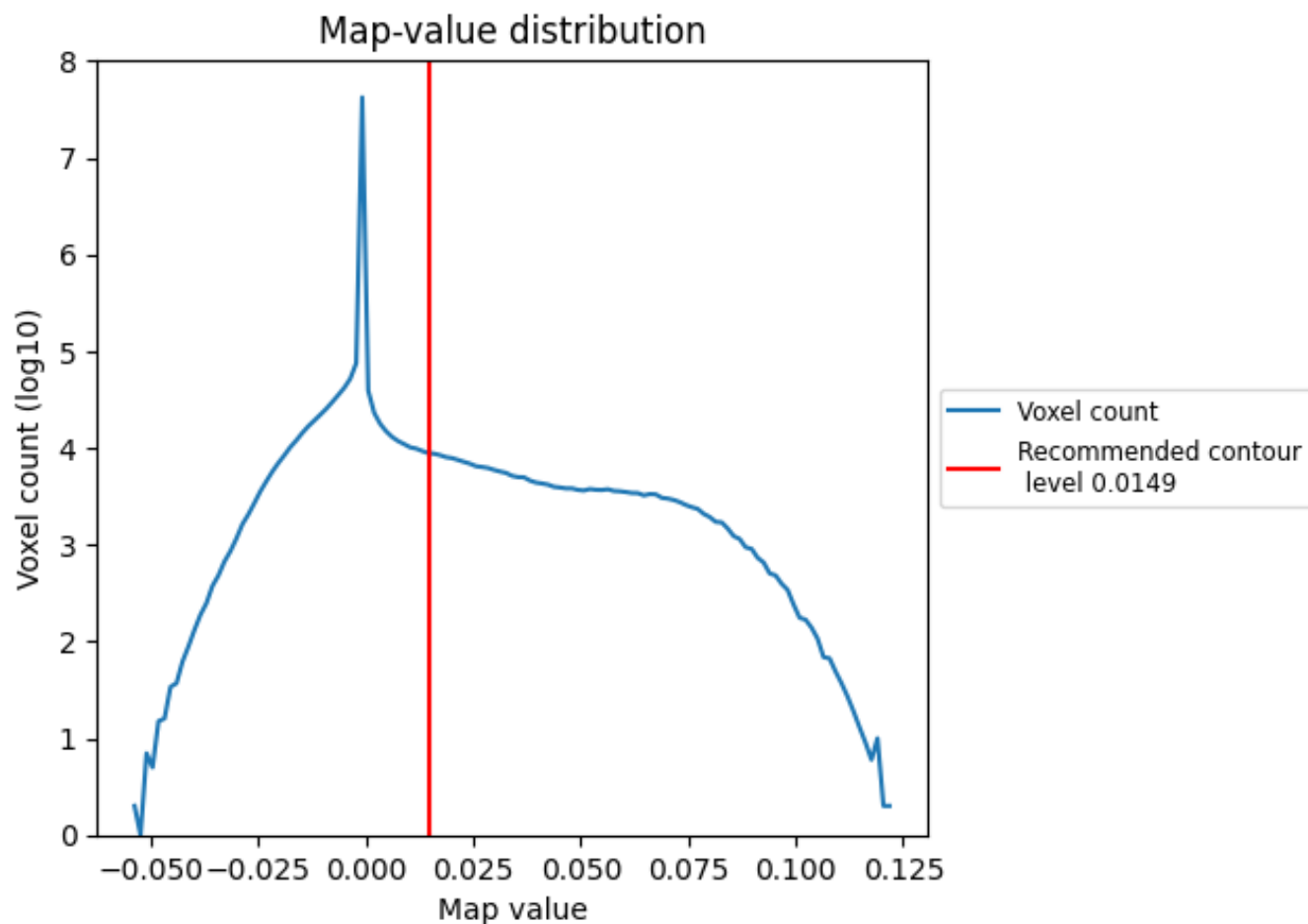


Z

7 Map analysis [i](#)

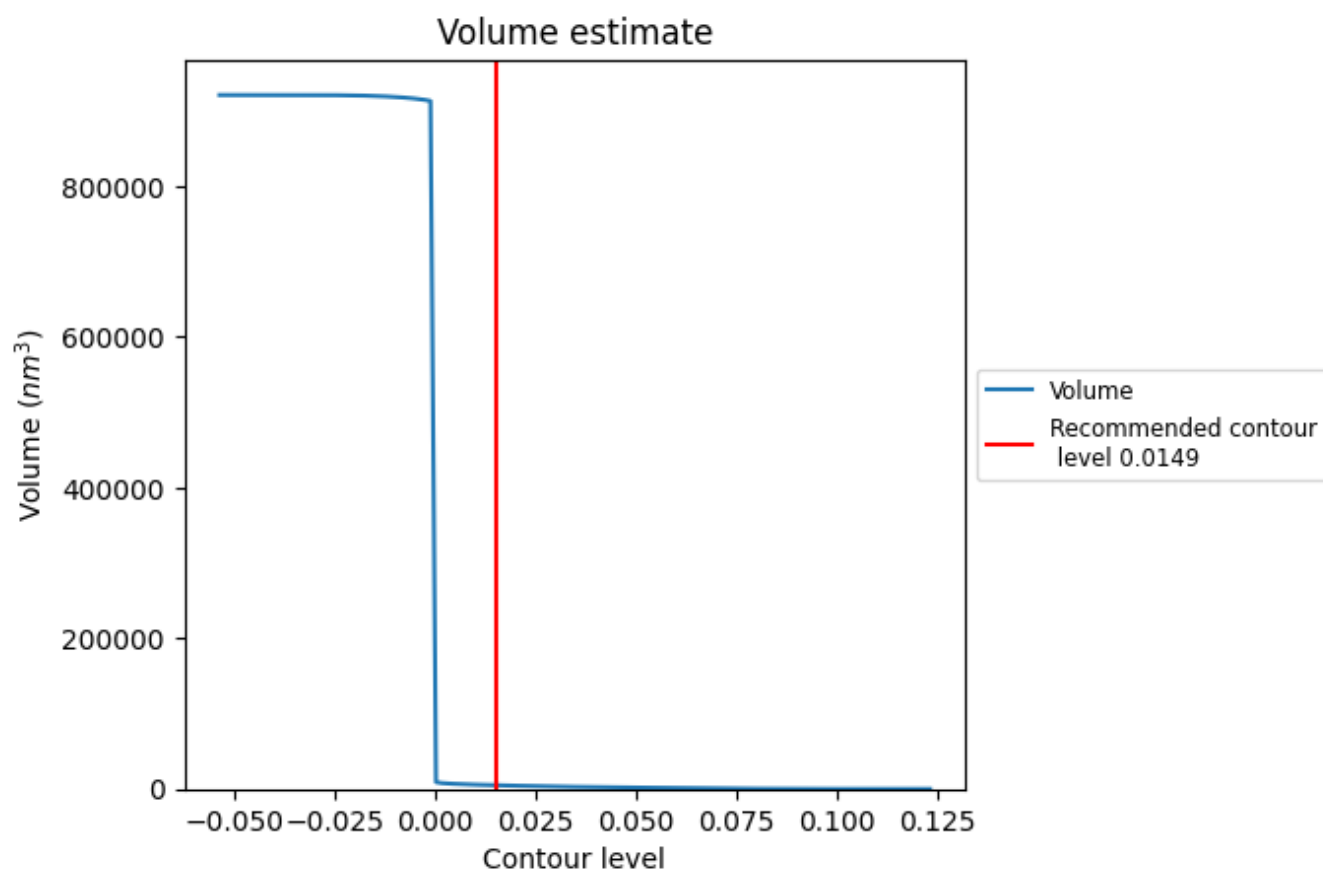
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

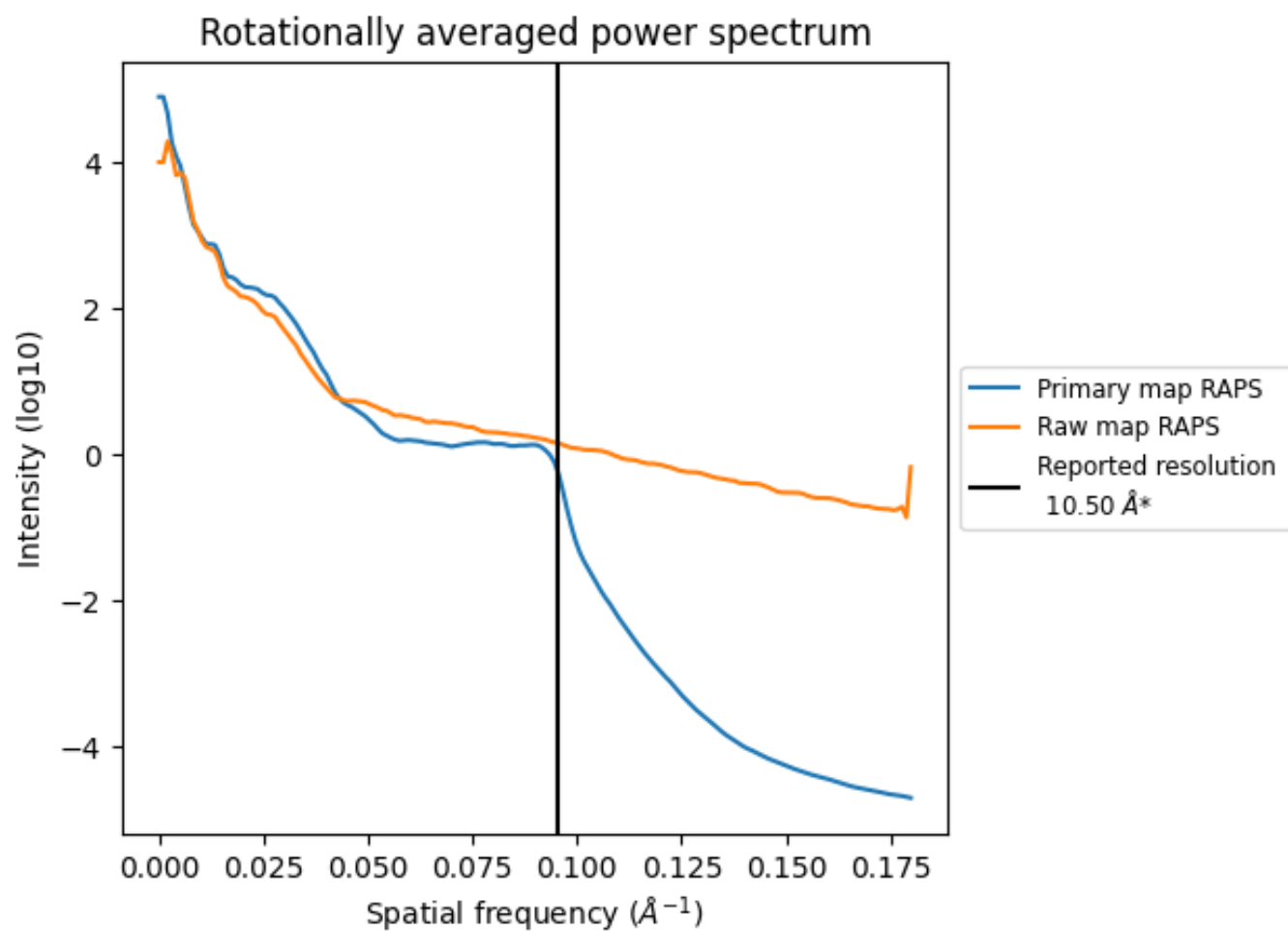
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4970 nm^3 ; this corresponds to an approximate mass of 4490 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 ⓘ

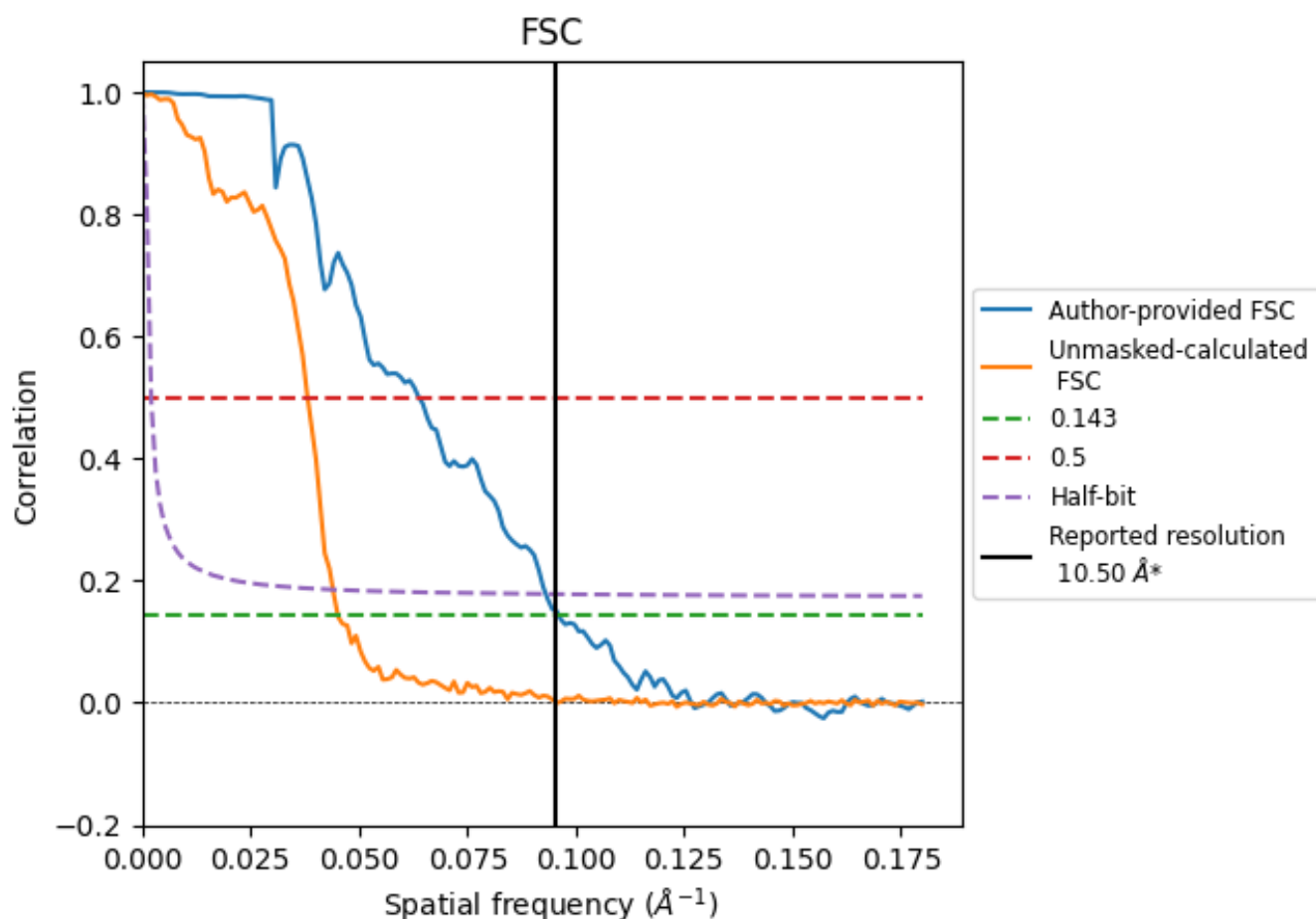


*Reported resolution corresponds to spatial frequency of 0.095 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.095 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

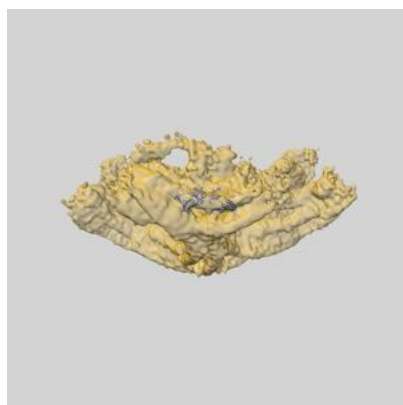
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	10.50	-	-
Author-provided FSC curve	10.41	15.65	10.74
Unmasked-calculated*	22.12	26.18	22.73

*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 22.12 differs from the reported value 10.5 by more than 10 %

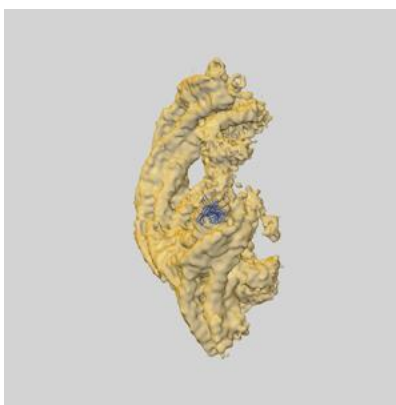
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12984 and PDB model 7OM8. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

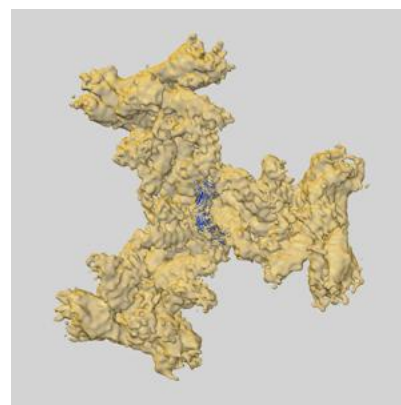
9.1 Map-model overlay [i](#)



X



Y



Z

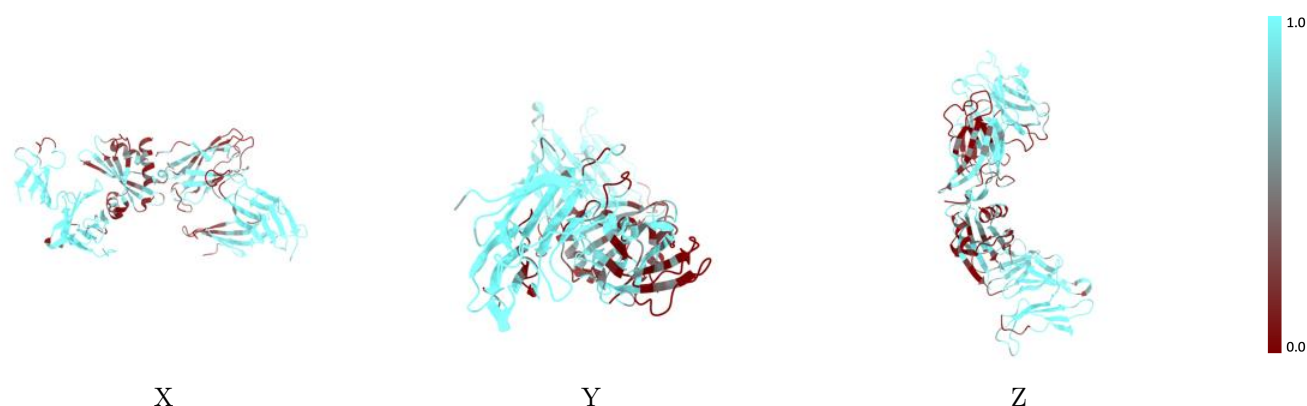
The images above show the 3D surface view of the map at the recommended contour level 0.0149 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



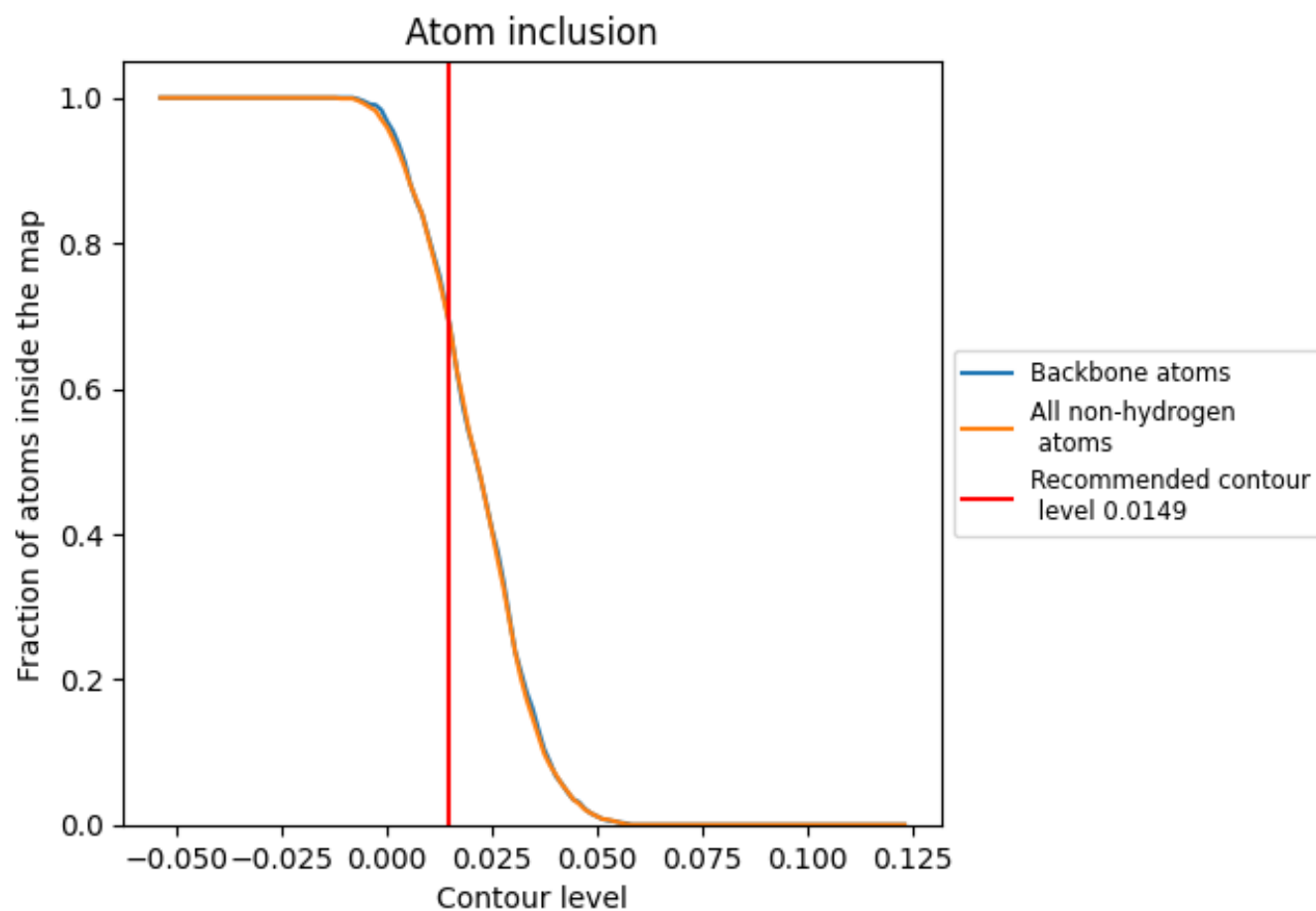
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0149).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 69% 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 (0.0149) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6890	0.0220
B	0.5000	0.0280
Y	0.7940	0.0110
Z	0.8680	0.0260

