



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 03:54 AM UTC

PDB ID : 9CJK / pdb_00009cjk
EMDB ID : EMD-45634
Title : Human TMED9 octamer structure
Authors : Le, X.; Xiong, P.
Deposited on : 2024-07-06
Resolution : 3.70 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
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

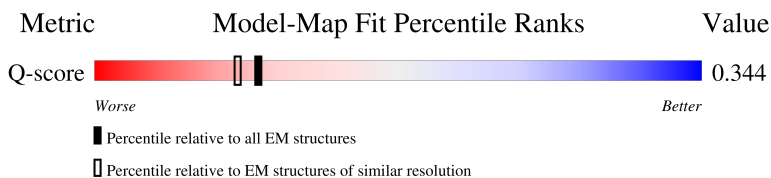
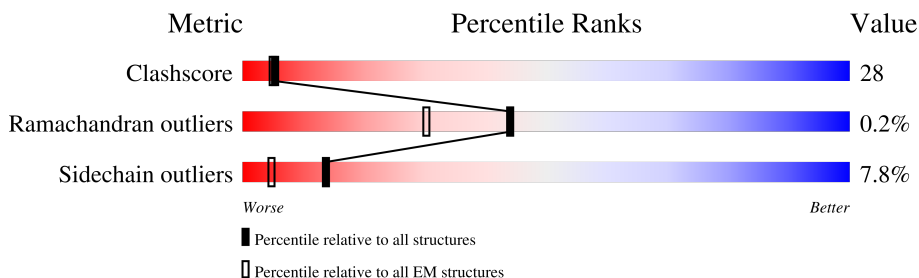
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

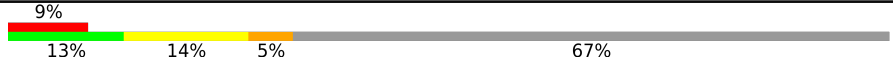
The reported resolution of this entry is 3.70 Å.

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	11569 (3.20 - 4.20)

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

Mol	Chain	Length	Quality of chain
1	A	235	
1	B	235	
1	C	235	
1	D	235	

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Mol	Chain	Length	Quality of chain
1	E	235	7%17%13%• 66%
1	F	235	12%18%11%•• 67%
1	G	235	5%8%6%• 84%
1	H	235	•11%• 84%

2 Entry composition

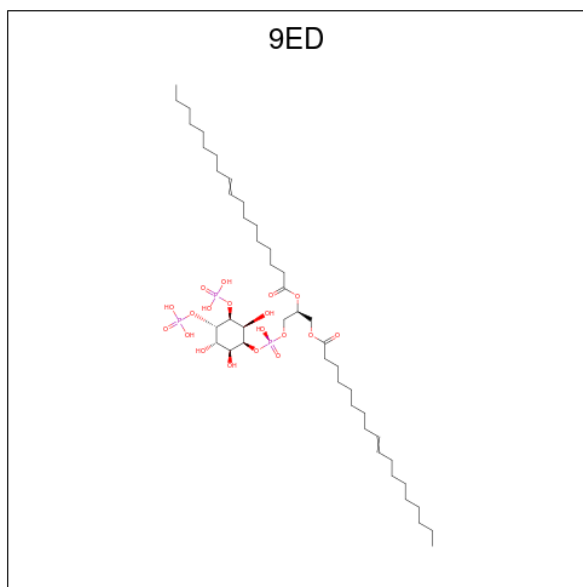
There are 2 unique types of molecules in this entry. The entry contains 4781 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

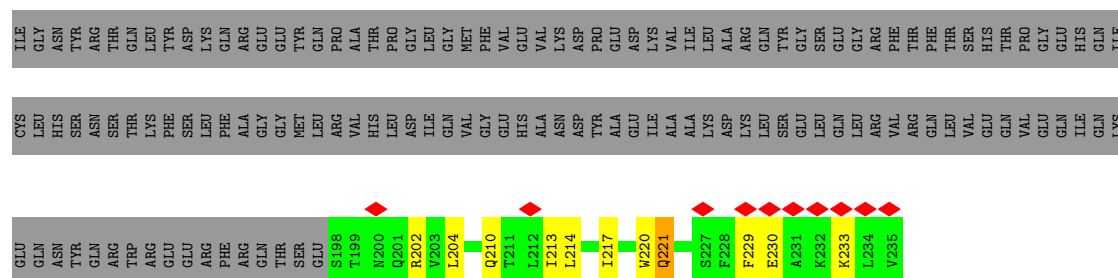
- Molecule 1 is a protein called Transmembrane emp24 domain-containing protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	77	Total	C	N	O	S	0	0
			673	430	125	117	1		
1	F	77	Total	C	N	O	S	0	0
			673	430	125	117	1		
1	H	38	Total	C	N	O	S	0	0
			321	215	56	49	1		
1	E	80	Total	C	N	O	S	0	0
			692	442	129	120	1		
1	A	77	Total	C	N	O	S	0	0
			673	430	125	117	1		
1	C	77	Total	C	N	O	S	0	0
			673	430	125	117	1		
1	G	38	Total	C	N	O	S	0	0
			321	215	56	49	1		
1	B	80	Total	C	N	O	S	0	0
			692	442	129	120	1		

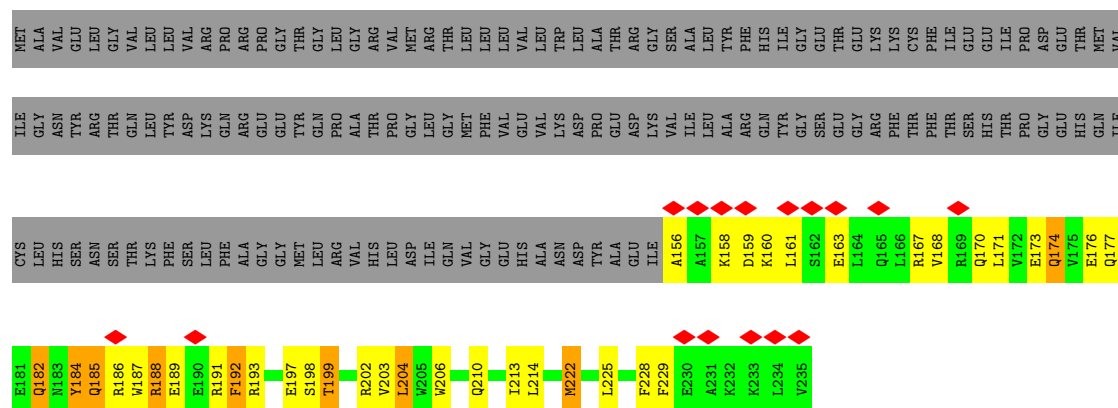
- Molecule 2 is [(2R)-2-[(E)-octadec-9-enoyl]oxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phosphoryl]oxy-propyl] (E)-octadec-9-enoate (CCD ID: 9ED) (formula: C₄₅H₈₅O₁₉P₃).



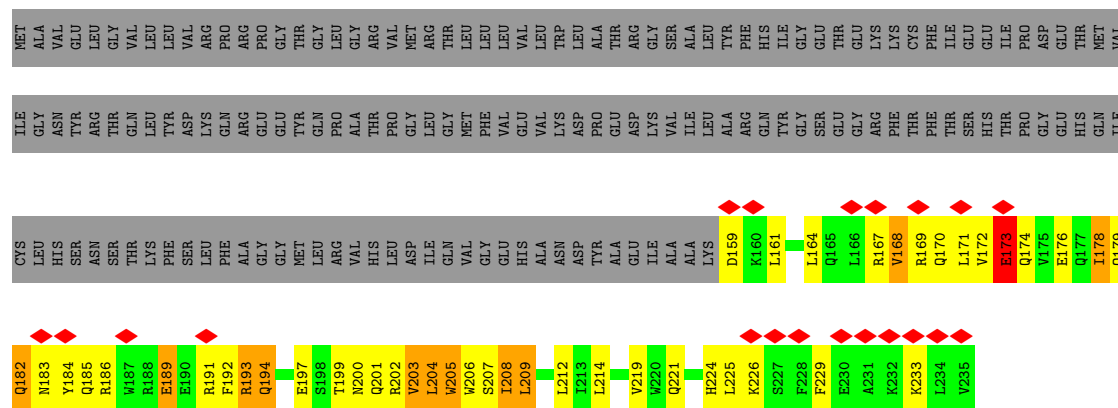
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
2	A	1	63	45	16	2	0



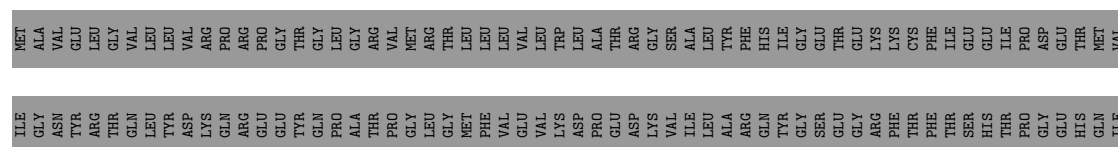
• Molecule 1: Transmembrane emp24 domain-containing protein 9

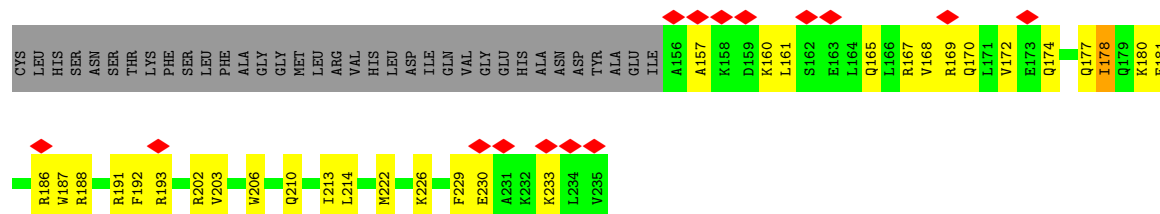


• Molecule 1: Transmembrane emp24 domain-containing protein 9



• Molecule 1: Transmembrane emp24 domain-containing protein 9





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	233493	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 ($e^-/\text{\AA}^2$)	43.2	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.183	Depositor
Minimum map value	-0.141	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	264.0, 264.0, 264.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 9ED

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	1.65	16/685 (2.3%)	1.45	12/921 (1.3%)
1	B	1.06	4/704 (0.6%)	0.98	3/946 (0.3%)
1	C	1.55	10/685 (1.5%)	1.36	7/921 (0.8%)
1	D	1.41	14/685 (2.0%)	1.27	8/921 (0.9%)
1	E	1.24	8/704 (1.1%)	1.15	7/946 (0.7%)
1	F	1.14	5/685 (0.7%)	1.17	7/921 (0.8%)
1	G	1.23	5/329 (1.5%)	1.19	3/445 (0.7%)
1	H	0.64	1/329 (0.3%)	0.74	2/445 (0.4%)
All	All	1.31	63/4806 (1.3%)	1.21	49/6466 (0.8%)

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	210	GLN	CA-C	-8.53	1.43	1.52
1	B	180	LYS	CA-C	-7.22	1.43	1.52
1	A	183	ASN	C-O	-7.13	1.16	1.23
1	D	202	ARG	C-O	-7.04	1.15	1.24
1	A	202	ARG	C-O	-6.94	1.16	1.24
1	C	182	GLN	CA-C	-6.85	1.44	1.52
1	E	206	TRP	CA-C	-6.38	1.44	1.52
1	E	192	PHE	C-O	-6.36	1.16	1.24
1	D	183	ASN	CG-ND2	-6.29	1.20	1.33
1	D	182	GLN	CD-NE2	-6.15	1.20	1.33
1	A	182	GLN	CD-NE2	-6.11	1.20	1.33
1	C	174	GLN	C-O	-6.08	1.16	1.24
1	B	187	TRP	C-O	-6.01	1.16	1.24
1	A	168	VAL	C-O	-5.99	1.17	1.24
1	E	192	PHE	CA-C	-5.97	1.45	1.52
1	E	206	TRP	C-O	-5.97	1.16	1.24
1	A	184	TYR	CA-C	-5.96	1.44	1.52
1	F	178	ILE	C-O	-5.91	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	163	GLU	C-O	-5.78	1.16	1.24
1	E	184	TYR	C-O	-5.77	1.17	1.24
1	A	194	GLN	CA-C	-5.76	1.45	1.52
1	D	161	LEU	CA-C	-5.63	1.45	1.52
1	G	210	GLN	CD-NE2	-5.62	1.21	1.33
1	A	221	GLN	N-CA	-5.59	1.39	1.46
1	E	185	GLN	C-O	-5.51	1.17	1.24
1	F	181	GLU	C-O	-5.47	1.17	1.24
1	D	184	TYR	C-O	-5.43	1.17	1.24
1	B	170	GLN	CD-NE2	-5.43	1.21	1.33
1	C	181	GLU	C-O	-5.42	1.17	1.24
1	C	171	LEU	C-O	-5.41	1.17	1.24
1	A	179	GLN	C-O	-5.40	1.17	1.24
1	F	185	GLN	C-O	-5.40	1.17	1.24
1	C	206	TRP	CA-C	-5.36	1.46	1.52
1	C	178	ILE	C-O	-5.36	1.18	1.24
1	E	170	GLN	CA-C	5.32	1.59	1.52
1	C	185	GLN	CD-NE2	-5.31	1.22	1.33
1	D	187	TRP	C-O	-5.31	1.18	1.24
1	C	202	ARG	C-O	-5.30	1.17	1.24
1	C	179	GLN	CD-NE2	-5.29	1.22	1.33
1	A	174	GLN	CD-NE2	-5.29	1.22	1.33
1	E	184	TYR	CA-C	-5.26	1.46	1.52
1	D	223	ARG	C-O	-5.26	1.18	1.24
1	C	185	GLN	CA-C	-5.25	1.46	1.52
1	G	224	HIS	ND1-CE1	5.25	1.37	1.32
1	D	202	ARG	CA-C	-5.24	1.46	1.52
1	A	184	TYR	C-O	-5.22	1.17	1.24
1	A	199	THR	C-O	-5.21	1.18	1.24
1	A	200	ASN	CG-ND2	-5.20	1.22	1.33
1	A	186	ARG	CA-C	-5.13	1.46	1.52
1	F	179	GLN	CD-NE2	-5.13	1.22	1.33
1	D	201	GLN	CD-OE1	5.12	1.33	1.23
1	G	221	GLN	CD-OE1	5.09	1.33	1.23
1	A	170	GLN	CD-NE2	-5.09	1.22	1.33
1	A	189	GLU	CA-C	-5.09	1.46	1.52
1	D	161	LEU	C-O	-5.08	1.18	1.24
1	B	177	GLN	CD-OE1	5.08	1.33	1.23
1	F	217	ILE	C-O	-5.08	1.18	1.24
1	H	221	GLN	CD-OE1	5.05	1.33	1.23
1	A	174	GLN	C-O	-5.05	1.17	1.24
1	D	217	ILE	C-O	-5.04	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	206	TRP	C-O	-5.04	1.18	1.24
1	D	176	GLU	C-O	-5.03	1.18	1.24
1	D	174	GLN	CD-OE1	5.02	1.33	1.23

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	210	GLN	N-CA-C	-10.97	98.08	112.68
1	A	183	ASN	N-CA-C	-10.28	95.10	111.04
1	A	209	LEU	N-CA-C	-10.14	100.30	111.36
1	F	215	VAL	N-CA-C	9.97	120.79	110.72
1	A	202	ARG	N-CA-C	-9.04	101.00	111.03
1	F	176	GLU	N-CA-C	-8.51	101.97	111.07
1	A	176	GLU	N-CA-C	-8.50	101.97	111.07
1	D	190	GLU	N-CA-C	-8.04	101.34	112.12
1	E	206	TRP	N-CA-C	-8.04	101.28	112.45
1	A	183	ASN	CB-CA-C	-7.78	99.02	111.39
1	D	165	GLN	N-CA-C	-7.59	102.95	111.07
1	A	205	TRP	N-CA-C	-7.14	104.83	113.97
1	B	178	ILE	CB-CA-C	-7.03	101.73	111.65
1	A	178	ILE	CB-CA-C	-7.00	103.01	111.97
1	C	160	LYS	N-CA-C	-6.91	102.81	111.11
1	G	224	HIS	CB-CG-CD2	-6.63	122.58	131.20
1	B	210	GLN	N-CA-C	-6.38	103.84	111.69
1	F	209	LEU	N-CA-C	-6.32	102.94	112.04
1	E	163	GLU	N-CA-C	-6.28	104.44	111.28
1	F	180	LYS	N-CA-C	-6.20	102.07	111.56
1	E	170	GLN	CB-CA-C	6.17	121.34	110.85
1	C	218	GLY	N-CA-C	-6.17	105.03	112.49
1	F	226	LYS	CG-CD-CE	6.13	125.40	111.30
1	D	221	GLN	N-CA-C	-6.11	104.53	111.07
1	E	161	LEU	N-CA-C	-6.06	104.59	111.14
1	D	178	ILE	CB-CA-C	-6.00	104.29	111.97
1	D	173	GLU	N-CA-C	-5.99	104.69	112.23
1	F	216	ALA	N-CA-C	-5.93	104.82	111.28
1	C	182	GLN	N-CA-C	-5.83	104.84	111.07
1	G	224	HIS	CB-CG-ND1	5.70	131.24	122.70
1	E	189	GLU	N-CA-C	-5.68	106.28	113.43
1	A	219	VAL	O-C-N	5.66	127.46	121.91
1	B	193	ARG	N-CA-C	-5.57	106.33	113.23
1	A	174	GLN	N-CA-C	-5.56	106.38	112.72
1	C	173	GLU	N-CA-C	-5.51	105.19	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	184	TYR	CB-CA-C	-5.50	102.25	110.88
1	F	169	ARG	O-C-N	5.43	128.57	122.22
1	D	164	LEU	N-CA-C	-5.28	105.60	111.36
1	D	175	VAL	CB-CA-C	-5.27	104.95	112.22
1	C	222	MET	CB-CG-SD	-5.25	96.94	112.70
1	A	194	GLN	CB-CA-C	-5.24	102.42	110.81
1	D	187	TRP	N-CA-C	-5.19	105.27	111.03
1	C	178	ILE	N-CA-C	-5.18	105.45	110.42
1	H	221	GLN	CA-C-N	5.17	128.87	120.60
1	H	221	GLN	C-N-CA	5.17	128.87	120.60
1	A	173	GLU	N-CA-C	-5.16	107.03	113.38
1	C	209	LEU	N-CA-C	-5.13	105.58	111.07
1	A	184	TYR	N-CA-C	5.08	118.25	111.75
1	E	158	LYS	N-CA-C	-5.01	105.27	111.33

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	673	0	688	76	0
1	B	692	0	711	69	0
1	C	673	0	688	57	0
1	D	673	0	688	52	0
1	E	692	0	711	70	0
1	F	673	0	688	42	0
1	G	321	0	341	26	0
1	H	321	0	341	18	0
2	A	63	0	0	2	0
All	All	4781	0	4856	272	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 28.

All (272) 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:F:221:GLN:HG2	1:E:222:MET:SD	1.72	1.28
1:F:221:GLN:CG	1:E:222:MET:SD	2.27	1.23
1:E:174:GLN:HE22	1:B:174:GLN:NE2	1.39	1.17
1:C:176:GLU:O	1:C:180:LYS:HG2	1.52	1.07
1:D:161:LEU:CD1	1:F:161:LEU:HD11	1.85	1.06
1:C:185:GLN:NE2	1:B:186:ARG:HG2	1.70	1.04
1:D:161:LEU:HD13	1:F:161:LEU:HD11	1.35	1.03
1:A:172:VAL:HG22	1:A:172:VAL:O	1.55	1.03
1:C:185:GLN:HE22	1:B:186:ARG:HG2	1.29	0.96
1:E:174:GLN:NE2	1:B:174:GLN:NE2	2.15	0.95
1:C:211:THR:HG21	1:G:210:GLN:HG3	1.49	0.94
1:F:221:GLN:HG3	1:E:222:MET:SD	2.08	0.93
1:A:204:LEU:HD12	1:B:203:VAL:HG23	1.51	0.93
1:E:174:GLN:NE2	1:B:174:GLN:HE22	1.68	0.92
1:C:211:THR:CG2	1:G:210:GLN:HG3	1.99	0.92
1:C:185:GLN:NE2	1:B:186:ARG:CG	2.34	0.90
1:E:174:GLN:HE22	1:B:174:GLN:HE22	1.18	0.88
1:D:208:ILE:CD1	1:A:208:ILE:HD13	2.04	0.87
1:A:164:LEU:CD2	1:C:164:LEU:HD23	2.05	0.87
1:D:226:LYS:CD	1:E:228:PHE:CE1	2.58	0.86
1:F:192:PHE:CZ	1:E:192:PHE:HE2	1.94	0.86
1:E:188:ARG:HD2	1:E:188:ARG:O	1.76	0.85
1:D:208:ILE:HD11	1:A:208:ILE:HD13	1.59	0.85
1:A:203:VAL:HG23	1:G:204:LEU:HD23	1.57	0.84
1:F:211:THR:OG1	1:H:210:GLN:CG	2.26	0.84
1:A:172:VAL:O	1:A:172:VAL:CG2	2.26	0.84
1:A:204:LEU:CD1	1:B:203:VAL:HA	2.07	0.84
1:F:211:THR:O	1:F:215:VAL:HG13	1.80	0.81
1:G:199:THR:HA	1:G:202:ARG:HG3	1.65	0.79
1:D:194:GLN:OE1	1:B:188:ARG:NH2	2.16	0.79
1:D:225:LEU:O	1:D:225:LEU:HD23	1.85	0.77
1:E:184:TYR:CE1	1:E:187:TRP:CE3	2.72	0.77
1:F:173:GLU:O	1:F:177:GLN:HG2	1.85	0.77
1:D:180:LYS:HB2	1:D:180:LYS:NZ	2.00	0.76
1:D:226:LYS:HD2	1:E:228:PHE:CE1	2.21	0.76
1:A:193:ARG:NH1	1:B:188:ARG:HG3	2.00	0.75
1:E:187:TRP:CH2	1:A:194:GLN:NE2	2.54	0.74
1:E:184:TYR:O	1:E:187:TRP:HB3	1.87	0.74
1:A:161:LEU:HD21	1:B:160:LYS:HE2	1.69	0.74
1:D:224:HIS:ND1	1:D:224:HIS:O	2.21	0.73
1:G:208:ILE:HD13	1:G:208:ILE:N	2.03	0.73
1:D:180:LYS:HB2	1:D:180:LYS:HZ2	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:VAL:HG12	1:G:217:ILE:HG13	1.70	0.72
1:A:164:LEU:HD21	1:C:164:LEU:CD2	2.20	0.72
1:D:205:TRP:CG	1:B:202:ARG:HD3	2.25	0.72
1:F:187:TRP:HH2	1:F:191:ARG:HH11	1.34	0.71
1:A:181:GLU:OE1	1:A:181:GLU:HA	1.89	0.71
1:F:211:THR:OG1	1:H:210:GLN:HG3	1.89	0.71
1:F:185:GLN:NE2	1:E:186:ARG:HG3	2.06	0.71
1:A:164:LEU:HD21	1:C:164:LEU:HD23	1.74	0.70
1:C:219:VAL:O	1:C:223:ARG:HG3	1.91	0.70
1:G:201:GLN:OE1	1:G:201:GLN:HA	1.91	0.70
1:A:206:TRP:CD1	1:A:209:LEU:HD12	2.27	0.70
1:E:193:ARG:HD3	1:E:197:GLU:OE2	1.92	0.69
1:B:165:GLN:O	1:B:169:ARG:HG3	1.92	0.69
1:F:187:TRP:HH2	1:F:191:ARG:NH1	1.90	0.69
1:E:198:SER:OG	1:E:202:ARG:NH1	2.26	0.69
1:G:210:GLN:O	1:G:213:ILE:HG22	1.92	0.69
1:A:161:LEU:CD2	1:B:160:LYS:HE2	2.23	0.69
1:A:164:LEU:HD11	1:C:168:VAL:HG21	1.74	0.69
1:C:185:GLN:CD	1:B:186:ARG:HG2	2.18	0.69
1:C:185:GLN:NE2	1:B:186:ARG:CD	2.55	0.68
1:A:185:GLN:CD	1:C:186:ARG:HG2	2.19	0.68
1:A:189:GLU:OE2	1:A:189:GLU:HA	1.94	0.68
1:C:181:GLU:OE1	1:B:186:ARG:NH1	2.26	0.68
1:E:204:LEU:HD23	1:E:204:LEU:C	2.19	0.67
1:A:173:GLU:O	1:A:173:GLU:HG2	1.94	0.67
1:C:229:PHE:CE2	1:B:229:PHE:HD2	2.12	0.67
1:C:181:GLU:O	1:C:181:GLU:HG3	1.95	0.66
1:D:226:LYS:HD3	1:E:228:PHE:CE1	2.31	0.66
1:A:206:TRP:HD1	1:A:209:LEU:HD12	1.59	0.66
1:A:161:LEU:HD21	1:B:160:LYS:HG3	1.78	0.66
1:D:204:LEU:HD13	1:E:203:VAL:HG22	1.79	0.65
1:F:181:GLU:O	1:F:181:GLU:HG3	1.93	0.65
1:G:200:ASN:N	1:G:200:ASN:OD1	2.28	0.65
1:F:187:TRP:CH2	1:F:191:ARG:NH1	2.62	0.65
1:A:204:LEU:HD11	1:B:203:VAL:HA	1.79	0.64
1:E:176:GLU:HA	1:E:176:GLU:OE2	1.97	0.64
1:C:215:VAL:CG1	1:G:217:ILE:HG13	2.28	0.64
1:F:210:GLN:O	1:F:214:LEU:HG	1.98	0.63
1:F:211:THR:OG1	1:H:210:GLN:HG2	1.98	0.63
1:C:230:GLU:OE1	1:C:230:GLU:HA	1.99	0.63
1:D:205:TRP:CD2	1:B:202:ARG:HG2	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:LEU:CD1	1:F:161:LEU:CD1	2.72	0.63
1:C:211:THR:CG2	1:G:210:GLN:CG	2.75	0.63
1:B:226:LYS:O	1:B:230:GLU:HG3	1.98	0.62
1:G:217:ILE:HG22	1:G:221:GLN:OE1	1.99	0.62
1:C:185:GLN:HE22	1:B:186:ARG:CG	2.03	0.62
1:A:185:GLN:OE1	1:C:186:ARG:HG2	1.99	0.62
1:F:185:GLN:HE21	1:E:186:ARG:CG	2.13	0.61
1:F:185:GLN:HE21	1:E:186:ARG:HG3	1.62	0.61
1:F:208:ILE:HG22	1:F:208:ILE:O	2.01	0.61
1:E:187:TRP:CH2	1:A:194:GLN:OE1	2.54	0.61
1:G:208:ILE:O	1:G:208:ILE:HG22	1.99	0.61
1:D:186:ARG:O	1:D:190:GLU:HB2	2.00	0.61
1:C:211:THR:HG22	1:G:210:GLN:CG	2.30	0.61
1:D:221:GLN:OE1	1:D:221:GLN:HA	2.00	0.61
1:C:174:GLN:O	1:C:174:GLN:HG2	1.99	0.60
1:B:174:GLN:O	1:B:178:ILE:HG13	2.01	0.60
1:D:176:GLU:OE1	1:E:174:GLN:OE1	2.20	0.60
1:C:181:GLU:OE1	1:B:186:ARG:CZ	2.49	0.59
1:E:213:ILE:HD11	1:A:212:LEU:HD21	1.85	0.59
1:E:187:TRP:CH2	1:A:194:GLN:CD	2.80	0.59
1:D:205:TRP:CE2	1:B:202:ARG:HG2	2.36	0.59
1:C:229:PHE:HZ	1:B:229:PHE:HB2	1.68	0.59
1:D:226:LYS:HD2	1:E:228:PHE:HE1	1.65	0.59
1:G:209:LEU:HD23	1:G:209:LEU:O	2.03	0.58
1:D:226:LYS:HG3	1:E:228:PHE:CZ	2.38	0.58
1:A:161:LEU:HD13	1:B:161:LEU:HD13	1.85	0.58
1:C:211:THR:HG22	1:G:210:GLN:HG3	1.85	0.58
1:D:212:LEU:HD21	1:B:213:ILE:HD11	1.85	0.58
1:E:193:ARG:HD2	1:E:193:ARG:C	2.27	0.58
1:E:199:THR:HA	1:E:202:ARG:HH11	1.69	0.58
1:A:203:VAL:HG13	1:A:203:VAL:O	2.03	0.58
1:D:175:VAL:HG11	1:E:174:GLN:HG2	1.86	0.58
1:E:156:ALA:O	1:E:159:ASP:HB3	2.04	0.58
1:C:221:GLN:NE2	1:B:222:MET:HB2	2.18	0.57
1:A:197:GLU:HA	1:A:197:GLU:OE1	2.03	0.57
1:C:192:PHE:CZ	1:B:192:PHE:CE2	2.92	0.57
1:A:225:LEU:O	1:A:229:PHE:CB	2.52	0.57
1:F:229:PHE:HE2	1:E:229:PHE:HD2	1.50	0.57
1:A:205:TRP:CE3	1:A:208:ILE:HG21	2.40	0.57
1:D:205:TRP:HB2	1:B:202:ARG:HD3	1.86	0.56
1:E:187:TRP:HH2	1:A:194:GLN:CD	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:GLN:HB3	1:B:191:ARG:HD3	1.87	0.56
1:E:191:ARG:HD3	1:A:194:GLN:NE2	2.20	0.56
1:F:192:PHE:CZ	1:E:192:PHE:CE2	2.85	0.56
1:D:161:LEU:HA	1:D:164:LEU:HD12	1.88	0.56
1:D:201:GLN:OE1	1:A:201:GLN:NE2	2.39	0.56
1:B:157:ALA:HA	1:B:160:LYS:HB3	1.88	0.56
1:E:184:TYR:CE1	1:E:187:TRP:CZ3	2.93	0.55
1:C:192:PHE:CZ	1:B:192:PHE:HE2	2.24	0.55
1:A:225:LEU:O	1:A:229:PHE:HB3	2.06	0.55
1:H:202:ARG:O	1:H:202:ARG:HG2	2.06	0.55
1:D:210:GLN:NE2	1:H:210:GLN:OE1	2.25	0.55
1:E:187:TRP:HH2	1:A:194:GLN:OE1	1.90	0.55
1:C:185:GLN:NE2	1:B:186:ARG:HD2	2.22	0.54
1:D:160:LYS:O	1:D:164:LEU:HG	2.07	0.54
1:A:204:LEU:CD1	1:B:203:VAL:CA	2.82	0.54
1:H:217:ILE:HG22	1:H:221:GLN:OE1	2.08	0.54
1:D:205:TRP:CB	1:B:202:ARG:HD3	2.37	0.54
1:B:165:GLN:HA	1:B:168:VAL:HG12	1.88	0.54
1:A:204:LEU:CD1	1:B:203:VAL:HG23	2.33	0.54
1:C:229:PHE:CZ	1:B:229:PHE:HD2	2.26	0.53
1:C:192:PHE:CD1	1:C:192:PHE:C	2.86	0.53
1:A:182:GLN:NE2	1:B:181:GLU:HG2	2.24	0.53
1:A:225:LEU:C	1:A:225:LEU:HD23	2.34	0.53
1:A:226:LYS:O	1:A:226:LYS:HG2	2.08	0.53
1:D:161:LEU:HD13	1:F:161:LEU:CD1	2.22	0.53
1:F:210:GLN:OE1	1:F:214:LEU:HD11	2.09	0.53
1:H:229:PHE:CZ	1:E:229:PHE:HZ	2.27	0.53
1:D:225:LEU:HD22	1:E:225:LEU:HD11	1.91	0.53
1:A:203:VAL:HG23	1:G:204:LEU:CD2	2.34	0.52
1:A:189:GLU:HG2	1:C:189:GLU:OE1	2.08	0.52
1:D:201:GLN:HB3	1:B:202:ARG:HH12	1.74	0.52
1:C:222:MET:HE1	1:G:220:TRP:HZ3	1.75	0.52
1:A:164:LEU:CD2	1:C:164:LEU:CD2	2.79	0.52
1:A:193:ARG:HH11	1:B:188:ARG:HG3	1.72	0.51
1:D:214:LEU:HD13	1:E:214:LEU:HD11	1.92	0.51
1:A:161:LEU:HD13	1:B:161:LEU:CD1	2.40	0.51
2:A:301:9ED:O06	2:A:301:9ED:O13	2.28	0.51
1:C:229:PHE:HZ	1:B:229:PHE:CB	2.23	0.51
1:E:188:ARG:HD2	1:E:188:ARG:C	2.33	0.51
1:A:214:LEU:HD13	1:B:214:LEU:HD11	1.92	0.51
1:A:167:ARG:O	1:A:171:LEU:HG	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:LEU:O	1:A:225:LEU:HD23	2.11	0.51
1:A:192:PHE:CD1	1:A:192:PHE:C	2.88	0.50
1:G:229:PHE:CZ	1:B:229:PHE:HZ	2.29	0.50
1:D:180:LYS:NZ	1:D:180:LYS:CB	2.73	0.50
1:C:171:LEU:HD12	1:B:172:VAL:HG22	1.93	0.50
1:F:185:GLN:HE22	1:E:182:GLN:HG3	1.77	0.50
1:E:184:TYR:OH	1:E:187:TRP:HZ3	1.94	0.50
1:D:178:ILE:HD11	1:F:175:VAL:HG13	1.94	0.49
1:D:208:ILE:CD1	1:A:208:ILE:CD1	2.85	0.49
1:E:184:TYR:O	1:E:187:TRP:N	2.39	0.49
1:E:184:TYR:OH	1:E:187:TRP:CZ3	2.66	0.49
1:F:219:VAL:HG22	1:H:220:TRP:CH2	2.47	0.49
1:E:184:TYR:HH	1:E:187:TRP:HZ3	1.57	0.48
1:E:193:ARG:C	1:E:193:ARG:CD	2.85	0.48
1:F:168:VAL:O	1:F:172:VAL:HG23	2.13	0.48
1:H:210:GLN:HA	1:H:213:ILE:HG22	1.94	0.48
1:E:185:GLN:C	1:E:187:TRP:H	2.21	0.48
1:A:193:ARG:HG3	1:B:192:PHE:CE2	2.49	0.48
1:C:183:ASN:HA	1:C:186:ARG:CZ	2.44	0.48
1:A:205:TRP:CE3	1:A:205:TRP:HA	2.48	0.48
1:D:172:VAL:HG21	1:E:167:ARG:HH22	1.78	0.47
1:E:187:TRP:CZ3	1:A:194:GLN:NE2	2.80	0.47
1:C:214:LEU:HA	1:C:214:LEU:HD23	1.46	0.47
1:D:160:LYS:O	1:D:164:LEU:N	2.44	0.47
1:H:213:ILE:O	1:H:217:ILE:HG12	2.15	0.47
1:H:229:PHE:CZ	1:E:229:PHE:CZ	3.03	0.47
1:A:178:ILE:HD11	1:C:175:VAL:HG13	1.97	0.47
1:D:224:HIS:ND1	1:D:224:HIS:C	2.72	0.47
1:G:213:ILE:O	1:G:217:ILE:HG12	2.15	0.47
1:E:184:TYR:CZ	1:E:187:TRP:CZ3	3.03	0.47
1:E:173:GLU:CD	1:E:173:GLU:C	2.82	0.46
1:E:167:ARG:CD	1:B:167:ARG:HD3	2.46	0.46
1:E:202:ARG:HD2	1:A:201:GLN:OE1	2.15	0.46
1:H:202:ARG:O	1:H:202:ARG:CG	2.63	0.46
1:A:225:LEU:O	1:A:229:PHE:HB2	2.16	0.46
1:B:192:PHE:O	1:B:192:PHE:CG	2.68	0.46
1:F:167:ARG:HA	1:F:170:GLN:HB3	1.98	0.46
1:A:178:ILE:HD13	1:A:178:ILE:HG21	1.66	0.45
1:E:185:GLN:C	1:E:187:TRP:N	2.75	0.45
1:C:221:GLN:HE21	1:B:222:MET:HB2	1.81	0.45
1:D:206:TRP:CE3	1:H:204:LEU:HD12	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:HIS:O	1:D:224:HIS:CG	2.70	0.44
1:D:174:GLN:NE2	1:F:179:GLN:OE1	2.50	0.44
1:E:167:ARG:NE	1:B:167:ARG:CD	2.79	0.44
1:C:190:GLU:HA	1:C:193:ARG:HD3	1.99	0.44
1:E:187:TRP:O	1:E:187:TRP:CD2	2.70	0.44
1:D:164:LEU:CD1	1:F:161:LEU:HD12	2.48	0.44
1:E:213:ILE:HD11	1:A:212:LEU:CD2	2.48	0.44
1:C:190:GLU:C	1:C:190:GLU:CD	2.85	0.44
1:A:185:GLN:NE2	1:C:186:ARG:HG2	2.32	0.44
1:F:186:ARG:O	1:F:186:ARG:HG2	2.17	0.44
1:A:182:GLN:O	1:A:182:GLN:HG2	2.17	0.44
1:C:219:VAL:CG1	1:C:223:ARG:NE	2.81	0.44
1:G:230:GLU:OE1	1:G:230:GLU:N	2.50	0.44
1:E:171:LEU:O	1:E:174:GLN:HB3	2.17	0.43
1:D:178:ILE:CD1	1:F:175:VAL:HG13	2.48	0.43
1:G:229:PHE:CZ	1:B:229:PHE:CZ	3.05	0.43
1:B:233:LYS:HD2	1:B:233:LYS:HA	1.86	0.43
1:C:176:GLU:O	1:C:180:LYS:CG	2.44	0.43
1:A:169:ARG:HA	1:A:172:VAL:HG12	2.00	0.43
1:A:233:LYS:NZ	1:G:233:LYS:HE2	2.34	0.43
1:D:233:LYS:NZ	1:H:233:LYS:HE2	2.33	0.43
1:C:198:SER:O	1:C:202:ARG:HG3	2.18	0.43
1:C:185:GLN:O	1:C:189:GLU:HG2	2.19	0.43
1:F:179:GLN:O	1:F:179:GLN:HG2	2.18	0.43
1:E:191:ARG:NE	1:A:194:GLN:OE1	2.52	0.43
1:C:185:GLN:HE21	1:B:186:ARG:HD2	1.83	0.42
1:A:204:LEU:HD13	1:B:203:VAL:HB	2.01	0.42
1:B:160:LYS:HD2	1:B:160:LYS:O	2.19	0.42
1:E:187:TRP:CD2	1:E:187:TRP:C	2.97	0.42
1:B:214:LEU:HA	1:B:214:LEU:HD23	1.77	0.42
1:C:229:PHE:CZ	1:B:229:PHE:CD2	3.06	0.42
1:D:212:LEU:CD2	1:B:213:ILE:HD11	2.49	0.42
1:C:181:GLU:OE1	1:B:186:ARG:HD2	2.20	0.42
1:D:186:ARG:O	1:D:186:ARG:HG2	2.19	0.42
1:E:214:LEU:HD23	1:E:214:LEU:HA	1.77	0.42
1:A:171:LEU:HD21	1:C:172:VAL:HG22	2.02	0.42
1:A:205:TRP:CZ3	1:A:208:ILE:HG21	2.55	0.42
1:H:230:GLU:N	1:H:230:GLU:OE1	2.50	0.41
1:A:159:ASP:OD1	1:A:159:ASP:O	2.38	0.41
1:F:170:GLN:O	1:F:170:GLN:HG2	2.20	0.41
1:F:221:GLN:HG3	1:E:222:MET:CG	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:PHE:CZ	1:B:229:PHE:CB	3.02	0.41
1:D:176:GLU:OE2	1:D:179:GLN:HG2	2.20	0.41
1:D:229:PHE:CE1	1:H:229:PHE:CD2	3.08	0.41
2:A:301:9ED:O06	2:A:301:9ED:P02	2.79	0.41
1:F:209:LEU:HD22	1:F:209:LEU:HA	1.74	0.41
1:B:160:LYS:O	1:B:160:LYS:CG	2.68	0.41
1:C:164:LEU:HD12	1:C:164:LEU:HA	1.91	0.41
1:D:201:GLN:HB3	1:B:202:ARG:NH1	2.34	0.41
1:F:217:ILE:O	1:F:220:TRP:HB3	2.21	0.41
1:A:207:SER:HB3	1:B:206:TRP:CD1	2.56	0.41
1:E:174:GLN:O	1:E:178:ILE:HG13	2.20	0.41
1:G:214:LEU:HA	1:G:214:LEU:HD23	1.83	0.41
1:H:214:LEU:HD23	1:H:214:LEU:HA	1.83	0.41
1:E:184:TYR:O	1:E:187:TRP:CB	2.64	0.41
1:A:168:VAL:HA	1:A:171:LEU:HD12	2.03	0.41
1:A:205:TRP:HA	1:A:205:TRP:HE3	1.84	0.40
1:C:222:MET:HE1	1:G:220:TRP:CZ3	2.55	0.40
1:H:229:PHE:CE1	1:E:229:PHE:CZ	3.10	0.40
1:A:161:LEU:CD1	1:B:161:LEU:CD1	3.00	0.40
1:F:167:ARG:O	1:F:170:GLN:HB3	2.21	0.40
1:A:229:PHE:CE1	1:G:229:PHE:CD2	3.09	0.40
1:F:170:GLN:O	1:F:170:GLN:CG	2.70	0.40
1:F:211:THR:O	1:F:215:VAL:CG1	2.60	0.40
1:E:187:TRP:CH2	1:A:191:ARG:HG2	2.57	0.40
1:A:197:GLU:OE1	1:A:197:GLU:CA	2.69	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	75/235 (32%)	72 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	78/235 (33%)	78 (100%)	0	0	100	100
1	C	75/235 (32%)	73 (97%)	1 (1%)	1 (1%)	9	38
1	D	75/235 (32%)	74 (99%)	1 (1%)	0	100	100
1	E	78/235 (33%)	77 (99%)	1 (1%)	0	100	100
1	F	75/235 (32%)	75 (100%)	0	0	100	100
1	G	36/235 (15%)	35 (97%)	1 (3%)	0	100	100
1	H	36/235 (15%)	36 (100%)	0	0	100	100
All	All	528/1880 (28%)	520 (98%)	7 (1%)	1 (0%)	44	72

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	174	GLN

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	74/207 (36%)	67 (90%)	7 (10%)	8	31
1	B	75/207 (36%)	75 (100%)	0	100	100
1	C	74/207 (36%)	66 (89%)	8 (11%)	6	27
1	D	74/207 (36%)	70 (95%)	4 (5%)	20	46
1	E	75/207 (36%)	65 (87%)	10 (13%)	4	20
1	F	74/207 (36%)	66 (89%)	8 (11%)	6	27
1	G	35/207 (17%)	32 (91%)	3 (9%)	10	34
1	H	35/207 (17%)	35 (100%)	0	100	100
All	All	516/1656 (31%)	476 (92%)	40 (8%)	14	37

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	173	GLU
1	D	179	GLN
1	D	180	LYS
1	D	190	GLU
1	F	193	ARG
1	F	209	LEU
1	F	210	GLN
1	F	211	THR
1	F	212	LEU
1	F	215	VAL
1	F	219	VAL
1	F	227	SER
1	E	160	LYS
1	E	168	VAL
1	E	174	GLN
1	E	177	GLN
1	E	182	GLN
1	E	188	ARG
1	E	199	THR
1	E	204	LEU
1	E	210	GLN
1	E	222	MET
1	A	173	GLU
1	A	181	GLU
1	A	193	ARG
1	A	203	VAL
1	A	204	LEU
1	A	208	ILE
1	A	224	HIS
1	C	161	LEU
1	C	180	LYS
1	C	210	GLN
1	C	212	LEU
1	C	225	LEU
1	C	226	LYS
1	C	230	GLU
1	C	232	LYS
1	G	200	ASN
1	G	203	VAL
1	G	208	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	179	GLN
1	F	185	GLN
1	F	224	HIS
1	H	201	GLN
1	E	210	GLN
1	A	179	GLN
1	A	210	GLN
1	C	165	GLN
1	C	185	GLN
1	C	201	GLN
1	B	165	GLN
1	B	174	GLN
1	B	177	GLN
1	B	182	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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	9ED	A	301	-	63,63,67	1.60	11 (17%)	75,78,85	2.25	13 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	9ED	A	301	-	-	29/59/83/88	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	9ED	C63-C62	4.27	1.56	1.31
2	A	301	9ED	C61-C60	4.18	1.55	1.31
2	A	301	9ED	P02-O05	3.78	1.66	1.59
2	A	301	9ED	P01-O04	3.47	1.69	1.59
2	A	301	9ED	C43-C41	-3.31	1.35	1.51
2	A	301	9ED	O19-C32	3.15	1.43	1.34
2	A	301	9ED	O20-C35	3.12	1.42	1.33
2	A	301	9ED	C24-C23	2.59	1.59	1.52
2	A	301	9ED	P01-O10	2.13	1.67	1.59
2	A	301	9ED	C33-C32	2.03	1.56	1.50
2	A	301	9ED	O19-C30	-2.00	1.41	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	9ED	C47-C52-C56	-7.44	78.11	113.86
2	A	301	9ED	O07-C26-C25	-7.10	91.73	109.94
2	A	301	9ED	O07-C26-C23	-7.01	91.96	109.94
2	A	301	9ED	C28-C27-C24	-6.39	99.62	110.83
2	A	301	9ED	C26-C23-C24	-5.67	102.99	110.86
2	A	301	9ED	C36-C34-C33	5.28	132.53	113.13
2	A	301	9ED	O04-C25-C28	3.99	117.19	108.73
2	A	301	9ED	O08-C27-C28	3.94	119.67	110.38
2	A	301	9ED	C25-C26-C23	3.78	116.77	109.11
2	A	301	9ED	O19-C32-C33	3.59	119.26	111.48
2	A	301	9ED	C43-C41-C38	3.28	130.97	114.37
2	A	301	9ED	O20-C35-C37	2.69	120.05	111.83
2	A	301	9ED	C52-C47-C48	2.31	126.05	114.37

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	9ED	C29-O10-P01-O04
2	A	301	9ED	C29-O10-P01-O11
2	A	301	9ED	C24-C23-O05-P02
2	A	301	9ED	C26-C23-O05-P02
2	A	301	9ED	O21-C32-O19-C30
2	A	301	9ED	C38-C41-C43-C46
2	A	301	9ED	C33-C32-O19-C30
2	A	301	9ED	C35-C37-C39-C40
2	A	301	9ED	C53-C49-C50-C3
2	A	301	9ED	C49-C53-C57-C63
2	A	301	9ED	C52-C47-C48-C54
2	A	301	9ED	C44-C45-C51-C62
2	A	301	9ED	C51-C62-C63-C57
2	A	301	9ED	C36-C38-C41-C43
2	A	301	9ED	C37-C39-C40-C42
2	A	301	9ED	C50-C3-C4-C5
2	A	301	9ED	C41-C43-C46-C60
2	A	301	9ED	C47-C48-C54-C58
2	A	301	9ED	C39-C40-C42-C44
2	A	301	9ED	C4-C3-C50-C49
2	A	301	9ED	C48-C54-C58-C1
2	A	301	9ED	C42-C44-C45-C51
2	A	301	9ED	C3-C4-C5-C6
2	A	301	9ED	C29-O10-P01-O16
2	A	301	9ED	C37-C35-O20-C31
2	A	301	9ED	O22-C35-O20-C31
2	A	301	9ED	C50-C49-C53-C57
2	A	301	9ED	C34-C36-C38-C41
2	A	301	9ED	C33-C34-C36-C38

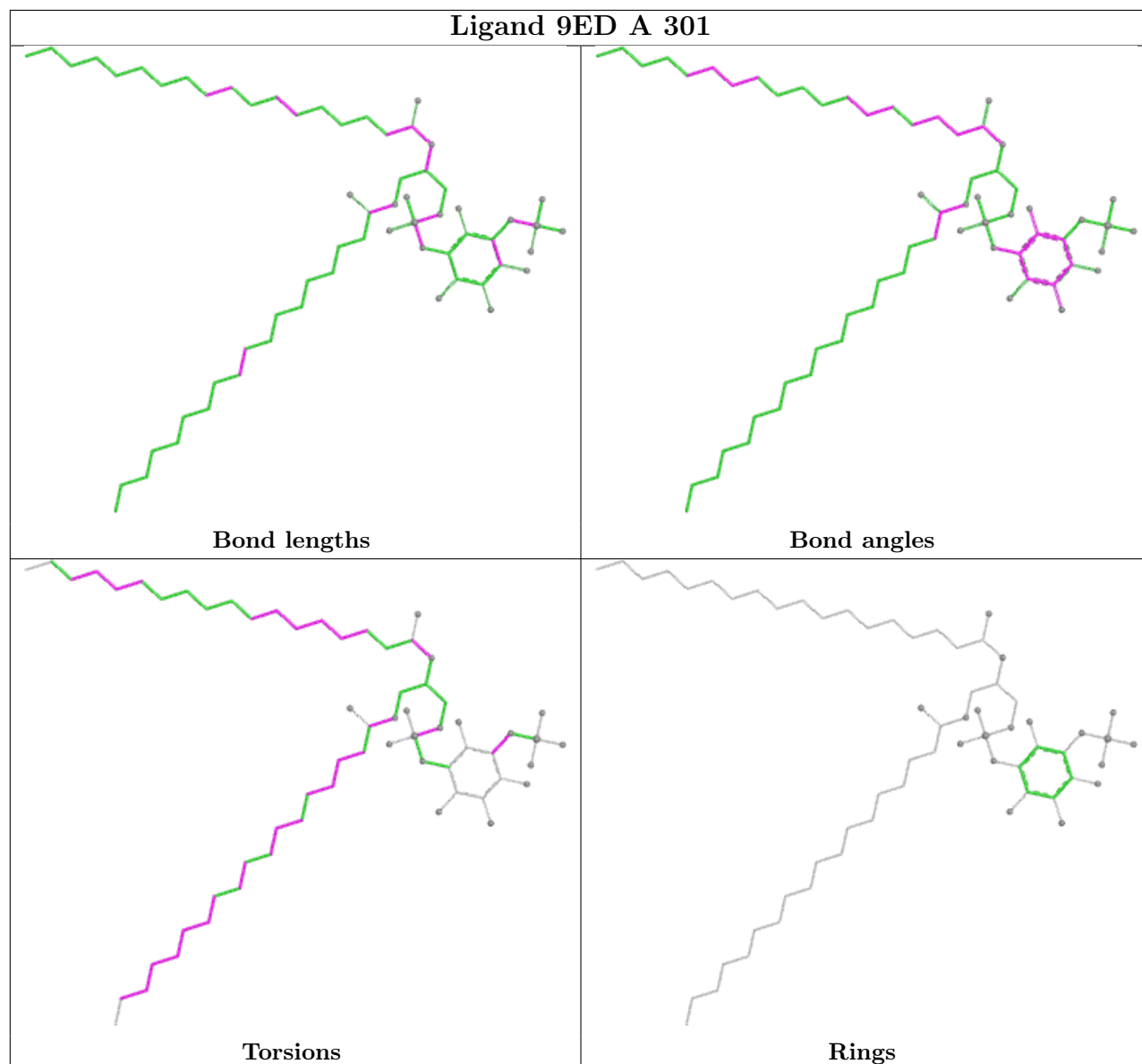
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	9ED	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

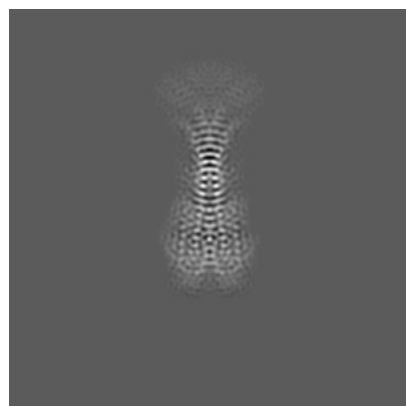
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45634. These allow visual inspection of the internal detail of the map and identification of artifacts.

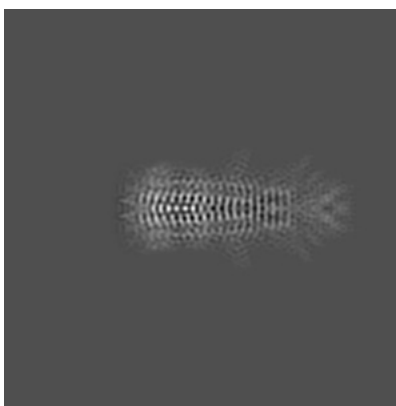
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

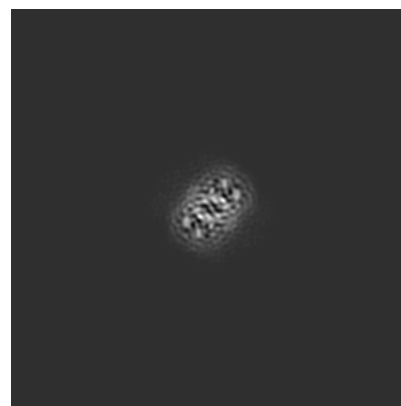
6.1.1 Primary map



X

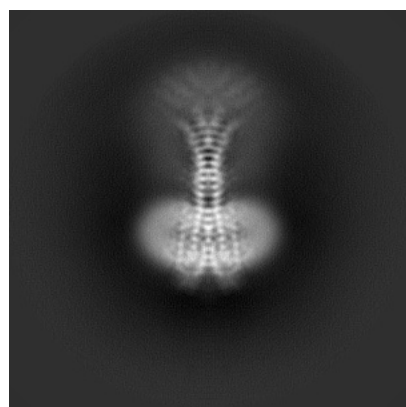


Y

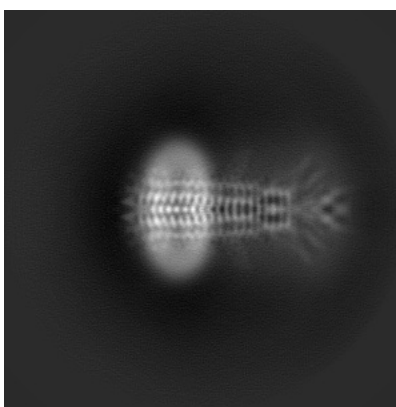


Z

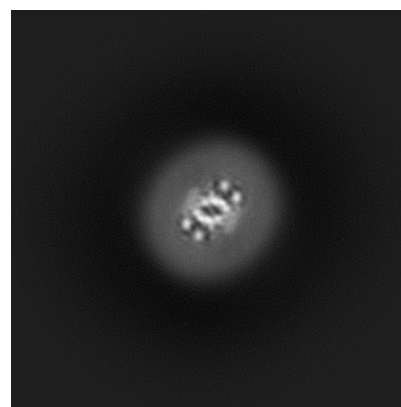
6.1.2 Raw map



X



Y

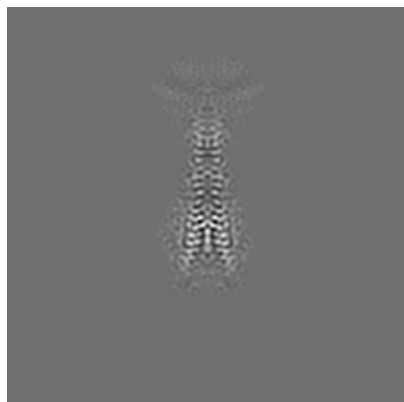


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 160

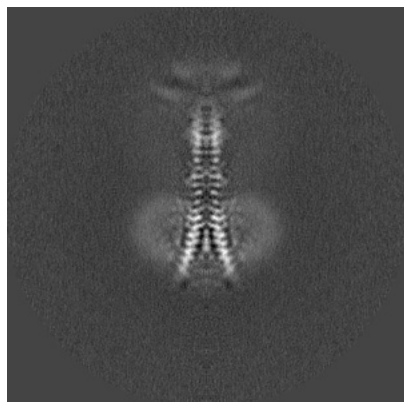


Y Index: 160

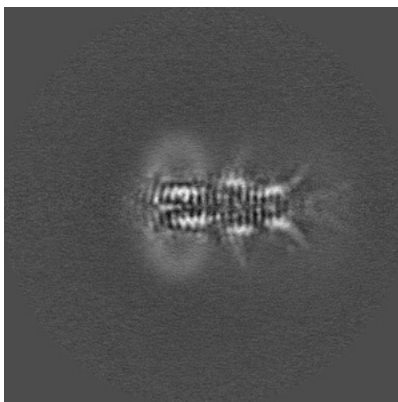


Z Index: 160

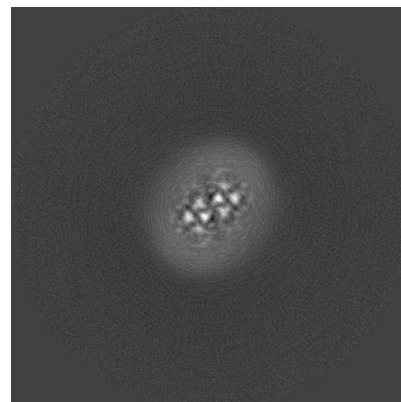
6.2.2 Raw map



X Index: 160



Y Index: 160

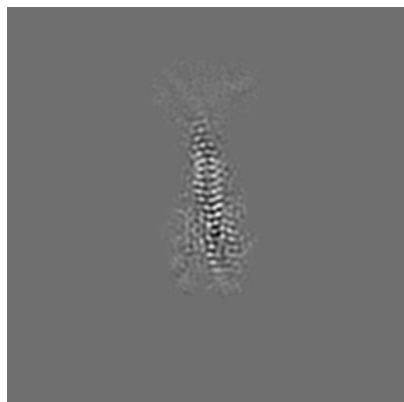


Z Index: 160

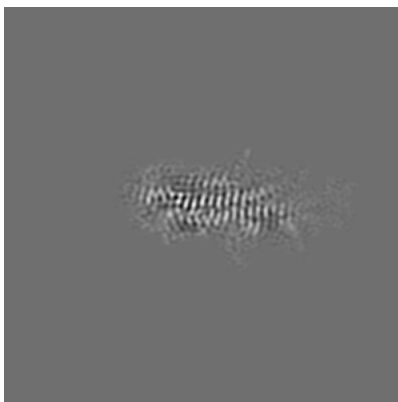
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 166

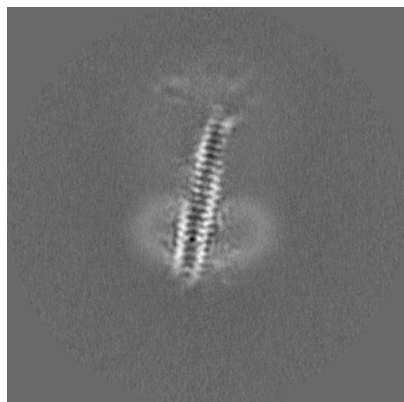


Y Index: 165

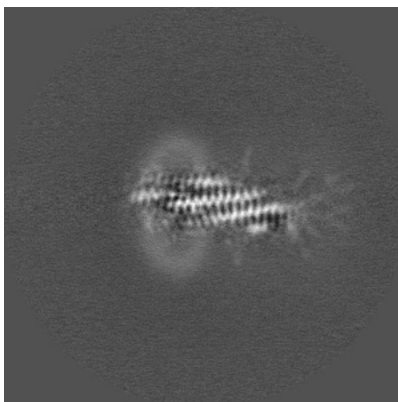


Z Index: 138

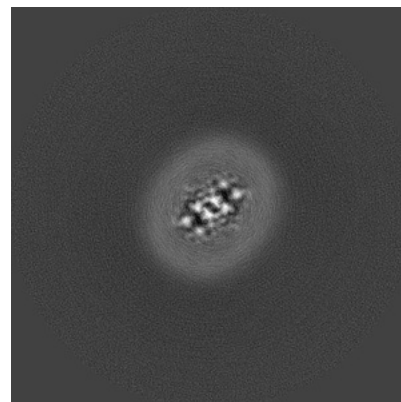
6.3.2 Raw map



X Index: 150



Y Index: 166

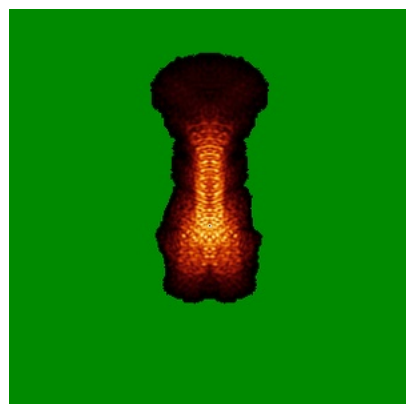


Z Index: 152

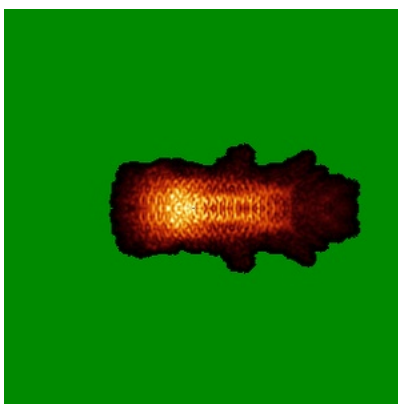
The images above show the largest variance slices of the map in three orthogonal directions.

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

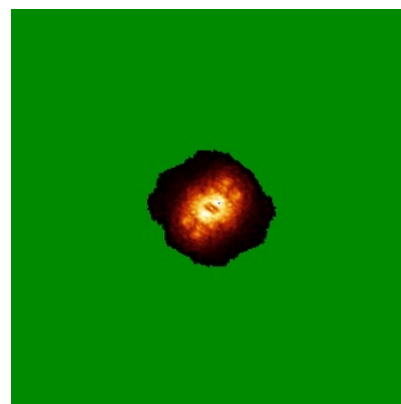
6.4.1 Primary map



X

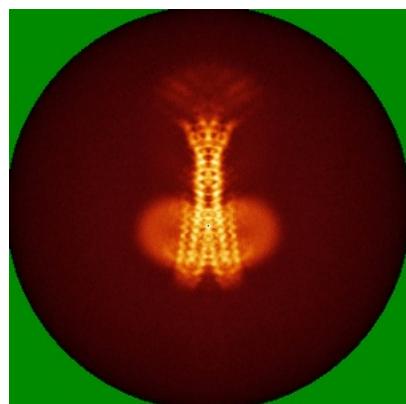


Y

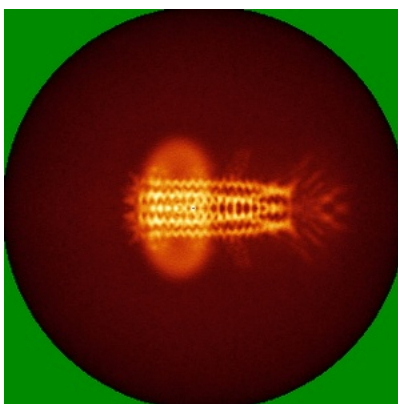


Z

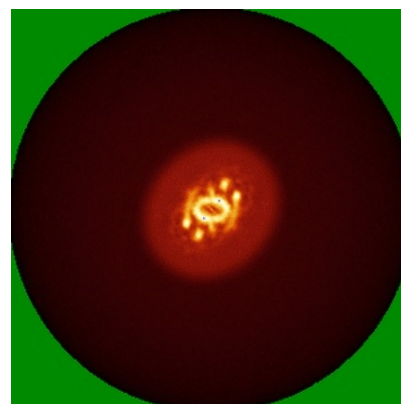
6.4.2 Raw map



X



Y

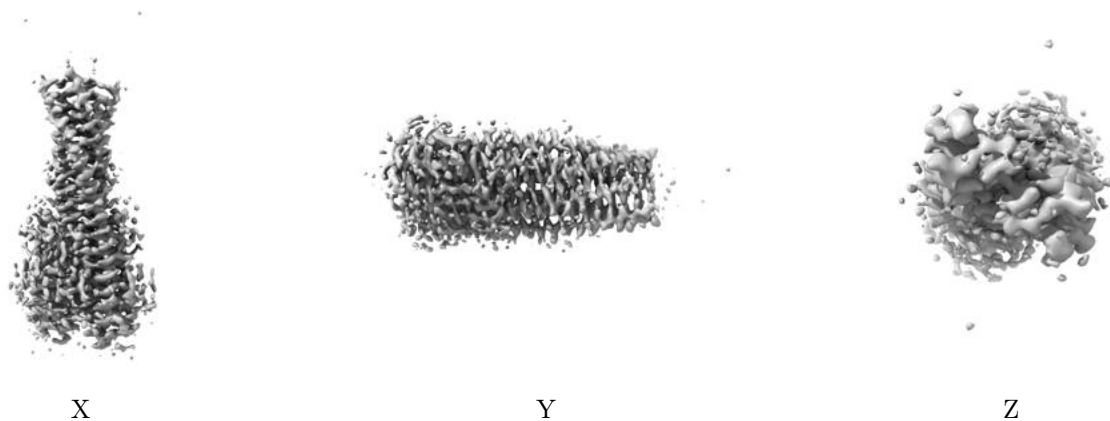


Z

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.

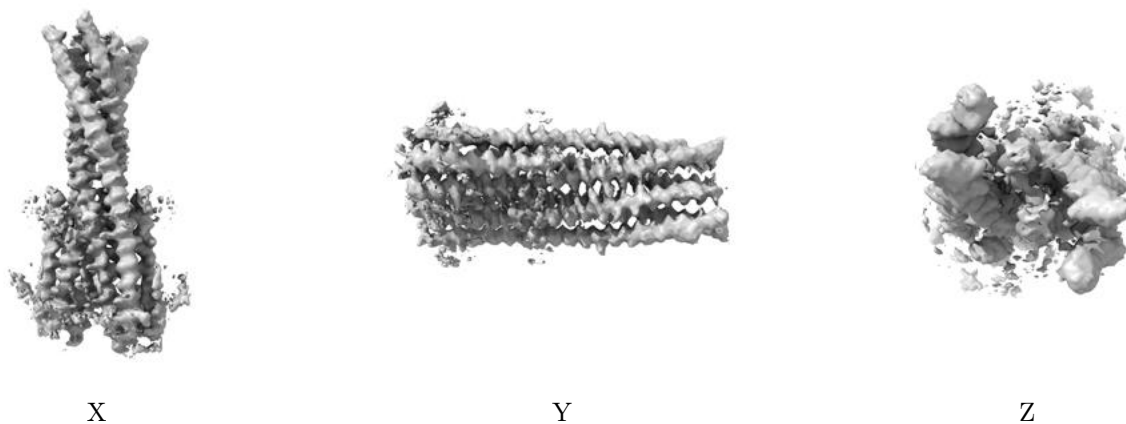
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. 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.

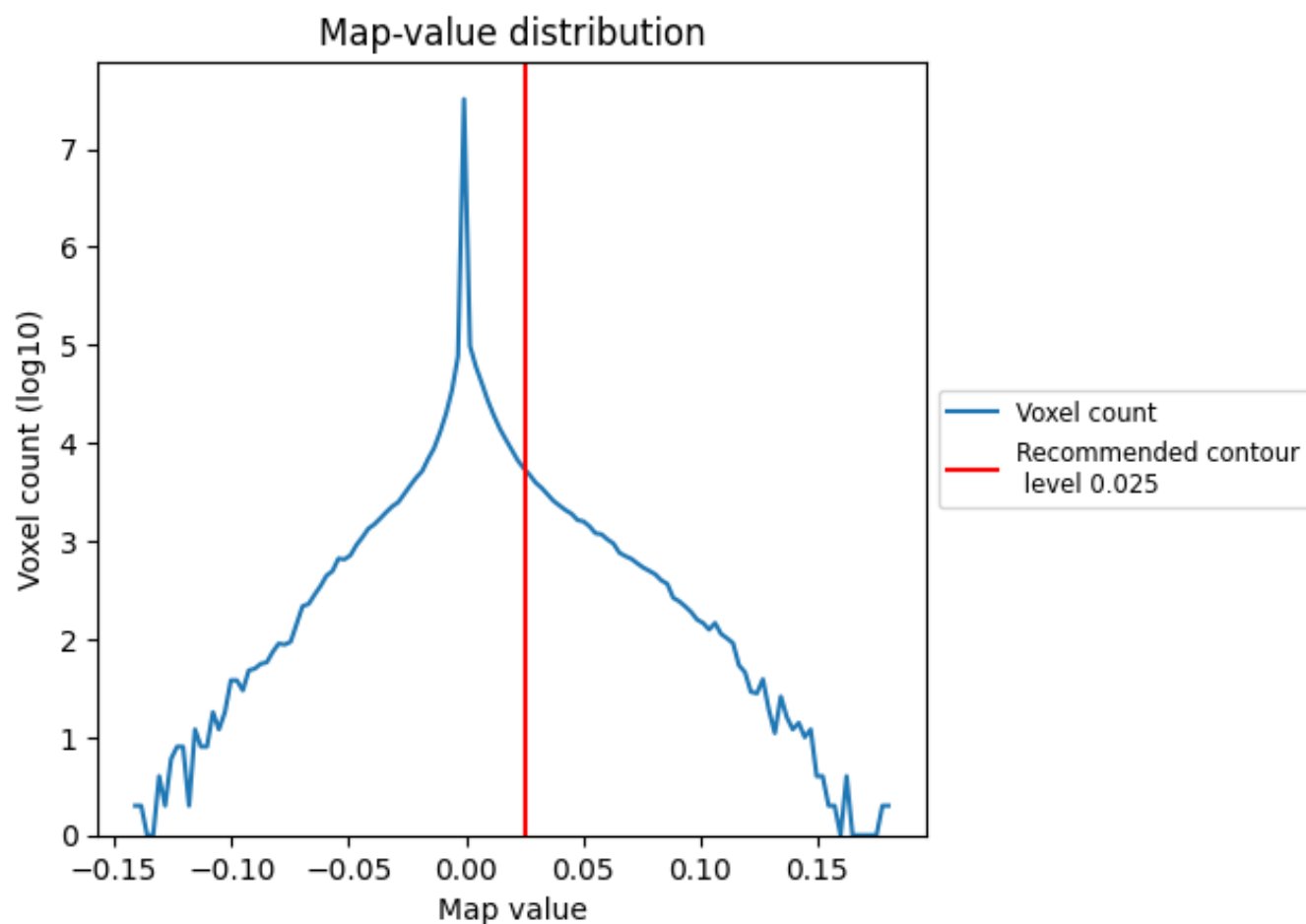
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

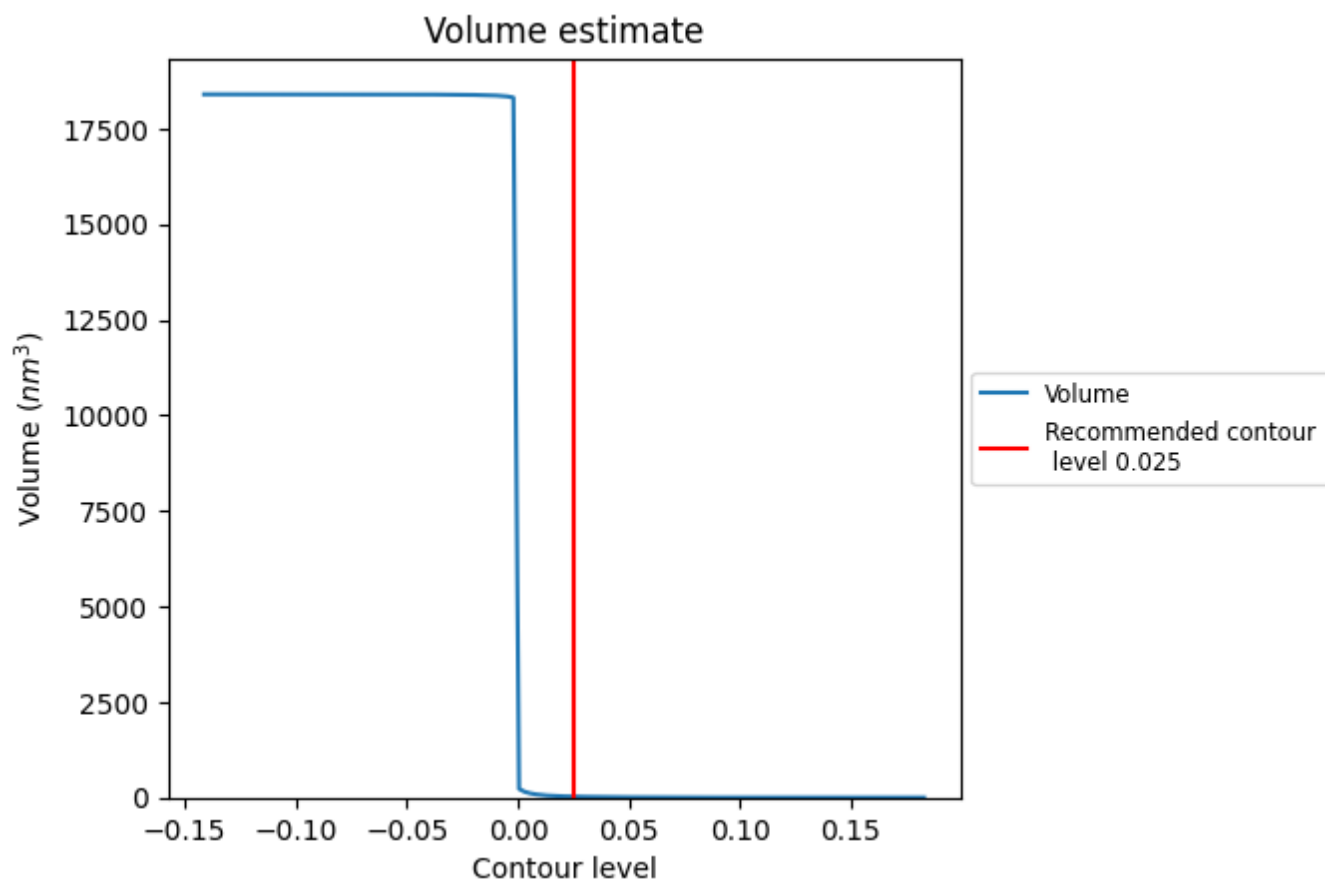
This section contains the results of statistical analysis of the map.

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.

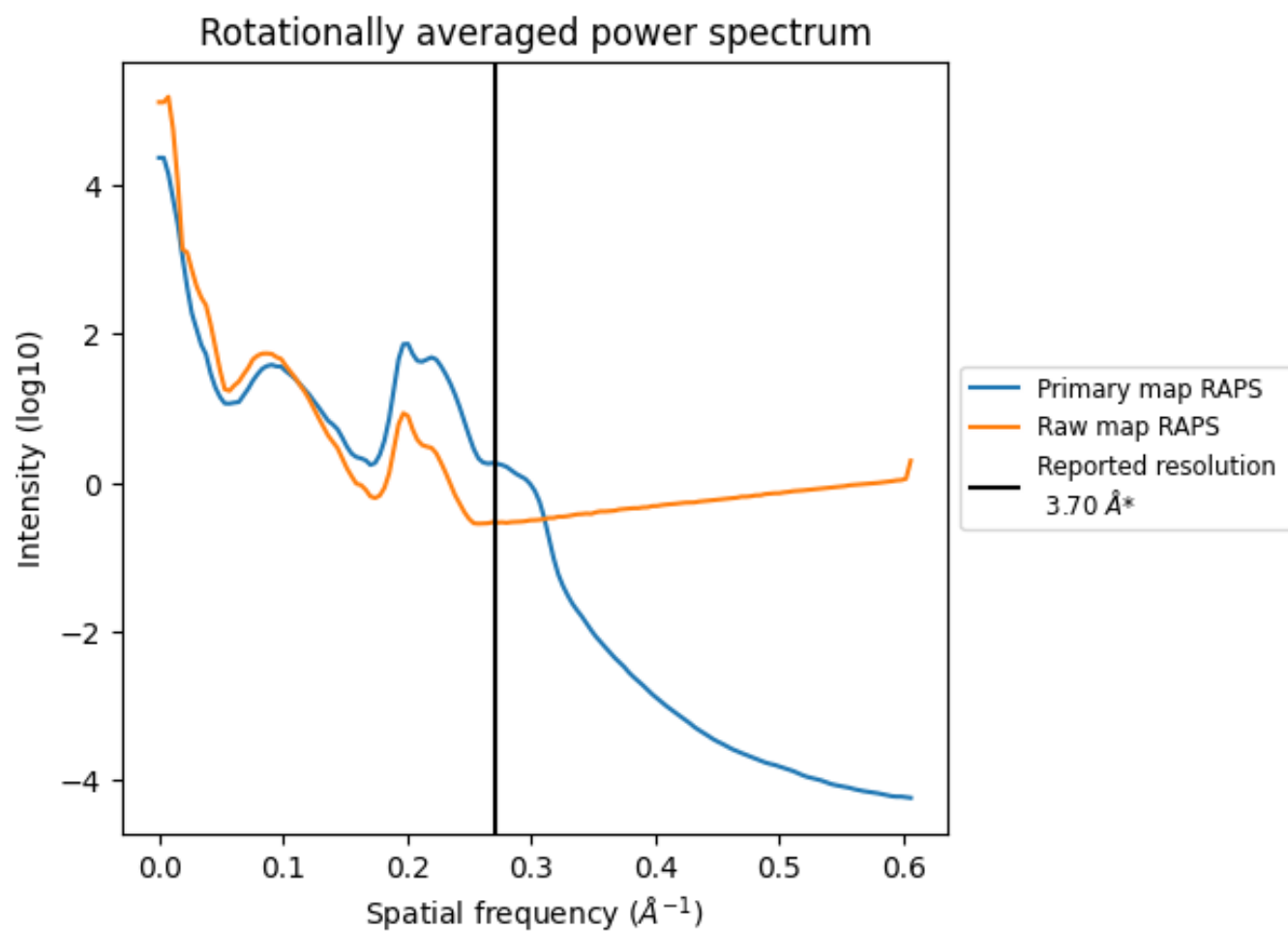
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 25 nm³; this corresponds to an approximate mass of 23 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 ⓘ

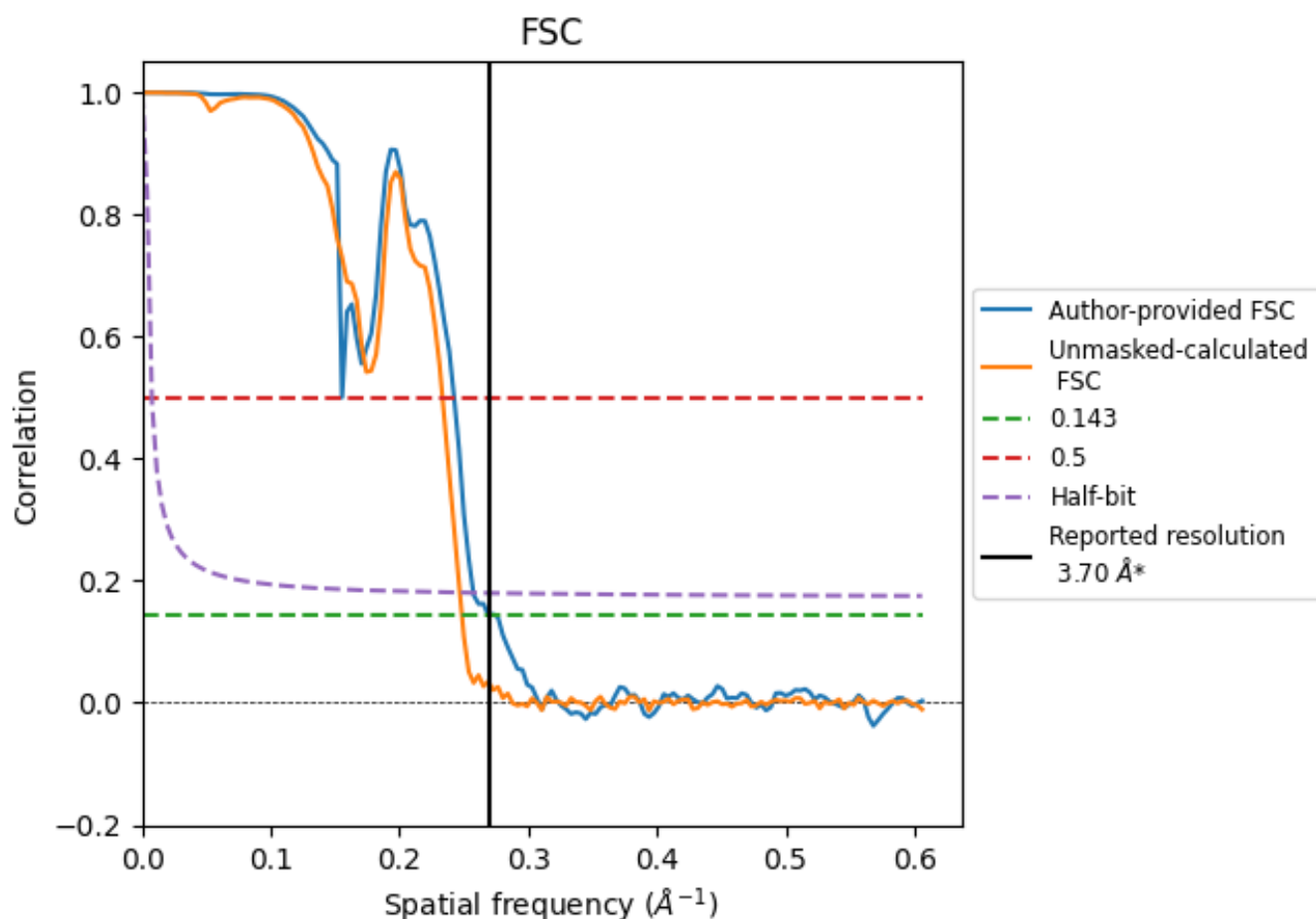


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

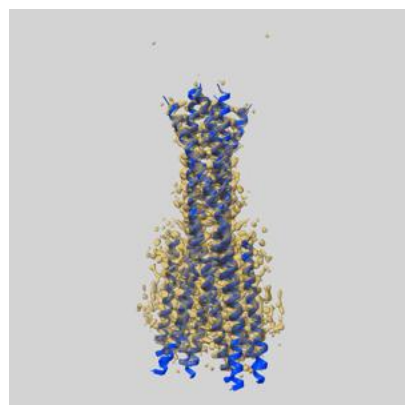
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.64	4.13	3.89
Unmasked-calculated*	4.02	4.29	4.05

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

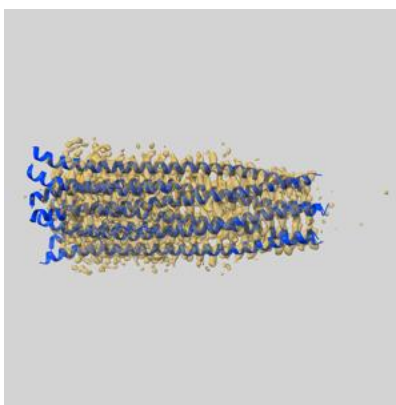
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-45634 and PDB model 9CJK. Per-residue inclusion information can be found in section [3](#) on page [6](#).

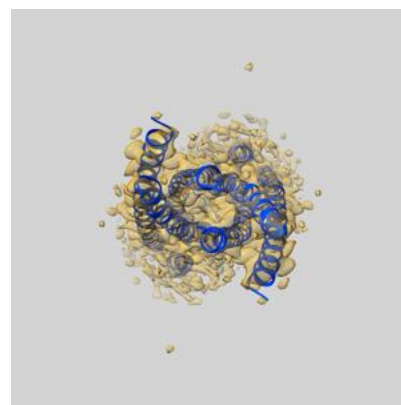
9.1 Map-model overlay [i](#)



X



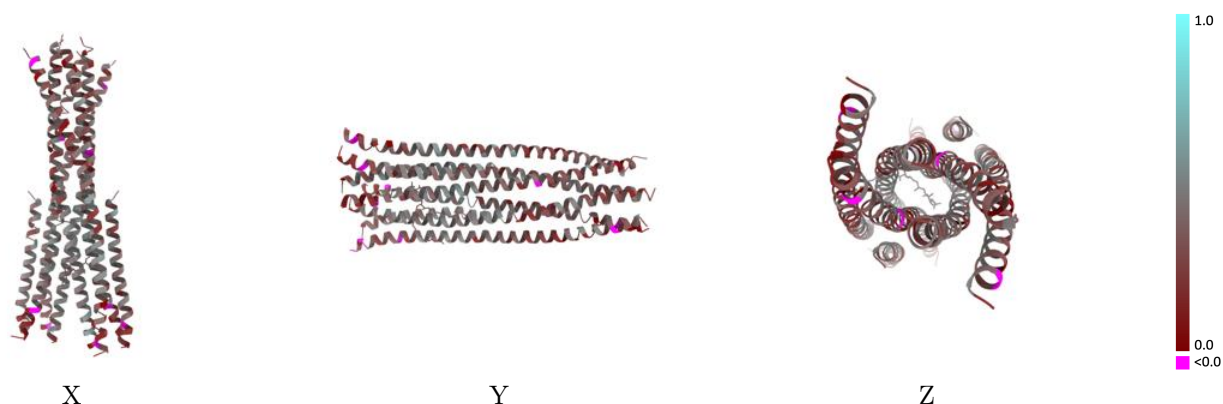
Y



Z

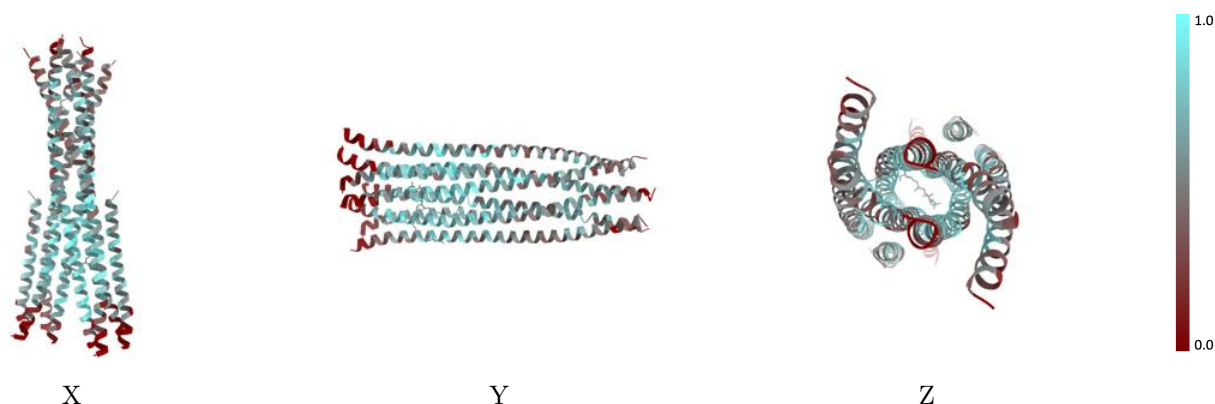
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



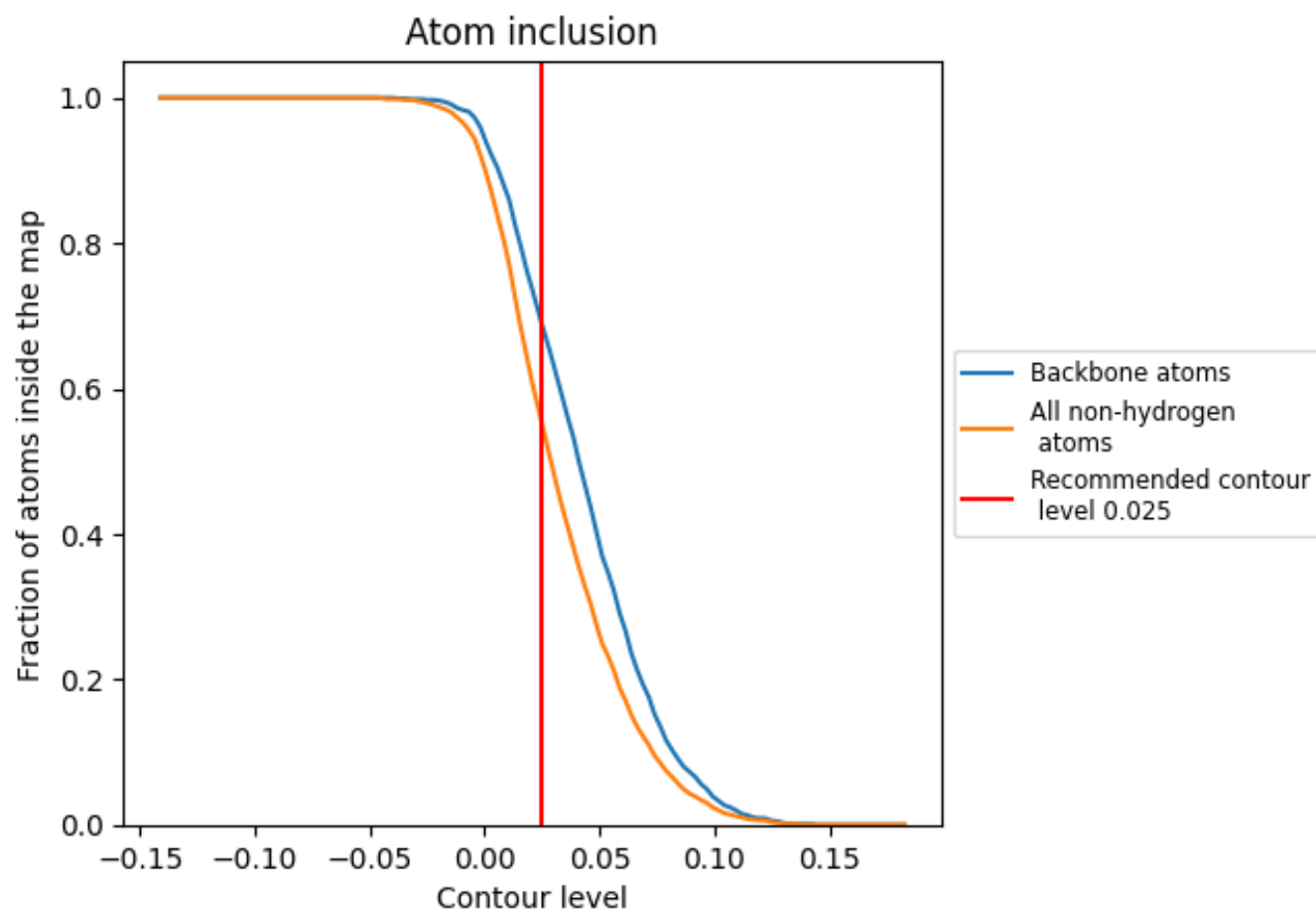
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 55% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5510	0.3440
A	0.5620	0.3200
B	0.6050	0.3870
C	0.4820	0.2850
D	0.5770	0.3390
E	0.6360	0.3940
F	0.4950	0.3290
G	0.4970	0.3520
H	0.4900	0.3520

1.0

0.0

<0.0