



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 10:05 PM UTC

PDB ID : 6N2P / pdb_00006n2p
EMDB ID : EMD-9332
Title : Helical assembly of the CARD9 CARD
Authors : Holliday, M.J.; Rohou, A.; Arthur, C.P.; Dueber, E.C.; Fairbrother, W.J.
Deposited on : 2018-11-13
Resolution : 4.00 Å(reported)
Based on initial model : 6E26

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

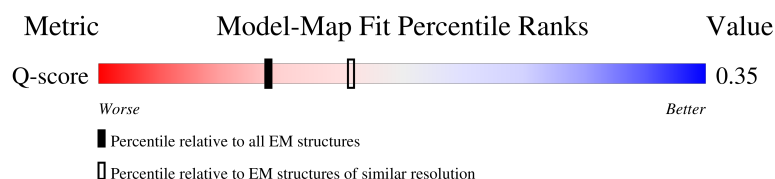
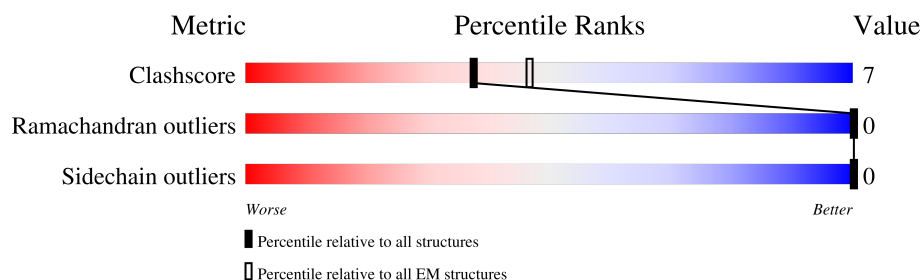
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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	7587 (3.50 - 4.50)

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	152	15% 45% 12% 42%
1	B	152	14% 46% 12% 42%
1	C	152	17% 46% 12% 42%
1	D	152	16% 47% 11% 42%

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Mol	Chain	Length	Quality of chain
1	E	152	
1	F	152	
1	G	152	
1	H	152	
1	I	152	
1	J	152	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14570 atoms, of which 7380 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 Caspase recruitment domain-containing protein 9.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	88	Total	C	H	N	O	S	0	0
			1457	463	738	121	133	2		
1	B	88	Total	C	H	N	O	S	0	0
			1457	463	738	121	133	2		
1	C	88	Total	C	H	N	O	S	0	0
			1457	463	738	121	133	2		
1	D	88	Total	C	H	N	O	S	0	0
			1457	463	738	121	133	2		
1	E	88	Total	C	H	N	O	S	0	0
			1457	463	738	121	133	2		
1	F	88	Total	C	H	N	O	S	0	0
			1457	463	738	121	133	2		
1	G	88	Total	C	H	N	O	S	0	0
			1457	463	738	121	133	2		
1	H	88	Total	C	H	N	O	S	0	0
			1457	463	738	121	133	2		
1	I	88	Total	C	H	N	O	S	0	0
			1457	463	738	121	133	2		
1	J	88	Total	C	H	N	O	S	0	0
			1457	463	738	121	133	2		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q9H257
A	107	GLU	ILE	engineered mutation	UNP Q9H257
B	1	GLY	-	expression tag	UNP Q9H257
B	107	GLU	ILE	engineered mutation	UNP Q9H257
C	1	GLY	-	expression tag	UNP Q9H257
C	107	GLU	ILE	engineered mutation	UNP Q9H257
D	1	GLY	-	expression tag	UNP Q9H257
D	107	GLU	ILE	engineered mutation	UNP Q9H257
E	1	GLY	-	expression tag	UNP Q9H257
E	107	GLU	ILE	engineered mutation	UNP Q9H257

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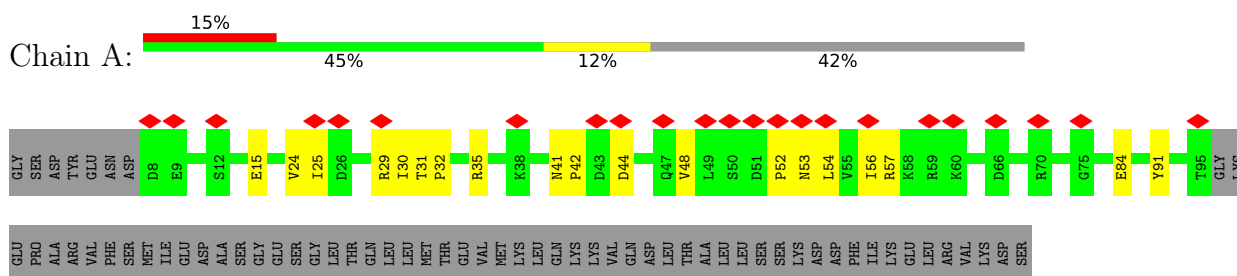
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Chain	Residue	Modelled	Actual	Comment	Reference
F	1	GLY	-	expression tag	UNP Q9H257
F	107	GLU	ILE	engineered mutation	UNP Q9H257
G	1	GLY	-	expression tag	UNP Q9H257
G	107	GLU	ILE	engineered mutation	UNP Q9H257
H	1	GLY	-	expression tag	UNP Q9H257
H	107	GLU	ILE	engineered mutation	UNP Q9H257
I	1	GLY	-	expression tag	UNP Q9H257
I	107	GLU	ILE	engineered mutation	UNP Q9H257
J	1	GLY	-	expression tag	UNP Q9H257
J	107	GLU	ILE	engineered mutation	UNP Q9H257

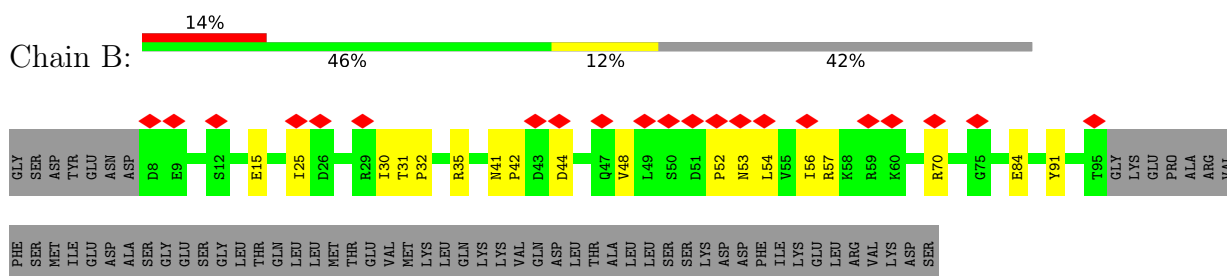
3 Residue-property plots [i](#)

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.

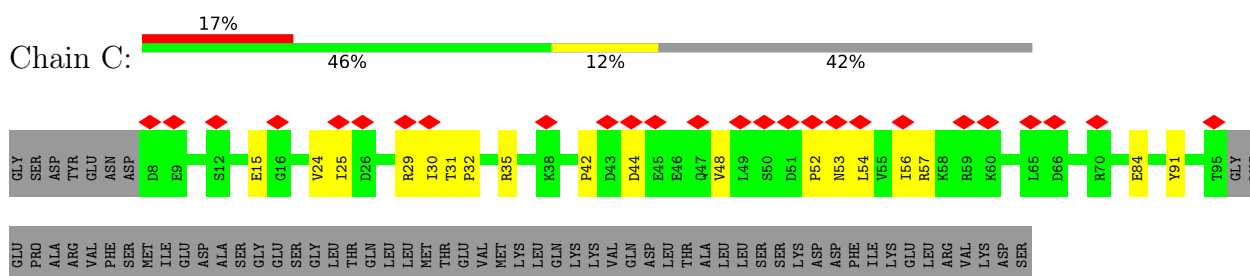
- Molecule 1: Caspase recruitment domain-containing protein 9



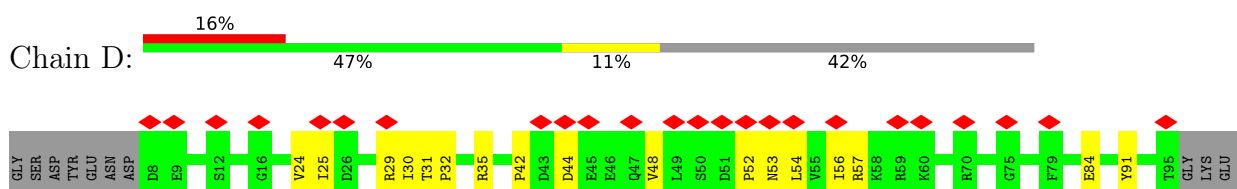
- Molecule 1: Caspase recruitment domain-containing protein 9



- Molecule 1: Caspase recruitment domain-containing protein 9



- Molecule 1: Caspase recruitment domain-containing protein 9



ALA ARG VAL PHE SER MET ILE GLU ASP ALA SER GLY SER GLY LEU THR GLN LEU LEU MET THR GLU VAL MET LYS LEU GLN LYS LYS VAL GLN ASP LEU THR ALA LEU LEU SER SER LYS ASP ASP PHE ILE LYS LYS LEU ARG VAL LYS ASP SER

• Molecule 1: Caspase recruitment domain-containing protein 9



GLY SER ASP TYR GLU ASN ASP D8 E9 S12 I25 D26 R29 I30 T31 P32 R35 P42 D43 D44 E45 E46 Q47 V48 L49 S50 D51 P52 N53 L54 V55 I56 R57 K58 R59 K60 L65 R70 G75 F79 E84 Y91 K92 K93 V94 T95 GLY LYS GLU

• Molecule 1: Caspase recruitment domain-containing protein 9



GLY SER ASP TYR GLU ASN ASP D8 E9 S12 G16 V24 I25 D26 R29 I30 T31 P32 R35 K38 P42 D43 D44 E45 E46 Q47 V48 L49 S50 D51 P52 N53 L54 V55 I56 R57 K58 R59 K60 D66 R70 G75 F79 E84 Y91 K92 K93

• Molecule 1: Caspase recruitment domain-containing protein 9



GLY SER ASP TYR GLU ASN ASP D8 E9 S12 E15 I25 D26 R29 I30 T31 P32 R35 K38 N41 P42 D43 D44 E45 E46 Q47 V48 L49 S50 D51 P52 N53 L54 V55 I56 R57 K58 R59 K60 R70 G75 E84 Y91 T95 GLY LYS GLU PRO

• Molecule 1: Caspase recruitment domain-containing protein 9



GLY SER ASP TYR GLU ASN ASP D8 E9 S12 E15 I25 D26 R29 I30 T31 P32 R35 K38 N41 P42 D43 D44 E45 E46 Q47 V48 L49 S50 D51 P52 N53 L54 V55 I56 R57 K58 R59 K60 D66 R70 G75 E84 Y91 T95 GLY LYS

• Molecule 1: Caspase recruitment domain-containing protein 9



GLY SER ASP TYR GLU ASN ASP D8 E9 S12 E15 I25 D26 R29 I30 T31 P32 R35 K38 P42 D43 D44 Q47 V48 L49 S50 D51 P52 N53 L54 V55 I56 R57 K58 R59 K60 R70 G75 E84 Y91 T95 GLY LYS GLU PRO ALA ARG

VAL	PHE	SER	MET	ILE	GLU	ASP	ALA	SER	GLY	GLU	SER	GLY	LEU	THR	GLN	LEU	MET	THR	GLU	VAL	MET	LYS	LEU	GLN	LYS	VAL	GLN	ASP	LEU	THR	ALA	LEU	LEU	SER	SER	LYS	ASP	ASP	PHE	ILE	LYS	GLU	LEU	ARG	VAL	LYS	ASP	SER
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● Molecule 1: Caspase recruitment domain-containing protein 9



GLY	SER	ASP	TYR	GLU	ASN	ASP	D8	E9	S12	E15	I25	D26	R29	I30	T31	P32	R35	K38	M41	P42	D43	D44	E45	E46	Q47	V48	L49	S50	D51	P52	N53	L54	V55	I56	R57	K58	R59	R70	G75	E84	Y91	T95	GLY	LYS	GLU	PRO	ALA
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ARG	VAL	PHE	SER	ILE	GLU	ASP	ALA	SER	GLY	GLU	SER	GLY	LEU	THR	GLN	LEU	LEU	MET	THR	GLU	VAL	MET	LYS	LEU	GLN	LYS	LYS	VAL	GLN	ASP	LEU	THR	ALA	LEU	LEU	SER	SER	LYS	ASP	ASP	PHE	ILE	LYS	GLU	LEU	ARG	VAL	LYS	ASP	SER
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4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-101.6°, rise=5.11 Å, axial sym=C1	Depositor
Number of segments used	31908	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 ($e^-/\text{Å}^2$)	50.9	Depositor
Minimum defocus (nm)	1250	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.061	Depositor
Minimum map value	-0.014	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.033	Depositor
Map size (Å)	325.5, 325.5, 325.5	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.085, 1.085, 1.085	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.36	0/733	0.49	0/995
1	B	0.36	0/733	0.49	0/995
1	C	0.36	0/733	0.49	0/995
1	D	0.36	0/733	0.49	0/995
1	E	0.36	0/733	0.49	0/995
1	F	0.36	0/733	0.49	0/995
1	G	0.36	0/733	0.49	0/995
1	H	0.36	0/733	0.49	0/995
1	I	0.36	0/733	0.49	0/995
1	J	0.36	0/733	0.49	0/995
All	All	0.36	0/7330	0.49	0/9950

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	719	738	738	17	0
1	B	719	738	738	14	0
1	C	719	738	738	15	0
1	D	719	738	738	14	0
1	E	719	738	738	13	0
1	F	719	738	738	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	719	738	738	15	0
1	H	719	738	738	14	0
1	I	719	738	738	11	0
1	J	719	738	738	13	0
All	All	7190	7380	7380	109	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 (109) 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:B:15:GLU:OE2	1:E:35:ARG:NE	2.20	0.75
1:A:15:GLU:OE2	1:D:35:ARG:NE	2.22	0.72
1:B:35:ARG:NE	1:H:15:GLU:OE2	2.23	0.72
1:D:53:ASN:ND2	1:E:52:PRO:O	2.24	0.69
1:C:15:GLU:OE2	1:F:35:ARG:NE	2.26	0.69
1:E:53:ASN:ND2	1:F:52:PRO:O	2.27	0.67
1:C:35:ARG:NE	1:G:15:GLU:OE2	2.29	0.65
1:A:53:ASN:ND2	1:B:52:PRO:O	2.29	0.64
1:A:35:ARG:NE	1:I:15:GLU:OE2	2.31	0.64
1:G:35:ARG:NE	1:J:15:GLU:OE2	2.30	0.64
1:H:52:PRO:O	1:I:53:ASN:ND2	2.30	0.64
1:G:52:PRO:O	1:H:53:ASN:ND2	2.32	0.62
1:A:52:PRO:O	1:G:53:ASN:ND2	2.34	0.60
1:B:53:ASN:ND2	1:C:52:PRO:O	2.34	0.59
1:C:53:ASN:ND2	1:D:52:PRO:O	2.35	0.59
1:E:57:ARG:O	1:E:57:ARG:HD2	2.09	0.53
1:A:57:ARG:O	1:A:57:ARG:HD2	2.09	0.53
1:G:57:ARG:O	1:G:57:ARG:HD2	2.09	0.53
1:J:57:ARG:O	1:J:57:ARG:HD2	2.09	0.53
1:B:57:ARG:O	1:B:57:ARG:HD2	2.09	0.53
1:F:57:ARG:O	1:F:57:ARG:HD2	2.09	0.53
1:H:57:ARG:O	1:H:57:ARG:HD2	2.09	0.53
1:I:52:PRO:O	1:J:53:ASN:ND2	2.42	0.52
1:C:57:ARG:O	1:C:57:ARG:HD2	2.09	0.52
1:I:57:ARG:O	1:I:57:ARG:HD2	2.09	0.52
1:D:57:ARG:HD2	1:D:57:ARG:O	2.09	0.52
1:D:29:ARG:NH1	1:G:41:ASN:OD1	2.42	0.52
1:E:31:THR:HB	1:E:32:PRO:HD3	1.93	0.51
1:A:31:THR:HB	1:A:32:PRO:HD3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:THR:HB	1:D:32:PRO:HD3	1.93	0.51
1:J:31:THR:HB	1:J:32:PRO:HD3	1.93	0.51
1:I:31:THR:HB	1:I:32:PRO:HD3	1.93	0.50
1:B:31:THR:HB	1:B:32:PRO:HD3	1.93	0.50
1:G:31:THR:HB	1:G:32:PRO:HD3	1.93	0.50
1:C:29:ARG:NH1	1:H:41:ASN:OD1	2.45	0.50
1:C:31:THR:HB	1:C:32:PRO:HD3	1.93	0.50
1:F:31:THR:HB	1:F:32:PRO:HD3	1.93	0.49
1:H:31:THR:HB	1:H:32:PRO:HD3	1.93	0.49
1:A:29:ARG:NH1	1:J:41:ASN:OD1	2.47	0.48
1:D:29:ARG:NH2	1:G:41:ASN:HB2	2.29	0.47
1:C:56:ILE:HG22	1:C:56:ILE:O	2.15	0.47
1:H:56:ILE:O	1:H:56:ILE:HG22	2.15	0.47
1:I:56:ILE:HG22	1:I:56:ILE:O	2.15	0.46
1:E:56:ILE:HG22	1:E:56:ILE:O	2.15	0.46
1:A:54:LEU:H	1:A:54:LEU:HD23	1.81	0.46
1:B:56:ILE:HG22	1:B:56:ILE:O	2.15	0.46
1:J:56:ILE:HG22	1:J:56:ILE:O	2.15	0.46
1:A:56:ILE:HG22	1:A:56:ILE:O	2.15	0.46
1:J:54:LEU:HD23	1:J:54:LEU:H	1.81	0.46
1:A:29:ARG:NH2	1:J:41:ASN:HB2	2.31	0.45
1:F:56:ILE:HG22	1:F:56:ILE:O	2.15	0.45
1:D:56:ILE:O	1:D:56:ILE:HG22	2.15	0.45
1:G:54:LEU:H	1:G:54:LEU:HD23	1.81	0.45
1:I:54:LEU:H	1:I:54:LEU:HD23	1.81	0.45
1:D:54:LEU:H	1:D:54:LEU:HD23	1.81	0.45
1:H:54:LEU:H	1:H:54:LEU:HD23	1.81	0.45
1:A:41:ASN:OD1	1:E:29:ARG:NH1	2.50	0.44
1:E:54:LEU:H	1:E:54:LEU:HD23	1.81	0.44
1:G:56:ILE:HG22	1:G:56:ILE:O	2.15	0.44
1:J:84:GLU:HB3	1:J:91:TYR:CD1	2.53	0.44
1:F:54:LEU:HD23	1:F:54:LEU:H	1.81	0.44
1:H:84:GLU:HB3	1:H:91:TYR:CD1	2.53	0.44
1:F:84:GLU:HB3	1:F:91:TYR:CD1	2.53	0.44
1:G:84:GLU:HB3	1:G:91:TYR:CD1	2.53	0.44
1:B:54:LEU:HD23	1:B:54:LEU:H	1.81	0.44
1:A:84:GLU:HB3	1:A:91:TYR:CD1	2.53	0.44
1:C:54:LEU:HD23	1:C:54:LEU:H	1.81	0.44
1:B:84:GLU:HB3	1:B:91:TYR:CD1	2.53	0.44
1:E:84:GLU:HB3	1:E:91:TYR:CD1	2.53	0.43
1:I:84:GLU:HB3	1:I:91:TYR:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:GLU:HB3	1:C:91:TYR:CD1	2.53	0.43
1:D:84:GLU:HB3	1:D:91:TYR:CD1	2.53	0.43
1:C:29:ARG:NH2	1:H:41:ASN:HB2	2.34	0.42
1:D:24:VAL:O	1:G:70:ARG:HD2	2.19	0.42
1:B:25:ILE:HD11	1:B:30:ILE:HG13	2.02	0.42
1:E:25:ILE:HD11	1:E:30:ILE:HG13	2.02	0.42
1:C:35:ARG:NH2	1:C:42:PRO:HG3	2.35	0.42
1:A:41:ASN:HB2	1:E:29:ARG:NH2	2.35	0.42
1:F:35:ARG:NH2	1:F:42:PRO:HG3	2.35	0.42
1:H:25:ILE:HD11	1:H:30:ILE:HG13	2.02	0.42
1:B:35:ARG:NH2	1:B:42:PRO:HG3	2.35	0.42
1:I:25:ILE:HD11	1:I:30:ILE:HG13	2.02	0.42
1:J:35:ARG:NH2	1:J:42:PRO:HG3	2.35	0.42
1:A:35:ARG:NH2	1:A:42:PRO:HG3	2.35	0.42
1:C:44:ASP:O	1:C:48:VAL:HG23	2.20	0.42
1:D:44:ASP:O	1:D:48:VAL:HG23	2.20	0.42
1:F:25:ILE:HD11	1:F:30:ILE:HG13	2.02	0.42
1:H:35:ARG:NH2	1:H:42:PRO:HG3	2.35	0.42
1:J:44:ASP:O	1:J:48:VAL:HG23	2.20	0.42
1:A:25:ILE:HD11	1:A:30:ILE:HG13	2.02	0.41
1:D:35:ARG:NH2	1:D:42:PRO:HG3	2.35	0.41
1:E:35:ARG:NH2	1:E:42:PRO:HG3	2.35	0.41
1:A:24:VAL:O	1:J:70:ARG:HD2	2.21	0.41
1:A:44:ASP:O	1:A:48:VAL:HG23	2.20	0.41
1:C:25:ILE:HD11	1:C:30:ILE:HG13	2.02	0.41
1:H:44:ASP:O	1:H:48:VAL:HG23	2.20	0.41
1:B:70:ARG:HD2	1:F:24:VAL:O	2.21	0.41
1:G:44:ASP:O	1:G:48:VAL:HG23	2.20	0.41
1:B:44:ASP:O	1:B:48:VAL:HG23	2.20	0.41
1:G:35:ARG:NH2	1:G:42:PRO:HG3	2.35	0.41
1:I:35:ARG:NH2	1:I:42:PRO:HG3	2.35	0.41
1:B:41:ASN:OD1	1:F:29:ARG:NH1	2.53	0.41
1:D:25:ILE:HD11	1:D:30:ILE:HG13	2.02	0.41
1:E:44:ASP:O	1:E:48:VAL:HG23	2.20	0.41
1:F:44:ASP:O	1:F:48:VAL:HG23	2.20	0.41
1:I:44:ASP:O	1:I:48:VAL:HG23	2.20	0.41
1:G:25:ILE:HD11	1:G:30:ILE:HG13	2.02	0.41
1:J:25:ILE:HD11	1:J:30:ILE:HG13	2.02	0.41
1:C:24:VAL:O	1:H:70:ARG:HD2	2.21	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	86/152 (57%)	75 (87%)	11 (13%)	0	100	100
1	B	86/152 (57%)	75 (87%)	11 (13%)	0	100	100
1	C	86/152 (57%)	75 (87%)	11 (13%)	0	100	100
1	D	86/152 (57%)	75 (87%)	11 (13%)	0	100	100
1	E	86/152 (57%)	75 (87%)	11 (13%)	0	100	100
1	F	86/152 (57%)	75 (87%)	11 (13%)	0	100	100
1	G	86/152 (57%)	75 (87%)	11 (13%)	0	100	100
1	H	86/152 (57%)	75 (87%)	11 (13%)	0	100	100
1	I	86/152 (57%)	75 (87%)	11 (13%)	0	100	100
1	J	86/152 (57%)	75 (87%)	11 (13%)	0	100	100
All	All	860/1520 (57%)	750 (87%)	110 (13%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	83/140 (59%)	83 (100%)	0	100	100
1	B	83/140 (59%)	83 (100%)	0	100	100
1	C	83/140 (59%)	83 (100%)	0	100	100
1	D	83/140 (59%)	83 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	83/140 (59%)	83 (100%)	0	100	100
1	F	83/140 (59%)	83 (100%)	0	100	100
1	G	83/140 (59%)	83 (100%)	0	100	100
1	H	83/140 (59%)	83 (100%)	0	100	100
1	I	83/140 (59%)	83 (100%)	0	100	100
1	J	83/140 (59%)	83 (100%)	0	100	100
All	All	830/1400 (59%)	830 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

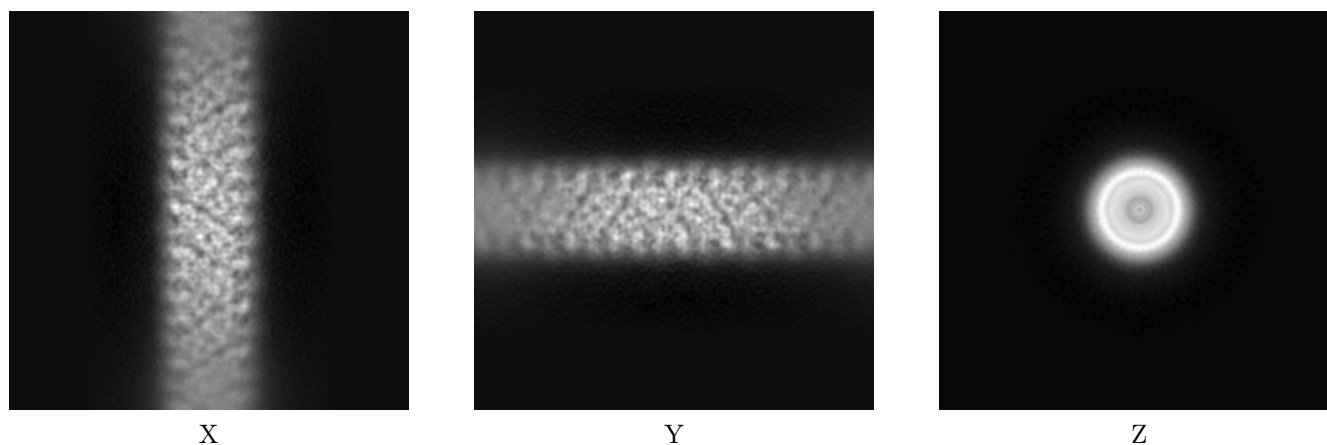
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9332. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

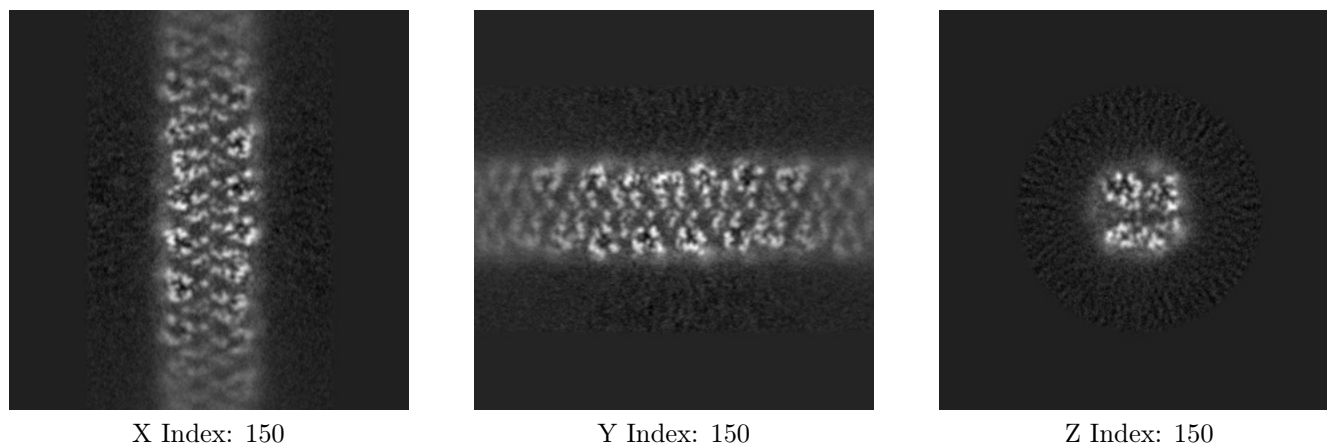
6.1.1 Primary map



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

6.2 Central slices [i](#)

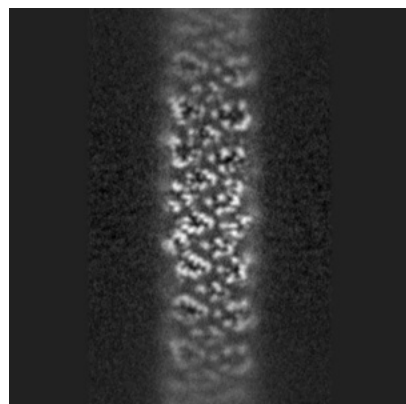
6.2.1 Primary map



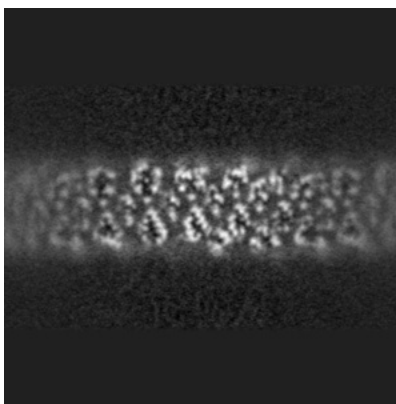
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

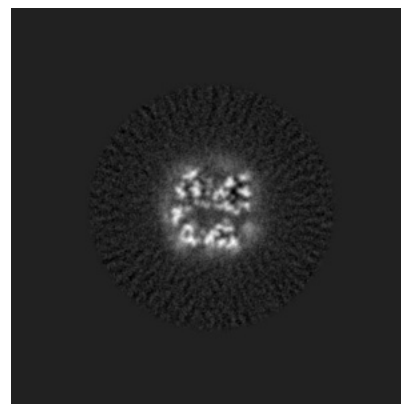
6.3.1 Primary map



X Index: 164



Y Index: 137

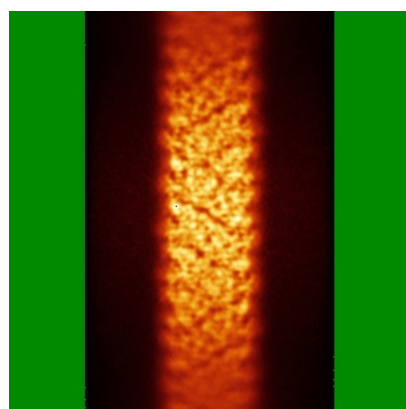


Z Index: 153

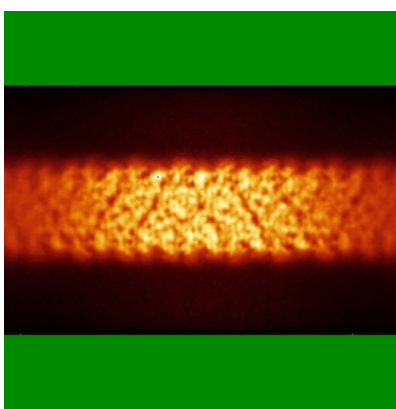
The images above show the largest variance slices of the map in three orthogonal directions.

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

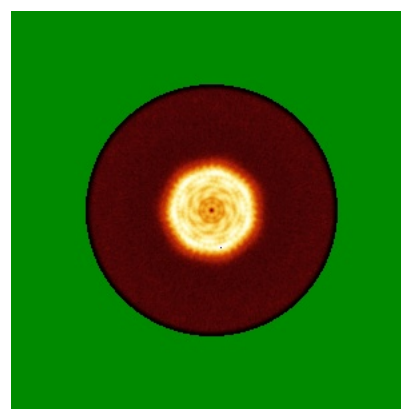
6.4.1 Primary map



X



Y

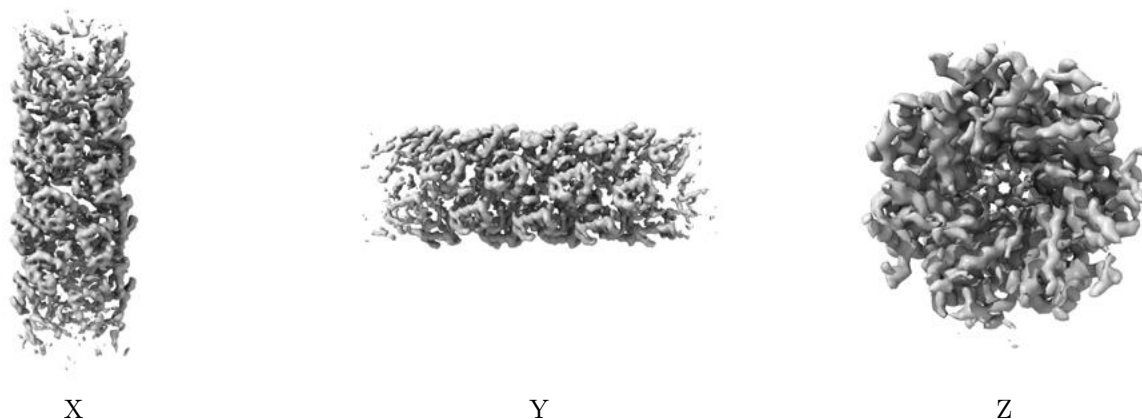


Z

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 0.033. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

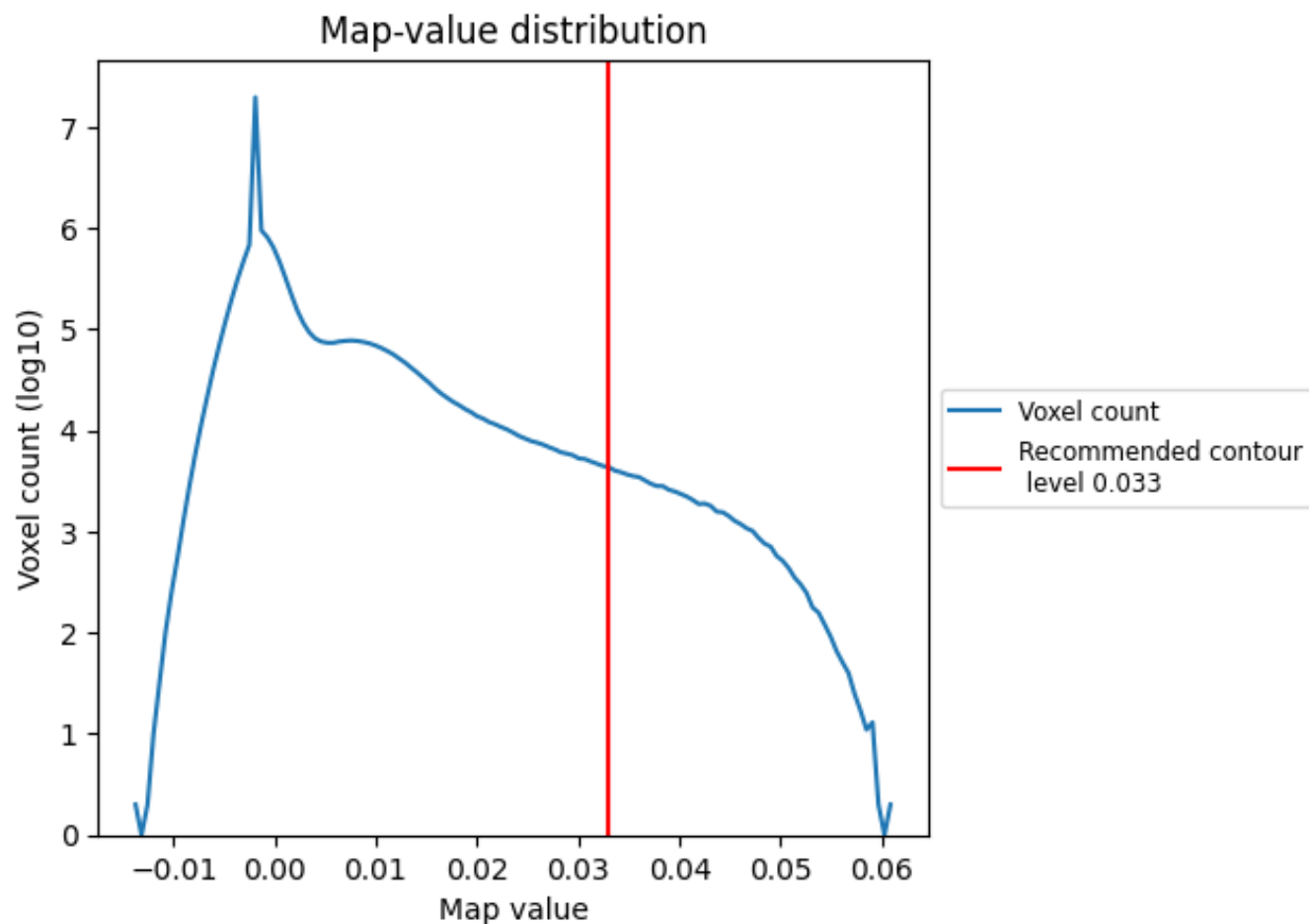
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

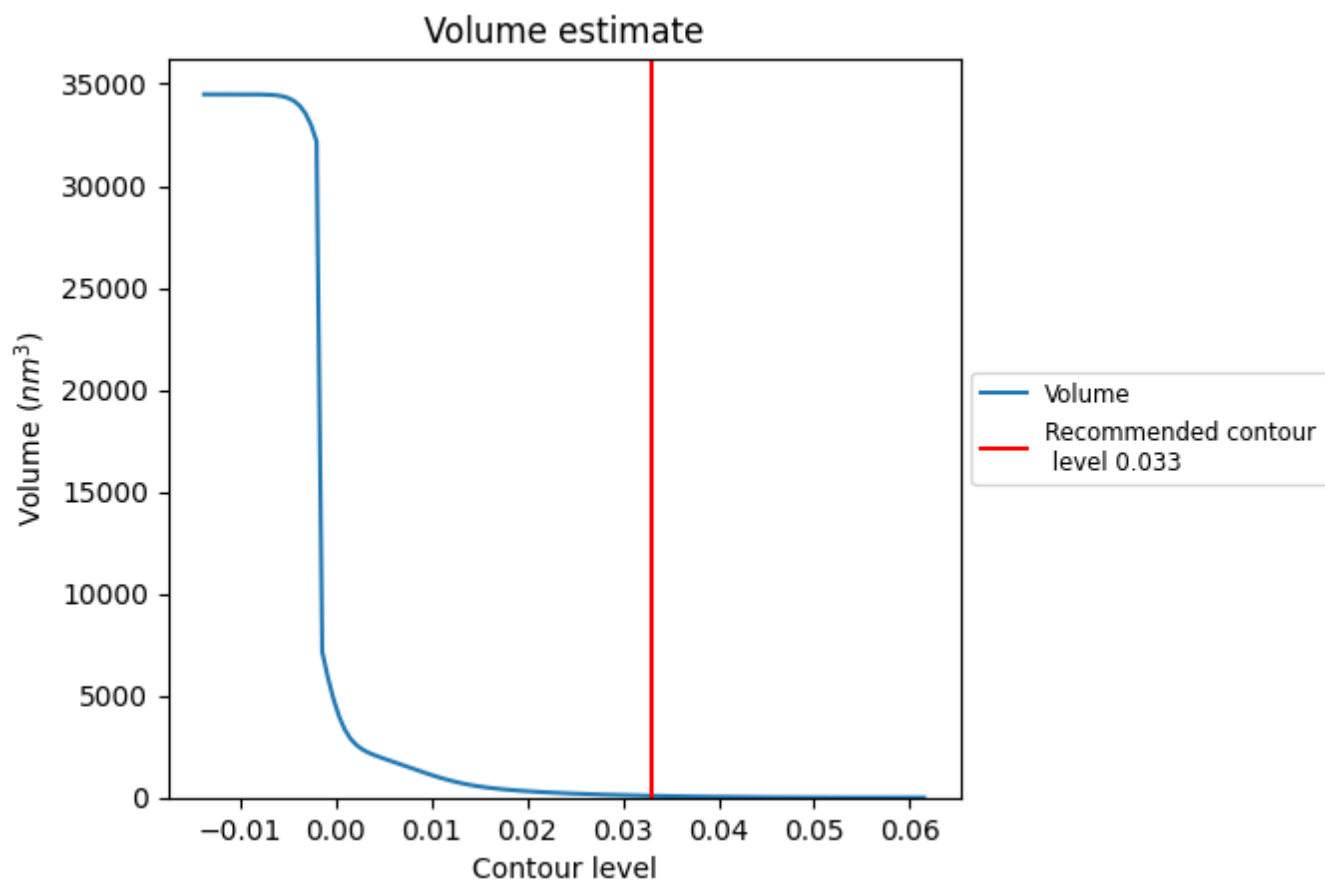
This section contains the results of statistical analysis of the map.

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.

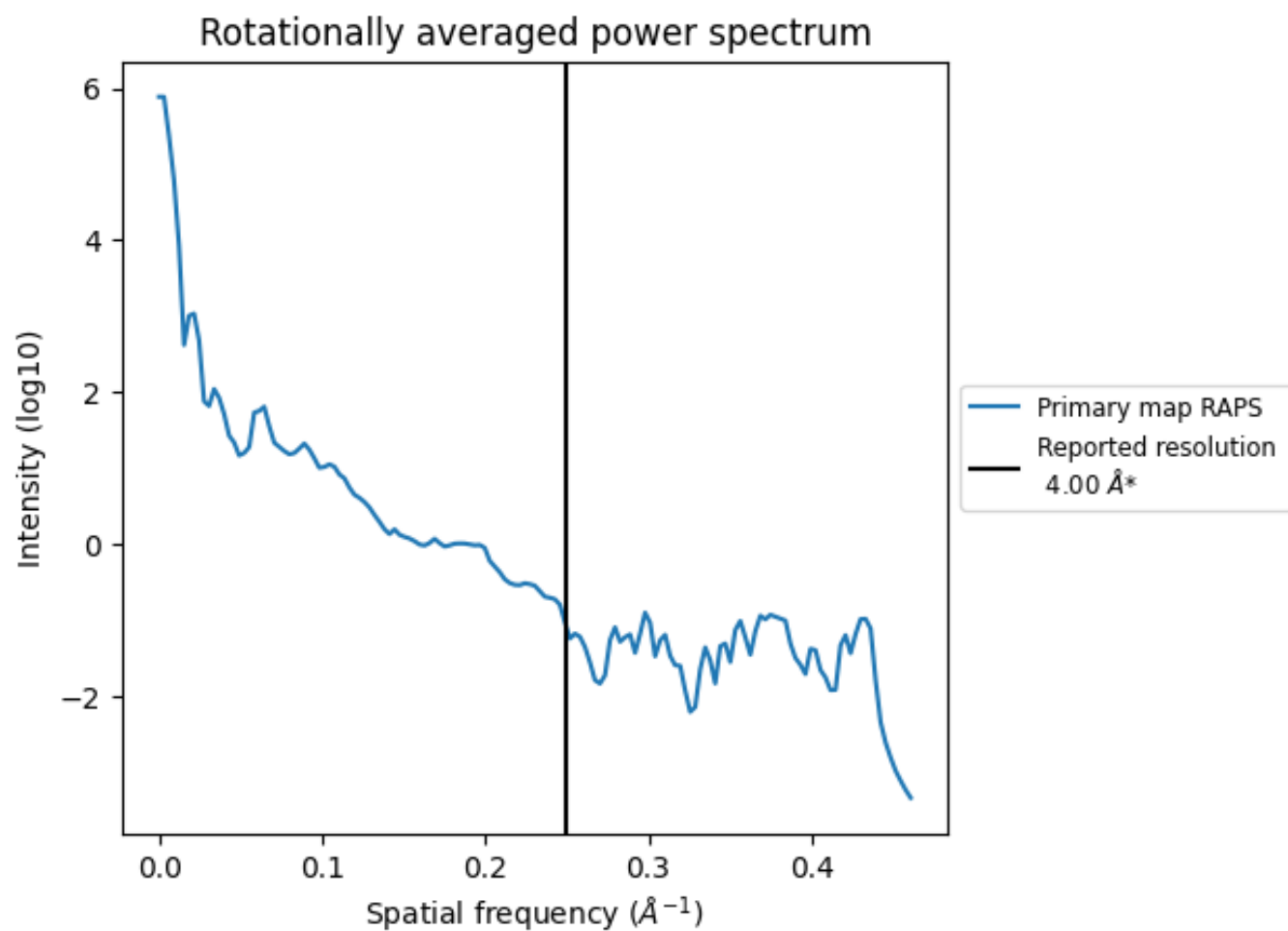
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 86 nm³; this corresponds to an approximate mass of 77 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 ⓘ

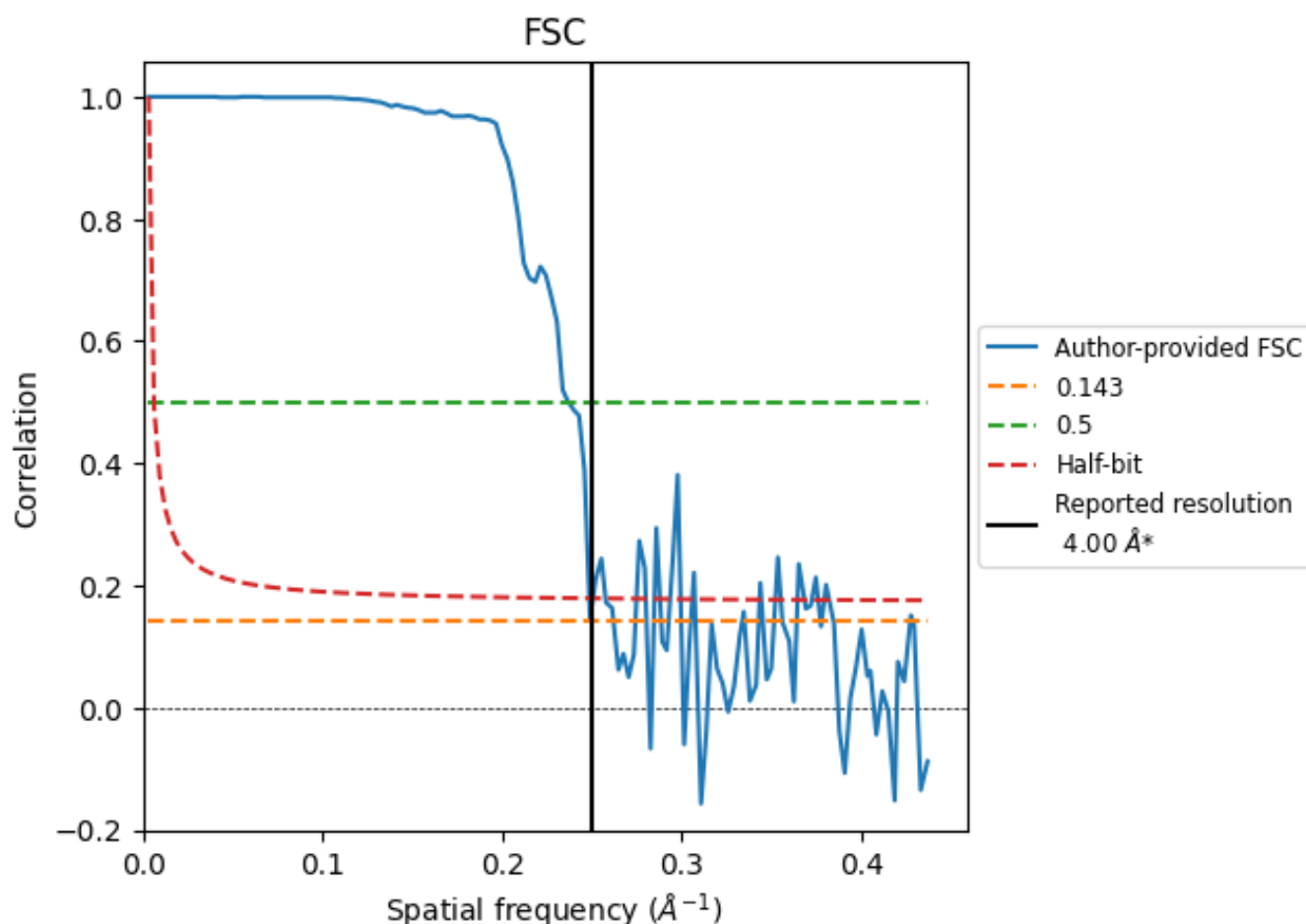


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

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 0.250 Å⁻¹

8.2 Resolution estimates [i](#)

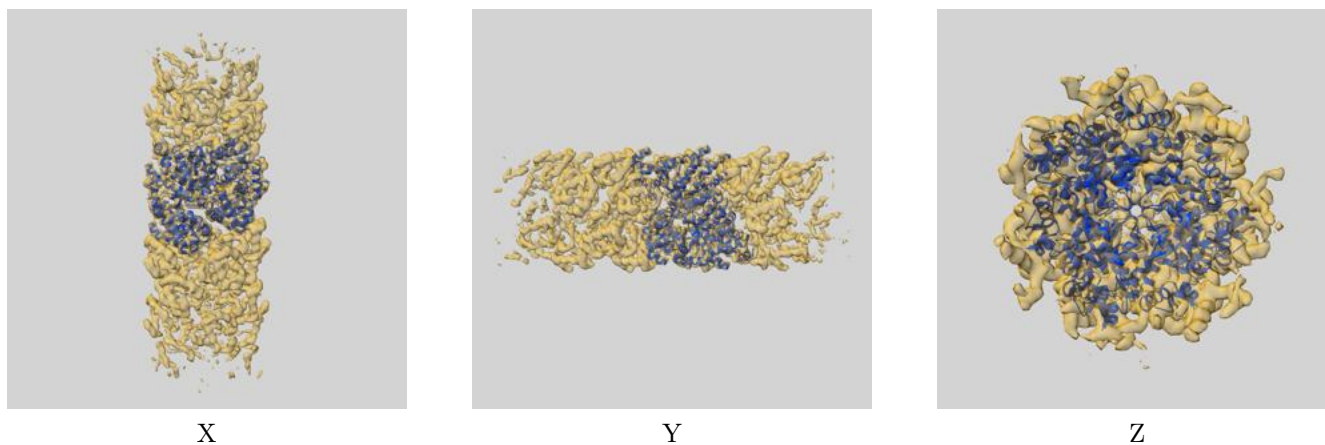
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.82	4.22	4.03
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

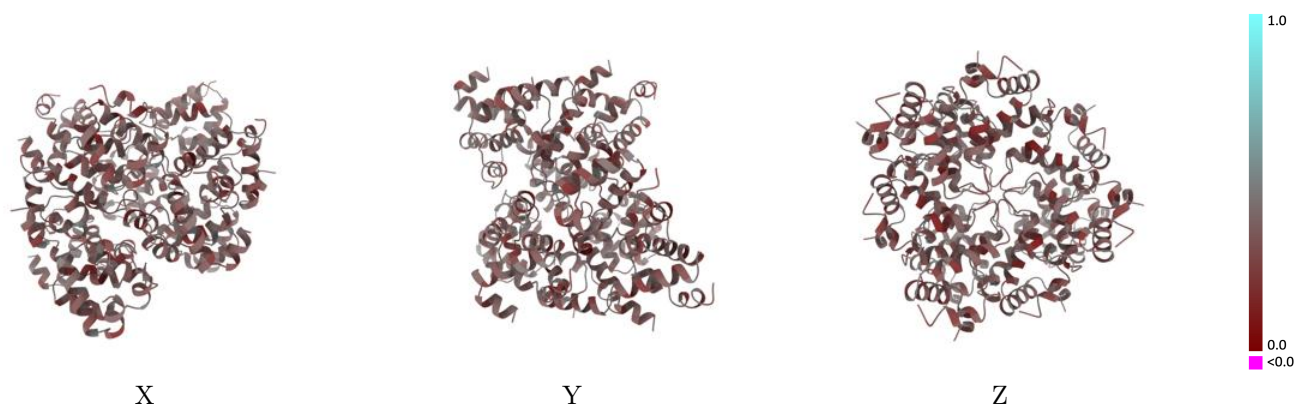
This section contains information regarding the fit between EMDB map EMD-9332 and PDB model 6N2P. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



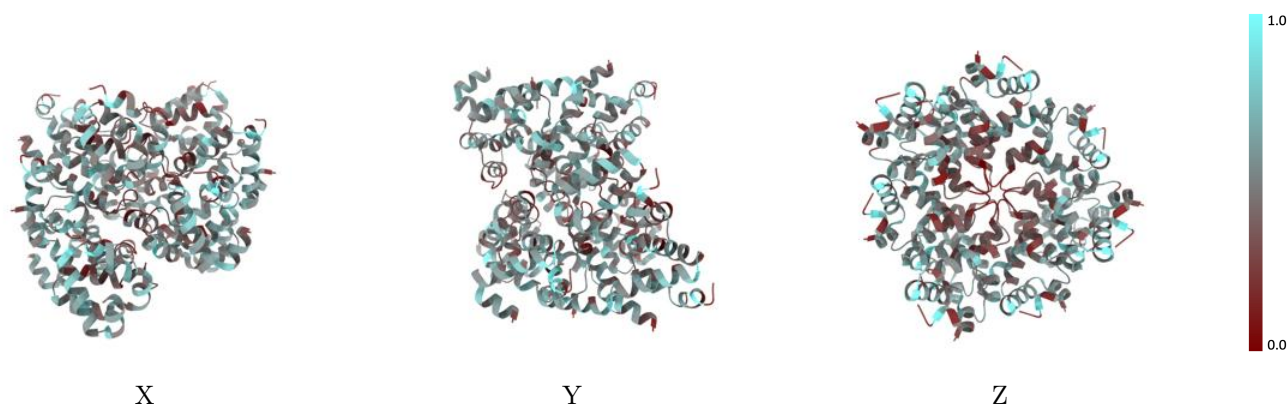
The images above show the 3D surface view of the map at the recommended contour level 0.033 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



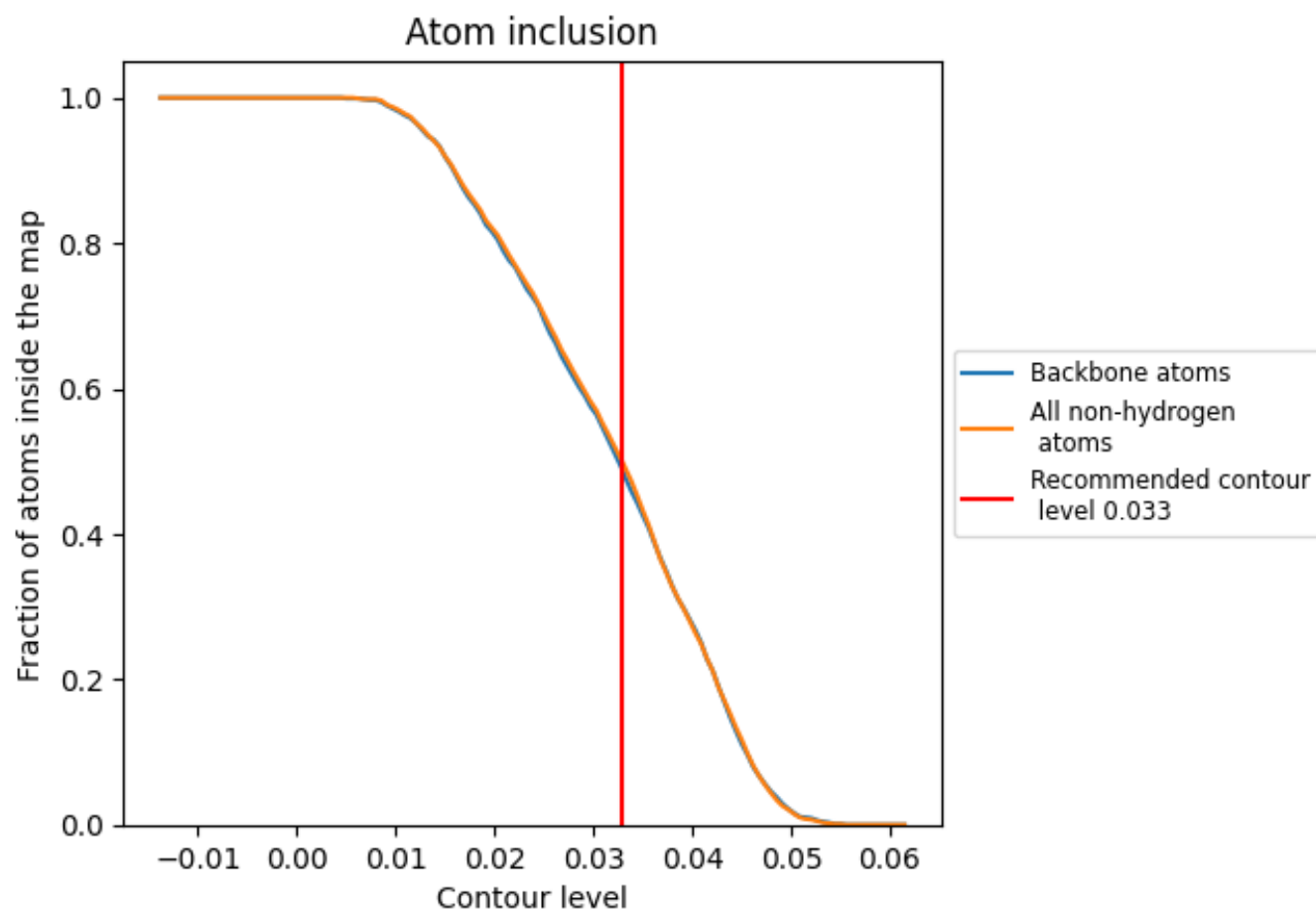
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.033).

9.4 Atom inclusion [i](#)



At the recommended contour level, 49% of all backbone atoms, 50% 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 (0.033) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4980	0.3500
A	0.5230	0.3490
B	0.5260	0.3430
C	0.5150	0.3470
D	0.5050	0.3500
E	0.5010	0.3470
F	0.4840	0.3470
G	0.5260	0.3530
H	0.5310	0.3540
I	0.5220	0.3510
J	0.5280	0.3580

1.0

0.0

<0.0