



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 12:34 AM UTC

PDB ID : 8P4I / pdb_00008p4i
EMDB ID : EMD-17409
Title : Cyanide dihydratase from *Bacillus pumilus* C1
Authors : Mulelu, A.E.; Reitz, J.; van Rooyen, J.M.; Scheffer, M.; Frangakis, A.S.;
Dlamini, L.S.; Woodward, J.D.; Benedik, M.J.; Sewell, B.T.
Deposited on : 2023-05-22
Resolution : 3.83 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:

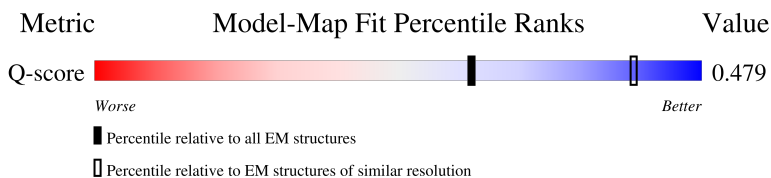
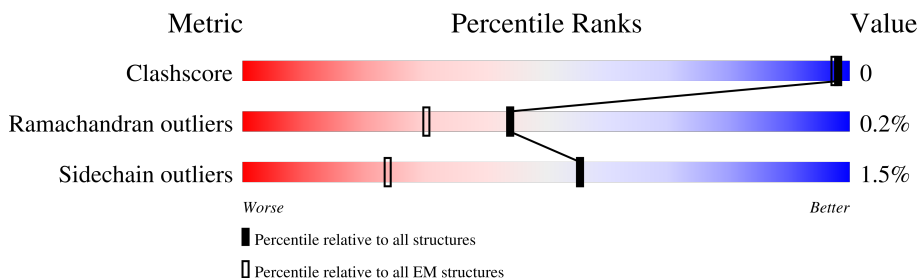
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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

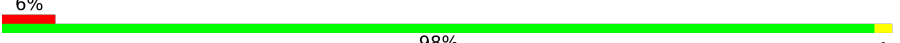
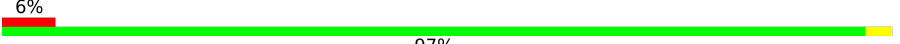
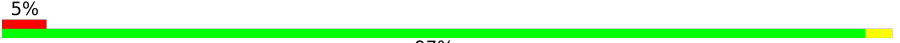
The reported resolution of this entry is 3.83 Å.

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.



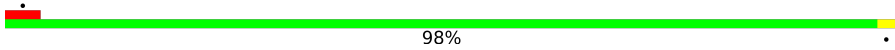
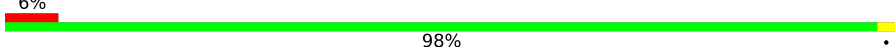
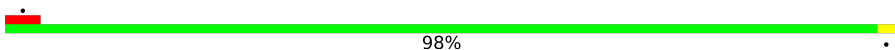
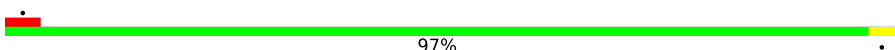
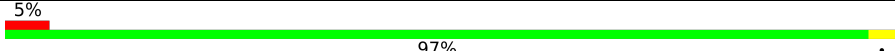
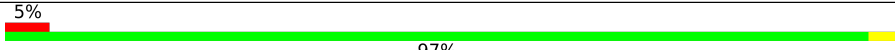
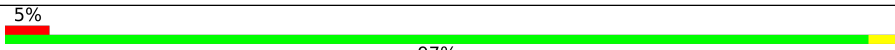
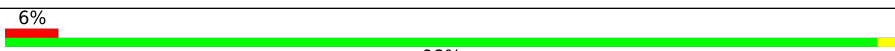
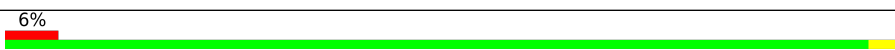
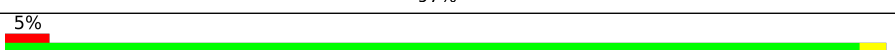
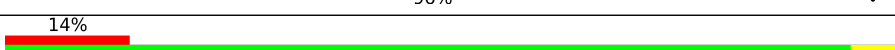
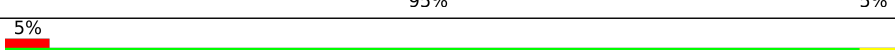
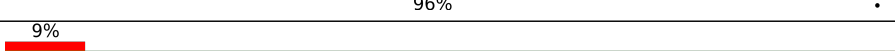
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	9087 (3.33 - 4.33)

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	B	317	 6% 98%
1	D	317	 6% 97%
1	F	317	 5% 97%
1	G	317	 6% 98%

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Mol	Chain	Length	Quality of chain
1	H	317	 98% .
1	I	317	 98% .
1	J	317	 98% .
1	K	317	 97% .
1	L	317	 97% .
1	M	317	 97% .
1	N	317	 97% .
1	O	317	 98% .
1	P	317	 97% .
1	Q	317	 96% .
1	R	317	 95% 5%
1	S	317	 96% .
1	U	317	 95% 5%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 42976 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.

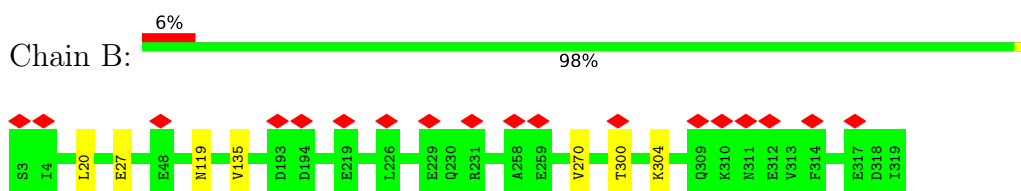
- Molecule 1 is a protein called Cyanide dihydratase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	317	Total	C	N	O	S	0	0
			2528	1616	410	485	17		
1	D	317	Total	C	N	O	S	0	0
			2528	1616	410	485	17		
1	F	317	Total	C	N	O	S	0	0
			2528	1616	410	485	17		
1	G	317	Total	C	N	O	S	0	0
			2528	1616	410	485	17		
1	H	317	Total	C	N	O	S	0	0
			2528	1616	410	485	17		
1	I	317	Total	C	N	O	S	0	0
			2528	1616	410	485	17		
1	J	317	Total	C	N	O	S	0	0
			2528	1616	410	485	17		
1	K	317	Total	C	N	O	S	0	0
			2528	1616	410	485	17		
1	L	317	Total	C	N	O	S	0	0
			2528	1616	410	485	17		
1	M	317	Total	C	N	O	S	0	0
			2528	1616	410	485	17		
1	N	317	Total	C	N	O	S	0	0
			2528	1616	410	485	17		
1	O	317	Total	C	N	O	S	0	0
			2528	1616	410	485	17		
1	P	317	Total	C	N	O	S	0	0
			2528	1616	410	485	17		
1	Q	317	Total	C	N	O	S	0	0
			2528	1616	410	485	17		
1	R	317	Total	C	N	O	S	0	0
			2528	1616	410	485	17		
1	S	317	Total	C	N	O	S	0	0
			2528	1616	410	485	17		
1	U	317	Total	C	N	O	S	0	0
			2528	1616	410	485	17		

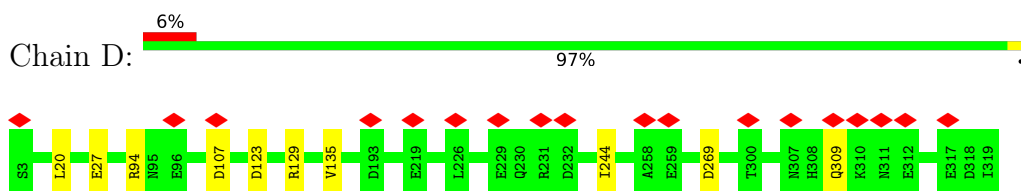
3 Residue-property plots [i](#)

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.

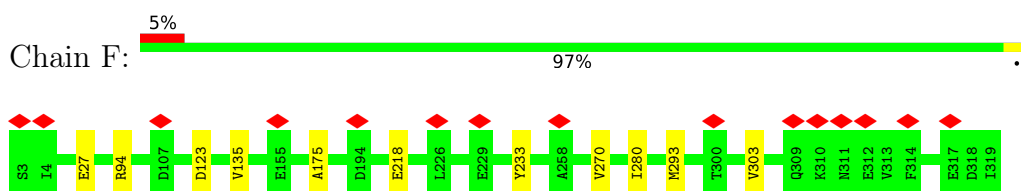
- Molecule 1: Cyanide dihydratase



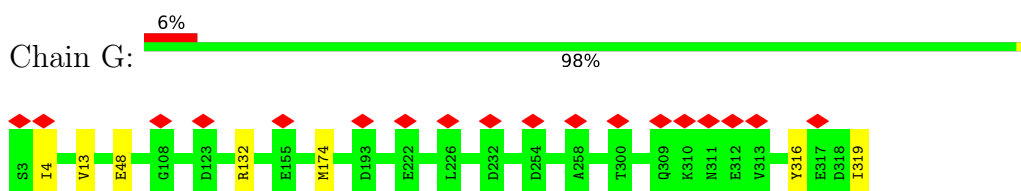
- Molecule 1: Cyanide dihydratase



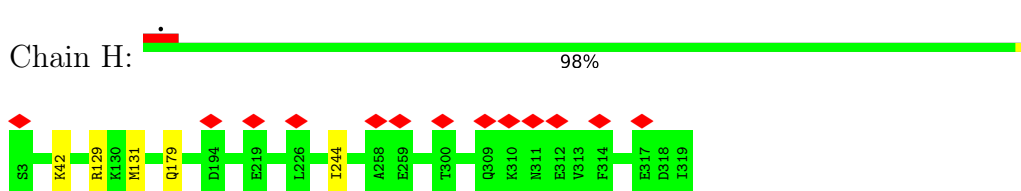
- Molecule 1: Cyanide dihydratase



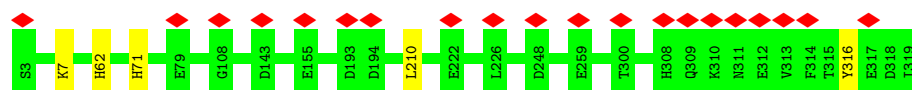
- Molecule 1: Cyanide dihydratase



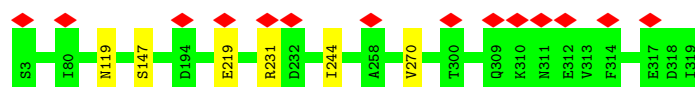
- Molecule 1: Cyanide dihydratase



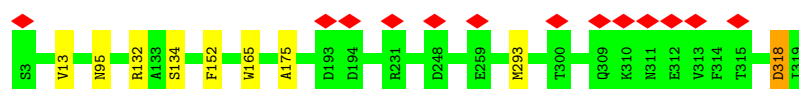
● Molecule 1: Cyanide dihydratase



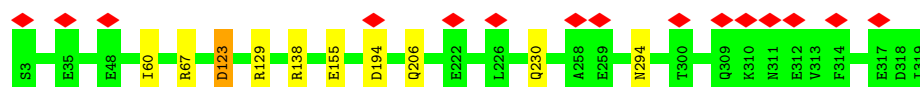
● Molecule 1: Cyanide dihydratase



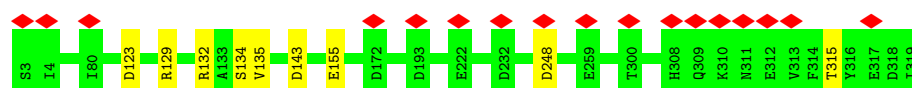
● Molecule 1: Cyanide dihydratase



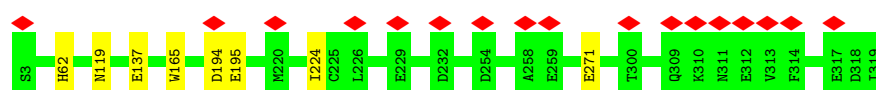
● Molecule 1: Cyanide dihydratase



● Molecule 1: Cyanide dihydratase

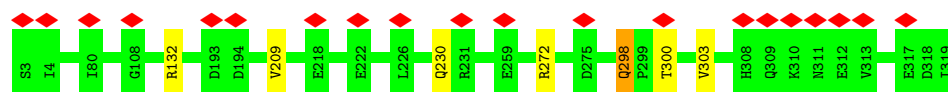


● Molecule 1: Cyanide dihydratase

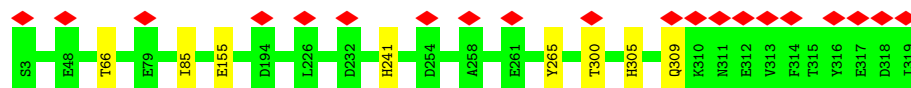


● Molecule 1: Cyanide dihydratase

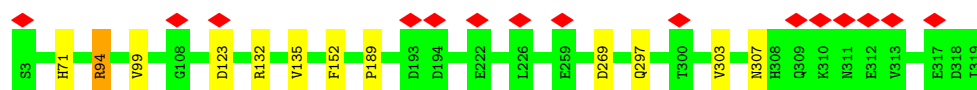




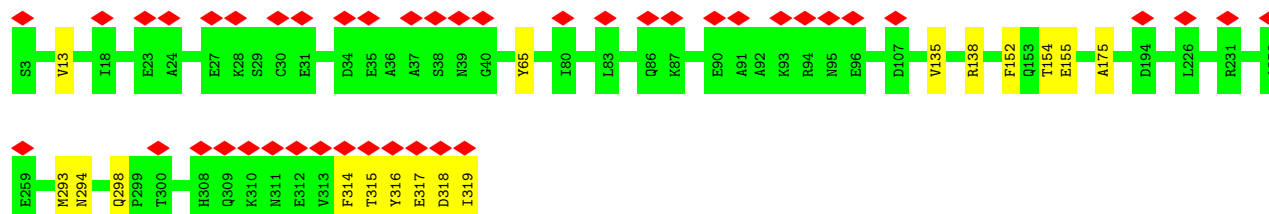
- Molecule 1: Cyanide dihydratase



- Molecule 1: Cyanide dihydratase



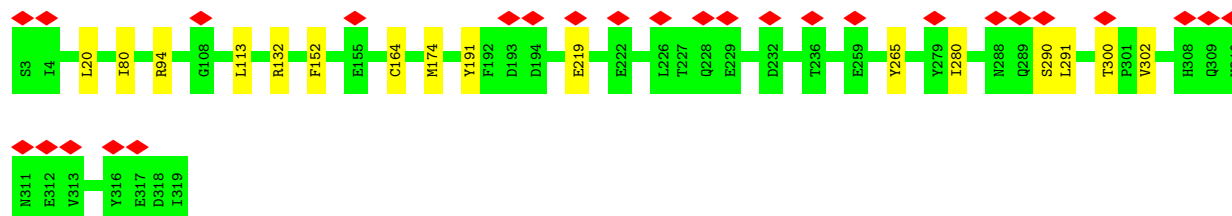
- Molecule 1: Cyanide dihydratase



- Molecule 1: Cyanide dihydratase



- Molecule 1: Cyanide dihydratase



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-77°, rise=16.9 Å, axial sym=C2	Depositor
Number of segments used	120943	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	59.4	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.048	Depositor
Minimum map value	-0.021	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0119	Depositor
Map size (Å)	315.0, 315.0, 315.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	B	0.69	0/2597	1.18	1/3525 (0.0%)
1	D	0.68	0/2597	1.18	5/3525 (0.1%)
1	F	0.68	0/2597	1.16	3/3525 (0.1%)
1	G	0.70	0/2597	1.19	1/3525 (0.0%)
1	H	0.70	0/2597	1.22	2/3525 (0.1%)
1	I	0.71	0/2597	1.20	1/3525 (0.0%)
1	J	0.70	0/2597	1.20	1/3525 (0.0%)
1	K	0.74	0/2597	1.20	1/3525 (0.0%)
1	L	0.73	1/2597 (0.0%)	1.24	5/3525 (0.1%)
1	M	0.72	0/2597	1.21	2/3525 (0.1%)
1	N	0.70	0/2597	1.20	6/3525 (0.2%)
1	O	0.71	0/2597	1.22	2/3525 (0.1%)
1	P	0.72	1/2597 (0.0%)	1.21	3/3525 (0.1%)
1	Q	0.72	0/2597	1.21	7/3525 (0.2%)
1	R	0.72	1/2597 (0.0%)	1.20	2/3525 (0.1%)
1	S	0.72	1/2597 (0.0%)	1.20	1/3525 (0.0%)
1	U	0.70	0/2597	1.20	1/3525 (0.0%)
All	All	0.71	4/44149 (0.0%)	1.20	44/59925 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	305	HIS	ND1-CE1	5.31	1.37	1.32
1	L	294	ASN	CG-OD1	5.03	1.33	1.23
1	R	294	ASN	CG-OD1	5.01	1.33	1.23
1	S	297	GLN	CD-OE1	5.01	1.33	1.23

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	131	MET	N-CA-C	7.53	119.17	110.97
1	K	132	ARG	NE-CZ-NH2	6.75	125.28	119.20
1	M	135	VAL	N-CA-C	6.61	117.30	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	305	HIS	CB-CG-CD2	-6.59	122.63	131.20
1	G	132	ARG	NE-CZ-NH2	6.51	125.06	119.20
1	Q	132	ARG	NE-CZ-NH2	6.41	124.97	119.20
1	Q	99	VAL	N-CA-C	6.31	117.18	107.78
1	F	233	TYR	N-CA-C	-6.27	104.53	111.36
1	Q	135	VAL	N-CA-C	6.08	116.26	110.42
1	O	132	ARG	NE-CZ-NH2	6.02	124.62	119.20
1	L	194	ASP	CA-CB-CG	5.91	118.51	112.60
1	D	135	VAL	N-CA-C	5.82	116.28	110.23
1	P	305	HIS	CB-CG-ND1	5.67	131.20	122.70
1	D	269	ASP	CA-CB-CG	5.66	118.25	112.60
1	F	135	VAL	N-CA-C	5.57	116.03	110.23
1	L	129	ARG	NE-CZ-NH2	5.57	124.21	119.20
1	H	129	ARG	NE-CZ-NH2	5.52	124.17	119.20
1	P	241	HIS	CB-CG-CD2	-5.50	124.05	131.20
1	B	119	ASN	CA-CB-CG	5.45	118.05	112.60
1	J	119	ASN	N-CA-CB	-5.45	103.44	110.03
1	D	107	ASP	CA-CB-CG	5.44	118.04	112.60
1	F	123	ASP	CA-CB-CG	5.32	117.92	112.60
1	N	137	GLU	CA-C-N	5.28	128.09	120.38
1	N	137	GLU	C-N-CA	5.28	128.09	120.38
1	L	138	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	M	129	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	Q	123	ASP	CA-CB-CG	5.21	117.81	112.60
1	I	71	HIS	CB-CG-CD2	-5.21	124.42	131.20
1	L	67	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	Q	71	HIS	CB-CG-CD2	-5.16	124.49	131.20
1	N	62	HIS	CA-C-N	5.15	124.86	119.82
1	N	62	HIS	C-N-CA	5.15	124.86	119.82
1	O	272	ARG	NE-CZ-NH2	5.15	123.83	119.20
1	N	119	ASN	CA-CB-CG	5.14	117.74	112.60
1	S	94	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	R	135	VAL	N-CA-C	5.11	115.72	110.36
1	R	138	ARG	NE-CZ-NH2	5.08	123.78	119.20
1	U	94	ARG	NE-CZ-NH2	5.08	123.77	119.20
1	D	123	ASP	CA-CB-CG	5.07	117.67	112.60
1	N	194	ASP	CA-CB-CG	5.05	117.66	112.60
1	Q	94	ARG	NE-CZ-NH2	5.05	123.74	119.20
1	L	123	ASP	CA-CB-CG	5.03	117.63	112.60
1	D	129	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	Q	269	ASP	CA-CB-CG	5.01	117.61	112.60

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	B	2528	0	2411	2	0
1	D	2528	0	2411	0	0
1	F	2528	0	2411	2	0
1	G	2528	0	2411	2	0
1	H	2528	0	2411	0	0
1	I	2528	0	2411	0	0
1	J	2528	0	2411	1	0
1	K	2528	0	2411	2	0
1	L	2528	0	2411	4	0
1	M	2528	0	2411	1	0
1	N	2528	0	2411	0	0
1	O	2528	0	2411	2	0
1	P	2528	0	2411	1	0
1	Q	2528	0	2411	3	0
1	R	2528	0	2411	8	0
1	S	2528	0	2411	5	0
1	U	2528	0	2411	4	0
All	All	42976	0	40987	34	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 0.

All (34) 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:L:60:ILE:O	1:L:60:ILE:HG22	1.91	0.71
1:R:314:PHE:O	1:R:315:THR:HG22	1.90	0.70
1:R:315:THR:HG23	1:R:317:GLU:HG2	1.74	0.70
1:Q:297:GLN:OE1	1:S:308:HIS:CE1	2.50	0.64
1:U:300:THR:O	1:U:300:THR:HG23	2.02	0.58
1:R:318:ASP:OD1	1:R:319:ILE:N	2.35	0.58
1:S:175:ALA:HB2	1:S:293:MET:HE1	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:305:HIS:HB3	1:S:308:HIS:HD2	1.69	0.56
1:L:60:ILE:HG22	1:L:230:GLN:HG2	1.89	0.55
1:R:314:PHE:O	1:R:315:THR:CG2	2.55	0.55
1:S:283:ALA:O	1:U:302:VAL:HG21	2.07	0.55
1:S:305:HIS:HB3	1:S:308:HIS:CD2	2.42	0.54
1:G:316:TYR:HA	1:G:319:ILE:HG12	1.90	0.54
1:L:60:ILE:O	1:L:60:ILE:CG2	2.54	0.53
1:U:174:MET:HA	1:U:174:MET:HE2	1.90	0.53
1:P:300:THR:O	1:P:300:THR:OG1	2.26	0.52
1:K:318:ASP:OD1	1:K:318:ASP:N	2.41	0.51
1:R:316:TYR:CG	1:R:316:TYR:O	2.64	0.51
1:G:174:MET:HA	1:G:174:MET:HE2	1.95	0.48
1:R:314:PHE:C	1:R:315:THR:HG22	2.39	0.48
1:Q:307:ASN:O	1:Q:307:ASN:CG	2.57	0.47
1:M:132:ARG:NH2	1:M:143:ASP:OD2	2.48	0.47
1:O:300:THR:O	1:O:300:THR:OG1	2.32	0.46
1:R:318:ASP:OD1	1:R:319:ILE:HG12	2.16	0.46
1:L:60:ILE:CG2	1:L:230:GLN:HG2	2.46	0.46
1:O:298:GLN:HB2	1:Q:307:ASN:ND2	2.31	0.45
1:K:175:ALA:HB2	1:K:293:MET:HE1	2.02	0.41
1:F:303:VAL:O	1:F:303:VAL:HG13	2.18	0.41
1:B:300:THR:O	1:B:300:THR:OG1	2.28	0.41
1:B:304:LYS:O	1:B:304:LYS:HG3	2.21	0.41
1:U:290:SER:OG	1:U:291:LEU:N	2.54	0.41
1:F:175:ALA:HB2	1:F:293:MET:HE1	2.03	0.41
1:R:175:ALA:HB2	1:R:293:MET:HE1	2.02	0.41
1:J:147:SER:O	1:J:147:SER:OG	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	315/317 (99%)	297 (94%)	16 (5%)	2 (1%)	21	55
1	D	315/317 (99%)	303 (96%)	11 (4%)	1 (0%)	36	69
1	F	315/317 (99%)	299 (95%)	16 (5%)	0	100	100
1	G	315/317 (99%)	301 (96%)	13 (4%)	1 (0%)	36	69
1	H	315/317 (99%)	300 (95%)	14 (4%)	1 (0%)	36	69
1	I	315/317 (99%)	301 (96%)	12 (4%)	2 (1%)	21	55
1	J	315/317 (99%)	299 (95%)	16 (5%)	0	100	100
1	K	315/317 (99%)	301 (96%)	13 (4%)	1 (0%)	36	69
1	L	315/317 (99%)	297 (94%)	18 (6%)	0	100	100
1	M	315/317 (99%)	296 (94%)	18 (6%)	1 (0%)	36	69
1	N	315/317 (99%)	303 (96%)	12 (4%)	0	100	100
1	O	315/317 (99%)	299 (95%)	16 (5%)	0	100	100
1	P	315/317 (99%)	298 (95%)	17 (5%)	0	100	100
1	Q	315/317 (99%)	295 (94%)	19 (6%)	1 (0%)	36	69
1	R	315/317 (99%)	298 (95%)	17 (5%)	0	100	100
1	S	315/317 (99%)	300 (95%)	14 (4%)	1 (0%)	36	69
1	U	315/317 (99%)	296 (94%)	17 (5%)	2 (1%)	21	55
All	All	5355/5389 (99%)	5083 (95%)	259 (5%)	13 (0%)	44	74

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	179	GLN
1	I	7	LYS
1	B	20	LEU
1	D	20	LEU
1	I	316	TYR
1	K	134	SER
1	B	135	VAL
1	Q	189	PRO
1	U	20	LEU
1	U	191	TYR
1	M	155	GLU
1	G	4	ILE
1	S	189	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	270/270 (100%)	268 (99%)	2 (1%)	76	78
1	D	270/270 (100%)	266 (98%)	4 (2%)	57	69
1	F	270/270 (100%)	265 (98%)	5 (2%)	50	66
1	G	270/270 (100%)	268 (99%)	2 (1%)	76	78
1	H	270/270 (100%)	268 (99%)	2 (1%)	76	78
1	I	270/270 (100%)	268 (99%)	2 (1%)	76	78
1	J	270/270 (100%)	266 (98%)	4 (2%)	57	69
1	K	270/270 (100%)	265 (98%)	5 (2%)	50	66
1	L	270/270 (100%)	267 (99%)	3 (1%)	65	73
1	M	270/270 (100%)	266 (98%)	4 (2%)	57	69
1	N	270/270 (100%)	266 (98%)	4 (2%)	57	69
1	O	270/270 (100%)	266 (98%)	4 (2%)	57	69
1	P	270/270 (100%)	265 (98%)	5 (2%)	50	66
1	Q	270/270 (100%)	267 (99%)	3 (1%)	65	73
1	R	270/270 (100%)	264 (98%)	6 (2%)	45	64
1	S	270/270 (100%)	264 (98%)	6 (2%)	45	64
1	U	270/270 (100%)	262 (97%)	8 (3%)	36	57
All	All	4590/4590 (100%)	4521 (98%)	69 (2%)	55	69

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	27	GLU
1	B	270	VAL
1	D	27	GLU
1	D	94	ARG
1	D	244	ILE
1	D	309	GLN
1	F	27	GLU

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Mol	Chain	Res	Type
1	F	94	ARG
1	F	218	GLU
1	F	270	VAL
1	F	280	ILE
1	G	13	VAL
1	G	48	GLU
1	H	42	LYS
1	H	244	ILE
1	I	62	HIS
1	I	210	LEU
1	J	219	GLU
1	J	231	ARG
1	J	244	ILE
1	J	270	VAL
1	K	13	VAL
1	K	95	ASN
1	K	152	PHE
1	K	165	TRP
1	K	318	ASP
1	L	123	ASP
1	L	155	GLU
1	L	206	GLN
1	M	123	ASP
1	M	134	SER
1	M	248	ASP
1	M	315	THR
1	N	165	TRP
1	N	195	GLU
1	N	224	ILE
1	N	271	GLU
1	O	209	VAL
1	O	230	GLN
1	O	298	GLN
1	O	303	VAL
1	P	66	THR
1	P	85	ILE
1	P	155	GLU
1	P	265	TYR
1	P	309	GLN
1	Q	94	ARG
1	Q	152	PHE
1	Q	303	VAL

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Mol	Chain	Res	Type
1	R	13	VAL
1	R	65	TYR
1	R	152	PHE
1	R	154	THR
1	R	155	GLU
1	R	298	GLN
1	S	123	ASP
1	S	151	VAL
1	S	265	TYR
1	S	289	GLN
1	S	308	HIS
1	S	315	THR
1	U	80	ILE
1	U	113	LEU
1	U	132	ARG
1	U	152	PHE
1	U	164	CYS
1	U	219	GLU
1	U	265	TYR
1	U	280	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	62	HIS
1	B	158	ASN
1	B	167	HIS
1	D	158	ASN
1	D	167	HIS
1	D	241	HIS
1	F	158	ASN
1	F	297	GLN
1	F	298	GLN
1	G	184	HIS
1	G	297	GLN
1	H	86	GLN
1	H	158	ASN
1	H	298	GLN
1	I	14	GLN
1	I	158	ASN
1	I	297	GLN
1	J	86	GLN

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Mol	Chain	Res	Type
1	J	119	ASN
1	J	158	ASN
1	J	297	GLN
1	K	115	GLN
1	K	121	ASN
1	K	158	ASN
1	K	177	ASN
1	K	179	GLN
1	L	14	GLN
1	L	121	ASN
1	L	158	ASN
1	L	308	HIS
1	M	76	ASN
1	M	95	ASN
1	M	121	ASN
1	M	158	ASN
1	M	180	ASN
1	M	182	GLN
1	M	285	HIS
1	N	158	ASN
1	N	184	HIS
1	O	158	ASN
1	O	241	HIS
1	O	294	ASN
1	O	309	GLN
1	P	158	ASN
1	P	184	HIS
1	P	294	ASN
1	P	309	GLN
1	Q	86	GLN
1	Q	119	ASN
1	Q	180	ASN
1	Q	182	GLN
1	Q	184	HIS
1	Q	307	ASN
1	Q	309	GLN
1	R	95	ASN
1	R	121	ASN
1	R	177	ASN
1	R	184	HIS
1	R	298	GLN
1	S	86	GLN

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Mol	Chain	Res	Type
1	S	121	ASN
1	S	158	ASN
1	S	177	ASN
1	S	297	GLN
1	S	305	HIS
1	U	158	ASN
1	U	179	GLN
1	U	228	GLN
1	U	230	GLN
1	U	305	HIS
1	U	309	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.

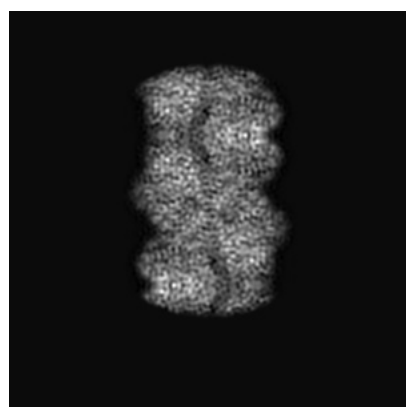
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17409. These allow visual inspection of the internal detail of the map and identification of artifacts.

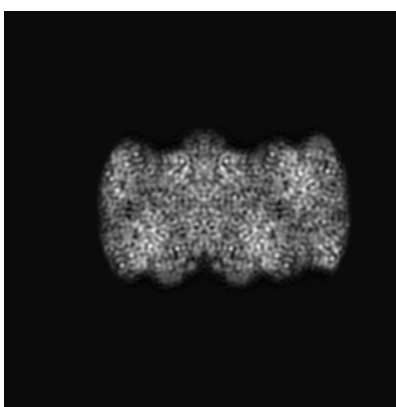
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

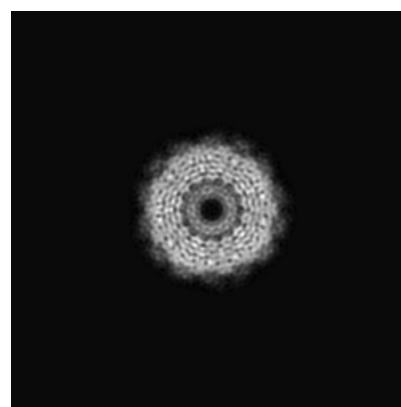
6.1.1 Primary map



X



Y



Z

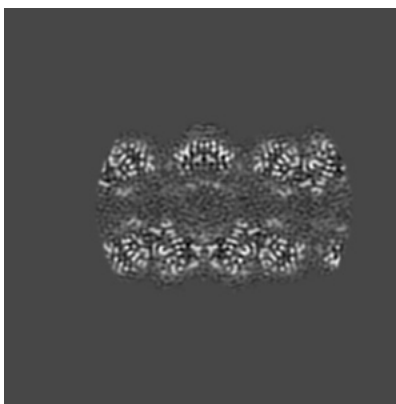
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

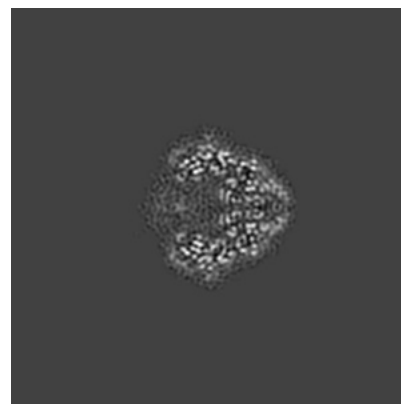
6.2.1 Primary map



X Index: 150



Y Index: 150

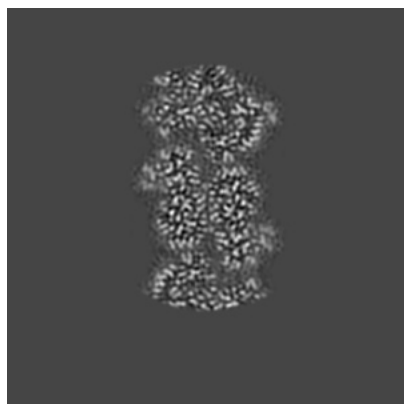


Z Index: 150

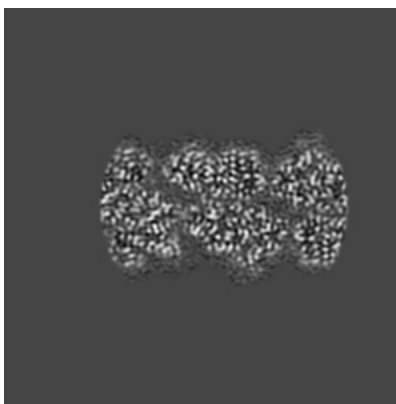
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

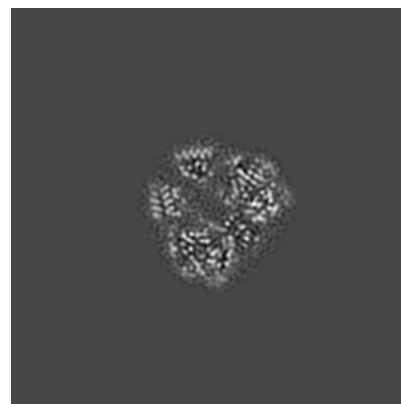
6.3.1 Primary map



X Index: 177



Y Index: 125

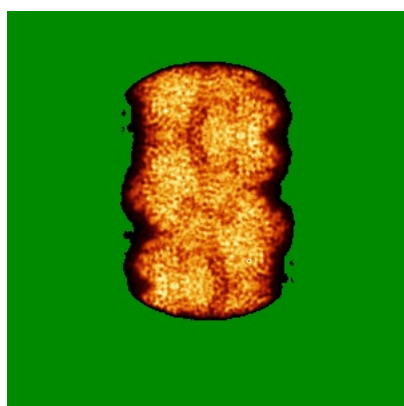


Z Index: 157

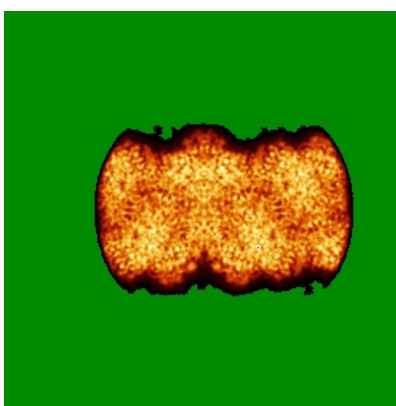
The images above show the largest variance slices of the map in three orthogonal directions.

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

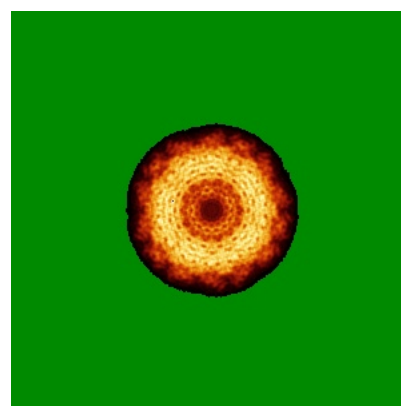
6.4.1 Primary map



X



Y

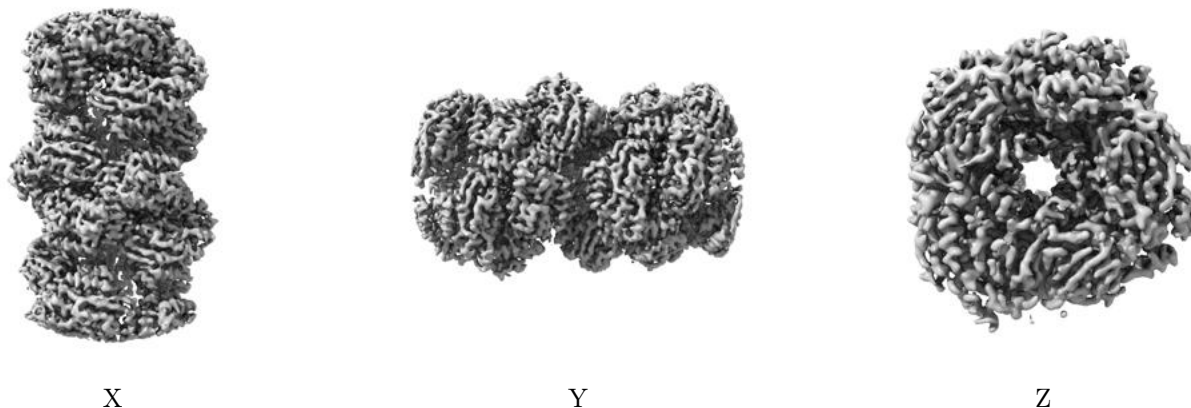


Z

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 0.0119. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

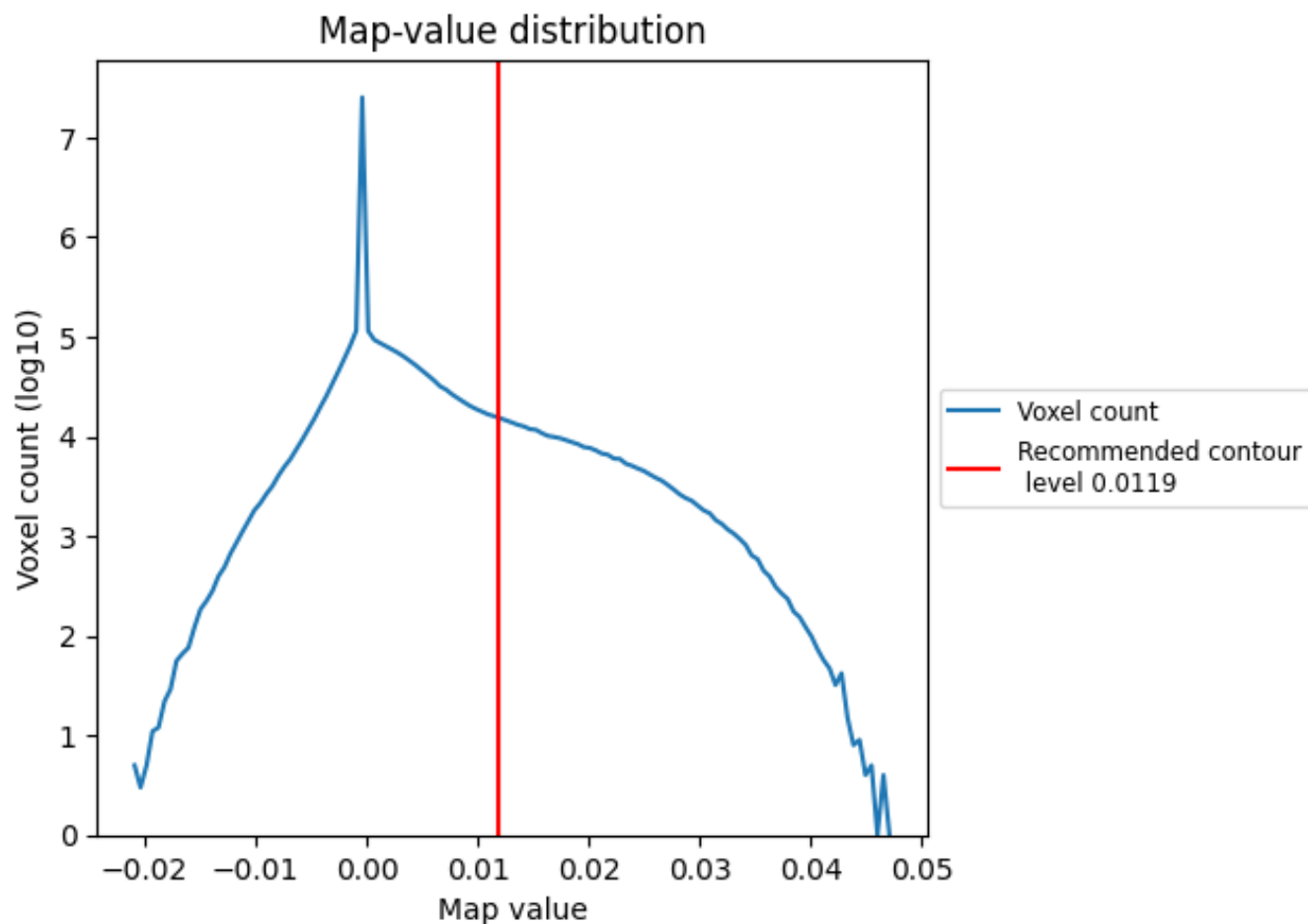
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

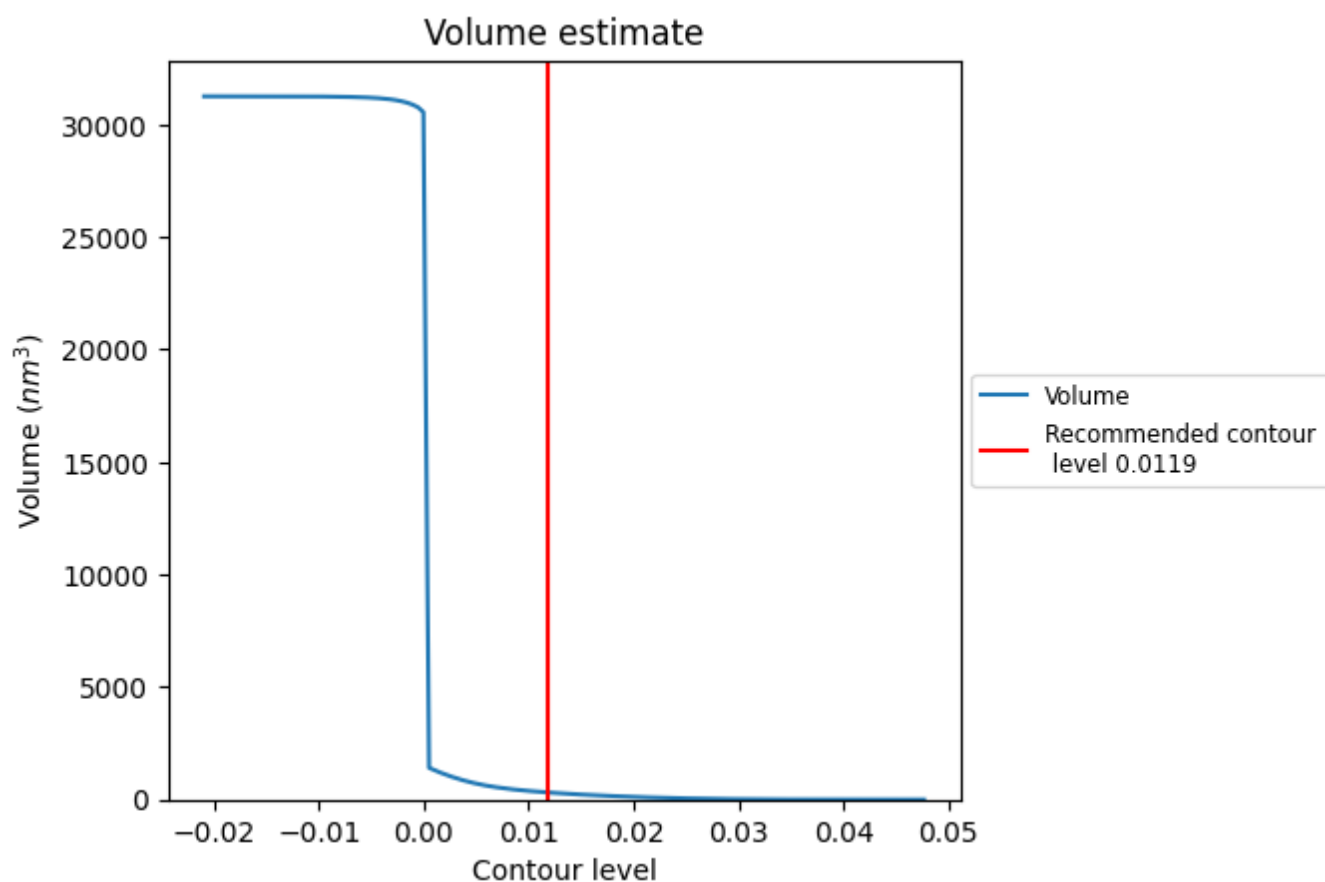
This section contains the results of statistical analysis of the map.

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.

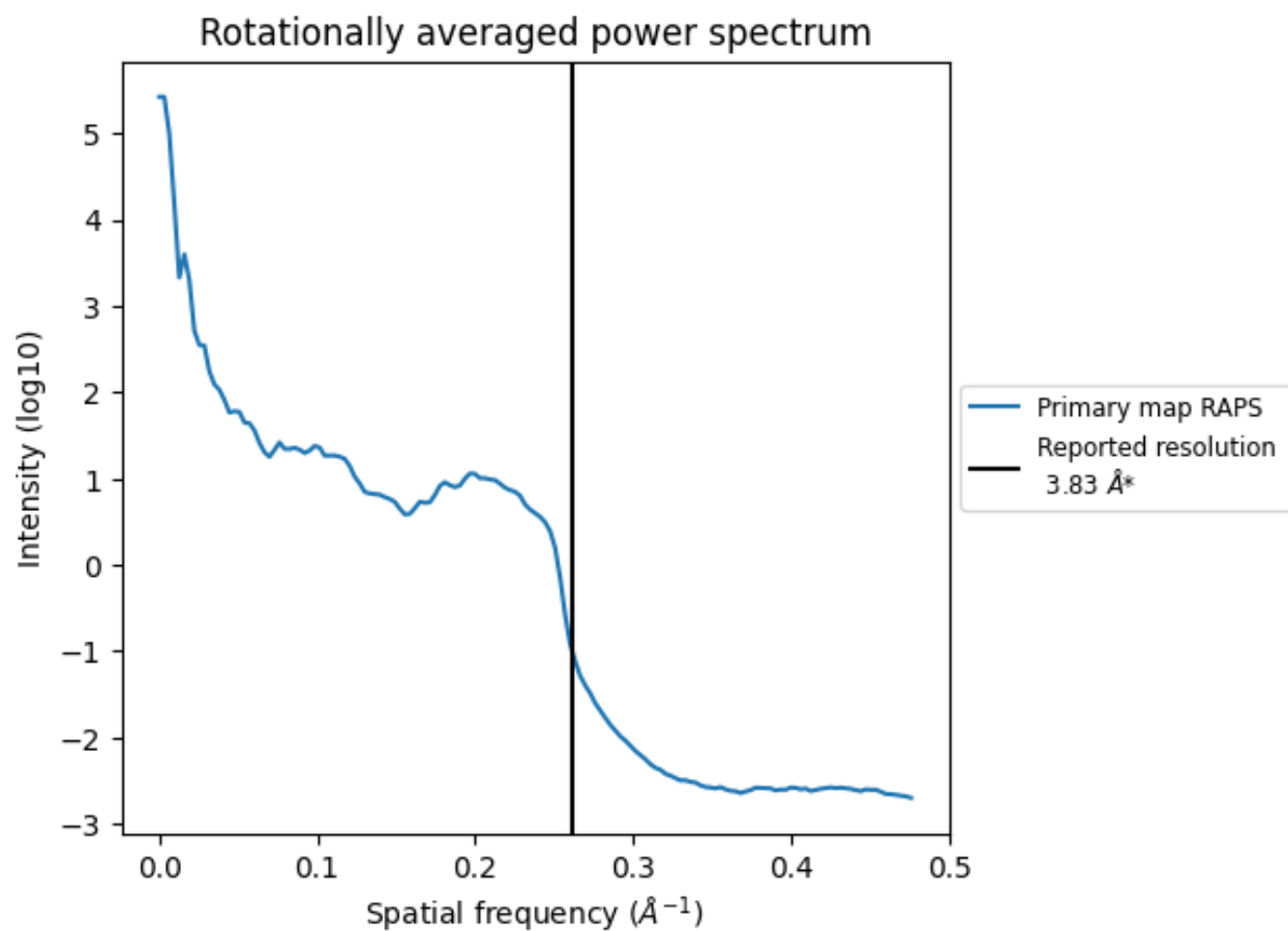
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 314 nm³; this corresponds to an approximate mass of 284 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 0.261 Å⁻¹

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

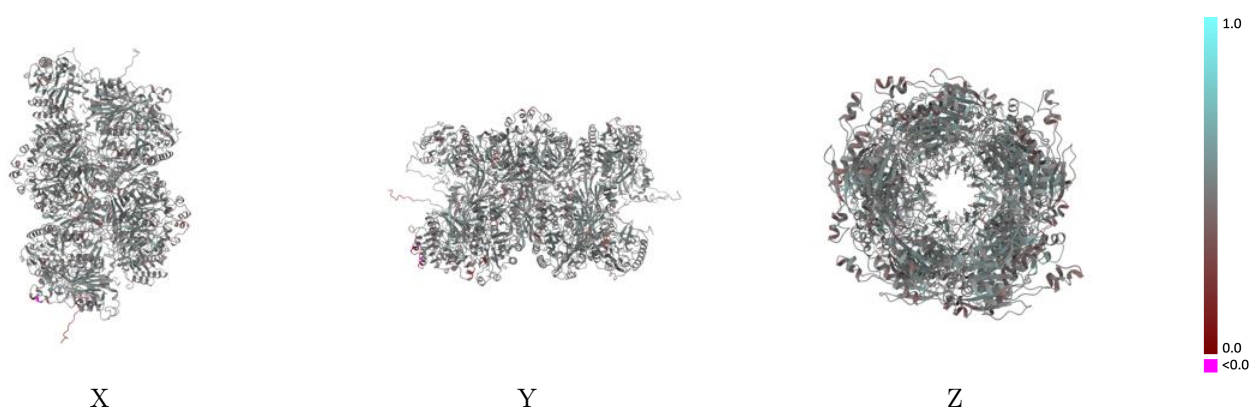
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-17409 and PDB model 8P4I. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)

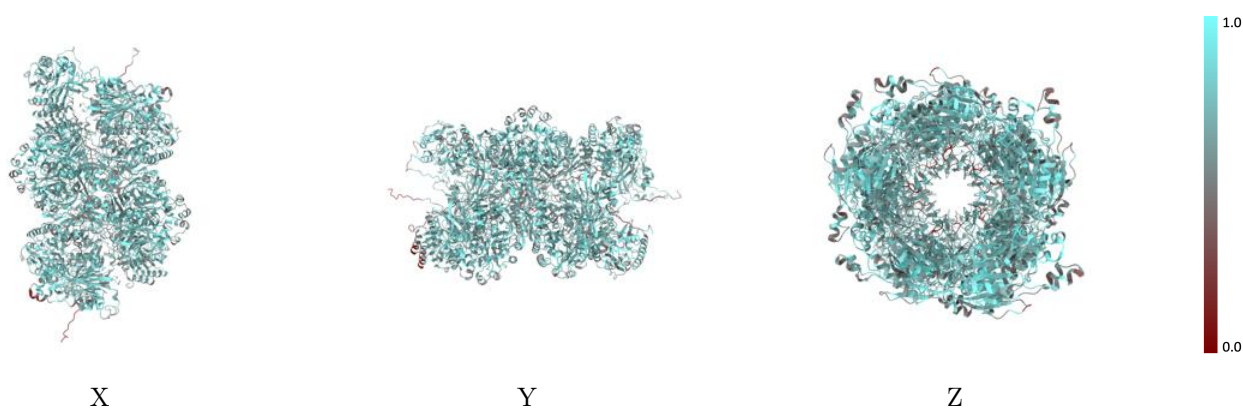
This section was not generated.

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



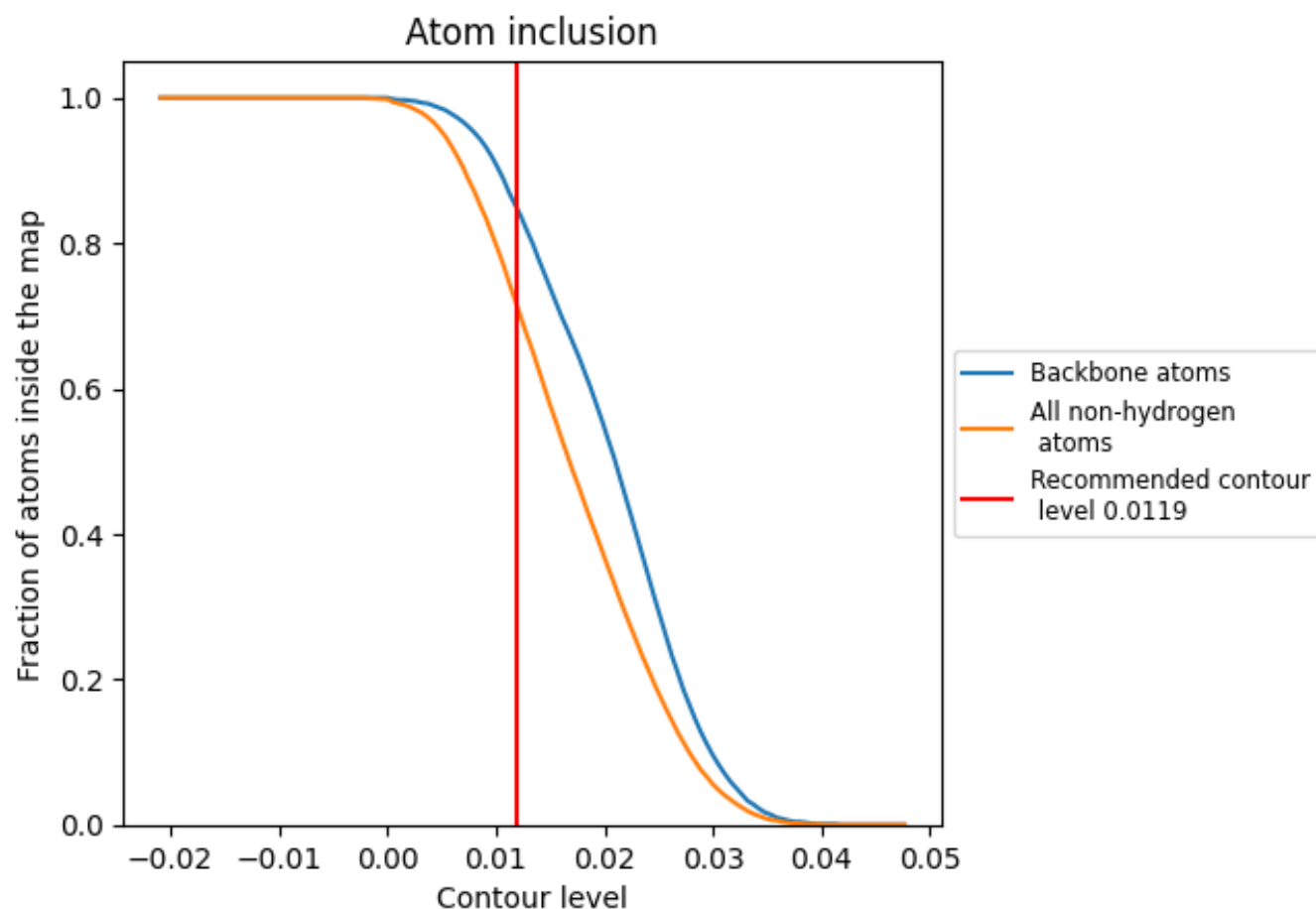
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0119).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 72% 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 (0.0119) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7160	0.4790
B	0.7160	0.4840
D	0.7120	0.4840
F	0.7200	0.4860
G	0.7180	0.4820
H	0.7270	0.4870
I	0.7210	0.4830
J	0.7240	0.4830
K	0.7340	0.4800
L	0.7190	0.4820
M	0.7270	0.4780
N	0.7150	0.4820
O	0.7260	0.4800
P	0.7050	0.4780
Q	0.7200	0.4810
R	0.6620	0.4380
S	0.7230	0.4780
U	0.6970	0.4750

1.0

0.0

<0.0