



Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 05:38 pm GMT

PDB ID : 4BLF
EMDB ID : EMD-2339
Title : Variable internal flexibility characterizes the helical capsid formed by Agrobacterium VirE2 protein on single-stranded DNA.
Authors : Bharat, T.A.M.; Zbaida, D.; Eisenstein, M.; Frankenstein, Z.; Mehlman, T.; Weiner, L.; Sorzano, C.O.S.; Barak, Y.; Albeck, S.; Briggs, J.A.G.; Wolf, S.G.; Elbaum, M.
Deposited on : 2013-05-02
Resolution : 20.00 Å (reported)
Based on initial model : 3BTP

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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

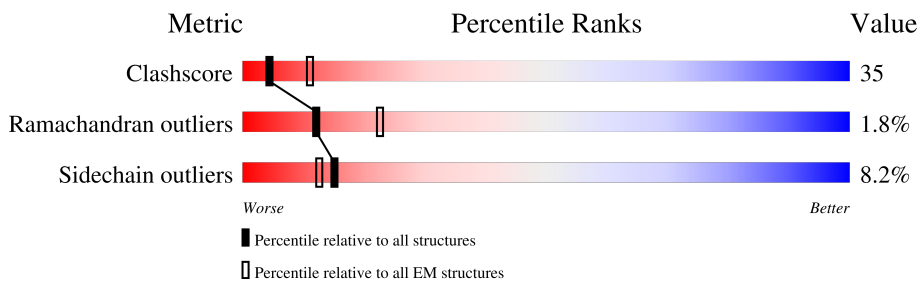
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 20.00 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	226	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1863 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 SINGLE-STRAND DNA-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	224	1863	1177	332	349	5	0	0

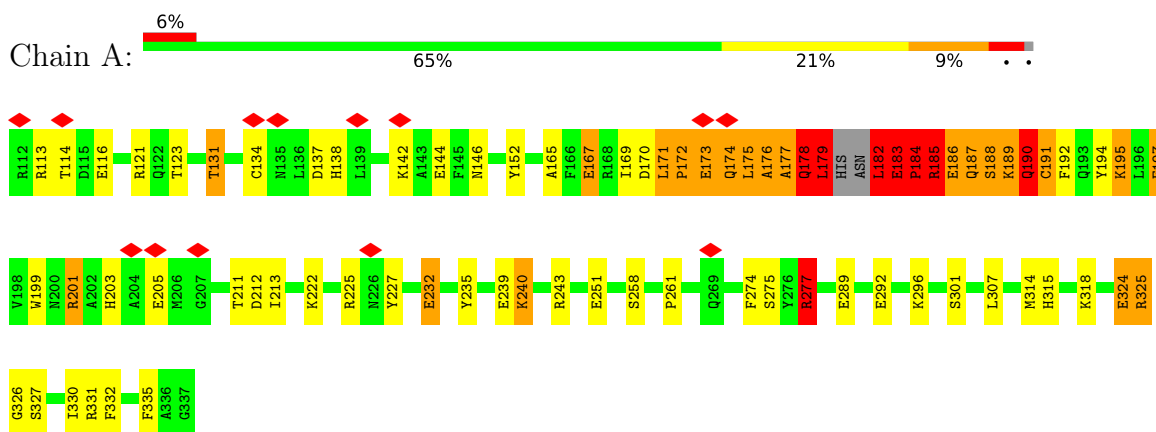
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	171	LEU	ILE	conflict	UNP P08062

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: SINGLE-STRAND DNA-BINDING PROTEIN



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of segments used	8019	Depositor
Resolution determination method	Not provided	
CTF correction method	PHASE-FLIPPING	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{Å}^2$)	20	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	50000	Depositor
Image detector	GENERIC TVIPS	Depositor
Maximum map value	0.054	Depositor
Minimum map value	-0.045	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	276.48, 276.48, 276.48	wwPDB
Map dimensions	64, 64, 64	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	4.32, 4.32, 4.32	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	3.00	137/1905 (7.2%)	1.34	16/2560 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (137) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	173	GLU	CG-CD	19.38	1.81	1.51
1	A	173	GLU	CD-OE2	18.99	1.46	1.25
1	A	186	GLU	CD-OE1	18.71	1.46	1.25
1	A	173	GLU	CD-OE1	17.70	1.45	1.25
1	A	188	SER	CA-CB	17.52	1.79	1.52
1	A	186	GLU	CG-CD	17.42	1.78	1.51
1	A	184	PRO	N-CD	17.28	1.72	1.47
1	A	173	GLU	CB-CG	17.09	1.84	1.52
1	A	185	ARG	NE-CZ	16.13	1.54	1.33
1	A	186	GLU	CD-OE2	15.91	1.43	1.25
1	A	183	GLU	CG-CD	15.13	1.74	1.51
1	A	185	ARG	CZ-NH2	14.81	1.52	1.33
1	A	177	ALA	N-CA	14.01	1.74	1.46
1	A	172	PRO	N-CA	13.91	1.70	1.47
1	A	173	GLU	N-CA	13.76	1.73	1.46
1	A	177	ALA	CA-CB	13.68	1.81	1.52
1	A	185	ARG	N-CA	13.65	1.73	1.46
1	A	179	LEU	N-CA	13.48	1.73	1.46
1	A	185	ARG	CD-NE	13.34	1.69	1.46
1	A	174	GLN	CG-CD	13.16	1.81	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	185	ARG	C-O	13.06	1.48	1.23
1	A	172	PRO	CA-C	12.96	1.78	1.52
1	A	183	GLU	CD-OE1	12.61	1.39	1.25
1	A	191	CYS	CB-SG	12.44	2.03	1.82
1	A	178	GLN	CG-CD	12.38	1.79	1.51
1	A	187	GLN	CG-CD	12.34	1.79	1.51
1	A	184	PRO	CA-C	12.30	1.77	1.52
1	A	183	GLU	CB-CG	12.27	1.75	1.52
1	A	167	GLU	C-N	12.00	1.61	1.34
1	A	176	ALA	N-CA	11.83	1.70	1.46
1	A	189	LYS	CD-CE	11.82	1.80	1.51
1	A	190	GLN	N-CA	11.62	1.69	1.46
1	A	172	PRO	N-CD	11.45	1.63	1.47
1	A	178	GLN	CA-CB	11.37	1.78	1.53
1	A	175	LEU	CA-CB	11.29	1.79	1.53
1	A	186	GLU	N-CA	11.13	1.68	1.46
1	A	174	GLN	CA-CB	11.02	1.78	1.53
1	A	183	GLU	CA-C	11.01	1.81	1.52
1	A	184	PRO	CA-CB	10.82	1.75	1.53
1	A	189	LYS	C-O	10.82	1.44	1.23
1	A	183	GLU	CD-OE2	10.80	1.37	1.25
1	A	183	GLU	CA-CB	10.49	1.77	1.53
1	A	177	ALA	C-O	10.44	1.43	1.23
1	A	176	ALA	CA-C	10.43	1.80	1.52
1	A	188	SER	N-CA	10.42	1.67	1.46
1	A	189	LYS	CA-C	10.31	1.79	1.52
1	A	187	GLN	C-O	10.28	1.42	1.23
1	A	182	LEU	C-N	10.27	1.57	1.34
1	A	190	GLN	CA-CB	10.06	1.76	1.53
1	A	190	GLN	C-O	10.01	1.42	1.23
1	A	173	GLU	C-O	9.92	1.42	1.23
1	A	174	GLN	C-N	9.74	1.56	1.34
1	A	182	LEU	N-CA	9.52	1.65	1.46
1	A	179	LEU	CA-CB	9.51	1.75	1.53
1	A	188	SER	C-O	9.42	1.41	1.23
1	A	174	GLN	CB-CG	9.35	1.77	1.52
1	A	176	ALA	C-N	9.35	1.55	1.34
1	A	175	LEU	CA-C	9.27	1.77	1.52
1	A	177	ALA	C-N	9.21	1.55	1.34
1	A	186	GLU	C-O	9.20	1.40	1.23
1	A	189	LYS	CE-NZ	8.99	1.71	1.49
1	A	178	GLN	C-N	8.93	1.54	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	184	PRO	C-N	8.81	1.54	1.34
1	A	185	ARG	CB-CG	8.81	1.76	1.52
1	A	174	GLN	C-O	8.77	1.40	1.23
1	A	172	PRO	CG-CD	8.62	1.79	1.50
1	A	178	GLN	CA-C	8.62	1.75	1.52
1	A	191	CYS	CA-C	8.56	1.75	1.52
1	A	173	GLU	CA-CB	8.55	1.72	1.53
1	A	179	LEU	CA-C	8.35	1.74	1.52
1	A	324	GLU	CG-CD	8.28	1.64	1.51
1	A	175	LEU	N-CA	8.27	1.62	1.46
1	A	189	LYS	N-CA	8.26	1.62	1.46
1	A	185	ARG	CA-C	8.23	1.74	1.52
1	A	170	ASP	N-CA	8.08	1.62	1.46
1	A	190	GLN	CG-CD	8.06	1.69	1.51
1	A	185	ARG	CA-CB	7.98	1.71	1.53
1	A	179	LEU	CB-CG	7.96	1.75	1.52
1	A	175	LEU	CG-CD2	7.90	1.81	1.51
1	A	187	GLN	CA-C	7.87	1.73	1.52
1	A	190	GLN	CD-NE2	7.85	1.52	1.32
1	A	174	GLN	CD-OE1	7.71	1.41	1.24
1	A	191	CYS	C-O	7.70	1.38	1.23
1	A	183	GLU	C-N	7.62	1.48	1.34
1	A	187	GLN	CA-CB	7.31	1.70	1.53
1	A	201	ARG	C-N	-7.29	1.17	1.34
1	A	188	SER	CB-OG	7.15	1.51	1.42
1	A	194	TYR	CD2-CE2	7.12	1.50	1.39
1	A	189	LYS	CB-CG	7.09	1.71	1.52
1	A	211	THR	C-N	6.98	1.50	1.34
1	A	195	LYS	C-N	6.96	1.50	1.34
1	A	175	LEU	CG-CD1	6.91	1.77	1.51
1	A	183	GLU	N-CA	6.90	1.60	1.46
1	A	182	LEU	CG-CD2	6.90	1.77	1.51
1	A	188	SER	CA-C	6.85	1.70	1.52
1	A	182	LEU	CA-CB	6.79	1.69	1.53
1	A	324	GLU	CB-CG	6.77	1.65	1.52
1	A	178	GLN	C-O	6.75	1.36	1.23
1	A	165	ALA	CA-CB	6.74	1.66	1.52
1	A	178	GLN	CD-NE2	6.69	1.49	1.32
1	A	176	ALA	C-O	6.46	1.35	1.23
1	A	170	ASP	CG-OD2	6.44	1.40	1.25
1	A	171	LEU	CB-CG	6.34	1.71	1.52
1	A	116	GLU	CG-CD	6.25	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	185	ARG	CZ-NH1	6.20	1.41	1.33
1	A	123	THR	C-N	6.18	1.44	1.33
1	A	172	PRO	C-O	6.06	1.35	1.23
1	A	171	LEU	CA-CB	6.02	1.67	1.53
1	A	170	ASP	CB-CG	5.82	1.64	1.51
1	A	185	ARG	CG-CD	5.81	1.66	1.51
1	A	175	LEU	CB-CG	5.77	1.69	1.52
1	A	324	GLU	CD-OE2	5.77	1.31	1.25
1	A	235	TYR	C-N	5.77	1.47	1.34
1	A	258	SER	CB-OG	5.74	1.49	1.42
1	A	187	GLN	CB-CG	5.73	1.68	1.52
1	A	194	TYR	CD1-CE1	5.70	1.48	1.39
1	A	175	LEU	C-O	5.68	1.34	1.23
1	A	194	TYR	CB-CG	5.65	1.60	1.51
1	A	171	LEU	CA-C	5.63	1.67	1.52
1	A	197	GLU	C-N	-5.58	1.21	1.34
1	A	186	GLU	CA-CB	5.57	1.66	1.53
1	A	191	CYS	C-N	-5.52	1.21	1.34
1	A	289	GLU	CG-CD	5.49	1.60	1.51
1	A	172	PRO	CA-CB	5.47	1.64	1.53
1	A	251	GLU	C-N	5.44	1.46	1.34
1	A	178	GLN	CD-OE1	5.42	1.35	1.24
1	A	172	PRO	CB-CG	5.42	1.77	1.50
1	A	185	ARG	C-N	5.41	1.46	1.34
1	A	184	PRO	C-O	5.36	1.33	1.23
1	A	318	LYS	CD-CE	5.32	1.64	1.51
1	A	227	TYR	C-N	5.32	1.46	1.34
1	A	197	GLU	CD-OE1	5.20	1.31	1.25
1	A	174	GLN	CA-C	5.20	1.66	1.52
1	A	182	LEU	CA-C	5.18	1.66	1.52
1	A	232	GLU	CG-CD	5.13	1.59	1.51
1	A	187	GLN	CD-OE1	5.09	1.35	1.24
1	A	170	ASP	C-N	5.08	1.45	1.34

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	ILE	O-C-N	-15.98	97.12	122.70
1	A	169	ILE	CA-C-N	10.26	139.78	117.20
1	A	185	ARG	NE-CZ-NH2	9.91	125.25	120.30
1	A	179	LEU	CA-CB-CG	8.46	134.75	115.30
1	A	183	GLU	N-CA-C	7.82	132.11	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	ARG	NE-CZ-NH1	-7.79	116.40	120.30
1	A	113	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	A	187	GLN	O-C-N	6.73	133.47	122.70
1	A	183	GLU	CA-C-N	6.44	135.14	117.10
1	A	201	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	A	183	GLU	O-C-N	-6.19	109.35	121.10
1	A	191	CYS	O-C-N	6.16	132.56	122.70
1	A	243	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	A	177	ALA	O-C-N	5.78	131.94	122.70
1	A	277	ARG	NE-CZ-NH2	5.69	123.15	120.30
1	A	182	LEU	CA-C-O	-5.03	109.53	120.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	171	LEU	Mainchain
1	A	182	LEU	Peptide

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	1863	0	1810	129	0
All	All	1863	0	1810	129	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 35.

All (129) 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:A:184:PRO:CA	1:A:184:PRO:CB	1.75	1.62
1:A:178:GLN:CA	1:A:178:GLN:CB	1.79	1.61
1:A:174:GLN:CA	1:A:174:GLN:CB	1.78	1.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:GLU:CB	1:A:183:GLU:CG	1.75	1.60
1:A:175:LEU:CA	1:A:175:LEU:CB	1.79	1.59
1:A:172:PRO:CD	1:A:172:PRO:CG	1.79	1.59
1:A:179:LEU:CB	1:A:179:LEU:CG	1.75	1.57
1:A:175:LEU:CG	1:A:175:LEU:CD1	1.77	1.57
1:A:177:ALA:CA	1:A:177:ALA:CB	1.81	1.56
1:A:179:LEU:CB	1:A:179:LEU:CA	1.75	1.56
1:A:183:GLU:CB	1:A:183:GLU:CA	1.77	1.56
1:A:185:ARG:CB	1:A:185:ARG:CG	1.76	1.56
1:A:190:GLN:CA	1:A:190:GLN:CB	1.76	1.56
1:A:189:LYS:CD	1:A:189:LYS:CE	1.80	1.55
1:A:172:PRO:CG	1:A:172:PRO:CB	1.77	1.55
1:A:174:GLN:CB	1:A:174:GLN:CG	1.77	1.55
1:A:173:GLU:CB	1:A:173:GLU:CG	1.84	1.55
1:A:182:LEU:CD2	1:A:182:LEU:CG	1.77	1.55
1:A:188:SER:CA	1:A:188:SER:CB	1.79	1.54
1:A:191:CYS:CA	1:A:191:CYS:C	1.75	1.54
1:A:176:ALA:CA	1:A:176:ALA:N	1.70	1.52
1:A:184:PRO:CA	1:A:184:PRO:C	1.77	1.52
1:A:178:GLN:CA	1:A:178:GLN:C	1.75	1.52
1:A:183:GLU:CG	1:A:183:GLU:CD	1.74	1.52
1:A:175:LEU:CA	1:A:175:LEU:C	1.77	1.52
1:A:175:LEU:CG	1:A:175:LEU:CD2	1.81	1.52
1:A:185:ARG:CD	1:A:185:ARG:NE	1.69	1.51
1:A:184:PRO:N	1:A:184:PRO:CD	1.72	1.51
1:A:189:LYS:CE	1:A:189:LYS:NZ	1.71	1.51
1:A:185:ARG:N	1:A:185:ARG:CA	1.73	1.51
1:A:190:GLN:CA	1:A:190:GLN:N	1.69	1.51
1:A:176:ALA:CA	1:A:176:ALA:C	1.80	1.51
1:A:179:LEU:CA	1:A:179:LEU:N	1.73	1.51
1:A:172:PRO:CA	1:A:172:PRO:N	1.70	1.50
1:A:178:GLN:CD	1:A:178:GLN:CG	1.79	1.50
1:A:186:GLU:N	1:A:186:GLU:CA	1.68	1.50
1:A:179:LEU:CA	1:A:179:LEU:C	1.74	1.50
1:A:189:LYS:CA	1:A:189:LYS:C	1.79	1.50
1:A:173:GLU:N	1:A:173:GLU:CA	1.73	1.49
1:A:172:PRO:CA	1:A:172:PRO:C	1.78	1.49
1:A:177:ALA:CA	1:A:177:ALA:N	1.74	1.48
1:A:187:GLN:CD	1:A:187:GLN:CG	1.79	1.47
1:A:191:CYS:CB	1:A:191:CYS:SG	2.03	1.46
1:A:186:GLU:CD	1:A:186:GLU:CG	1.78	1.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:GLN:CG	1:A:174:GLN:CD	1.81	1.45
1:A:183:GLU:CA	1:A:183:GLU:C	1.81	1.44
1:A:173:GLU:CG	1:A:173:GLU:CD	1.81	1.44
1:A:277:ARG:HH11	1:A:277:ARG:CG	1.62	1.11
1:A:325:ARG:HH11	1:A:325:ARG:CG	1.66	1.07
1:A:167:GLU:OE1	1:A:195:LYS:NZ	1.88	1.05
1:A:325:ARG:HH11	1:A:325:ARG:HG3	0.86	1.01
1:A:325:ARG:HG3	1:A:325:ARG:NH1	1.69	0.97
1:A:277:ARG:HG2	1:A:277:ARG:NH1	1.63	0.97
1:A:277:ARG:HH11	1:A:277:ARG:HG2	0.78	0.94
1:A:315:HIS:HD2	1:A:331:ARG:HH12	1.15	0.90
1:A:315:HIS:CD2	1:A:331:ARG:HH12	1.90	0.88
1:A:191:CYS:CA	1:A:192:PHE:N	2.39	0.85
1:A:137:ASP:OD1	1:A:138:HIS:HD2	1.62	0.82
1:A:183:GLU:C	1:A:183:GLU:HA	2.00	0.81
1:A:172:PRO:CG	1:A:172:PRO:CA	2.65	0.74
1:A:152:TYR:OH	1:A:203:HIS:HE1	1.76	0.69
1:A:189:LYS:CE	1:A:189:LYS:CG	2.70	0.68
1:A:121:ARG:HH12	1:A:131:THR:HG22	1.57	0.68
1:A:184:PRO:CB	1:A:184:PRO:N	2.50	0.66
1:A:178:GLN:CB	1:A:178:GLN:N	2.57	0.65
1:A:182:LEU:CD2	1:A:182:LEU:CB	2.75	0.64
1:A:172:PRO:CD	1:A:172:PRO:CA	2.76	0.63
1:A:184:PRO:CA	1:A:184:PRO:CD	2.63	0.63
1:A:146:ASN:HD21	1:A:212:ASP:H	1.47	0.63
1:A:175:LEU:C	1:A:176:ALA:CA	2.63	0.62
1:A:138:HIS:HE1	1:A:144:GLU:OE1	1.82	0.62
1:A:137:ASP:OD1	1:A:138:HIS:CD2	2.51	0.61
1:A:172:PRO:CD	1:A:172:PRO:CB	2.79	0.60
1:A:184:PRO:CA	1:A:184:PRO:CG	2.74	0.60
1:A:201:ARG:O	1:A:205:GLU:HG3	2.01	0.60
1:A:185:ARG:CG	1:A:185:ARG:CA	2.80	0.59
1:A:315:HIS:HD2	1:A:331:ARG:NH1	1.95	0.59
1:A:277:ARG:CD	1:A:332:PHE:O	2.51	0.58
1:A:239:GLU:HG2	1:A:240:LYS:HG3	1.86	0.58
1:A:179:LEU:CG	1:A:179:LEU:HB3	2.19	0.57
1:A:172:PRO:CG	1:A:172:PRO:N	2.66	0.56
1:A:189:LYS:C	1:A:190:GLN:CA	2.69	0.56
1:A:325:ARG:HD2	1:A:325:ARG:N	2.21	0.56
1:A:179:LEU:CA	1:A:179:LEU:HB3	2.19	0.55
1:A:179:LEU:CB	1:A:179:LEU:HG	2.18	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:THR:HB	1:A:134:CYS:HB3	1.88	0.55
1:A:174:GLN:CG	1:A:174:GLN:NE2	2.65	0.55
1:A:179:LEU:CA	1:A:179:LEU:HB2	2.19	0.54
1:A:172:PRO:CB	1:A:172:PRO:N	2.67	0.54
1:A:179:LEU:CB	1:A:179:LEU:CD2	2.80	0.53
1:A:296:LYS:HB2	1:A:301:SER:HA	1.90	0.53
1:A:190:GLN:CB	1:A:190:GLN:C	2.74	0.52
1:A:175:LEU:CB	1:A:175:LEU:CD1	2.83	0.52
1:A:179:LEU:CG	1:A:179:LEU:HB2	2.19	0.52
1:A:325:ARG:HD2	1:A:325:ARG:H	1.74	0.52
1:A:174:GLN:CB	1:A:174:GLN:HA	2.20	0.51
1:A:185:ARG:CB	1:A:185:ARG:CD	2.85	0.51
1:A:192:PHE:HE1	1:A:213:ILE:CD1	2.23	0.51
1:A:152:TYR:OH	1:A:203:HIS:CE1	2.62	0.50
1:A:277:ARG:HD3	1:A:332:PHE:O	2.11	0.50
1:A:175:LEU:CA	1:A:176:ALA:N	2.66	0.49
1:A:292:GLU:O	1:A:296:LYS:HG2	2.13	0.49
1:A:177:ALA:CB	1:A:177:ALA:C	2.72	0.47
1:A:199:TRP:CE2	1:A:203:HIS:NE2	2.82	0.47
1:A:315:HIS:CD2	1:A:331:ARG:NH1	2.73	0.47
1:A:326:GLY:O	1:A:330:ILE:HG13	2.13	0.47
1:A:176:ALA:N	1:A:176:ALA:CB	2.70	0.46
1:A:199:TRP:CZ2	1:A:203:HIS:NE2	2.83	0.46
1:A:121:ARG:NH1	1:A:131:THR:HG22	2.30	0.46
1:A:192:PHE:HE1	1:A:213:ILE:HD12	1.80	0.46
1:A:184:PRO:O	1:A:186:GLU:N	2.50	0.44
1:A:325:ARG:CG	1:A:325:ARG:NH1	2.40	0.44
1:A:277:ARG:HD3	1:A:335:PHE:HB2	2.00	0.43
1:A:182:LEU:CD2	1:A:182:LEU:CD1	2.87	0.43
1:A:175:LEU:CD1	1:A:175:LEU:CD2	2.93	0.43
1:A:178:GLN:O	1:A:179:LEU:HB2	2.19	0.43
1:A:296:LYS:HB3	1:A:296:LYS:HE2	1.75	0.43
1:A:324:GLU:HB3	1:A:327:SER:OG	2.19	0.43
1:A:176:ALA:C	1:A:176:ALA:CB	2.78	0.42
1:A:179:LEU:CB	1:A:179:LEU:CD1	2.87	0.42
1:A:146:ASN:ND2	1:A:212:ASP:H	2.14	0.42
1:A:174:GLN:CB	1:A:174:GLN:N	2.70	0.42
1:A:191:CYS:CA	1:A:191:CYS:SG	3.02	0.42
1:A:277:ARG:CG	1:A:277:ARG:NH1	2.39	0.41
1:A:189:LYS:C	1:A:189:LYS:CB	2.78	0.41
1:A:191:CYS:C	1:A:191:CYS:CB	2.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:GLU:N	1:A:187:GLN:N	2.69	0.40
1:A:261:PRO:HG2	1:A:274:PHE:HB3	2.03	0.40
1:A:187:GLN:CG	1:A:187:GLN:NE2	2.71	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	A	220/226 (97%)	210 (96%)	6 (3%)	4 (2%)	8 40

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	ARG
1	A	178	GLN
1	A	183	GLU
1	A	184	PRO

5.3.2 Protein sidechains [i](#)

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	195/197 (99%)	179 (92%)	16 (8%)	11 34

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	THR
1	A	142	LYS
1	A	178	GLN
1	A	179	LEU
1	A	182	LEU
1	A	190	GLN
1	A	197	GLU
1	A	222	LYS
1	A	225	ARG
1	A	232	GLU
1	A	240	LYS
1	A	275	SER
1	A	277	ARG
1	A	307	LEU
1	A	314	MET
1	A	325	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	HIS
1	A	146	ASN
1	A	174	GLN
1	A	200	ASN
1	A	203	HIS
1	A	270	ASN
1	A	315	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	167:GLU	C	168:ARG	N	1.61
1	A	201:ARG	C	202:ALA	N	1.17

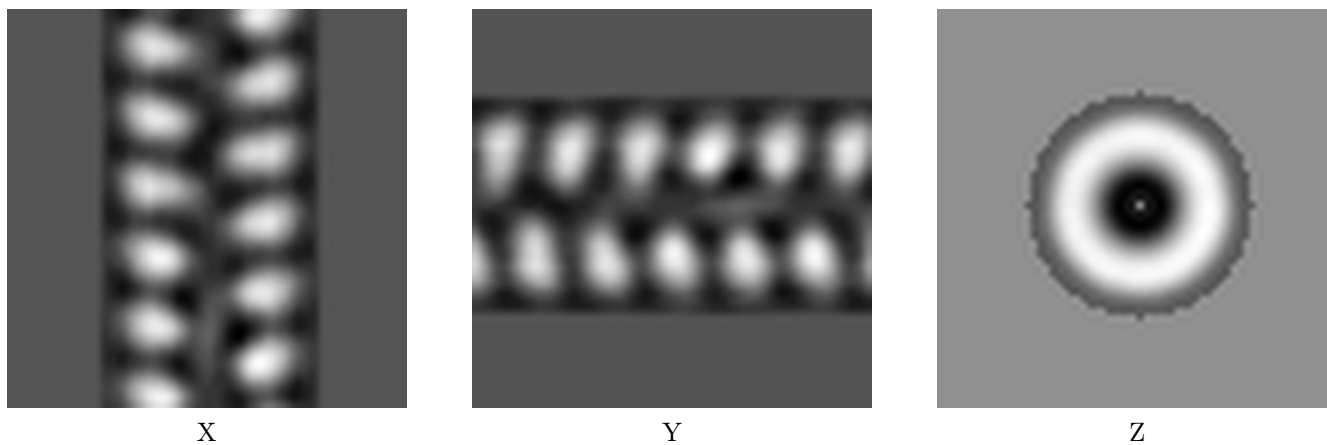
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2339. 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](#)

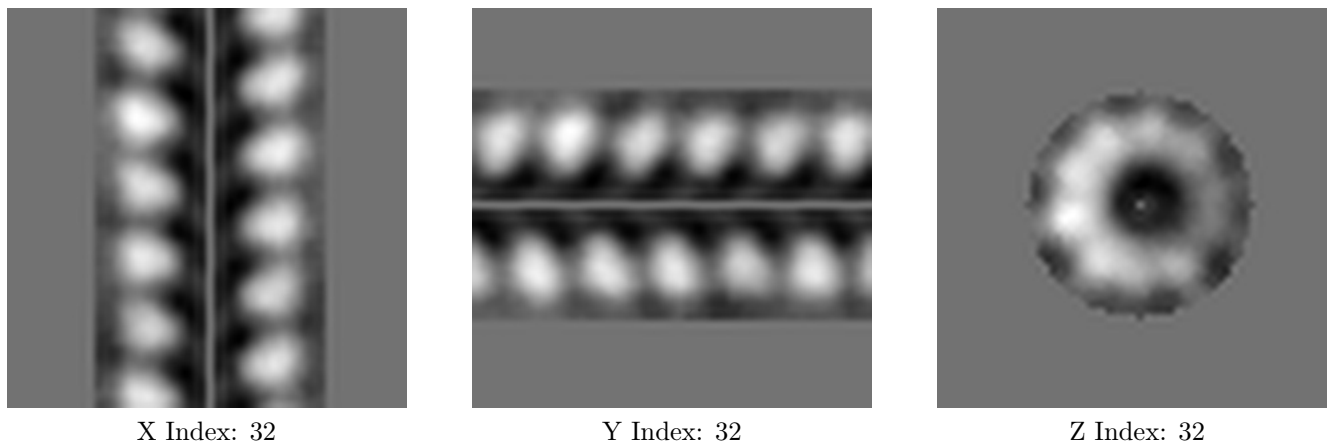
6.1.1 Primary map



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

6.2 Central slices [i](#)

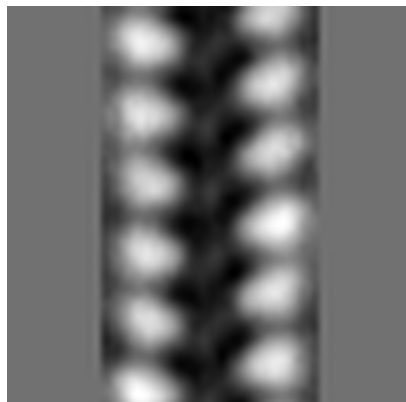
6.2.1 Primary map



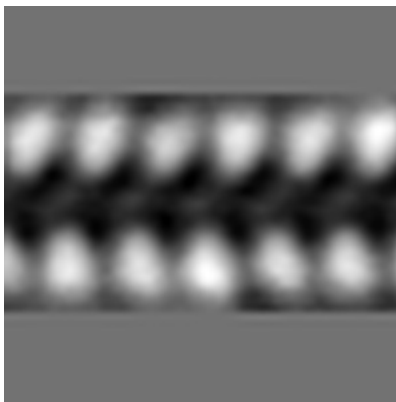
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

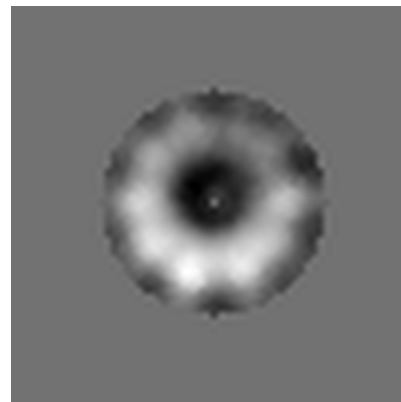
6.3.1 Primary map



X Index: 34



Y Index: 30



Z Index: 12

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

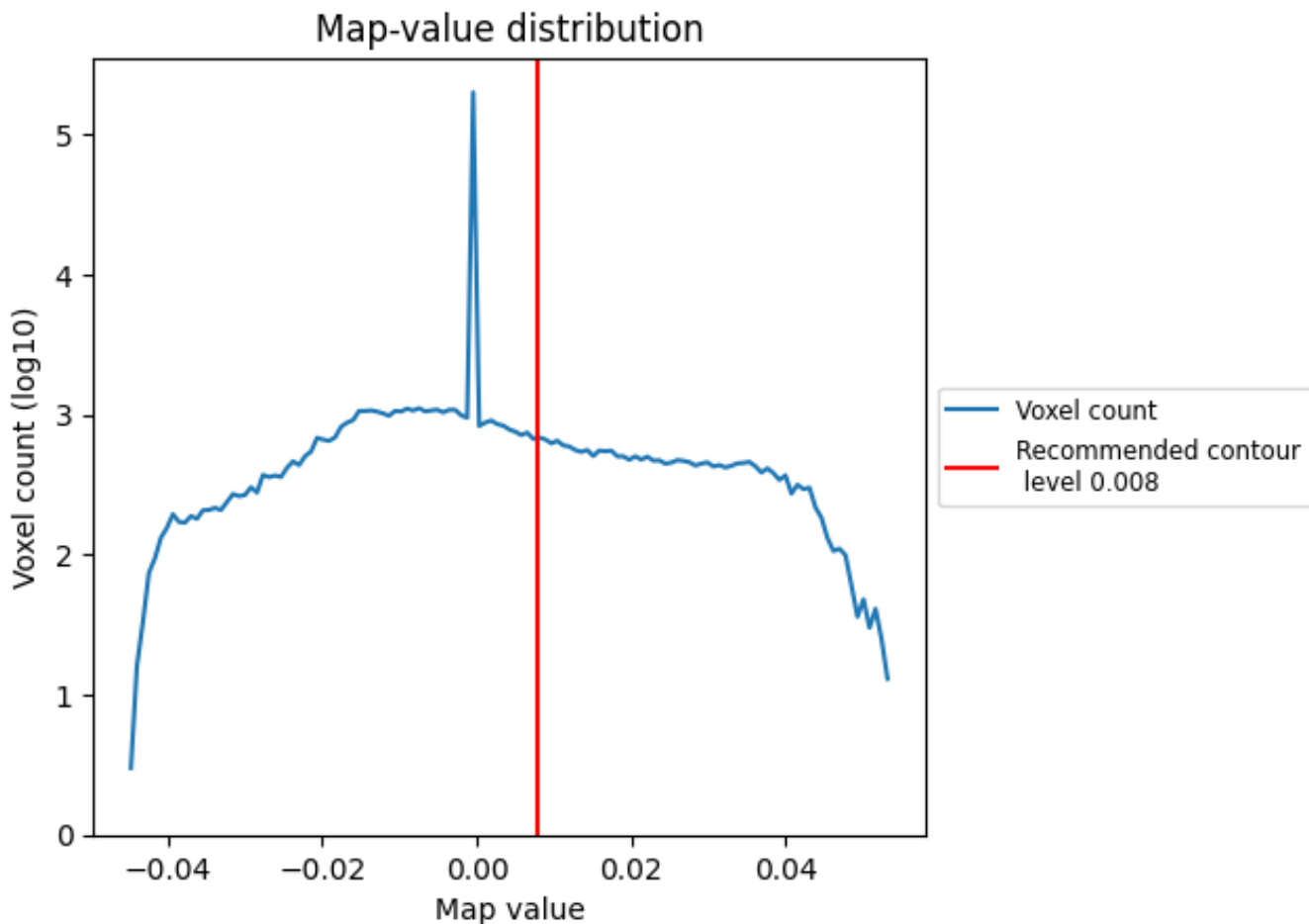
6.5 Mask visualisation

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

7 Map analysis [i](#)

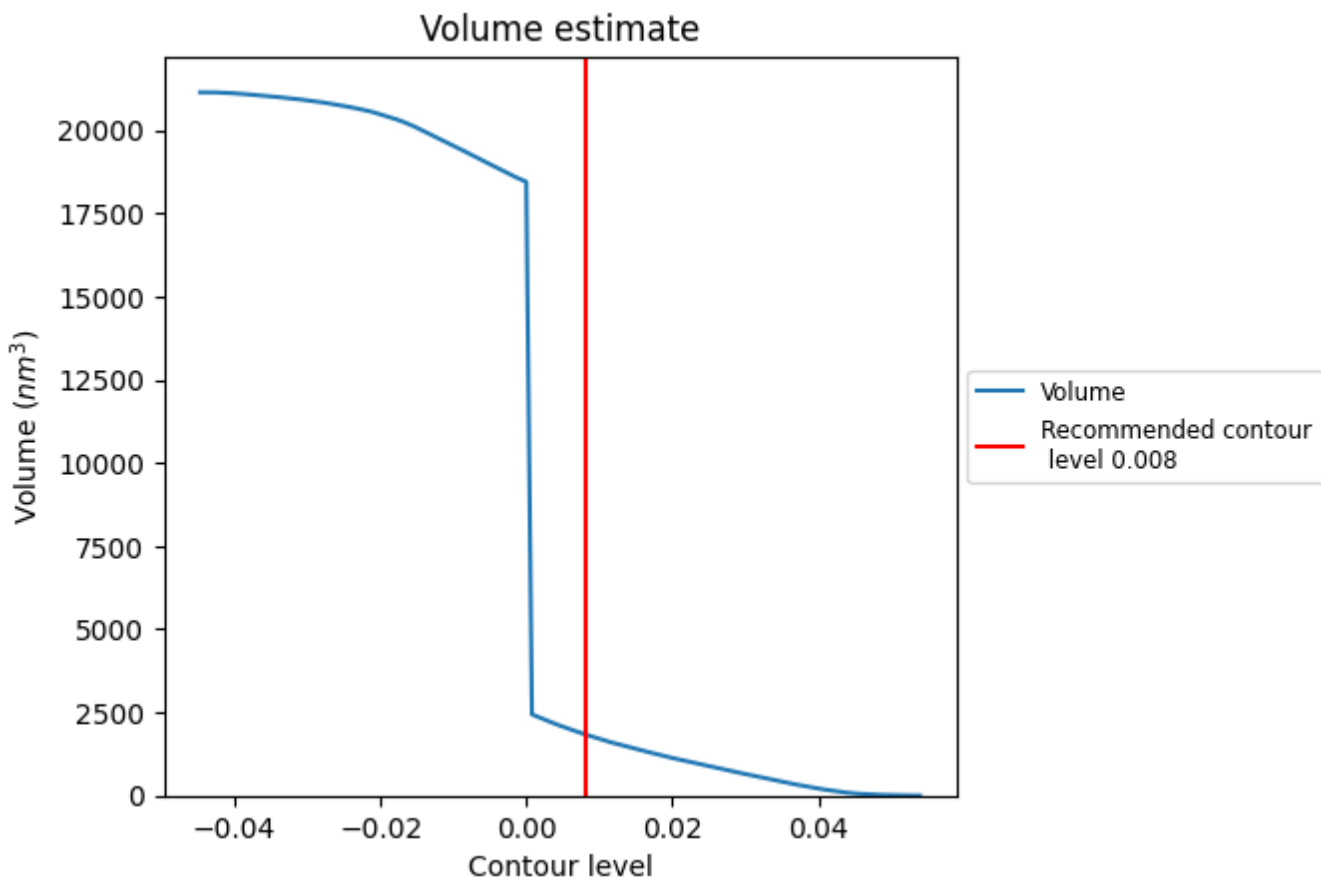
This section contains the results of statistical analysis of the map.

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.

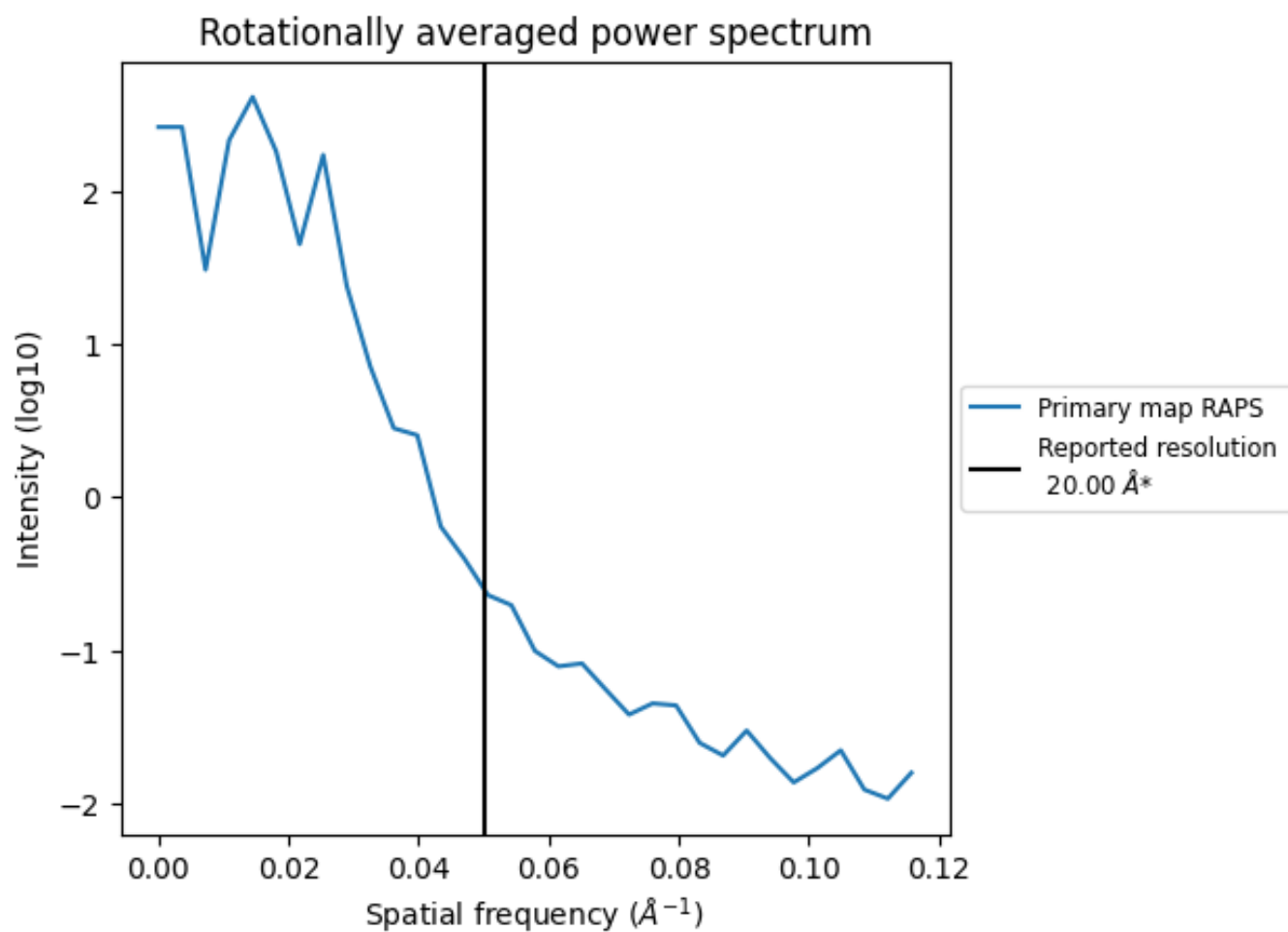
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1843 nm³; this corresponds to an approximate mass of 1665 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.050\AA^{-1}

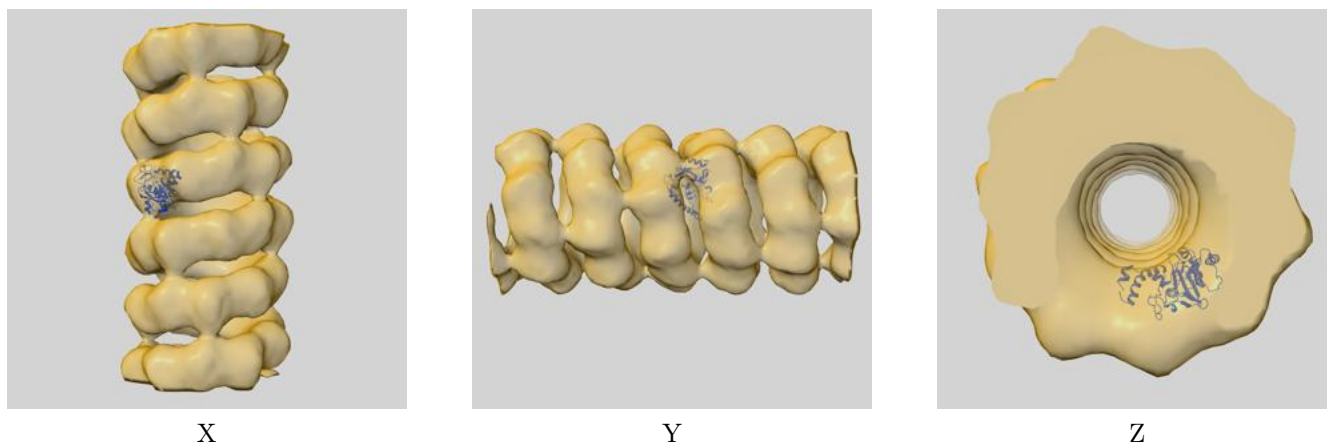
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

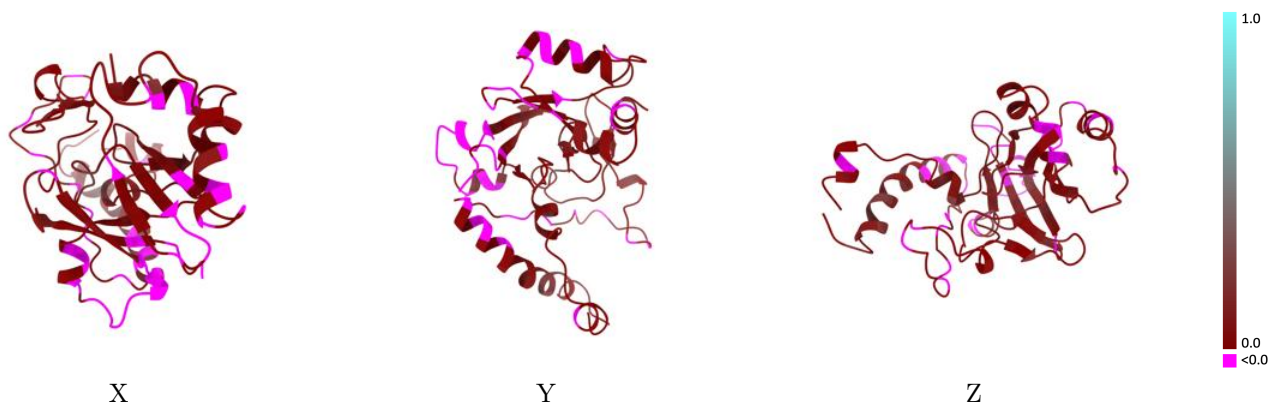
This section contains information regarding the fit between EMDB map EMD-2339 and PDB model 4BLF. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)



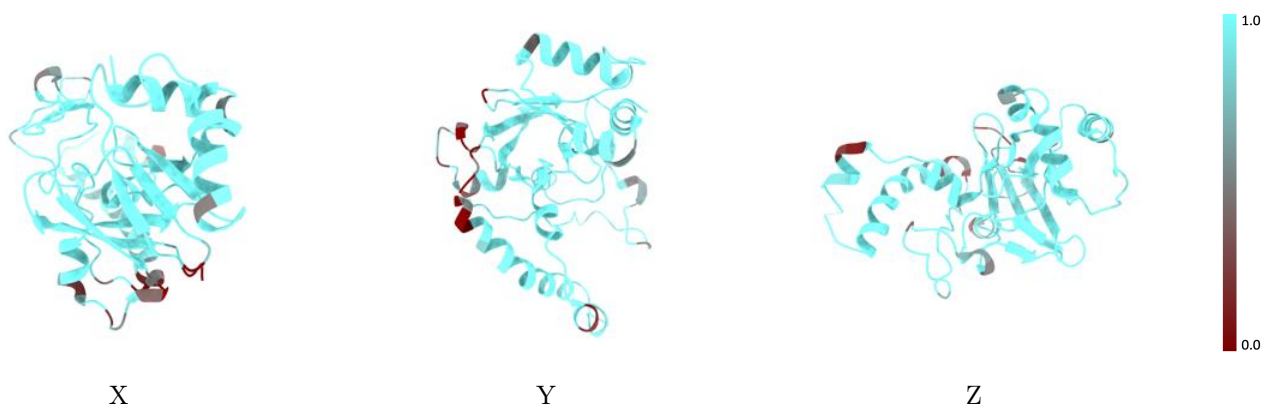
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



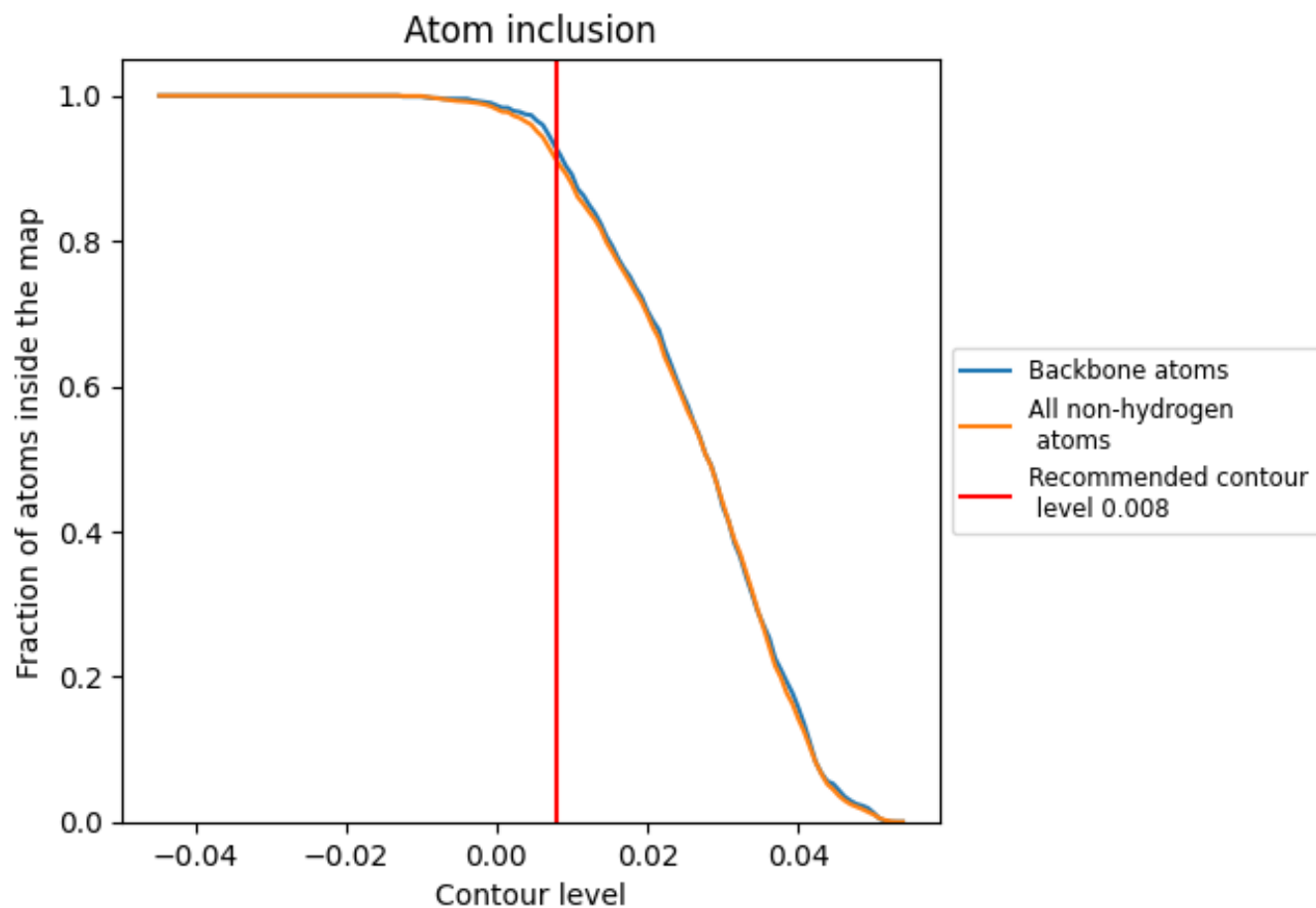
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.008).





9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9104	 0.0440
A	 0.9104	 0.0440

