



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 03:27 PM UTC

PDB ID : 6H3N / pdb_00006h3n
EMDB ID : EMD-0136
Title : Structure of VgrG1 in the Type VI secretion VgrG1-Tse6-EF-Tu complex embedded in lipid nanodiscs
Authors : Quentin, D.; Raunser, S.
Deposited on : 2018-07-19
Resolution : 3.25 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

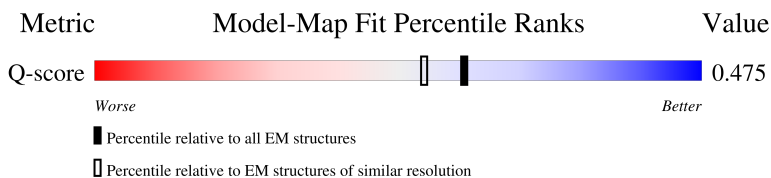
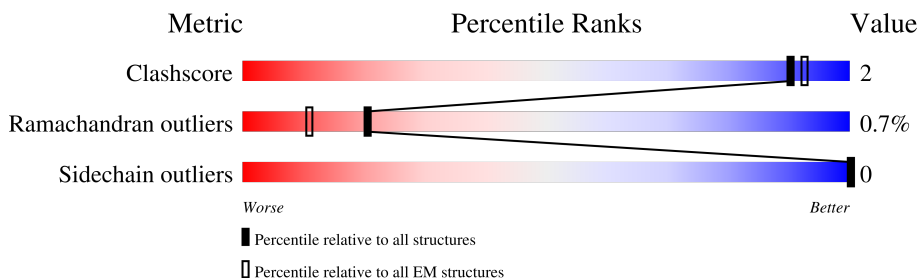
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.25 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	14599 (2.75 - 3.75)

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	643	14% 89% 8% .
1	B	643	15% 89% 8% .
1	C	643	14% 89% 8% .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 29319 atoms, of which 14388 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.

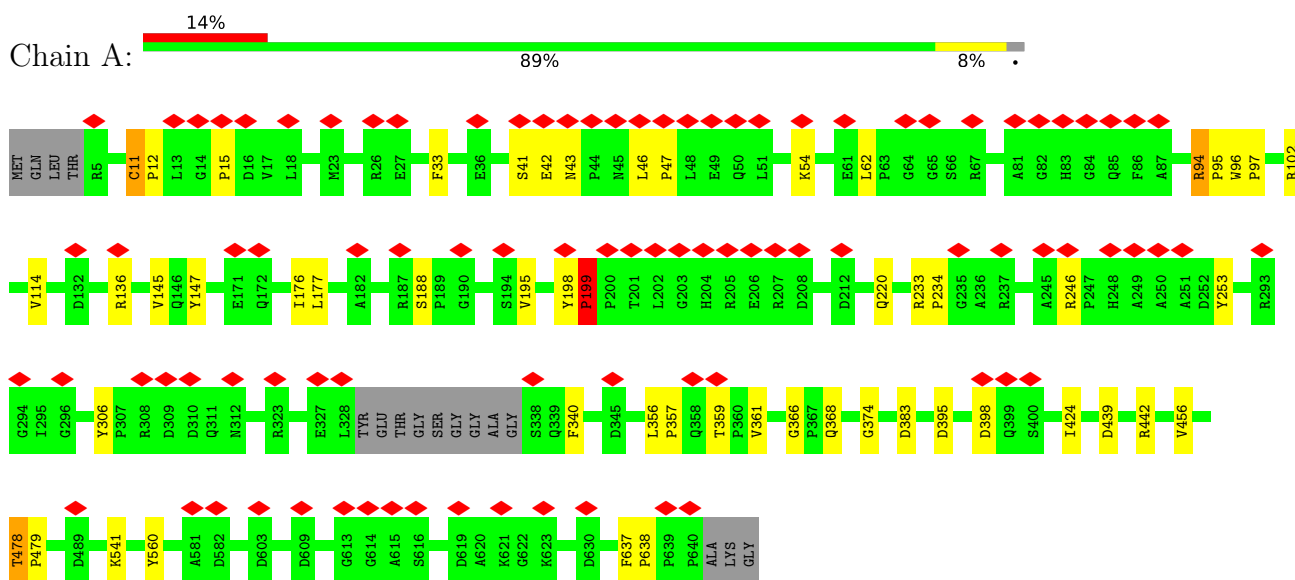
- Molecule 1 is a protein called VgrG1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	627	Total	C	H	N	O	S	0	0
			9773	3113	4796	910	939	15		
1	B	627	Total	C	H	N	O	S	0	0
			9773	3113	4796	910	939	15		
1	C	627	Total	C	H	N	O	S	0	0
			9773	3113	4796	910	939	15		

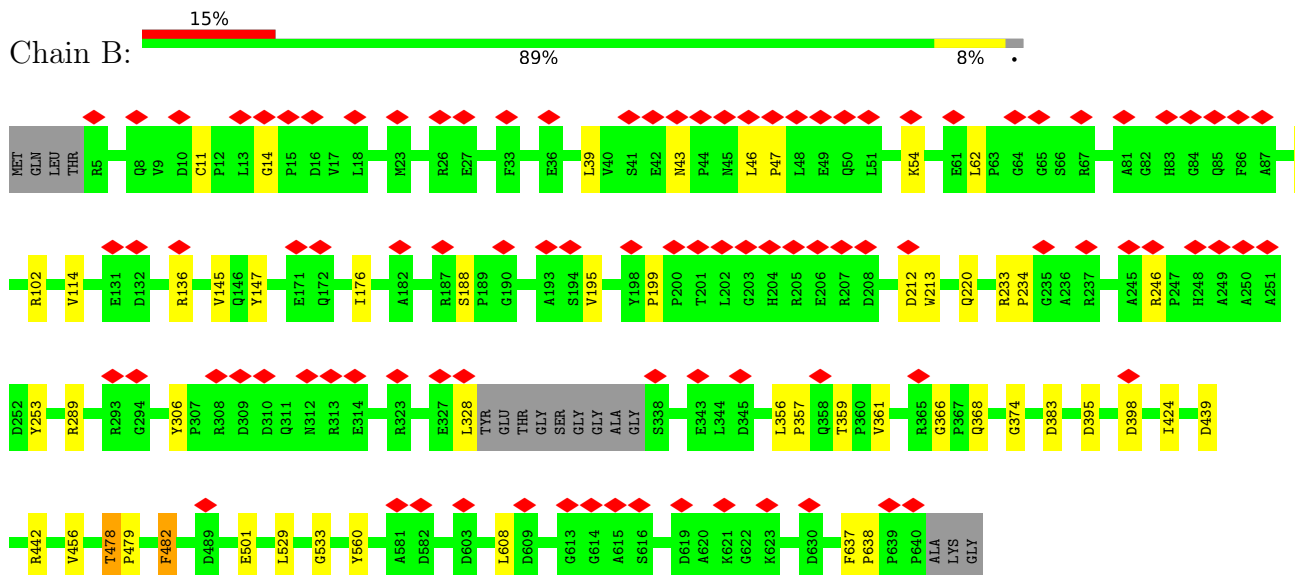
3 Residue-property plots [i](#)

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.

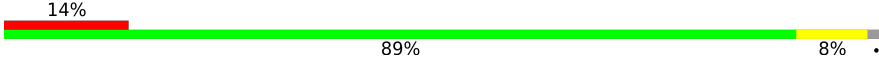
- Molecule 1: VgrG1

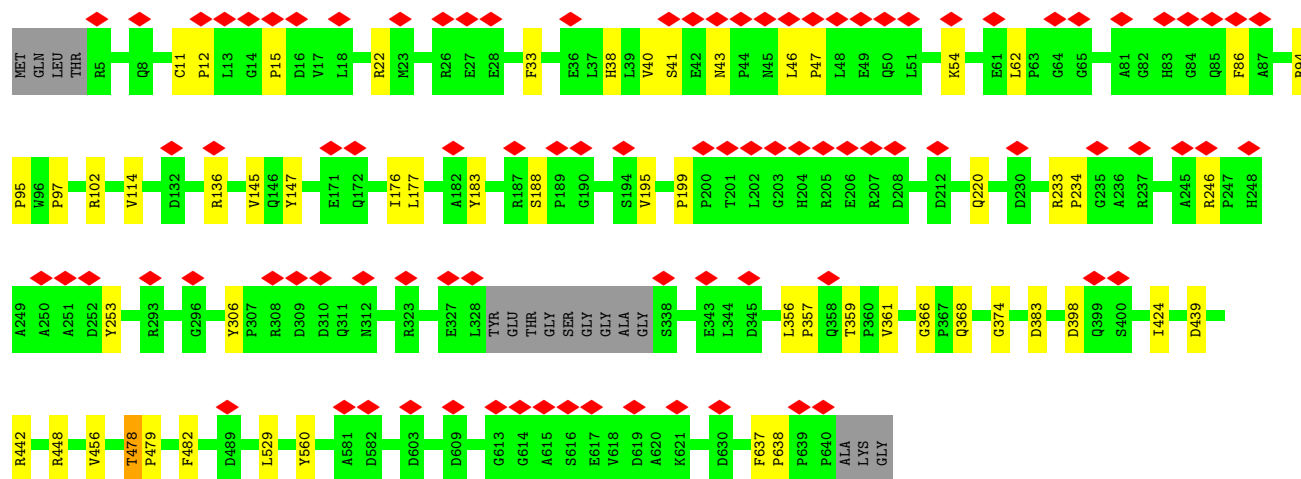


- Molecule 1: VgrG1



- Molecule 1: VgrG1

Chain C:  14% 89% 8%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	72000	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 ($e^-/\text{\AA}^2$)	91	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	59000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.127	Depositor
Minimum map value	-0.069	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.027	Depositor
Map size (Å)	396.0, 396.0, 396.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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	A	0.91	0/5095	1.18	61/6905 (0.9%)
1	B	0.90	0/5095	1.17	60/6905 (0.9%)
1	C	0.92	0/5095	1.15	58/6905 (0.8%)
All	All	0.91	0/15285	1.16	179/20715 (0.9%)

There are no bond length outliers.

All (179) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	638	PRO	CA-C-N	10.67	127.34	119.66
1	A	638	PRO	C-N-CA	10.67	127.34	119.66
1	A	637	PHE	CA-C-N	9.73	126.66	119.66
1	A	637	PHE	C-N-CA	9.73	126.66	119.66
1	B	637	PHE	CA-C-N	9.49	126.49	119.66
1	B	637	PHE	C-N-CA	9.49	126.49	119.66
1	B	374	GLY	CA-C-N	8.61	128.65	119.78
1	B	374	GLY	C-N-CA	8.61	128.65	119.78
1	C	374	GLY	CA-C-N	8.58	128.62	119.78
1	C	374	GLY	C-N-CA	8.58	128.62	119.78
1	A	374	GLY	CA-C-N	8.58	128.62	119.78
1	A	374	GLY	C-N-CA	8.58	128.62	119.78
1	B	456	VAL	CA-C-N	8.57	129.09	119.32
1	B	456	VAL	C-N-CA	8.57	129.09	119.32
1	B	94	ARG	CA-C-N	8.54	128.58	119.78
1	B	94	ARG	C-N-CA	8.54	128.58	119.78
1	B	199	PRO	CA-C-N	8.53	128.17	119.56
1	B	199	PRO	C-N-CA	8.53	128.17	119.56
1	B	14	GLY	CA-C-N	8.52	128.17	119.56
1	B	14	GLY	C-N-CA	8.52	128.17	119.56
1	C	199	PRO	CA-C-N	8.46	128.10	119.56
1	C	199	PRO	C-N-CA	8.46	128.10	119.56
1	A	456	VAL	CA-C-N	8.36	128.00	119.56
1	A	456	VAL	C-N-CA	8.36	128.00	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	456	VAL	CA-C-N	8.36	129.16	119.47
1	C	456	VAL	C-N-CA	8.36	129.16	119.47
1	B	43	ASN	CA-C-N	8.13	127.85	119.56
1	B	43	ASN	C-N-CA	8.13	127.85	119.56
1	A	246	ARG	CA-C-N	8.09	127.73	119.56
1	A	246	ARG	C-N-CA	8.09	127.73	119.56
1	C	246	ARG	CA-C-N	8.05	127.69	119.56
1	C	246	ARG	C-N-CA	8.05	127.69	119.56
1	B	246	ARG	CA-C-N	7.92	127.55	119.56
1	B	246	ARG	C-N-CA	7.92	127.55	119.56
1	A	43	ASN	CA-C-N	7.84	128.03	119.87
1	A	43	ASN	C-N-CA	7.84	128.03	119.87
1	A	253	TYR	CA-C-N	7.77	128.38	120.14
1	A	253	TYR	C-N-CA	7.77	128.38	120.14
1	C	43	ASN	CA-C-N	7.70	127.88	119.87
1	C	43	ASN	C-N-CA	7.70	127.88	119.87
1	C	54	LYS	CA-C-N	7.63	127.62	119.76
1	C	54	LYS	C-N-CA	7.63	127.62	119.76
1	B	253	TYR	CA-C-N	7.62	128.22	120.14
1	B	253	TYR	C-N-CA	7.62	128.22	120.14
1	B	54	LYS	CA-C-N	7.62	127.61	119.76
1	B	54	LYS	C-N-CA	7.62	127.61	119.76
1	C	424	ILE	CA-C-N	7.59	127.60	119.78
1	C	424	ILE	C-N-CA	7.59	127.60	119.78
1	B	220	GLN	CA-C-N	7.59	127.59	119.78
1	B	220	GLN	C-N-CA	7.59	127.59	119.78
1	A	442	ARG	CA-C-N	7.56	127.49	119.85
1	A	442	ARG	C-N-CA	7.56	127.49	119.85
1	A	94	ARG	CA-C-N	7.52	127.45	119.85
1	A	94	ARG	C-N-CA	7.52	127.45	119.85
1	B	424	ILE	CA-C-N	7.50	127.48	119.76
1	B	424	ILE	C-N-CA	7.50	127.48	119.76
1	B	442	ARG	CA-C-N	7.49	127.42	119.85
1	B	442	ARG	C-N-CA	7.49	127.42	119.85
1	A	439	ASP	CA-C-N	7.48	128.14	119.47
1	A	439	ASP	C-N-CA	7.48	128.14	119.47
1	A	366	GLY	CA-C-N	7.45	127.45	119.78
1	A	366	GLY	C-N-CA	7.45	127.45	119.78
1	C	253	TYR	CA-C-N	7.42	128.00	120.14
1	C	253	TYR	C-N-CA	7.42	128.00	120.14
1	B	638	PRO	CA-C-N	7.33	127.94	120.38
1	B	638	PRO	C-N-CA	7.33	127.94	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	195	VAL	CA-C-N	7.32	127.25	119.85
1	B	195	VAL	C-N-CA	7.32	127.25	119.85
1	C	94	ARG	CA-C-N	7.30	127.23	119.85
1	C	94	ARG	C-N-CA	7.30	127.23	119.85
1	B	11	CYS	CA-C-N	7.29	127.28	119.78
1	B	11	CYS	C-N-CA	7.29	127.28	119.78
1	A	220	GLN	CA-C-N	7.25	127.22	119.76
1	A	220	GLN	C-N-CA	7.25	127.22	119.76
1	B	145	VAL	N-CA-C	7.25	118.26	108.11
1	C	356	LEU	CA-C-N	7.25	128.90	119.84
1	C	356	LEU	C-N-CA	7.25	128.90	119.84
1	B	439	ASP	CA-C-N	7.21	127.83	119.47
1	B	439	ASP	C-N-CA	7.21	127.83	119.47
1	C	220	GLN	CA-C-N	7.16	127.15	119.78
1	C	220	GLN	C-N-CA	7.16	127.15	119.78
1	A	356	LEU	CA-C-N	7.14	128.77	119.84
1	A	356	LEU	C-N-CA	7.14	128.77	119.84
1	C	638	PRO	CA-C-N	7.11	127.71	120.38
1	C	638	PRO	C-N-CA	7.11	127.71	120.38
1	C	195	VAL	CA-C-N	7.10	127.03	119.85
1	C	195	VAL	C-N-CA	7.10	127.03	119.85
1	A	145	VAL	N-CA-C	7.09	118.04	108.11
1	C	439	ASP	CA-C-N	7.05	127.65	119.47
1	C	439	ASP	C-N-CA	7.05	127.65	119.47
1	A	199	PRO	CA-C-N	7.04	128.64	119.84
1	A	199	PRO	C-N-CA	7.04	128.64	119.84
1	C	442	ARG	CA-C-N	7.04	126.96	119.85
1	C	442	ARG	C-N-CA	7.04	126.96	119.85
1	A	195	VAL	CA-C-N	6.99	127.55	120.14
1	A	195	VAL	C-N-CA	6.99	127.55	120.14
1	C	136	ARG	CA-C-N	6.94	126.86	119.85
1	C	136	ARG	C-N-CA	6.94	126.86	119.85
1	B	306	TYR	CA-C-N	6.90	127.18	119.32
1	B	306	TYR	C-N-CA	6.90	127.18	119.32
1	A	11	CYS	CA-C-N	6.86	126.85	119.78
1	A	11	CYS	C-N-CA	6.86	126.85	119.78
1	B	188	SER	CA-C-N	6.73	126.71	119.78
1	B	188	SER	C-N-CA	6.73	126.71	119.78
1	A	359	THR	CA-C-N	6.68	126.64	119.76
1	A	359	THR	C-N-CA	6.68	126.64	119.76
1	B	361	VAL	CA-C-N	6.67	126.58	119.85
1	B	361	VAL	C-N-CA	6.67	126.58	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	145	VAL	N-CA-C	6.65	117.42	108.11
1	C	188	SER	CA-C-N	6.62	126.59	119.78
1	C	188	SER	C-N-CA	6.62	126.59	119.78
1	A	424	ILE	CA-C-N	6.56	126.48	119.85
1	A	424	ILE	C-N-CA	6.56	126.48	119.85
1	C	637	PHE	CA-C-N	6.47	127.04	120.38
1	C	637	PHE	C-N-CA	6.47	127.04	120.38
1	C	366	GLY	CA-C-N	6.46	126.43	120.03
1	C	366	GLY	C-N-CA	6.46	126.43	120.03
1	A	54	LYS	CA-C-N	6.44	126.39	119.76
1	A	54	LYS	C-N-CA	6.44	126.39	119.76
1	C	306	TYR	CA-C-N	6.43	127.88	119.84
1	C	306	TYR	C-N-CA	6.43	127.88	119.84
1	A	361	VAL	CA-C-N	6.33	126.09	119.76
1	A	361	VAL	C-N-CA	6.33	126.09	119.76
1	C	359	THR	CA-C-N	6.28	126.23	119.76
1	C	359	THR	C-N-CA	6.28	126.23	119.76
1	A	188	SER	CA-C-N	6.25	126.21	119.78
1	A	188	SER	C-N-CA	6.25	126.21	119.78
1	B	366	GLY	CA-C-N	6.20	126.17	120.03
1	B	366	GLY	C-N-CA	6.20	126.17	120.03
1	A	176	ILE	N-CA-C	6.19	116.84	108.17
1	A	306	TYR	CA-C-N	6.18	127.57	119.84
1	A	306	TYR	C-N-CA	6.18	127.57	119.84
1	B	62	LEU	CA-C-N	6.11	126.08	119.78
1	B	62	LEU	C-N-CA	6.11	126.08	119.78
1	B	136	ARG	CA-C-N	6.03	126.53	120.14
1	B	136	ARG	C-N-CA	6.03	126.53	120.14
1	B	11	CYS	N-CA-C	6.01	115.23	108.25
1	C	361	VAL	CA-C-N	6.01	125.78	119.76
1	C	361	VAL	C-N-CA	6.01	125.78	119.76
1	C	176	ILE	N-CA-C	5.98	116.55	108.17
1	A	136	ARG	CA-C-N	5.94	126.44	120.14
1	A	136	ARG	C-N-CA	5.94	126.44	120.14
1	C	478	THR	CA-C-N	5.93	127.25	119.84
1	C	478	THR	C-N-CA	5.93	127.25	119.84
1	A	62	LEU	CA-C-N	5.83	125.79	119.78
1	A	62	LEU	C-N-CA	5.83	125.79	119.78
1	B	114	VAL	CA-C-N	5.82	125.30	119.24
1	B	114	VAL	C-N-CA	5.82	125.30	119.24
1	A	46	LEU	CA-C-N	5.82	127.11	119.84
1	A	46	LEU	C-N-CA	5.82	127.11	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	176	ILE	N-CA-C	5.76	116.59	108.36
1	B	478	THR	CA-C-N	5.71	126.98	119.84
1	B	478	THR	C-N-CA	5.71	126.98	119.84
1	C	62	LEU	CA-C-N	5.67	125.62	119.78
1	C	62	LEU	C-N-CA	5.67	125.62	119.78
1	A	478	THR	CA-C-N	5.67	126.92	119.84
1	A	478	THR	C-N-CA	5.67	126.92	119.84
1	B	233	ARG	CA-C-N	5.65	126.90	119.84
1	B	233	ARG	C-N-CA	5.65	126.90	119.84
1	C	46	LEU	CA-C-N	5.64	126.89	119.84
1	C	46	LEU	C-N-CA	5.64	126.89	119.84
1	A	233	ARG	CA-C-N	5.55	126.78	119.84
1	A	233	ARG	C-N-CA	5.55	126.78	119.84
1	B	359	THR	CA-C-N	5.45	126.66	119.84
1	B	359	THR	C-N-CA	5.45	126.66	119.84
1	A	11	CYS	N-CA-C	5.35	114.29	108.14
1	B	356	LEU	CA-C-N	5.28	126.44	119.84
1	B	356	LEU	C-N-CA	5.28	126.44	119.84
1	C	41	SER	N-CA-C	5.21	116.98	108.76
1	A	114	VAL	CA-C-N	5.18	125.23	119.32
1	A	114	VAL	C-N-CA	5.18	125.23	119.32
1	A	96	TRP	CA-C-N	5.17	124.83	119.56
1	A	96	TRP	C-N-CA	5.17	124.83	119.56
1	C	114	VAL	CA-C-N	5.14	125.18	119.32
1	C	114	VAL	C-N-CA	5.14	125.18	119.32
1	C	424	ILE	N-CA-C	5.14	113.05	108.63
1	C	233	ARG	CA-C-N	5.03	126.13	119.84
1	C	233	ARG	C-N-CA	5.03	126.13	119.84
1	B	482	PHE	CA-CB-CG	-5.03	108.77	113.80

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	4977	4796	4794	16	0
1	B	4977	4796	4794	18	0
1	C	4977	4796	4794	16	0
All	All	14931	14388	14382	49	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 2.

All (49) 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:213:TRP:O	1:B:213:TRP:HE3	1.83	0.61
1:A:177:LEU:C	1:A:177:LEU:HD23	2.27	0.60
1:B:213:TRP:O	1:B:213:TRP:CE3	2.54	0.60
1:C:177:LEU:C	1:C:177:LEU:HD23	2.28	0.59
1:B:39:LEU:C	1:B:39:LEU:HD12	2.30	0.57
1:B:501:GLU:HA	1:B:501:GLU:OE1	2.09	0.52
1:B:213:TRP:CE3	1:B:213:TRP:C	2.88	0.51
1:A:33:PHE:CD1	1:A:33:PHE:C	2.88	0.51
1:A:398:ASP:OD1	1:A:398:ASP:C	2.52	0.50
1:B:398:ASP:C	1:B:398:ASP:OD1	2.56	0.49
1:A:198:TYR:O	1:A:199:PRO:C	2.55	0.48
1:B:608:LEU:C	1:B:608:LEU:HD23	2.37	0.48
1:B:328:LEU:O	1:B:328:LEU:HG	2.12	0.48
1:A:340:PHE:C	1:A:340:PHE:CD2	2.91	0.48
1:B:102:ARG:NE	1:B:102:ARG:HA	2.30	0.47
1:C:478:THR:HB	1:C:479:PRO:HD2	1.97	0.47
1:C:102:ARG:NE	1:C:102:ARG:HA	2.30	0.47
1:C:95:PRO:HB2	1:C:97:PRO:HD2	1.97	0.47
1:A:147:TYR:OH	1:A:368:GLN:NE2	2.48	0.46
1:C:33:PHE:C	1:C:33:PHE:CD1	2.93	0.46
1:A:41:SER:OG	1:A:42:GLU:N	2.49	0.46
1:B:395:ASP:OD1	1:B:395:ASP:C	2.56	0.46
1:A:102:ARG:NE	1:A:102:ARG:HA	2.31	0.45
1:A:478:THR:HB	1:A:479:PRO:HD2	1.99	0.45
1:B:478:THR:HB	1:B:479:PRO:HD2	1.99	0.45
1:A:95:PRO:HB2	1:A:97:PRO:HD2	1.98	0.44
1:B:482:PHE:CD1	1:B:482:PHE:C	2.96	0.44
1:B:147:TYR:OH	1:B:368:GLN:NE2	2.51	0.43
1:C:529:LEU:C	1:C:529:LEU:HD23	2.44	0.43
1:B:529:LEU:C	1:B:529:LEU:HD23	2.44	0.43
1:C:147:TYR:OH	1:C:368:GLN:NE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ARG:HB3	1:A:95:PRO:HD2	2.02	0.42
1:C:11:CYS:HB2	1:C:12:PRO:HD2	2.02	0.42
1:C:183:TYR:CD1	1:C:183:TYR:C	2.97	0.42
1:C:482:PHE:CD1	1:C:482:PHE:C	2.97	0.42
1:C:398:ASP:OD1	1:C:398:ASP:C	2.62	0.41
1:C:448:ARG:HD2	1:C:448:ARG:N	2.35	0.41
1:A:383:ASP:OD1	1:A:383:ASP:C	2.62	0.41
1:A:395:ASP:C	1:A:395:ASP:OD1	2.63	0.41
1:C:560:TYR:C	1:C:560:TYR:CD1	2.96	0.41
1:B:560:TYR:C	1:B:560:TYR:CD1	2.97	0.41
1:A:541:LYS:HB3	1:B:533:GLY:O	2.21	0.41
1:B:383:ASP:OD1	1:B:383:ASP:C	2.63	0.41
1:B:212:ASP:HB3	1:B:289:ARG:HB2	2.03	0.41
1:C:22:ARG:HG2	1:C:38:HIS:HB3	2.03	0.41
1:A:11:CYS:HB2	1:A:12:PRO:HD2	2.03	0.40
1:C:40:VAL:HB	1:C:86:PHE:HB3	2.02	0.40
1:A:560:TYR:C	1:A:560:TYR:CD1	2.97	0.40
1:C:383:ASP:OD1	1:C:383:ASP:C	2.62	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	623/643 (97%)	589 (94%)	29 (5%)	5 (1%)	16	44
1	B	623/643 (97%)	588 (94%)	31 (5%)	4 (1%)	21	51
1	C	623/643 (97%)	592 (95%)	27 (4%)	4 (1%)	21	51
All	All	1869/1929 (97%)	1769 (95%)	87 (5%)	13 (1%)	20	48

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	PRO
1	B	47	PRO
1	C	15	PRO
1	B	234	PRO
1	B	357	PRO
1	A	15	PRO
1	A	47	PRO
1	B	46	LEU
1	C	47	PRO
1	C	234	PRO
1	A	234	PRO
1	C	357	PRO
1	A	357	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	A	526/535 (98%)	526 (100%)	0	100	100
1	B	526/535 (98%)	526 (100%)	0	100	100
1	C	526/535 (98%)	526 (100%)	0	100	100
All	All	1578/1605 (98%)	1578 (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. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	454	GLN
1	A	466	GLN
1	B	112	GLN
1	B	204	HIS
1	B	326	GLN
1	B	466	GLN
1	C	112	GLN

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Mol	Chain	Res	Type
1	C	282	GLN
1	C	454	GLN
1	C	466	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.

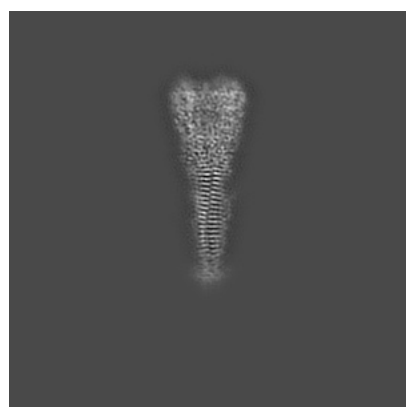
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0136. These allow visual inspection of the internal detail of the map and identification of artifacts.

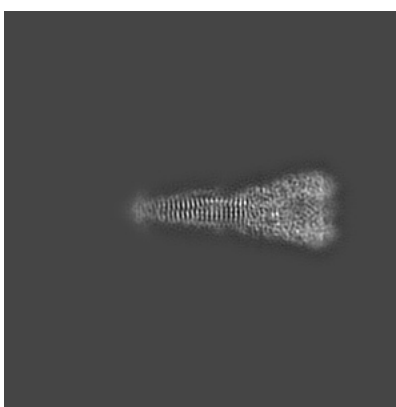
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

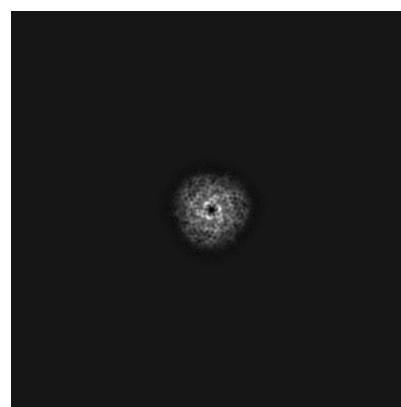
6.1.1 Primary map



X



Y



Z

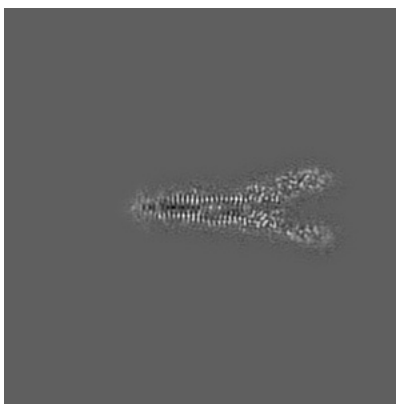
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

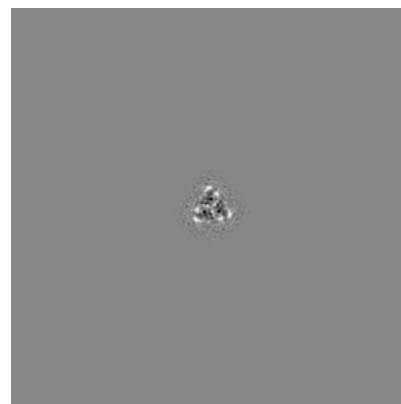
6.2.1 Primary map



X Index: 180



Y Index: 180



Z Index: 180

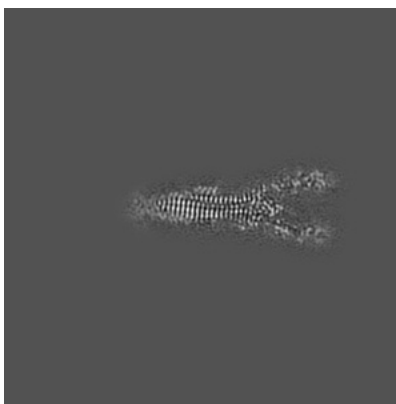
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

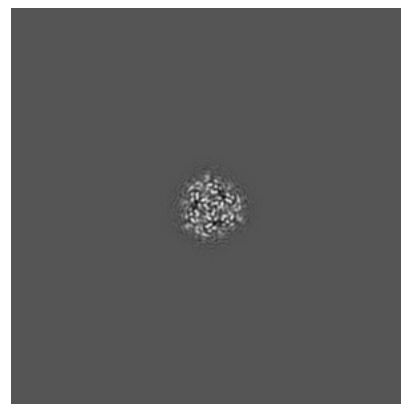
6.3.1 Primary map



X Index: 187



Y Index: 174

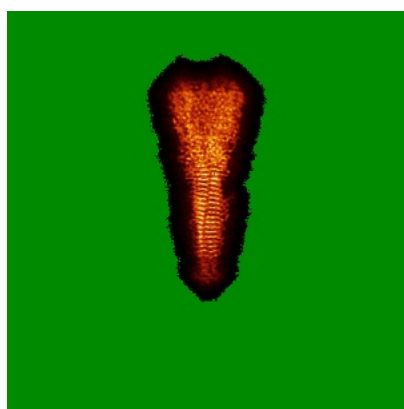


Z Index: 246

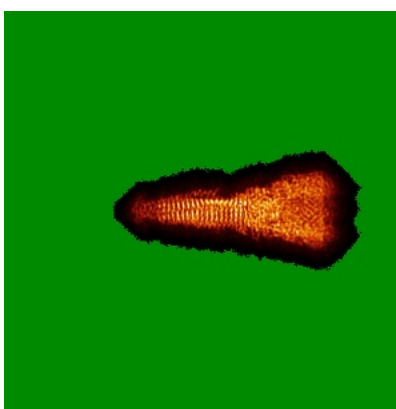
The images above show the largest variance slices of the map in three orthogonal directions.

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

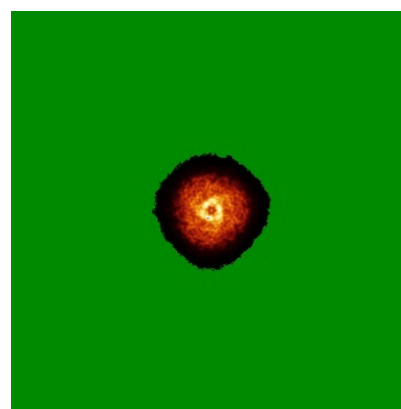
6.4.1 Primary map



X



Y

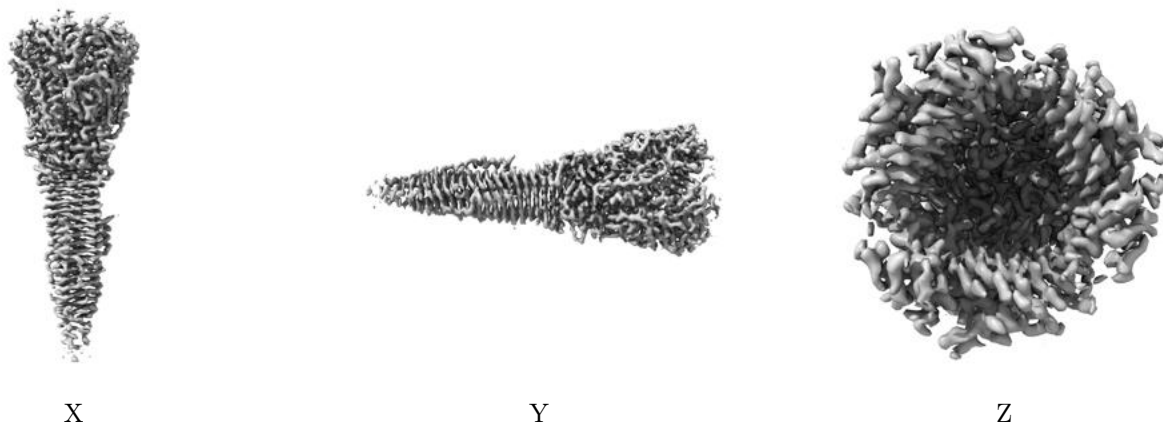


Z

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

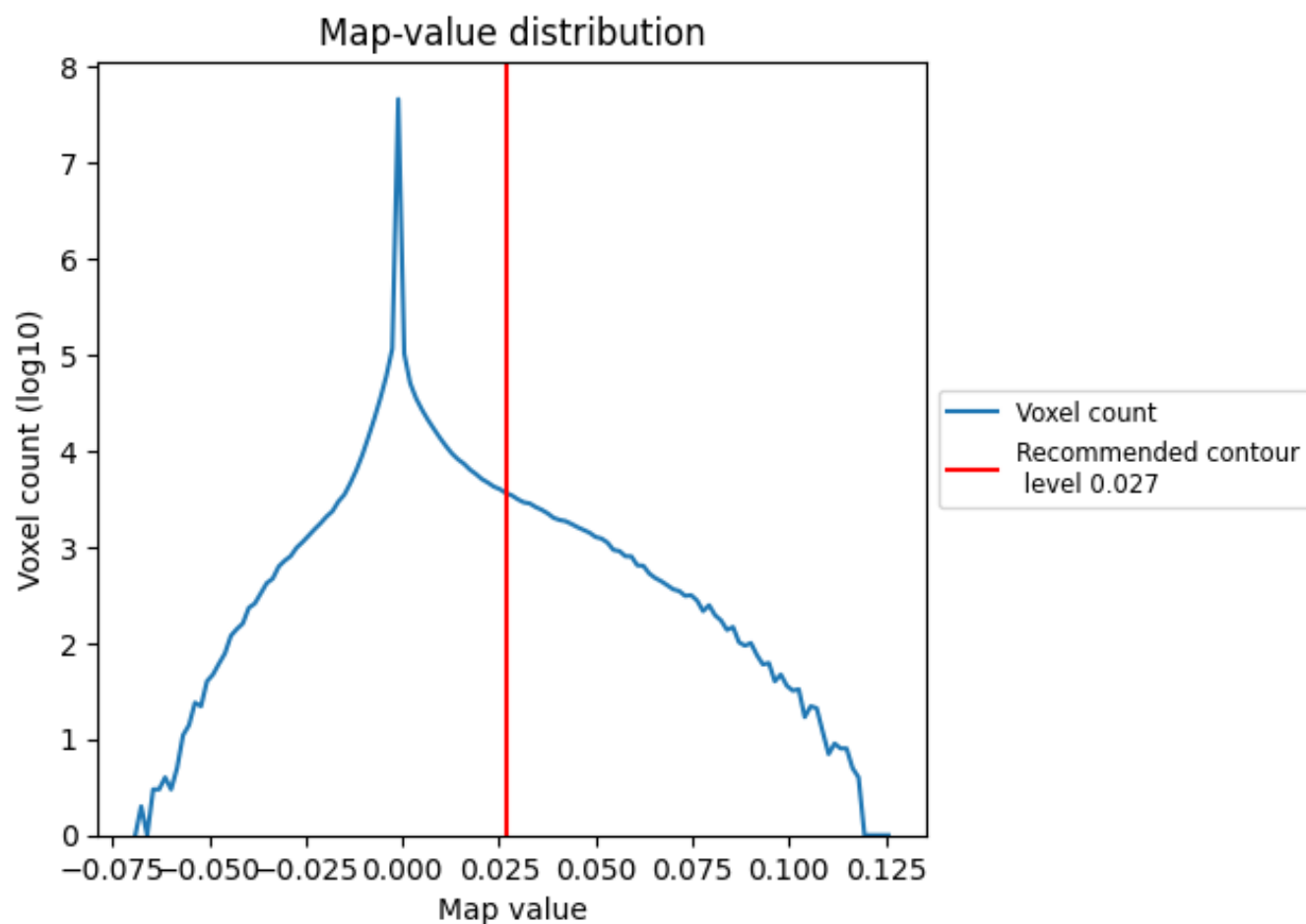
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

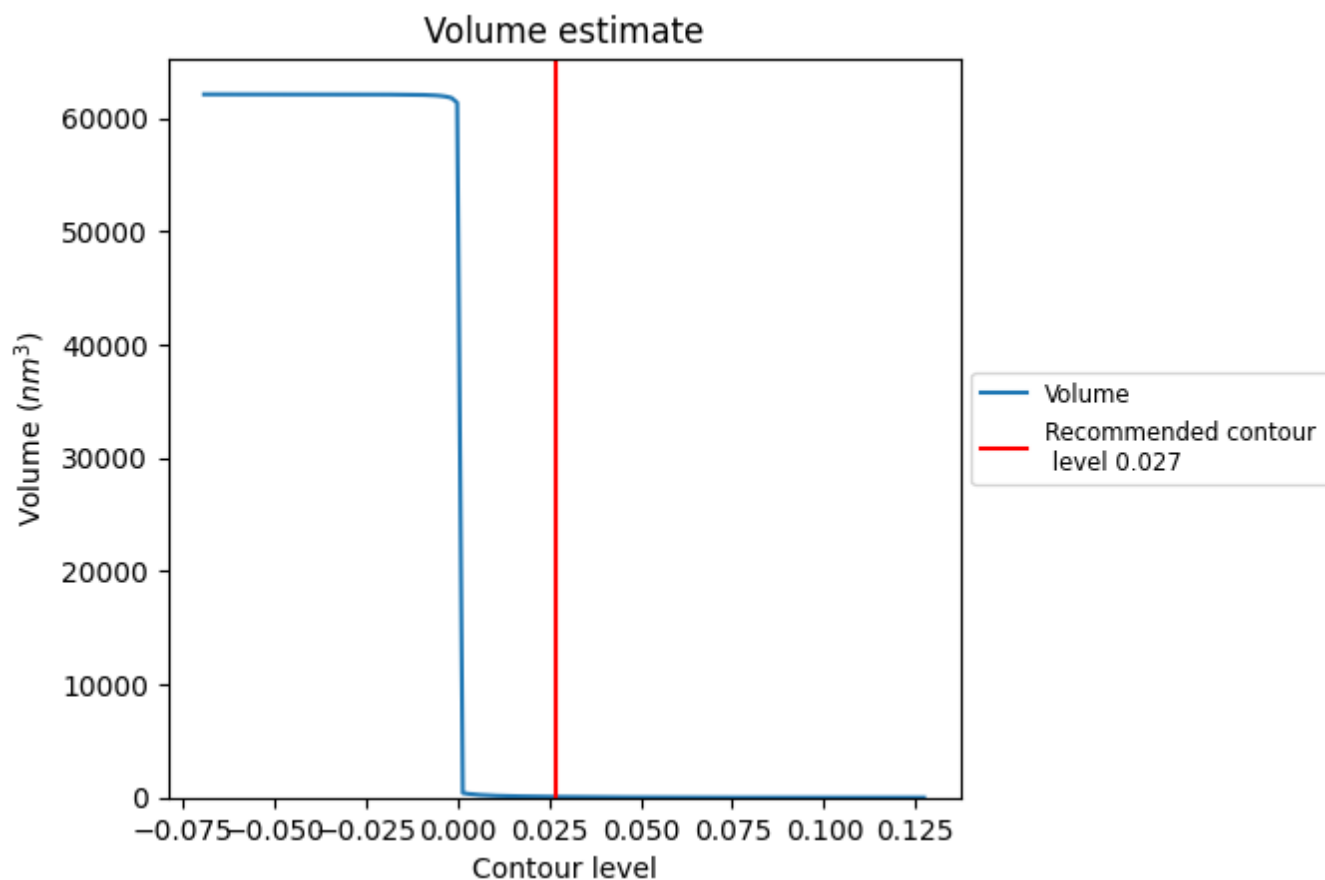
This section contains the results of statistical analysis of the map.

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.

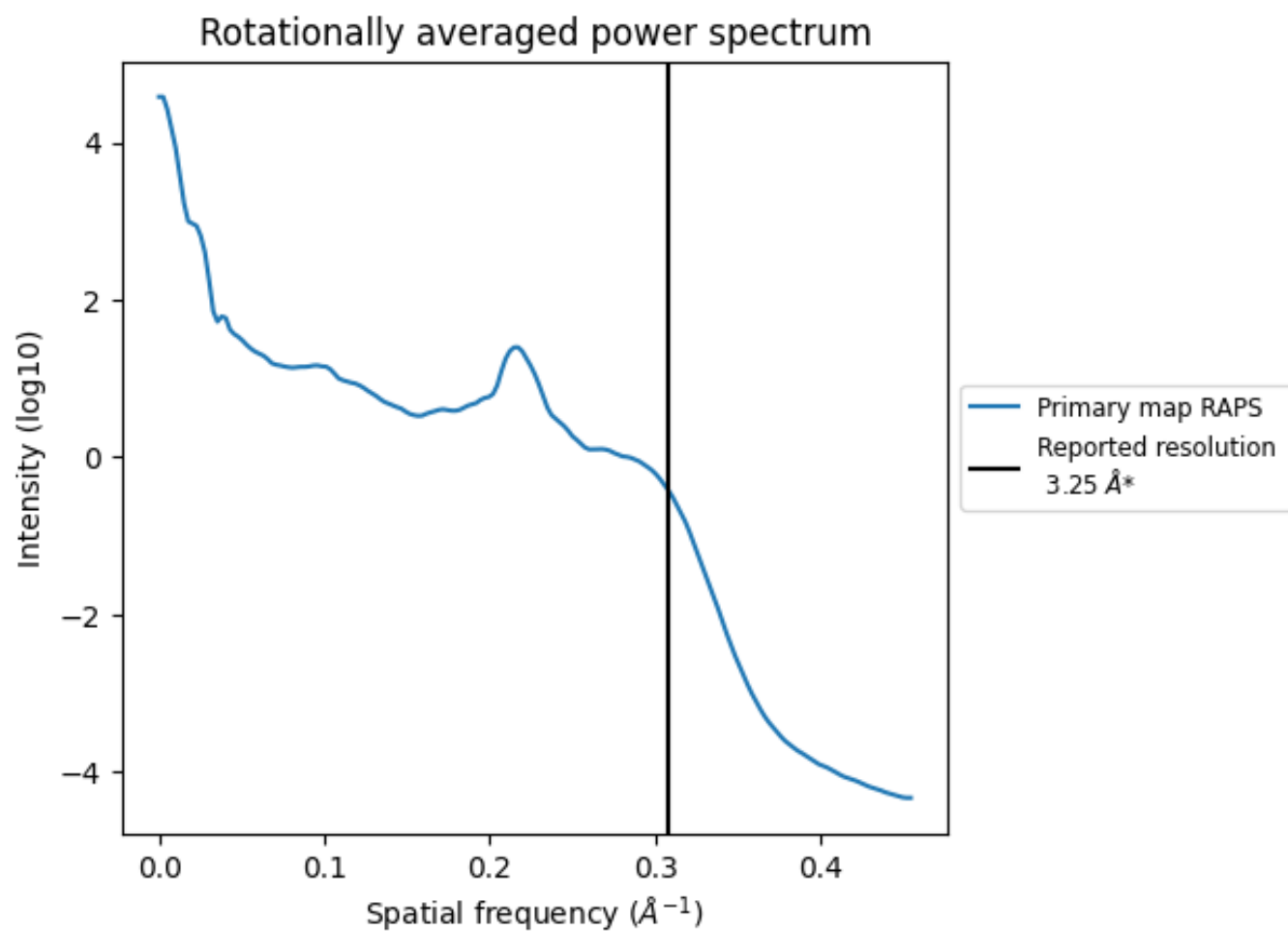
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 65 nm^3 ; this corresponds to an approximate mass of 58 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 0.308 Å⁻¹

8 Fourier-Shell correlation ⓘ

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

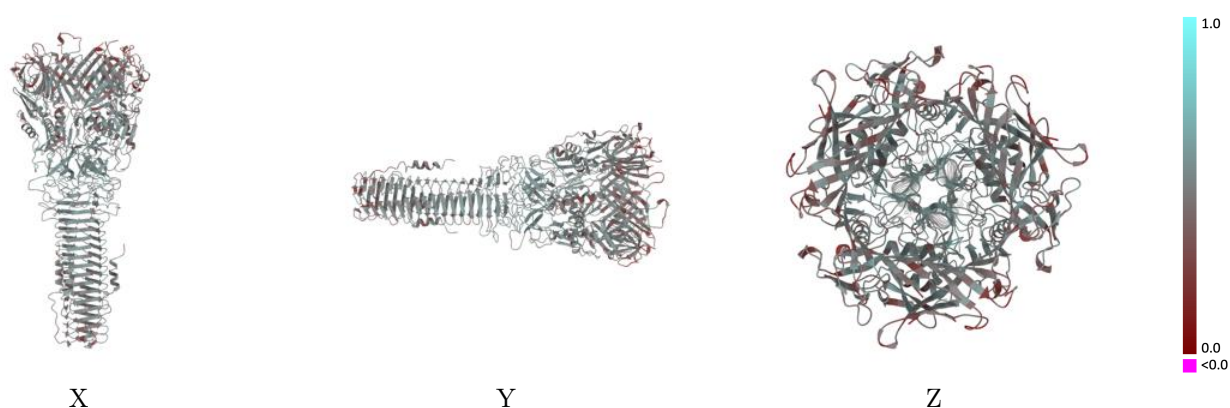
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0136 and PDB model 6H3N. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)

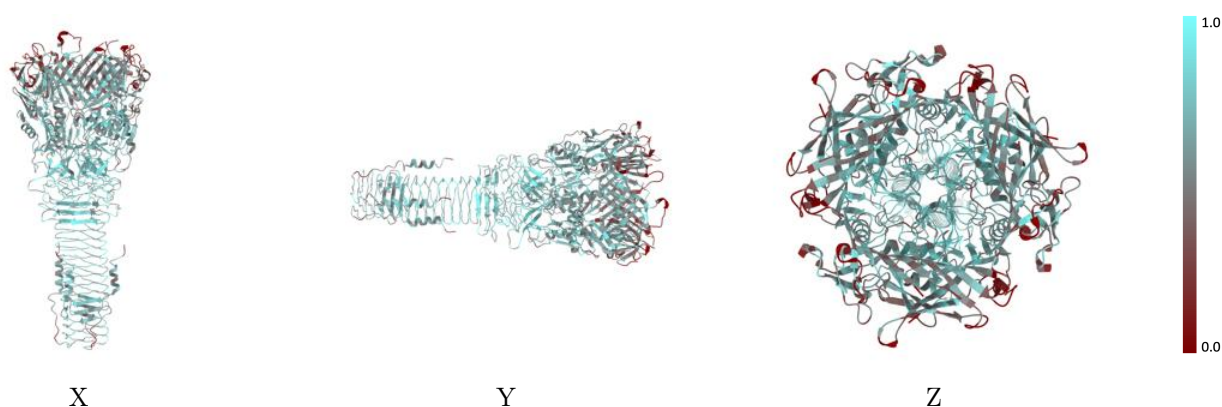
This section was not generated.

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



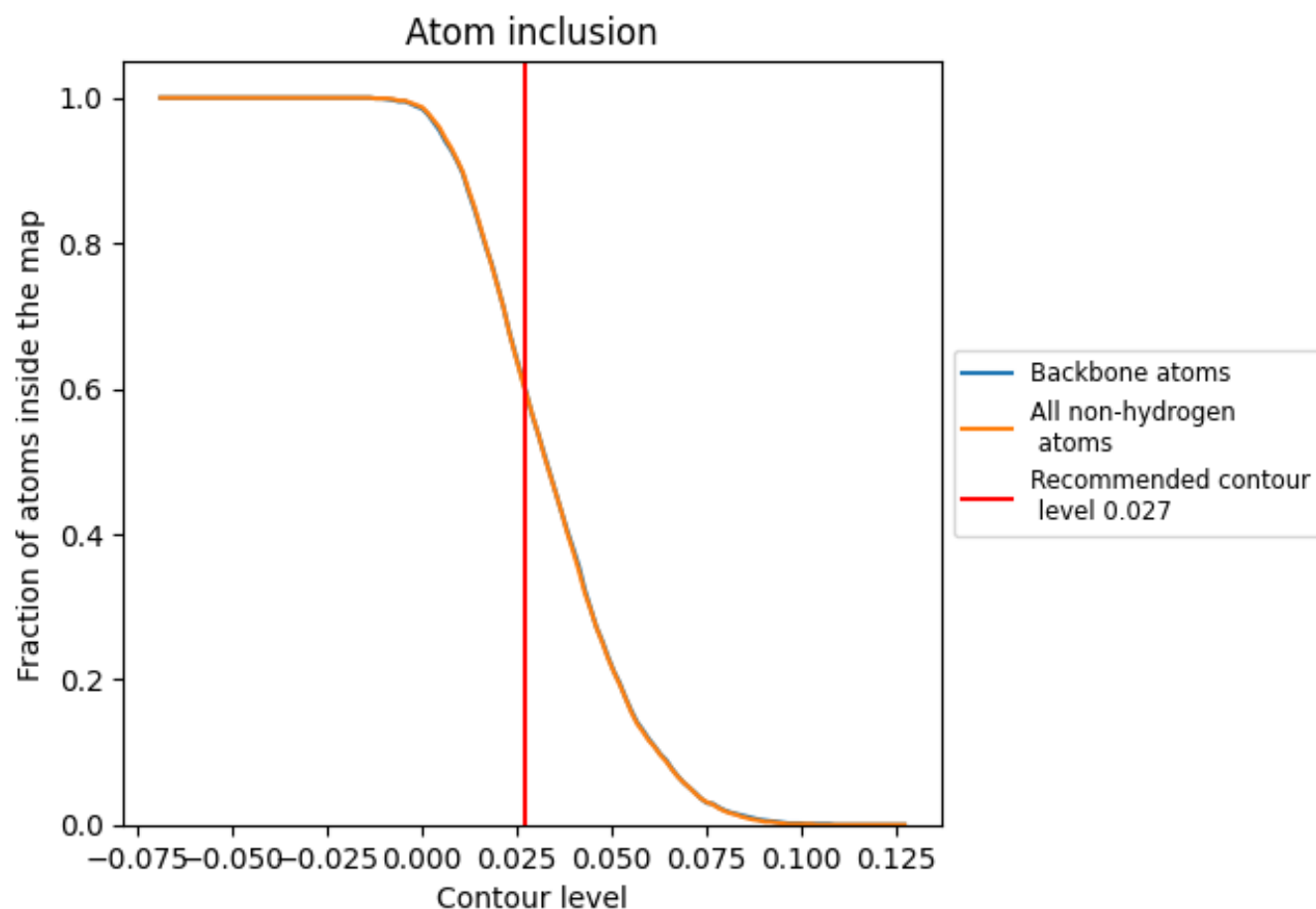
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.027).

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 60% 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 (0.027) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6000	0.4750
A	0.6120	0.4750
B	0.6130	0.4750
C	0.6160	0.4750

