



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 11:14 AM UTC

PDB ID : 8QOE / pdb_00008qoe
EMDB ID : EMD-18535
Title : Inward-facing conformation of the ABC transporter BmrA
Authors : Di Cesare, M.; Kaplan, E.; Valimehr, S.; Hanssen, E.; Orelle, C.; Jault, J.M.
Deposited on : 2023-09-28
Resolution : 3.16 Å(reported)
Based on initial model : 8CHB

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

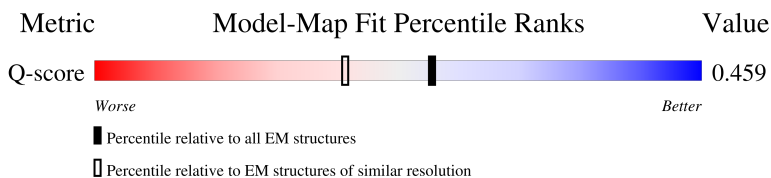
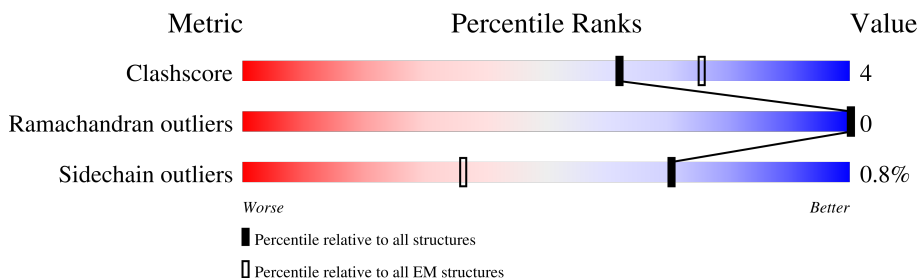
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.16 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	14474 (2.66 - 3.66)

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	604	13% 72% 21% • 6%
1	B	604	13% 72% 21% • 6%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 17816 atoms, of which 9072 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 Multidrug resistance ABC transporter ATP-binding/permease protein BmrA.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	B	568	Total	C	H	N	O	S	0	0
			8908	2806	4536	728	821	17		
1	A	568	Total	C	H	N	O	S	0	0
			8908	2806	4536	728	821	17		

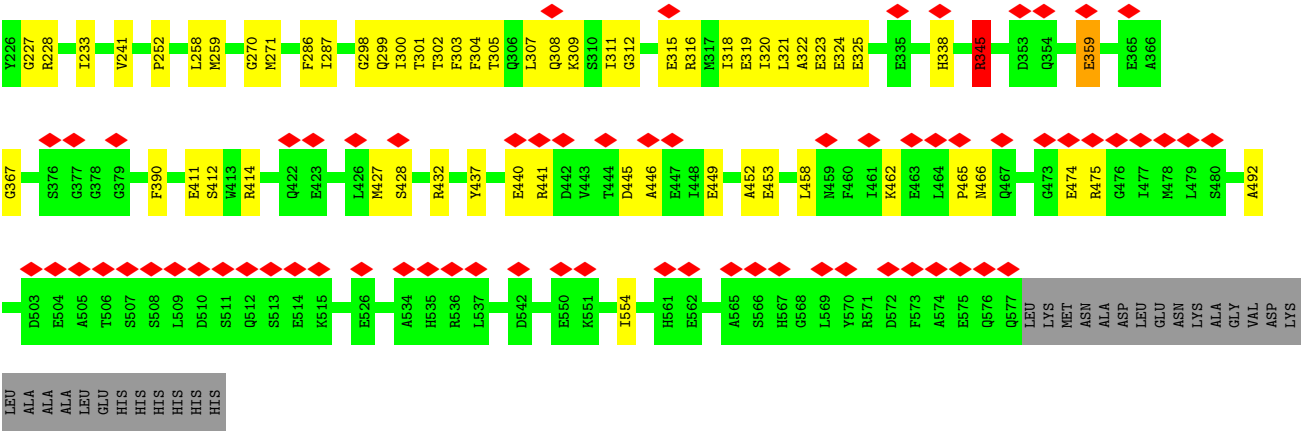
There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	590	VAL	-	expression tag	UNP O06967
B	591	ASP	-	expression tag	UNP O06967
B	592	LYS	-	expression tag	UNP O06967
B	593	LEU	-	expression tag	UNP O06967
B	594	ALA	-	expression tag	UNP O06967
B	595	ALA	-	expression tag	UNP O06967
B	596	ALA	-	expression tag	UNP O06967
B	597	LEU	-	expression tag	UNP O06967
B	598	GLU	-	expression tag	UNP O06967
B	599	HIS	-	expression tag	UNP O06967
B	600	HIS	-	expression tag	UNP O06967
B	601	HIS	-	expression tag	UNP O06967
B	602	HIS	-	expression tag	UNP O06967
B	603	HIS	-	expression tag	UNP O06967
B	604	HIS	-	expression tag	UNP O06967
A	590	VAL	-	expression tag	UNP O06967
A	591	ASP	-	expression tag	UNP O06967
A	592	LYS	-	expression tag	UNP O06967
A	593	LEU	-	expression tag	UNP O06967
A	594	ALA	-	expression tag	UNP O06967
A	595	ALA	-	expression tag	UNP O06967
A	596	ALA	-	expression tag	UNP O06967
A	597	LEU	-	expression tag	UNP O06967
A	598	GLU	-	expression tag	UNP O06967
A	599	HIS	-	expression tag	UNP O06967

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Chain	Residue	Modelled	Actual	Comment	Reference
A	600	HIS	-	expression tag	UNP O06967
A	601	HIS	-	expression tag	UNP O06967
A	602	HIS	-	expression tag	UNP O06967
A	603	HIS	-	expression tag	UNP O06967
A	604	HIS	-	expression tag	UNP O06967



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	1043614	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.891	Depositor
Minimum map value	-0.460	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	321.00003, 321.00003, 321.00003	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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	1.32	37/4439 (0.8%)	1.93	197/6009 (3.3%)
1	B	1.31	37/4439 (0.8%)	1.93	197/6009 (3.3%)
All	All	1.31	74/8878 (0.8%)	1.93	394/12018 (3.3%)

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	100	ARG	CZ-NH2	-17.32	1.10	1.33
1	A	100	ARG	CZ-NH2	-17.31	1.10	1.33
1	A	126	ARG	CZ-NH2	-17.09	1.11	1.33
1	B	126	ARG	CZ-NH2	-17.08	1.11	1.33
1	A	316	ARG	CZ-NH2	-16.88	1.11	1.33
1	B	316	ARG	CZ-NH2	-16.85	1.11	1.33
1	B	316	ARG	CZ-NH1	-15.60	1.10	1.32
1	A	316	ARG	CZ-NH1	-15.57	1.10	1.32
1	A	126	ARG	CZ-NH1	-15.57	1.10	1.32
1	B	126	ARG	CZ-NH1	-15.54	1.10	1.32
1	A	100	ARG	CZ-NH1	-15.38	1.11	1.32
1	B	100	ARG	CZ-NH1	-15.38	1.11	1.32
1	B	412	SER	CB-OG	-11.26	1.19	1.42
1	A	412	SER	CB-OG	-11.26	1.19	1.42
1	A	441	ARG	CZ-NH2	-10.14	1.20	1.33
1	B	441	ARG	CZ-NH2	-10.12	1.20	1.33
1	A	475	ARG	CZ-NH2	-9.88	1.20	1.33
1	B	475	ARG	CZ-NH2	-9.88	1.20	1.33
1	B	441	ARG	CZ-NH1	-9.22	1.19	1.32
1	A	441	ARG	CZ-NH1	-9.21	1.19	1.32
1	A	475	ARG	CZ-NH1	-8.88	1.20	1.32
1	B	475	ARG	CZ-NH1	-8.85	1.20	1.32
1	B	107	LEU	C-N	-8.15	1.25	1.34
1	A	107	LEU	C-N	-8.15	1.25	1.34
1	B	100	ARG	C-N	-7.20	1.24	1.33
1	A	100	ARG	C-N	-7.14	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	ARG	C-N	-6.94	1.25	1.33
1	B	259	MET	C-O	-6.92	1.15	1.24
1	A	259	MET	C-O	-6.91	1.15	1.24
1	B	126	ARG	C-N	-6.90	1.25	1.33
1	B	319	GLU	C-N	-6.85	1.25	1.33
1	A	319	GLU	C-N	-6.84	1.25	1.33
1	B	214	ARG	CA-C	-6.75	1.44	1.52
1	A	214	ARG	CA-C	-6.70	1.44	1.52
1	B	105	LYS	CA-C	-6.64	1.43	1.52
1	A	105	LYS	CA-C	-6.60	1.43	1.52
1	A	122	GLU	C-N	-6.57	1.25	1.33
1	B	122	GLU	C-N	-6.55	1.25	1.33
1	B	109	LYS	CA-CB	-6.44	1.44	1.53
1	A	100	ARG	NE-CZ	-6.42	1.25	1.33
1	B	100	ARG	NE-CZ	-6.42	1.25	1.33
1	A	109	LYS	CA-CB	-6.40	1.44	1.53
1	B	104	TRP	N-CA	-6.35	1.38	1.46
1	A	104	TRP	N-CA	-6.34	1.38	1.46
1	A	125	SER	C-N	-6.31	1.26	1.33
1	B	125	SER	C-N	-6.29	1.26	1.33
1	A	228	ARG	C-O	-6.28	1.15	1.24
1	B	228	ARG	C-O	-6.27	1.15	1.24
1	A	114	TYR	C-N	-6.21	1.25	1.33
1	B	114	TYR	C-N	-6.17	1.25	1.33
1	B	228	ARG	CA-C	-6.14	1.44	1.52
1	B	316	ARG	NE-CZ	-6.11	1.26	1.33
1	A	228	ARG	CA-C	-6.10	1.44	1.52
1	A	316	ARG	NE-CZ	-6.09	1.26	1.33
1	A	202	PHE	CA-C	-5.86	1.45	1.52
1	B	202	PHE	CA-C	-5.86	1.45	1.52
1	B	114	TYR	N-CA	-5.72	1.39	1.46
1	A	114	TYR	N-CA	-5.72	1.39	1.46
1	A	320	ILE	N-CA	-5.65	1.40	1.46
1	B	320	ILE	N-CA	-5.65	1.40	1.46
1	B	126	ARG	NE-CZ	-5.62	1.26	1.33
1	A	126	ARG	NE-CZ	-5.62	1.26	1.33
1	B	101	GLU	N-CA	-5.47	1.39	1.46
1	A	101	GLU	N-CA	-5.47	1.39	1.46
1	B	100	ARG	N-CA	-5.27	1.40	1.46
1	A	100	ARG	N-CA	-5.25	1.40	1.46
1	B	345	ARG	CA-C	-5.22	1.46	1.53
1	A	345	ARG	CA-C	-5.20	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	107	LEU	N-CA	-5.12	1.40	1.46
1	A	148	GLY	N-CA	-5.10	1.39	1.45
1	B	148	GLY	N-CA	-5.10	1.39	1.45
1	A	107	LEU	N-CA	-5.08	1.40	1.46
1	B	115	PHE	N-CA	-5.06	1.39	1.46
1	A	115	PHE	N-CA	-5.04	1.39	1.46

All (394) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	319	GLU	CA-C-N	13.18	138.03	120.77
1	B	319	GLU	C-N-CA	13.18	138.03	120.77
1	A	319	GLU	CA-C-N	13.15	138.00	120.77
1	A	319	GLU	C-N-CA	13.15	138.00	120.77
1	B	126	ARG	CA-C-N	12.58	136.83	120.60
1	B	126	ARG	C-N-CA	12.58	136.83	120.60
1	A	126	ARG	CA-C-N	12.58	136.82	120.60
1	A	126	ARG	C-N-CA	12.58	136.82	120.60
1	B	125	SER	CA-C-N	12.07	137.57	120.79
1	B	125	SER	C-N-CA	12.07	137.57	120.79
1	A	125	SER	CA-C-N	12.07	137.57	120.79
1	A	125	SER	C-N-CA	12.07	137.57	120.79
1	B	100	ARG	CA-C-N	11.58	136.17	120.54
1	B	100	ARG	C-N-CA	11.58	136.17	120.54
1	A	100	ARG	CA-C-N	11.56	136.15	120.54
1	A	100	ARG	C-N-CA	11.56	136.15	120.54
1	A	113	SER	CA-C-N	11.14	135.59	120.54
1	A	113	SER	C-N-CA	11.14	135.59	120.54
1	B	113	SER	CA-C-N	11.12	135.55	120.54
1	B	113	SER	C-N-CA	11.12	135.55	120.54
1	B	126	ARG	CD-NE-CZ	10.92	139.69	124.40
1	A	126	ARG	CD-NE-CZ	10.91	139.67	124.40
1	A	316	ARG	CD-NE-CZ	10.63	139.28	124.40
1	B	316	ARG	CD-NE-CZ	10.63	139.28	124.40
1	A	315	GLU	CA-C-N	10.60	135.55	120.28
1	A	315	GLU	C-N-CA	10.60	135.55	120.28
1	B	315	GLU	CA-C-N	10.59	135.53	120.28
1	B	315	GLU	C-N-CA	10.59	135.53	120.28
1	A	122	GLU	CA-C-N	10.39	134.57	120.54
1	A	122	GLU	C-N-CA	10.39	134.57	120.54
1	B	122	GLU	CA-C-N	10.38	134.56	120.54
1	B	122	GLU	C-N-CA	10.38	134.56	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	LEU	CA-C-N	9.79	137.21	120.86
1	A	107	LEU	C-N-CA	9.79	137.21	120.86
1	B	107	LEU	CA-C-N	9.77	137.17	120.86
1	B	107	LEU	C-N-CA	9.77	137.17	120.86
1	A	127	VAL	N-CA-CB	9.60	121.16	110.51
1	B	127	VAL	N-CA-CB	9.58	121.14	110.51
1	B	99	LEU	CA-C-N	9.11	132.84	120.54
1	B	99	LEU	C-N-CA	9.11	132.84	120.54
1	A	99	LEU	CA-C-N	9.11	132.83	120.54
1	A	99	LEU	C-N-CA	9.11	132.83	120.54
1	B	320	ILE	N-CA-CB	8.95	120.02	110.62
1	A	320	ILE	N-CA-CB	8.94	120.01	110.62
1	B	100	ARG	CD-NE-CZ	8.87	136.81	124.40
1	A	100	ARG	CD-NE-CZ	8.86	136.80	124.40
1	A	114	TYR	CA-C-N	8.78	138.56	121.18
1	A	114	TYR	C-N-CA	8.78	138.56	121.18
1	B	114	TYR	CA-C-N	8.76	138.52	121.18
1	B	114	TYR	C-N-CA	8.76	138.52	121.18
1	A	321	LEU	CA-C-N	8.39	135.82	121.14
1	A	321	LEU	C-N-CA	8.39	135.82	121.14
1	B	321	LEU	CA-C-N	8.38	135.81	121.14
1	B	321	LEU	C-N-CA	8.38	135.81	121.14
1	B	123	THR	N-CA-CB	8.34	122.36	109.94
1	A	123	THR	N-CA-CB	8.32	122.34	109.94
1	A	103	LEU	CA-C-N	8.20	131.10	120.44
1	A	103	LEU	C-N-CA	8.20	131.10	120.44
1	B	103	LEU	CA-C-N	8.18	131.08	120.44
1	B	103	LEU	C-N-CA	8.18	131.08	120.44
1	B	106	LYS	CA-C-N	7.80	132.52	120.82
1	B	106	LYS	C-N-CA	7.80	132.52	120.82
1	A	106	LYS	CA-C-N	7.79	132.50	120.82
1	A	106	LYS	C-N-CA	7.79	132.50	120.82
1	B	36	SER	CA-C-N	7.67	130.38	120.56
1	B	36	SER	C-N-CA	7.67	130.38	120.56
1	A	36	SER	CA-C-N	7.65	130.35	120.56
1	A	36	SER	C-N-CA	7.65	130.35	120.56
1	A	148	GLY	CA-C-N	7.57	130.17	120.70
1	A	148	GLY	C-N-CA	7.57	130.17	120.70
1	B	148	GLY	CA-C-N	7.53	130.11	120.70
1	B	148	GLY	C-N-CA	7.53	130.11	120.70
1	B	144	GLY	CA-C-N	7.45	130.48	120.65
1	B	144	GLY	C-N-CA	7.45	130.48	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	GLY	CA-C-N	7.40	130.41	120.65
1	A	144	GLY	C-N-CA	7.40	130.41	120.65
1	B	304	PHE	CA-C-N	7.39	130.05	120.44
1	B	304	PHE	C-N-CA	7.39	130.05	120.44
1	A	92	GLY	CA-C-N	7.35	130.13	120.28
1	A	92	GLY	C-N-CA	7.35	130.13	120.28
1	A	304	PHE	CA-C-N	7.35	130.00	120.44
1	A	304	PHE	C-N-CA	7.35	130.00	120.44
1	B	92	GLY	CA-C-N	7.33	130.10	120.28
1	B	92	GLY	C-N-CA	7.33	130.10	120.28
1	B	474	GLU	CA-C-N	7.33	134.09	122.59
1	B	474	GLU	C-N-CA	7.33	134.09	122.59
1	A	474	GLU	CA-C-N	7.33	134.09	122.59
1	A	474	GLU	C-N-CA	7.33	134.09	122.59
1	A	143	SER	CA-C-N	7.25	128.03	119.98
1	A	143	SER	C-N-CA	7.25	128.03	119.98
1	B	143	SER	CA-C-N	7.22	128.00	119.98
1	B	143	SER	C-N-CA	7.22	128.00	119.98
1	A	83	TYR	CA-C-N	7.17	129.89	120.28
1	A	83	TYR	C-N-CA	7.17	129.89	120.28
1	A	145	PHE	CA-C-N	7.17	129.59	120.56
1	A	145	PHE	C-N-CA	7.17	129.59	120.56
1	B	83	TYR	CA-C-N	7.17	129.88	120.28
1	B	83	TYR	C-N-CA	7.17	129.88	120.28
1	A	126	ARG	N-CA-CB	7.16	120.70	109.82
1	B	126	ARG	N-CA-CB	7.16	120.70	109.82
1	B	145	PHE	CA-C-N	7.16	129.57	120.56
1	B	145	PHE	C-N-CA	7.16	129.57	120.56
1	A	131	THR	CA-C-N	7.14	129.72	120.44
1	A	131	THR	C-N-CA	7.14	129.72	120.44
1	B	301	THR	CA-C-N	7.13	129.72	120.44
1	B	301	THR	C-N-CA	7.13	129.72	120.44
1	B	131	THR	CA-C-N	7.12	129.69	120.44
1	B	131	THR	C-N-CA	7.12	129.69	120.44
1	A	301	THR	CA-C-N	7.10	129.67	120.44
1	A	301	THR	C-N-CA	7.10	129.67	120.44
1	A	35	LEU	CA-C-N	7.07	129.75	120.28
1	A	35	LEU	C-N-CA	7.07	129.75	120.28
1	B	35	LEU	CA-C-N	7.05	129.73	120.28
1	B	35	LEU	C-N-CA	7.05	129.73	120.28
1	A	299	GLN	CA-C-N	7.02	129.47	120.70
1	A	299	GLN	C-N-CA	7.02	129.47	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	119	ALA	CA-C-N	7.02	130.01	120.54
1	B	119	ALA	C-N-CA	7.02	130.01	120.54
1	A	119	ALA	CA-C-N	7.02	130.01	120.54
1	A	119	ALA	C-N-CA	7.02	130.01	120.54
1	B	299	GLN	CA-C-N	7.00	129.45	120.70
1	B	299	GLN	C-N-CA	7.00	129.45	120.70
1	A	466	ASN	CA-CB-CG	6.92	119.52	112.60
1	B	85	THR	CA-C-N	6.92	129.43	120.44
1	B	85	THR	C-N-CA	6.92	129.43	120.44
1	A	85	THR	CA-C-N	6.91	129.42	120.44
1	A	85	THR	C-N-CA	6.91	129.42	120.44
1	B	466	ASN	CA-C-N	6.90	129.84	120.38
1	B	466	ASN	C-N-CA	6.90	129.84	120.38
1	A	466	ASN	CA-C-N	6.89	129.83	120.38
1	A	466	ASN	C-N-CA	6.89	129.83	120.38
1	B	466	ASN	CA-CB-CG	6.89	119.49	112.60
1	B	30	ALA	CA-C-N	6.85	129.47	120.28
1	B	30	ALA	C-N-CA	6.85	129.47	120.28
1	A	30	ALA	CA-C-N	6.85	129.46	120.28
1	A	30	ALA	C-N-CA	6.85	129.46	120.28
1	B	33	LEU	CA-C-N	6.83	129.76	120.54
1	B	33	LEU	C-N-CA	6.83	129.76	120.54
1	A	87	ALA	CA-C-N	6.83	129.32	120.44
1	A	87	ALA	C-N-CA	6.83	129.32	120.44
1	A	33	LEU	CA-C-N	6.83	129.76	120.54
1	A	33	LEU	C-N-CA	6.83	129.76	120.54
1	B	458	LEU	CA-C-N	6.82	130.09	120.28
1	B	458	LEU	C-N-CA	6.82	130.09	120.28
1	A	458	LEU	CA-C-N	6.81	130.09	120.28
1	A	458	LEU	C-N-CA	6.81	130.09	120.28
1	B	87	ALA	CA-C-N	6.80	129.28	120.44
1	B	87	ALA	C-N-CA	6.80	129.28	120.44
1	A	318	ILE	CA-C-N	6.78	134.50	121.54
1	A	318	ILE	C-N-CA	6.78	134.50	121.54
1	B	318	ILE	CA-C-N	6.77	134.47	121.54
1	B	318	ILE	C-N-CA	6.77	134.47	121.54
1	A	86	TYR	CA-C-N	6.76	129.34	120.28
1	A	86	TYR	C-N-CA	6.76	129.34	120.28
1	A	104	TRP	N-CA-CB	6.76	119.81	110.01
1	B	86	TYR	CA-C-N	6.75	129.33	120.28
1	B	86	TYR	C-N-CA	6.75	129.33	120.28
1	B	104	TRP	O-C-N	-6.75	115.12	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	TRP	O-C-N	-6.75	115.12	122.07
1	B	104	TRP	N-CA-CB	6.74	119.78	110.01
1	A	146	ILE	CA-C-N	6.74	129.31	120.28
1	A	146	ILE	C-N-CA	6.74	129.31	120.28
1	A	312	GLY	CA-C-N	6.74	129.63	120.54
1	A	312	GLY	C-N-CA	6.74	129.63	120.54
1	B	32	ALA	CA-C-N	6.73	129.19	120.44
1	B	32	ALA	C-N-CA	6.73	129.19	120.44
1	B	312	GLY	CA-C-N	6.71	129.60	120.54
1	B	312	GLY	C-N-CA	6.71	129.60	120.54
1	A	32	ALA	CA-C-N	6.71	129.16	120.44
1	A	32	ALA	C-N-CA	6.71	129.16	120.44
1	B	146	ILE	CA-C-N	6.71	129.27	120.28
1	B	146	ILE	C-N-CA	6.71	129.27	120.28
1	B	31	PHE	CA-C-N	6.70	129.26	120.28
1	B	31	PHE	C-N-CA	6.70	129.26	120.28
1	A	31	PHE	CA-C-N	6.70	129.25	120.28
1	A	31	PHE	C-N-CA	6.70	129.25	120.28
1	B	101	GLU	N-CA-CB	6.68	119.90	109.94
1	A	101	GLU	N-CA-CB	6.66	119.86	109.94
1	B	147	THR	CA-C-N	6.63	127.30	119.94
1	B	147	THR	C-N-CA	6.63	127.30	119.94
1	A	147	THR	CA-C-N	6.60	127.27	119.94
1	A	147	THR	C-N-CA	6.60	127.27	119.94
1	A	322	ALA	CA-C-N	6.59	130.69	120.75
1	A	322	ALA	C-N-CA	6.59	130.69	120.75
1	B	322	ALA	CA-C-N	6.58	130.69	120.75
1	B	322	ALA	C-N-CA	6.58	130.69	120.75
1	A	449	GLU	CA-C-N	6.58	129.10	120.28
1	A	449	GLU	C-N-CA	6.58	129.10	120.28
1	B	449	GLU	CA-C-N	6.58	129.09	120.28
1	B	449	GLU	C-N-CA	6.58	129.09	120.28
1	A	117	THR	CA-C-N	6.57	132.25	123.05
1	A	117	THR	C-N-CA	6.57	132.25	123.05
1	B	117	THR	CA-C-N	6.57	132.24	123.05
1	B	117	THR	C-N-CA	6.57	132.24	123.05
1	A	89	ASN	CA-C-N	6.55	129.30	120.65
1	A	89	ASN	C-N-CA	6.55	129.30	120.65
1	B	89	ASN	CA-C-N	6.55	129.29	120.65
1	B	89	ASN	C-N-CA	6.55	129.29	120.65
1	B	88	LEU	CA-C-N	6.54	128.94	120.44
1	B	88	LEU	C-N-CA	6.54	128.94	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	LEU	CA-C-N	6.52	128.92	120.44
1	A	88	LEU	C-N-CA	6.52	128.92	120.44
1	B	258	LEU	O-C-N	-6.49	114.75	122.15
1	A	114	TYR	O-C-N	-6.49	115.34	122.09
1	B	124	VAL	CA-C-N	6.46	129.59	120.28
1	B	124	VAL	C-N-CA	6.46	129.59	120.28
1	B	114	TYR	O-C-N	-6.46	115.37	122.09
1	A	258	LEU	O-C-N	-6.46	114.79	122.15
1	A	124	VAL	CA-C-N	6.45	129.56	120.28
1	A	124	VAL	C-N-CA	6.45	129.56	120.28
1	A	123	THR	CA-C-N	6.36	129.17	120.46
1	A	123	THR	C-N-CA	6.36	129.17	120.46
1	A	323	GLU	CA-C-N	6.35	129.85	120.95
1	A	323	GLU	C-N-CA	6.35	129.85	120.95
1	A	453	GLU	CA-C-N	6.35	128.79	120.28
1	A	453	GLU	C-N-CA	6.35	128.79	120.28
1	B	123	THR	CA-C-N	6.34	129.15	120.46
1	B	123	THR	C-N-CA	6.34	129.15	120.46
1	B	323	GLU	CA-C-N	6.34	129.83	120.95
1	B	323	GLU	C-N-CA	6.34	129.83	120.95
1	B	453	GLU	CA-C-N	6.33	128.76	120.28
1	B	453	GLU	C-N-CA	6.33	128.76	120.28
1	A	130	ASP	CA-C-N	6.33	128.76	120.28
1	A	130	ASP	C-N-CA	6.33	128.76	120.28
1	B	130	ASP	CA-C-N	6.31	128.73	120.28
1	B	130	ASP	C-N-CA	6.31	128.73	120.28
1	A	465	PRO	CA-C-N	6.31	132.71	122.81
1	A	465	PRO	C-N-CA	6.31	132.71	122.81
1	B	305	THR	CA-C-N	6.30	131.36	120.58
1	B	305	THR	C-N-CA	6.30	131.36	120.58
1	B	465	PRO	CA-C-N	6.30	132.71	122.81
1	B	465	PRO	C-N-CA	6.30	132.71	122.81
1	A	118	ASN	CA-C-N	6.30	130.35	121.02
1	A	118	ASN	C-N-CA	6.30	130.35	121.02
1	A	305	THR	CA-C-N	6.30	131.35	120.58
1	A	305	THR	C-N-CA	6.30	131.35	120.58
1	B	118	ASN	CA-C-N	6.30	130.34	121.02
1	B	118	ASN	C-N-CA	6.30	130.34	121.02
1	B	107	LEU	N-CA-CB	6.29	120.02	109.78
1	A	107	LEU	N-CA-CB	6.27	120.00	109.78
1	B	27	GLY	CA-C-N	6.26	129.83	120.31
1	B	27	GLY	C-N-CA	6.26	129.83	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	GLY	CA-C-N	6.25	129.81	120.31
1	A	27	GLY	C-N-CA	6.25	129.81	120.31
1	A	309	LYS	CA-C-N	6.24	129.15	120.29
1	A	309	LYS	C-N-CA	6.24	129.15	120.29
1	B	309	LYS	CA-C-N	6.23	129.13	120.29
1	B	309	LYS	C-N-CA	6.23	129.13	120.29
1	A	135	LYS	CA-C-N	6.20	128.59	120.28
1	A	135	LYS	C-N-CA	6.20	128.59	120.28
1	B	100	ARG	N-CA-CB	6.19	119.17	109.94
1	A	100	ARG	N-CA-CB	6.18	119.15	109.94
1	B	135	LYS	CA-C-N	6.16	128.53	120.28
1	B	135	LYS	C-N-CA	6.16	128.53	120.28
1	A	122	GLU	O-C-N	-6.10	115.20	122.15
1	A	96	ILE	CA-C-N	6.07	128.41	120.28
1	A	96	ILE	C-N-CA	6.07	128.41	120.28
1	B	96	ILE	CA-C-N	6.07	128.41	120.28
1	B	96	ILE	C-N-CA	6.07	128.41	120.28
1	B	462	LYS	CA-C-N	6.06	131.75	121.14
1	B	462	LYS	C-N-CA	6.06	131.75	121.14
1	B	122	GLU	O-C-N	-6.06	115.25	122.15
1	A	441	ARG	CD-NE-CZ	6.05	132.87	124.40
1	A	462	LYS	CA-C-N	6.05	131.72	121.14
1	A	462	LYS	C-N-CA	6.05	131.72	121.14
1	B	91	ASN	CA-C-N	6.04	126.69	119.98
1	B	91	ASN	C-N-CA	6.04	126.69	119.98
1	B	132	MET	CA-C-N	6.02	129.02	120.53
1	B	132	MET	C-N-CA	6.02	129.02	120.53
1	A	367	GLY	CA-C-N	6.02	131.96	122.21
1	A	367	GLY	C-N-CA	6.02	131.96	122.21
1	B	441	ARG	CD-NE-CZ	6.02	132.82	124.40
1	A	91	ASN	CA-C-N	6.01	126.66	119.98
1	A	91	ASN	C-N-CA	6.01	126.66	119.98
1	A	138	ILE	CA-C-N	6.01	128.83	120.29
1	A	138	ILE	C-N-CA	6.01	128.83	120.29
1	B	34	ALA	CA-C-N	6.01	128.94	120.28
1	B	34	ALA	C-N-CA	6.01	128.94	120.28
1	A	446	ALA	CA-C-N	6.01	130.85	120.58
1	A	446	ALA	C-N-CA	6.01	130.85	120.58
1	B	138	ILE	CA-C-N	6.00	128.82	120.29
1	B	138	ILE	C-N-CA	6.00	128.82	120.29
1	A	132	MET	CA-C-N	6.00	128.99	120.53
1	A	132	MET	C-N-CA	6.00	128.99	120.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	367	GLY	CA-C-N	6.00	131.92	122.21
1	B	367	GLY	C-N-CA	6.00	131.92	122.21
1	B	446	ALA	CA-C-N	5.99	130.83	120.58
1	B	446	ALA	C-N-CA	5.99	130.83	120.58
1	A	34	ALA	CA-C-N	5.99	128.91	120.28
1	A	34	ALA	C-N-CA	5.99	128.91	120.28
1	B	90	TYR	CA-C-N	5.84	128.11	120.28
1	B	90	TYR	C-N-CA	5.84	128.11	120.28
1	A	90	TYR	CA-C-N	5.84	128.10	120.28
1	A	90	TYR	C-N-CA	5.84	128.10	120.28
1	A	440	GLU	CA-C-N	5.83	131.34	122.08
1	A	440	GLU	C-N-CA	5.83	131.34	122.08
1	B	100	ARG	O-C-N	-5.82	116.04	122.09
1	A	100	ARG	O-C-N	-5.81	116.05	122.09
1	B	440	GLU	CA-C-N	5.80	131.30	122.08
1	B	440	GLU	C-N-CA	5.80	131.30	122.08
1	B	125	SER	O-C-N	-5.79	115.44	122.22
1	B	302	THR	CA-C-N	5.78	128.83	120.79
1	B	302	THR	C-N-CA	5.78	128.83	120.79
1	A	134	VAL	CA-C-N	5.78	127.96	120.44
1	A	134	VAL	C-N-CA	5.78	127.96	120.44
1	B	134	VAL	CA-C-N	5.77	127.94	120.44
1	B	134	VAL	C-N-CA	5.77	127.94	120.44
1	A	302	THR	CA-C-N	5.76	128.80	120.79
1	A	302	THR	C-N-CA	5.76	128.80	120.79
1	A	125	SER	O-C-N	-5.75	115.49	122.22
1	A	303	PHE	CA-C-N	5.75	127.99	120.28
1	A	303	PHE	C-N-CA	5.75	127.99	120.28
1	A	111	PRO	N-CA-CB	5.74	108.36	103.19
1	B	111	PRO	N-CA-CB	5.73	108.35	103.19
1	B	307	LEU	CA-C-N	5.72	127.94	120.28
1	B	307	LEU	C-N-CA	5.72	127.94	120.28
1	A	307	LEU	CA-C-N	5.72	127.94	120.28
1	A	307	LEU	C-N-CA	5.72	127.94	120.28
1	B	303	PHE	CA-C-N	5.72	127.94	120.28
1	B	303	PHE	C-N-CA	5.72	127.94	120.28
1	A	142	ILE	CA-C-N	5.72	127.94	120.28
1	A	142	ILE	C-N-CA	5.72	127.94	120.28
1	B	142	ILE	CA-C-N	5.70	127.92	120.28
1	B	142	ILE	C-N-CA	5.70	127.92	120.28
1	B	298	GLY	CA-C-N	5.62	128.86	120.31
1	B	298	GLY	C-N-CA	5.62	128.86	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	GLY	CA-C-N	5.62	128.84	120.31
1	A	298	GLY	C-N-CA	5.62	128.84	120.31
1	B	126	ARG	O-C-N	-5.60	116.09	122.08
1	A	107	LEU	O-C-N	-5.59	115.68	122.11
1	B	300	ILE	CA-C-N	5.59	128.22	120.29
1	B	300	ILE	C-N-CA	5.59	128.22	120.29
1	A	300	ILE	CA-C-N	5.57	128.20	120.29
1	A	300	ILE	C-N-CA	5.57	128.20	120.29
1	A	126	ARG	O-C-N	-5.56	116.13	122.08
1	B	107	LEU	O-C-N	-5.56	115.72	122.11
1	B	325	GLU	CA-C-N	5.51	130.25	121.66
1	B	325	GLU	C-N-CA	5.51	130.25	121.66
1	A	300	ILE	N-CA-CB	5.48	116.59	110.62
1	A	324	GLU	CA-C-N	5.48	130.48	121.39
1	A	324	GLU	C-N-CA	5.48	130.48	121.39
1	B	300	ILE	N-CA-CB	5.46	116.58	110.62
1	A	325	GLU	CA-C-N	5.46	130.18	121.66
1	A	325	GLU	C-N-CA	5.46	130.18	121.66
1	B	324	GLU	CA-C-N	5.46	130.45	121.39
1	B	324	GLU	C-N-CA	5.46	130.45	121.39
1	B	29	LEU	CA-C-N	5.46	127.53	120.44
1	B	29	LEU	C-N-CA	5.46	127.53	120.44
1	A	29	LEU	CA-C-N	5.44	127.51	120.44
1	A	29	LEU	C-N-CA	5.44	127.51	120.44
1	B	311	ILE	CA-C-N	5.32	125.89	119.98
1	B	311	ILE	C-N-CA	5.32	125.89	119.98
1	A	311	ILE	CA-C-N	5.32	125.88	119.98
1	A	311	ILE	C-N-CA	5.32	125.88	119.98
1	A	129	ASN	CA-C-N	5.31	127.39	120.28
1	A	129	ASN	C-N-CA	5.31	127.39	120.28
1	B	114	TYR	N-CA-CB	5.31	117.85	109.94
1	B	129	ASN	CA-C-N	5.30	127.38	120.28
1	B	129	ASN	C-N-CA	5.30	127.38	120.28
1	B	308	GLN	CA-C-N	5.30	129.64	120.58
1	B	308	GLN	C-N-CA	5.30	129.64	120.58
1	B	432	ARG	NE-CZ-NH2	5.30	123.97	119.20
1	A	114	TYR	N-CA-CB	5.30	117.83	109.94
1	B	390	PHE	CA-CB-CG	5.29	119.09	113.80
1	A	308	GLN	CA-C-N	5.29	129.62	120.58
1	A	308	GLN	C-N-CA	5.29	129.62	120.58
1	A	432	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	A	390	PHE	CA-CB-CG	5.27	119.07	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	453	GLU	N-CA-CB	5.27	117.60	109.91
1	B	452	ALA	CA-C-N	5.26	127.60	120.65
1	B	452	ALA	C-N-CA	5.26	127.60	120.65
1	A	453	GLU	N-CA-CB	5.26	117.59	109.91
1	A	475	ARG	CD-NE-CZ	5.26	131.76	124.40
1	B	475	ARG	CD-NE-CZ	5.24	131.73	124.40
1	B	492	ALA	CA-C-N	5.22	127.70	120.29
1	B	492	ALA	C-N-CA	5.22	127.70	120.29
1	B	445	ASP	CA-C-N	5.22	127.79	120.28
1	B	445	ASP	C-N-CA	5.22	127.79	120.28
1	A	452	ALA	CA-C-N	5.22	127.54	120.65
1	A	452	ALA	C-N-CA	5.22	127.54	120.65
1	A	492	ALA	CA-C-N	5.20	127.68	120.29
1	A	492	ALA	C-N-CA	5.20	127.68	120.29
1	A	445	ASP	CA-C-N	5.19	127.75	120.28
1	A	445	ASP	C-N-CA	5.19	127.75	120.28
1	B	414	ARG	NE-CZ-NH2	5.14	123.82	119.20
1	A	227	GLY	O-C-N	-5.14	116.80	122.24
1	B	227	GLY	O-C-N	-5.13	116.81	122.24
1	A	414	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	A	338	HIS	CB-CG-CD2	-5.10	124.57	131.20
1	B	338	HIS	CB-CG-CD2	-5.10	124.57	131.20
1	B	316	ARG	NE-CZ-NH1	5.05	126.55	121.50
1	B	100	ARG	NE-CZ-NH1	5.03	126.53	121.50
1	A	100	ARG	NE-CZ-NH1	5.02	126.52	121.50
1	A	316	ARG	NE-CZ-NH1	5.02	126.52	121.50

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	4372	4536	4535	72	0
1	B	4372	4536	4535	72	0
All	All	8744	9072	9070	77	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 4.

All (77) 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:212:GLU:CD	1:A:427:MET:HB3	1.63	1.22
1:B:220:ASN:ND2	1:A:411:GLU:OE2	1.79	1.15
1:B:101:GLU:HG3	1:A:233:ILE:CD1	1.77	1.15
1:B:212:GLU:OE2	1:A:427:MET:HB3	1.45	1.15
1:B:427:MET:HB3	1:A:212:GLU:CD	1.73	1.13
1:B:101:GLU:CG	1:A:233:ILE:HD11	1.77	1.13
1:B:411:GLU:OE2	1:A:220:ASN:ND2	1.81	1.13
1:B:212:GLU:OE2	1:A:427:MET:CB	1.99	1.11
1:B:271:MET:HE1	1:A:62:LEU:CD2	1.80	1.11
1:B:427:MET:HB3	1:A:212:GLU:OE2	1.51	1.09
1:B:62:LEU:CD2	1:A:271:MET:HE1	1.83	1.09
1:B:233:ILE:CD1	1:A:101:GLU:HG3	1.83	1.08
1:B:271:MET:HE1	1:A:62:LEU:HD21	1.35	1.08
1:B:233:ILE:HD11	1:A:101:GLU:CG	1.86	1.04
1:B:428:SER:OG	1:A:208:GLN:OE1	1.76	1.02
1:B:208:GLN:OE1	1:A:428:SER:OG	1.75	1.01
1:B:62:LEU:HD21	1:A:271:MET:HE1	1.41	1.01
1:B:212:GLU:OE1	1:A:427:MET:HB3	1.58	1.01
1:B:427:MET:CB	1:A:212:GLU:OE2	2.09	1.00
1:B:101:GLU:HG2	1:A:233:ILE:HD11	1.40	0.99
1:B:101:GLU:HG3	1:A:233:ILE:HD12	1.46	0.96
1:B:427:MET:HB3	1:A:212:GLU:OE1	1.64	0.94
1:B:233:ILE:HD11	1:A:101:GLU:HG2	1.52	0.92
1:B:287:ILE:HD13	1:A:287:ILE:HD13	1.51	0.92
1:B:101:GLU:CG	1:A:233:ILE:CD1	2.41	0.91
1:B:233:ILE:HD12	1:A:101:GLU:HG3	1.54	0.90
1:B:233:ILE:CD1	1:A:101:GLU:CG	2.49	0.85
1:B:212:GLU:CD	1:A:427:MET:CB	2.52	0.73
1:B:271:MET:HE2	1:A:57:PHE:CG	2.25	0.71
1:B:271:MET:HE3	1:A:57:PHE:HB2	1.71	0.70
1:B:212:GLU:OE2	1:A:427:MET:HB2	1.90	0.70
1:B:271:MET:CE	1:A:62:LEU:HD21	2.17	0.69
1:B:62:LEU:HD21	1:A:271:MET:CE	2.21	0.67
1:B:57:PHE:HB2	1:A:271:MET:HE3	1.76	0.66
1:B:57:PHE:CG	1:A:271:MET:HE2	2.33	0.64
1:B:212:GLU:OE1	1:A:427:MET:CB	2.42	0.60
1:B:104:TRP:CZ3	1:A:206:LEU:HG	2.39	0.57

Continued on next page...

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:MET:CE	1:A:57:PHE:CG	2.86	0.57
1:A:345:ARG:HG2	1:A:359:GLU:HG2	1.87	0.56
1:B:345:ARG:HG2	1:B:359:GLU:HG2	1.87	0.55
1:B:210:LEU:HD12	1:A:124:VAL:HG23	1.87	0.55
1:B:62:LEU:HD23	1:A:271:MET:HE1	1.86	0.54
1:A:345:ARG:HG2	1:A:359:GLU:CG	2.38	0.53
1:B:427:MET:HB2	1:A:212:GLU:OE2	2.05	0.53
1:B:345:ARG:HG2	1:B:359:GLU:CG	2.38	0.52
1:B:110:LEU:O	1:A:217:LYS:HE3	2.09	0.52
1:B:210:LEU:HD12	1:A:124:VAL:CG2	2.40	0.52
1:B:271:MET:HB3	1:A:57:PHE:CD2	2.46	0.51
1:B:437:TYR:OH	1:A:225:GLU:CD	2.54	0.51
1:B:271:MET:HE2	1:A:57:PHE:CD2	2.46	0.50
1:A:214:ARG:HB3	1:A:214:ARG:NH2	2.27	0.50
1:B:124:VAL:HG23	1:A:210:LEU:HD12	1.92	0.50
1:B:252:PRO:HG3	1:A:82:ALA:HB2	1.94	0.49
1:B:214:ARG:HB3	1:B:214:ARG:NH2	2.27	0.49
1:B:271:MET:HE1	1:A:62:LEU:HD23	1.82	0.49
1:B:187:LYS:HG2	1:B:188:MET:N	2.27	0.49
1:A:187:LYS:HG2	1:A:188:MET:N	2.27	0.48
1:B:217:LYS:HE3	1:A:110:LEU:O	2.14	0.48
1:B:57:PHE:CG	1:A:271:MET:CE	2.96	0.47
1:B:206:LEU:HG	1:A:104:TRP:CZ3	2.50	0.47
1:B:82:ALA:HB2	1:A:252:PRO:HG3	1.97	0.46
1:B:427:MET:CB	1:A:212:GLU:OE1	2.50	0.46
1:B:284:VAL:HG21	1:A:270:GLY:HA3	1.97	0.45
1:B:287:ILE:HD13	1:A:287:ILE:CD1	2.35	0.44
1:B:225:GLU:CD	1:A:437:TYR:OH	2.61	0.44
1:B:124:VAL:CG2	1:A:210:LEU:HD12	2.48	0.43
1:B:90:TYR:HD1	1:A:241:VAL:HG23	1.81	0.43
1:B:271:MET:HE3	1:A:57:PHE:CB	2.42	0.43
1:B:57:PHE:CD2	1:A:271:MET:HB3	2.53	0.42
1:B:54:VAL:HG13	1:A:270:GLY:C	2.44	0.42
1:B:270:GLY:C	1:A:54:VAL:HG13	2.45	0.41
1:B:159:LEU:HD22	1:B:286:PHE:CD2	2.56	0.41
1:A:159:LEU:HD22	1:A:286:PHE:CD2	2.56	0.41
1:B:112:VAL:HG23	1:A:213:ILE:HG23	2.03	0.41
1:B:233:ILE:CD1	1:A:101:GLU:HG2	2.32	0.40
1:B:427:MET:CB	1:A:212:GLU:CD	2.63	0.40
1:B:57:PHE:CD2	1:A:271:MET:HE2	2.55	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	566/604 (94%)	547 (97%)	19 (3%)	0	100	100
1	B	566/604 (94%)	547 (97%)	19 (3%)	0	100	100
All	All	1132/1208 (94%)	1094 (97%)	38 (3%)	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	479/509 (94%)	475 (99%)	4 (1%)	73	78
1	B	479/509 (94%)	475 (99%)	4 (1%)	73	78
All	All	958/1018 (94%)	950 (99%)	8 (1%)	70	78

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	187	LYS
1	B	345	ARG
1	B	359	GLU
1	B	554	ILE
1	A	187	LYS
1	A	345	ARG
1	A	359	GLU
1	A	554	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	91	ASN
1	B	141	HIS
1	B	272	GLN
1	B	292	GLN
1	B	485	GLN
1	A	52	GLN
1	A	66	GLN
1	A	77	GLN
1	A	91	ASN
1	A	141	HIS
1	A	272	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.

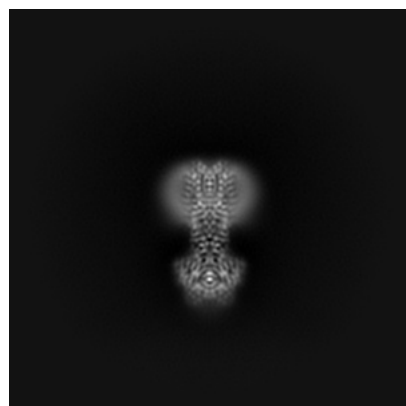
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18535. These allow visual inspection of the internal detail of the map and identification of artifacts.

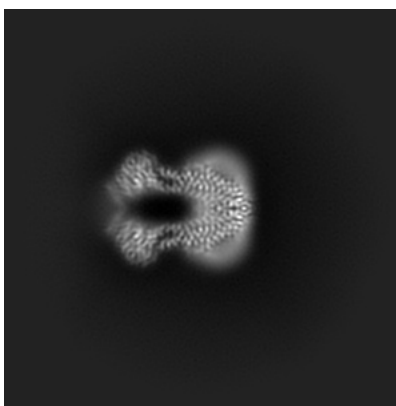
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

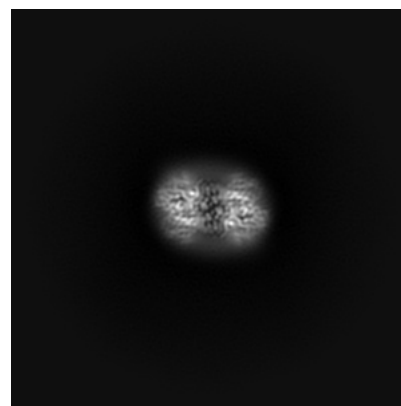
6.1.1 Primary map



X

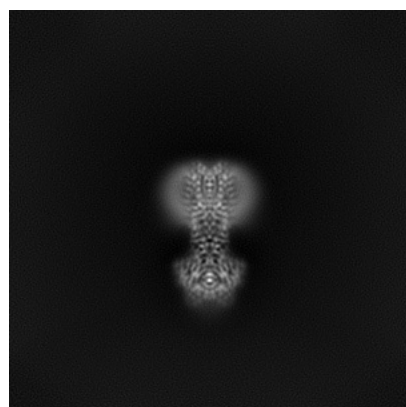


Y

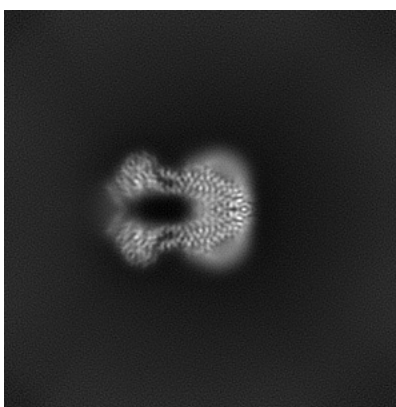


Z

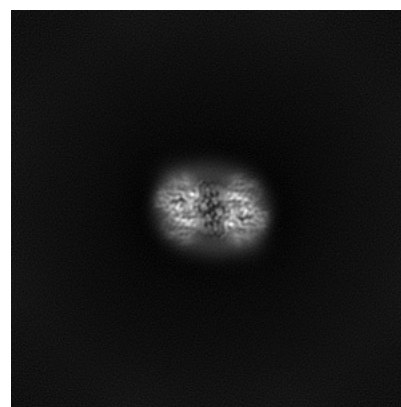
6.1.2 Raw map



X



Y

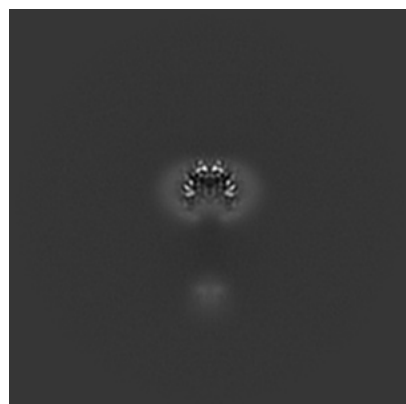


Z

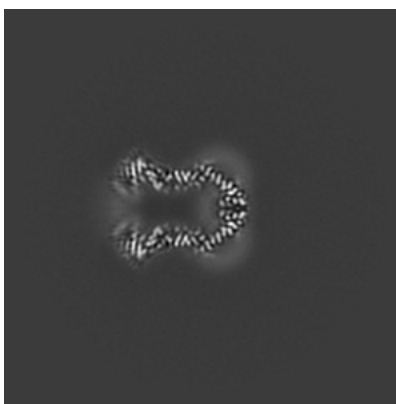
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

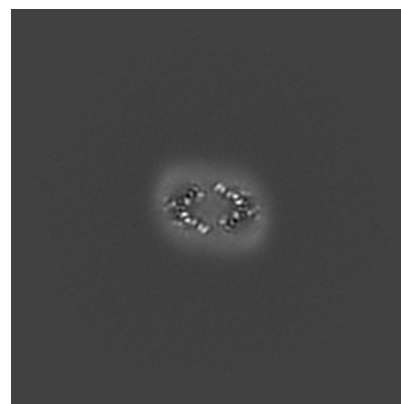
6.2.1 Primary map



X Index: 150

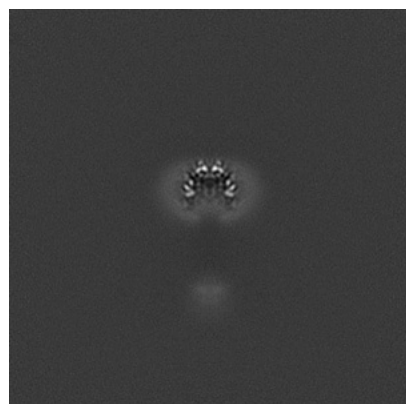


Y Index: 150

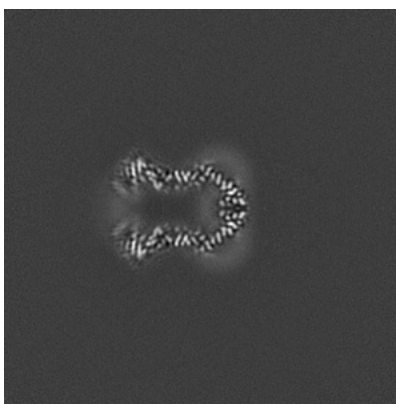


Z Index: 150

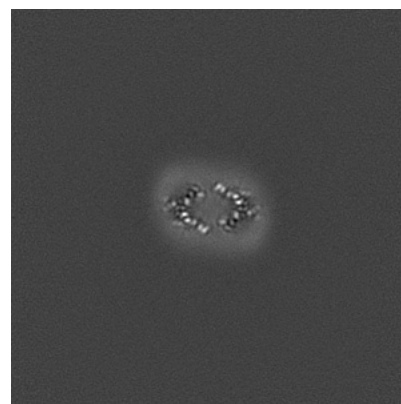
6.2.2 Raw map



X Index: 150



Y Index: 150

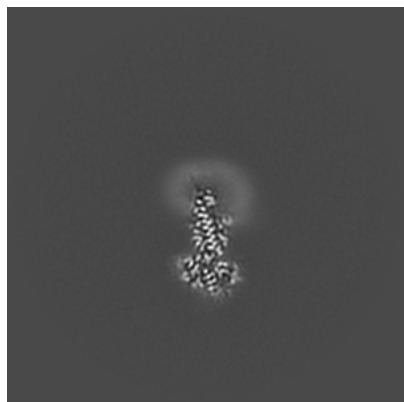


Z Index: 150

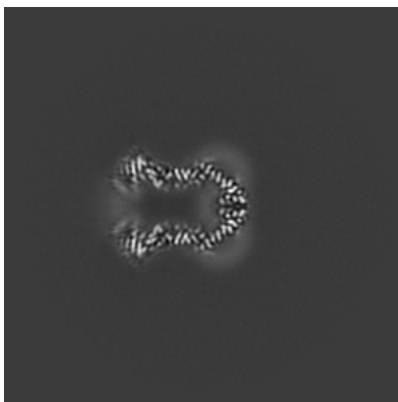
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

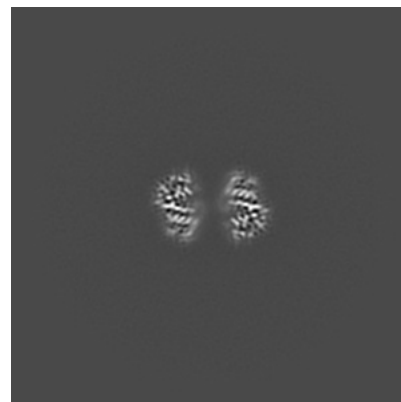
6.3.1 Primary map



X Index: 125

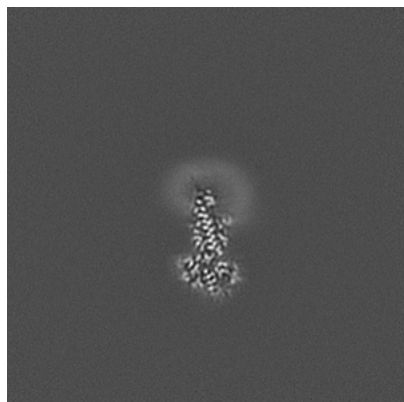


Y Index: 150

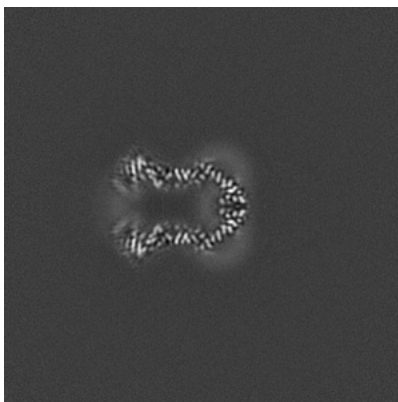


Z Index: 101

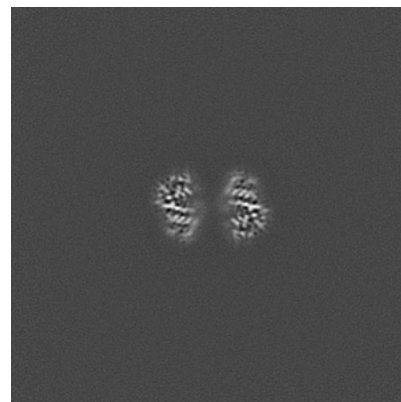
6.3.2 Raw map



X Index: 125



Y Index: 150

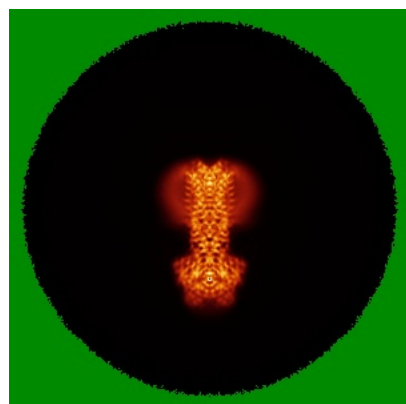


Z Index: 101

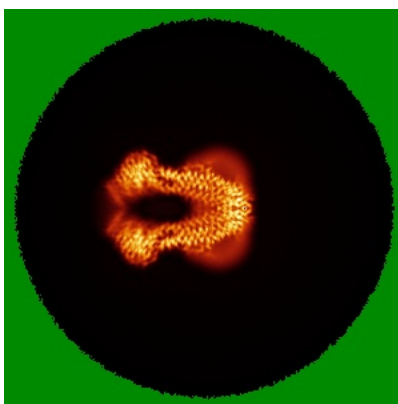
The images above show the largest variance slices of the map in three orthogonal directions.

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

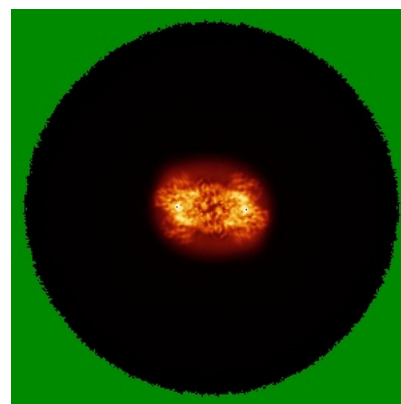
6.4.1 Primary map



X

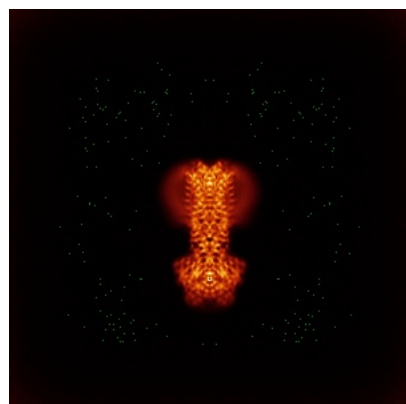


Y

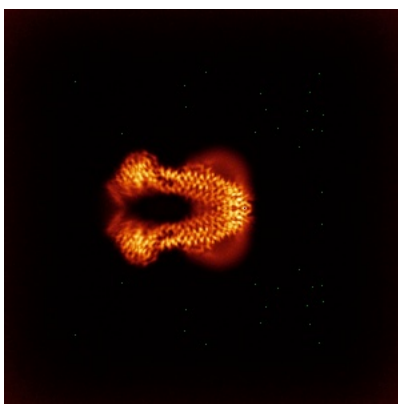


Z

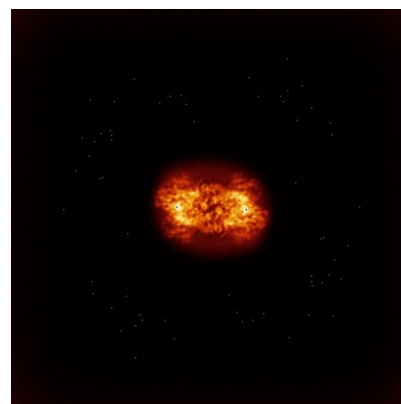
6.4.2 Raw map



X



Y

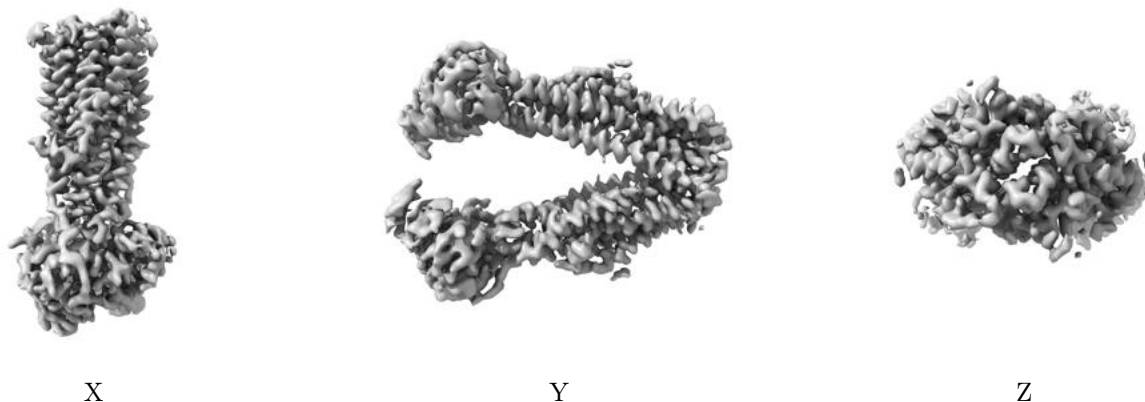


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

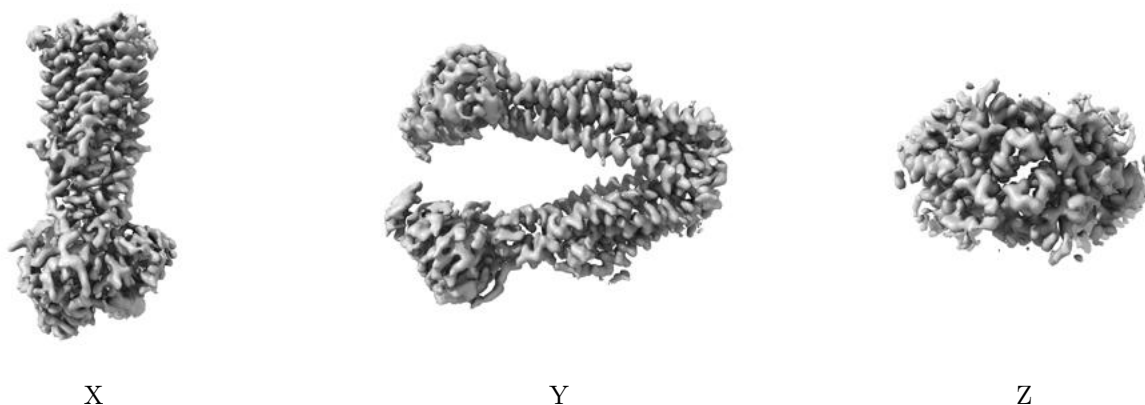
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

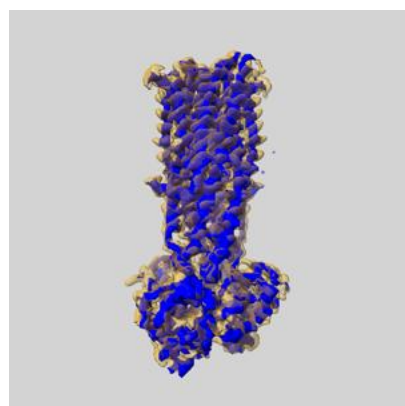
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

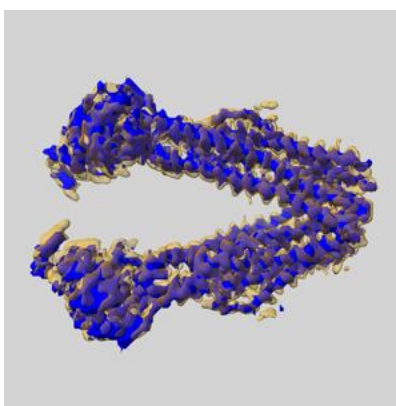
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

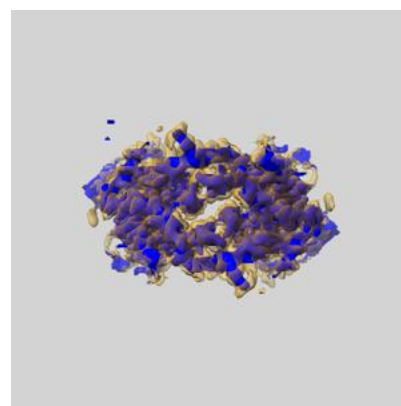
6.6.1 emd_18535_msk_1.map [i](#)



X



Y

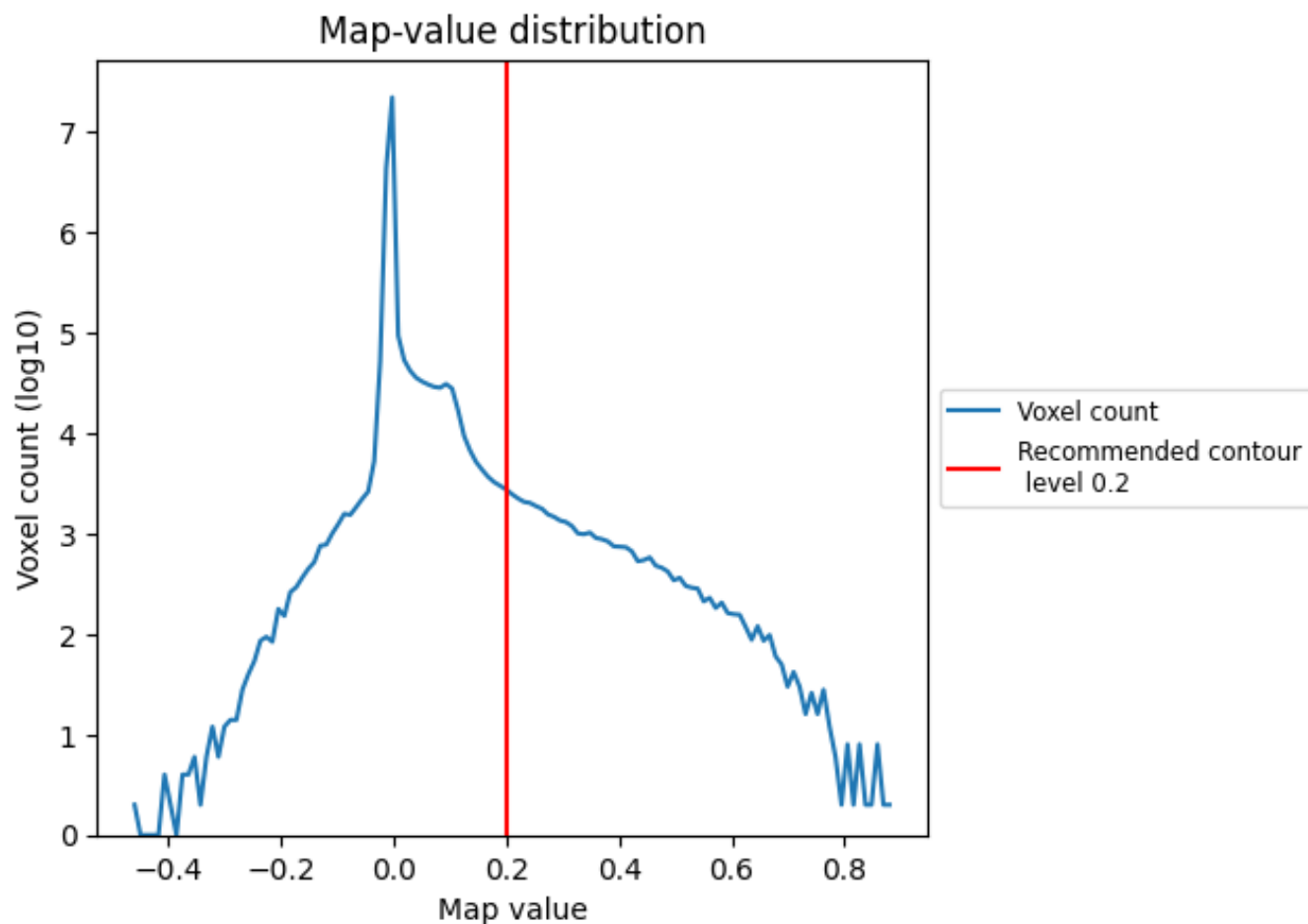


Z

7 Map analysis [i](#)

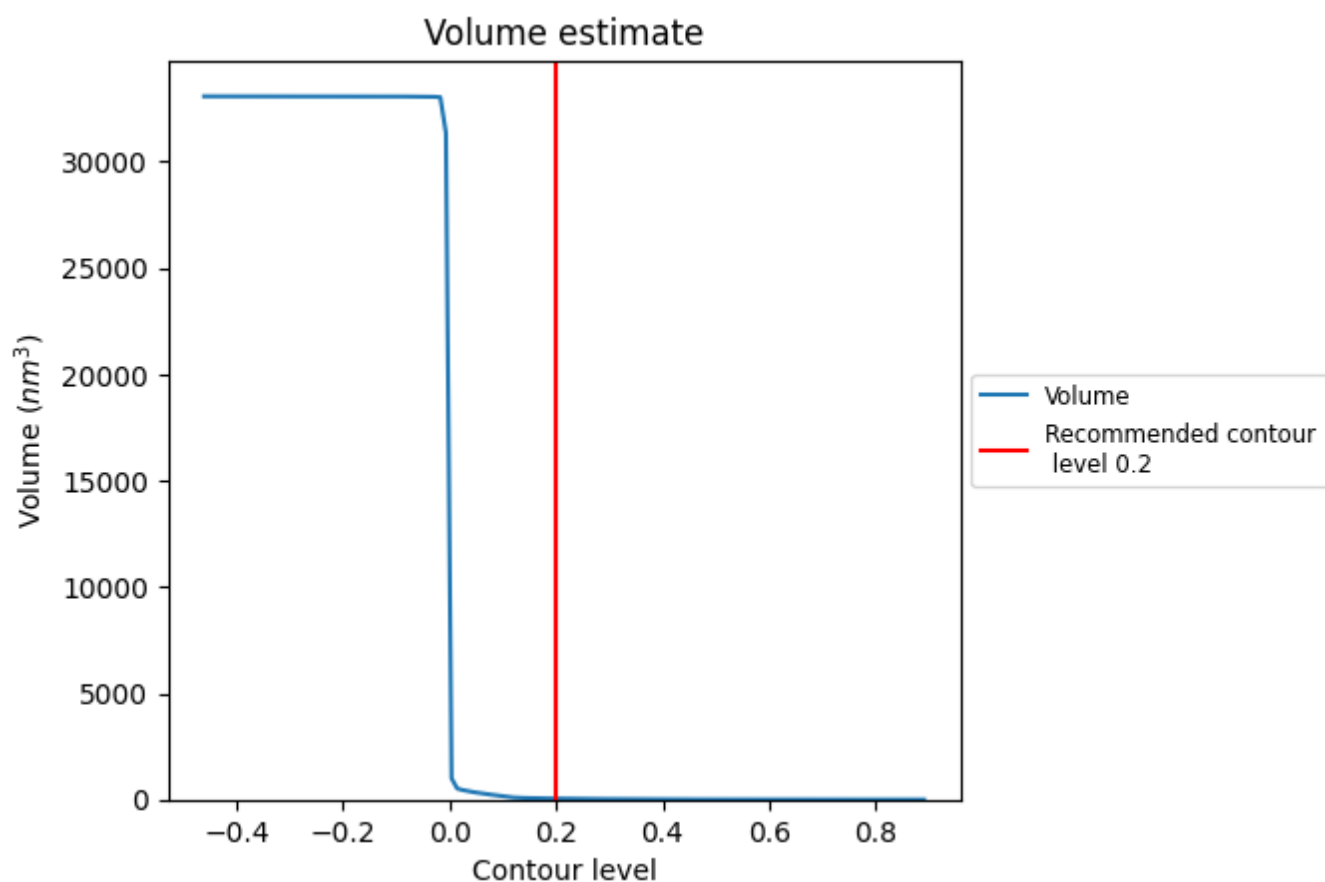
This section contains the results of statistical analysis of the map.

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.

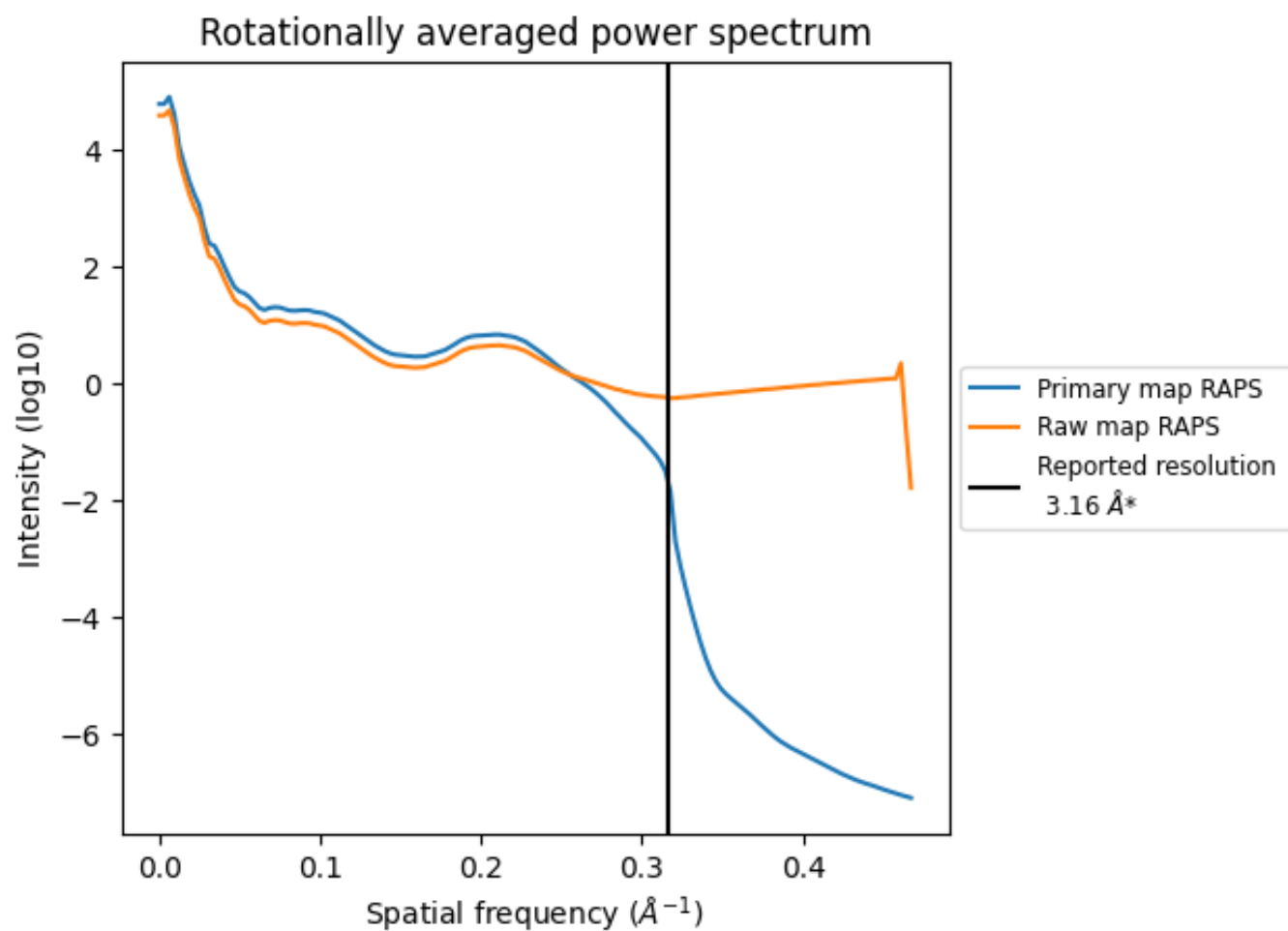
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 46 nm^3 ; this corresponds to an approximate mass of 41 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 ⓘ

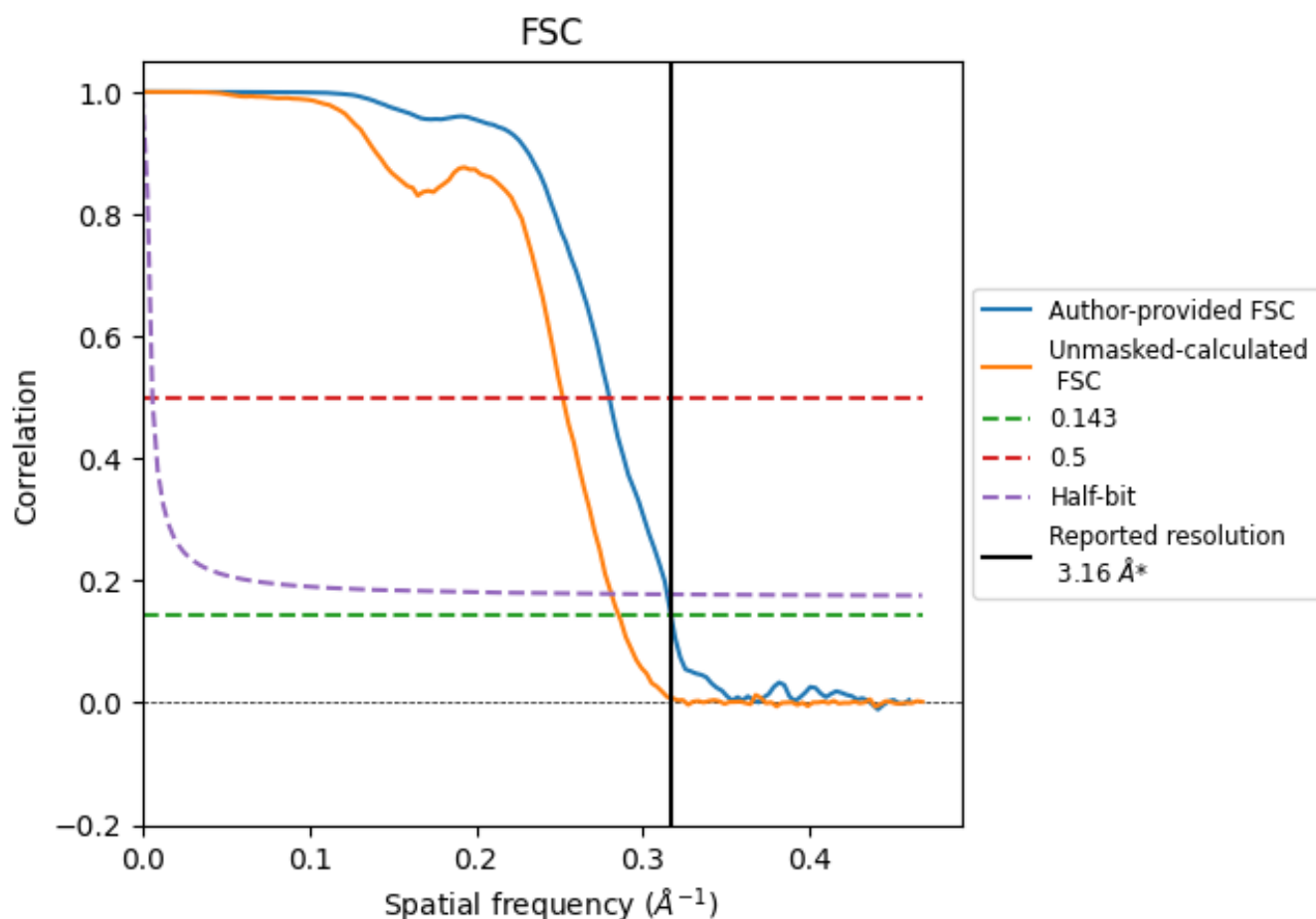


*Reported resolution corresponds to spatial frequency of $0.316 \text{ \AA}^{-1}$

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 0.316 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

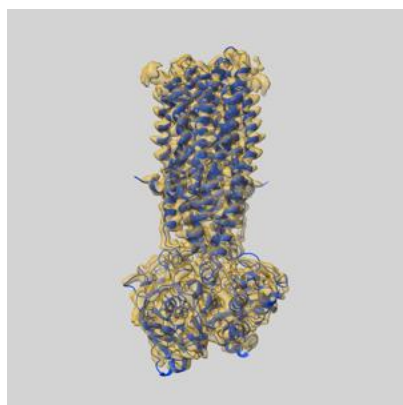
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.16	-	-
Author-provided FSC curve	3.16	3.57	3.18
Unmasked-calculated*	3.50	3.97	3.56

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.50 differs from the reported value 3.16 by more than 10 %

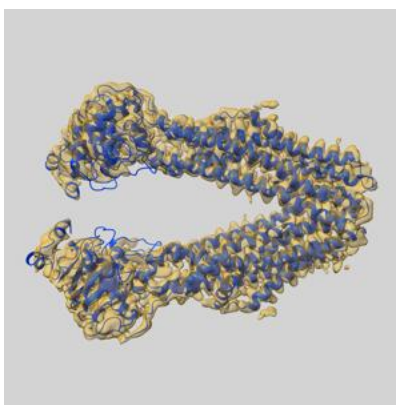
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18535 and PDB model 8QOE. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

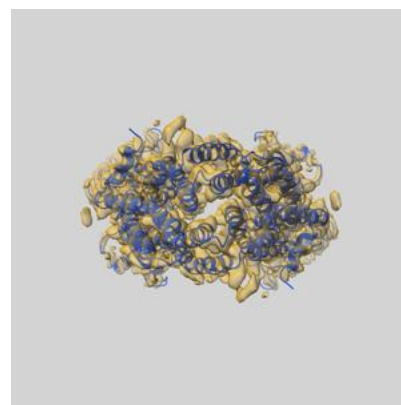
9.1 Map-model overlay [i](#)



X



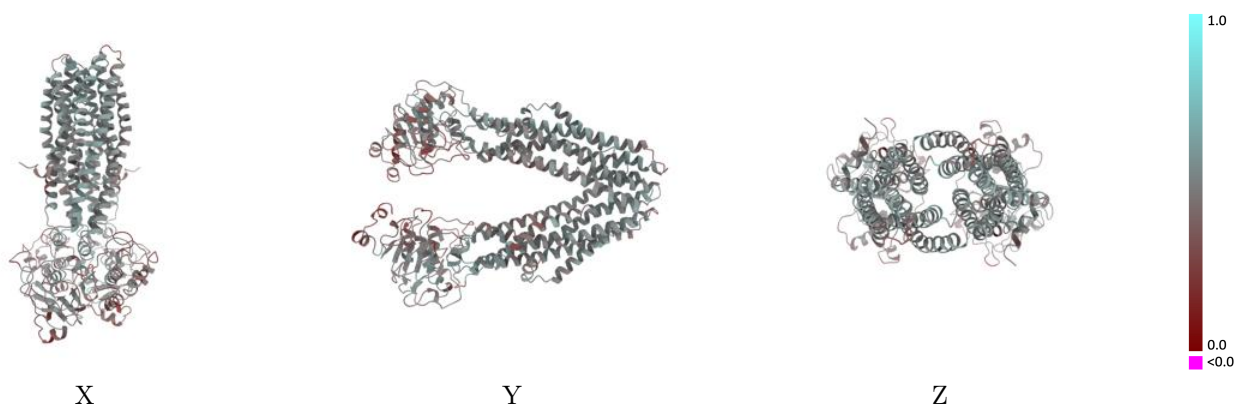
Y



Z

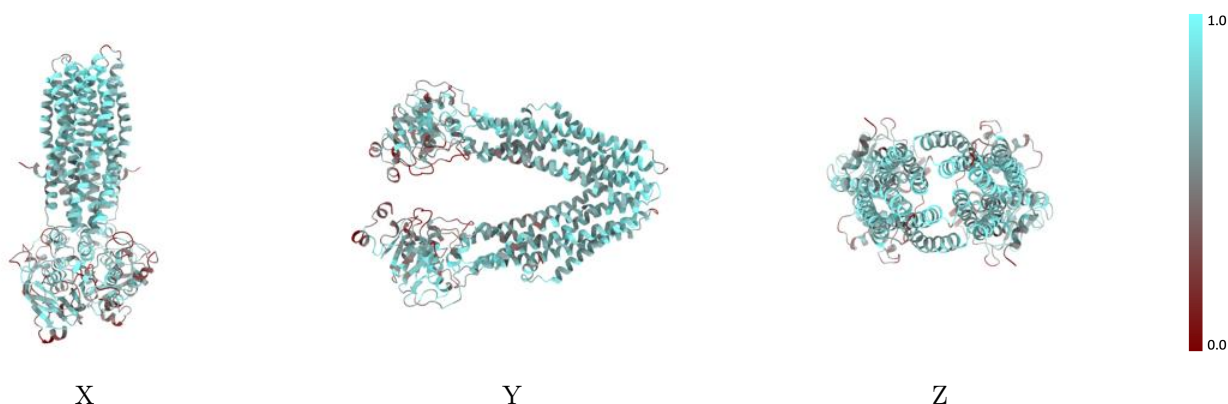
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



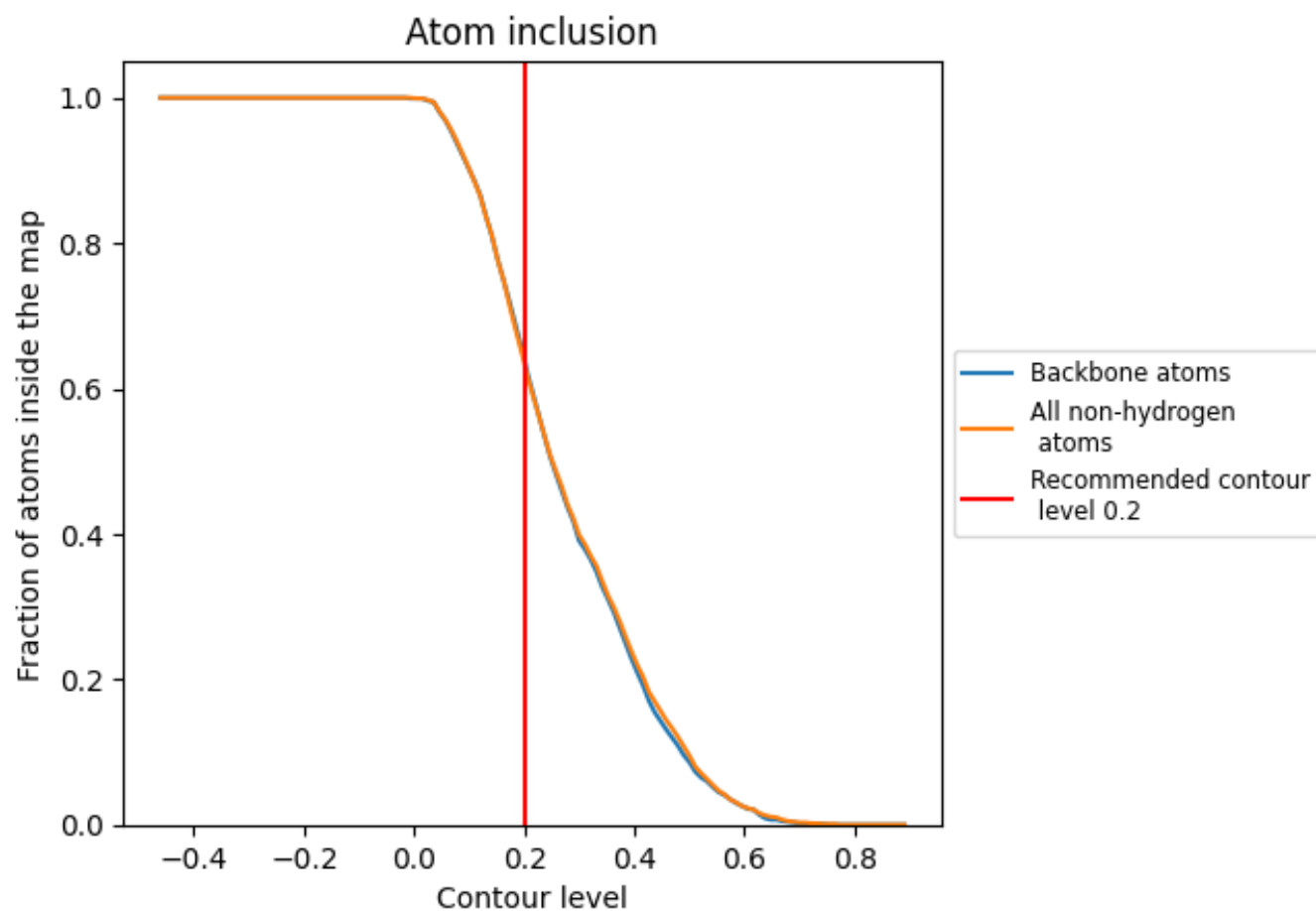
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 64% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6360	0.4590
A	0.6450	0.4560
B	0.6440	0.4620

