



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 04:24 PM UTC

PDB ID : 7SPJ / pdb_00007spj
EMDB ID : EMD-24772
Title : Models for C17 reconstruction of Outer Membrane Core Complex (OMCC) of Type IV Secretion System (T4SS) encoded by a plasmid overproducing TraV, TraK and TraB of pED208
Authors : Liu, X.; Khara, P.; Baker, M.L.; Christie, P.J.; Hu, B.
Deposited on : 2021-11-02
Resolution : 3.56 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:

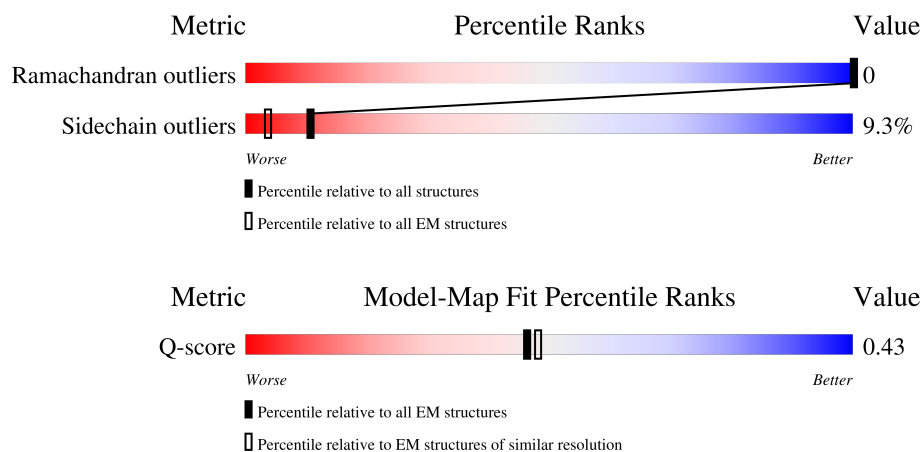
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.56 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.



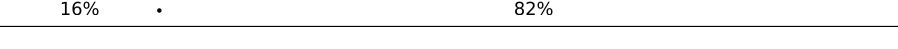
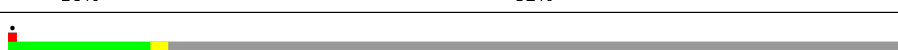
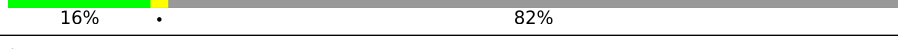
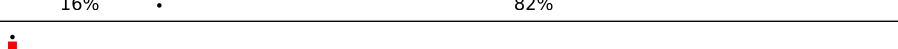
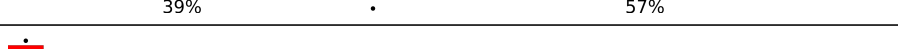
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12891 (3.04 - 4.04)

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	AB1	204	
1	AB10	204	
1	AB11	204	
1	AB12	204	
1	AB13	204	

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Mol	Chain	Length	Quality of chain
1	AB14	204	
1	AB15	204	
1	AB16	204	
1	AB17	204	
1	AB2	204	
1	AB3	204	
1	AB4	204	
1	AB5	204	
1	AB6	204	
1	AB7	204	
1	AB8	204	
1	AB9	204	
2	EF1	453	
2	EF10	453	
2	EF11	453	
2	EF12	453	
2	EF13	453	
2	EF14	453	
2	EF15	453	
2	EF16	453	
2	EF17	453	
2	EF2	453	
2	EF3	453	
2	EF4	453	
2	EF5	453	

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Mol	Chain	Length	Quality of chain
2	EF6	453	39% 57%
2	EF7	453	39% 57%
2	EF8	453	39% 57%
2	EF9	453	39% 57%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 29597 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 TraV.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AB1	37	Total	C	N	O	S	0	0
			261	153	47	56	5		
1	AB2	37	Total	C	N	O	S	0	0
			261	153	47	56	5		
1	AB3	37	Total	C	N	O	S	0	0
			261	153	47	56	5		
1	AB4	37	Total	C	N	O	S	0	0
			261	153	47	56	5		
1	AB5	37	Total	C	N	O	S	0	0
			261	153	47	56	5		
1	AB6	37	Total	C	N	O	S	0	0
			261	153	47	56	5		
1	AB7	37	Total	C	N	O	S	0	0
			261	153	47	56	5		
1	AB8	37	Total	C	N	O	S	0	0
			261	153	47	56	5		
1	AB9	37	Total	C	N	O	S	0	0
			261	153	47	56	5		
1	AB10	37	Total	C	N	O	S	0	0
			261	153	47	56	5		
1	AB11	37	Total	C	N	O	S	0	0
			261	153	47	56	5		
1	AB12	37	Total	C	N	O	S	0	0
			261	153	47	56	5		
1	AB13	37	Total	C	N	O	S	0	0
			261	153	47	56	5		
1	AB14	37	Total	C	N	O	S	0	0
			261	153	47	56	5		
1	AB15	37	Total	C	N	O	S	0	0
			261	153	47	56	5		
1	AB16	37	Total	C	N	O	S	0	0
			261	153	47	56	5		
1	AB17	37	Total	C	N	O	S	0	0
			261	153	47	56	5		

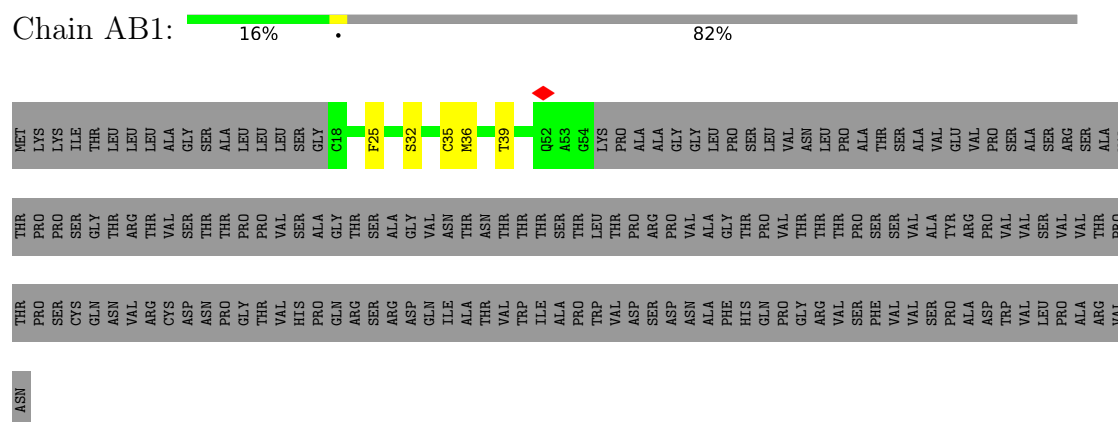
- Molecule 2 is a protein called TraB.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	EF1	196	Total	C	N	O	S	0	0
			1480	925	259	290	6		
2	EF2	196	Total	C	N	O	S	0	0
			1480	925	259	290	6		
2	EF3	196	Total	C	N	O	S	0	0
			1480	925	259	290	6		
2	EF4	196	Total	C	N	O	S	0	0
			1480	925	259	290	6		
2	EF5	196	Total	C	N	O	S	0	0
			1480	925	259	290	6		
2	EF6	196	Total	C	N	O	S	0	0
			1480	925	259	290	6		
2	EF7	196	Total	C	N	O	S	0	0
			1480	925	259	290	6		
2	EF8	196	Total	C	N	O	S	0	0
			1480	925	259	290	6		
2	EF9	196	Total	C	N	O	S	0	0
			1480	925	259	290	6		
2	EF10	196	Total	C	N	O	S	0	0
			1480	925	259	290	6		
2	EF11	196	Total	C	N	O	S	0	0
			1480	925	259	290	6		
2	EF12	196	Total	C	N	O	S	0	0
			1480	925	259	290	6		
2	EF13	196	Total	C	N	O	S	0	0
			1480	925	259	290	6		
2	EF14	196	Total	C	N	O	S	0	0
			1480	925	259	290	6		
2	EF15	196	Total	C	N	O	S	0	0
			1480	925	259	290	6		
2	EF16	196	Total	C	N	O	S	0	0
			1480	925	259	290	6		
2	EF17	196	Total	C	N	O	S	0	0
			1480	925	259	290	6		

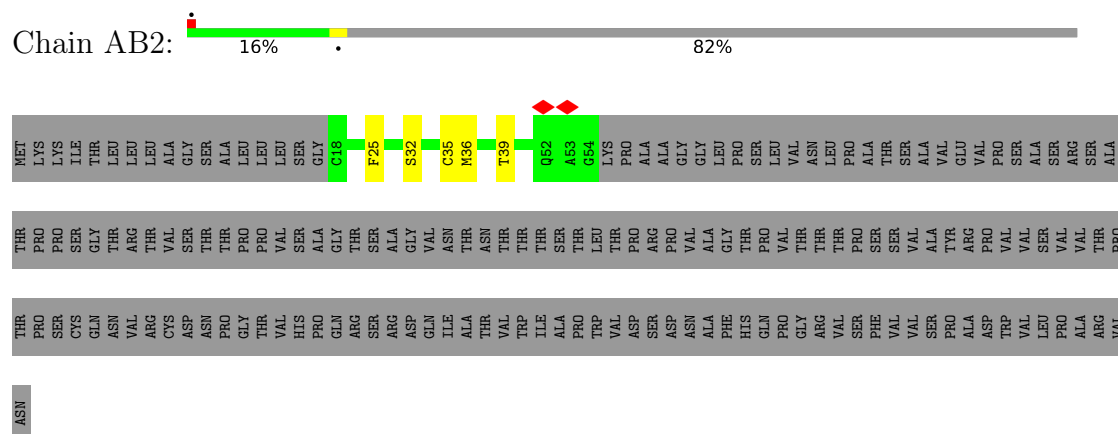
3 Residue-property plots [i](#)

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.

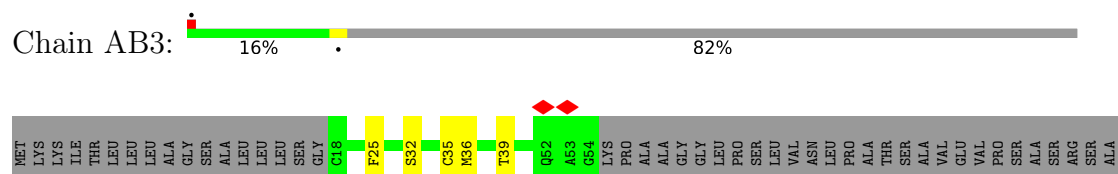
• Molecule 1: TraV

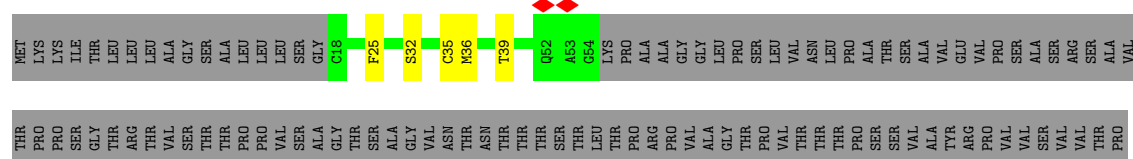


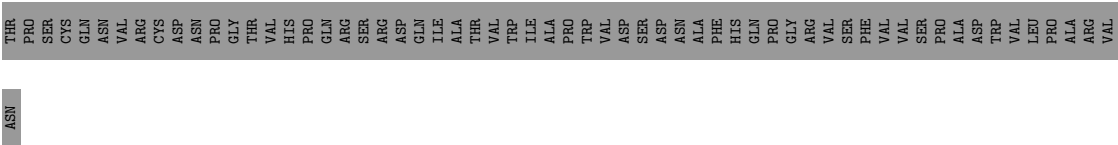
• Molecule 1: TraV



• Molecule 1: TraV

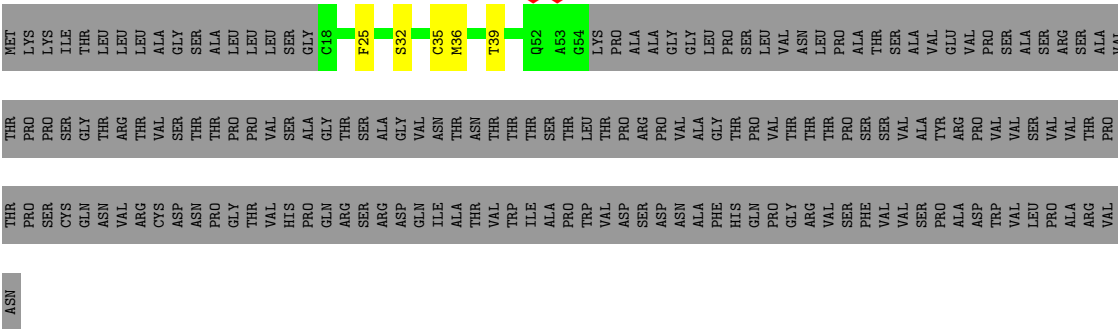






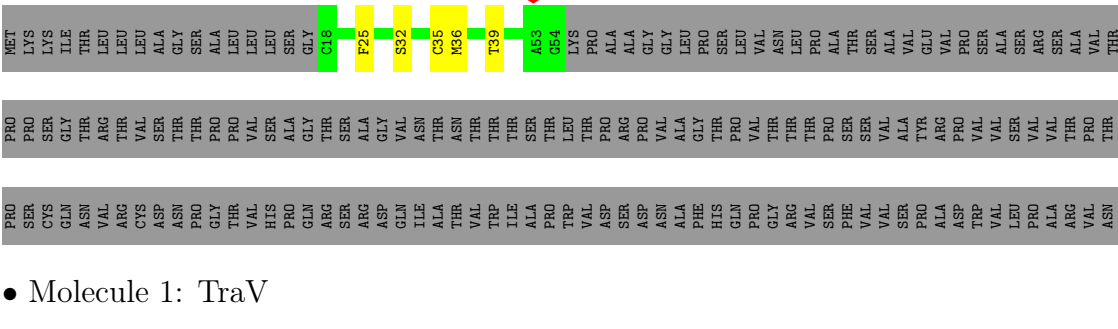
• Molecule 1: TraV

Chain AB14: 16% 82%



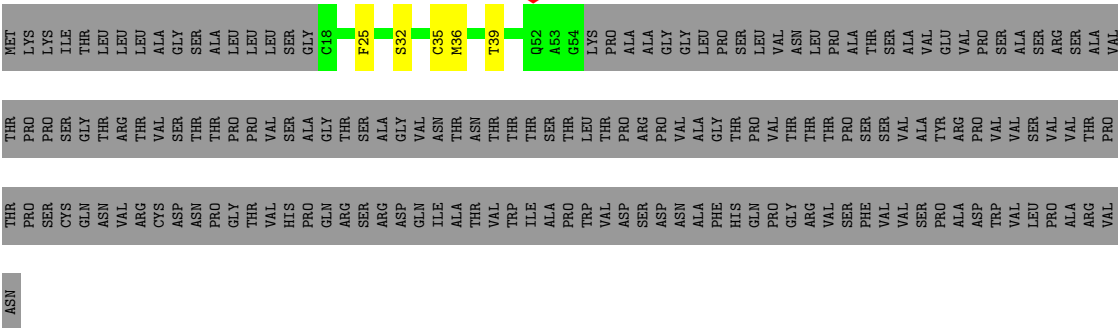
• Molecule 1: TraV

Chain AB15: 16% 82%



• Molecule 1: TraV

Chain AB16: 16% 82%

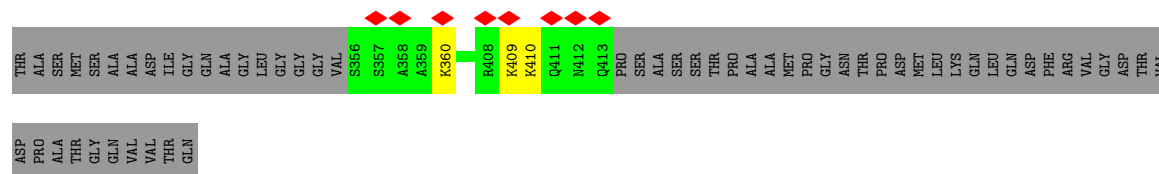
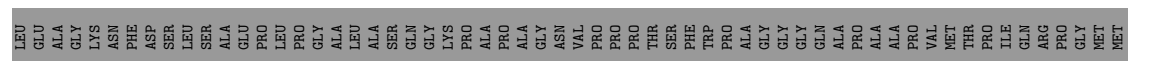
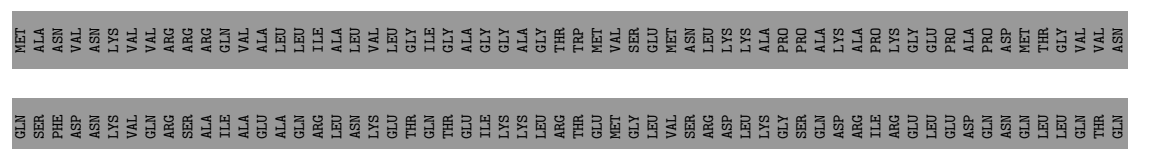


• Molecule 1: TraV

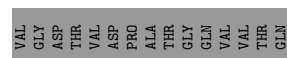
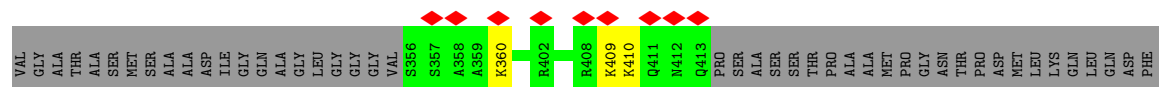
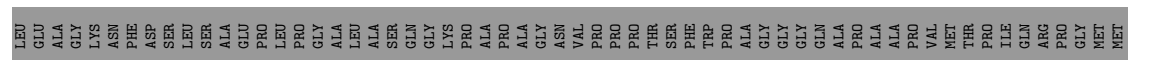
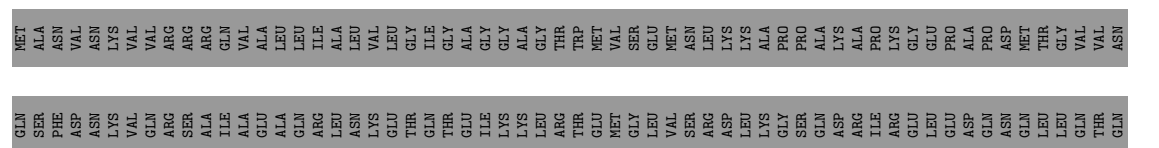
Chain AB17: 16% 82%



- Molecule 2: TraB



- Molecule 2: TraB



- Molecule 2: TraB

Response	Percentage
Yes	39%
No	57%

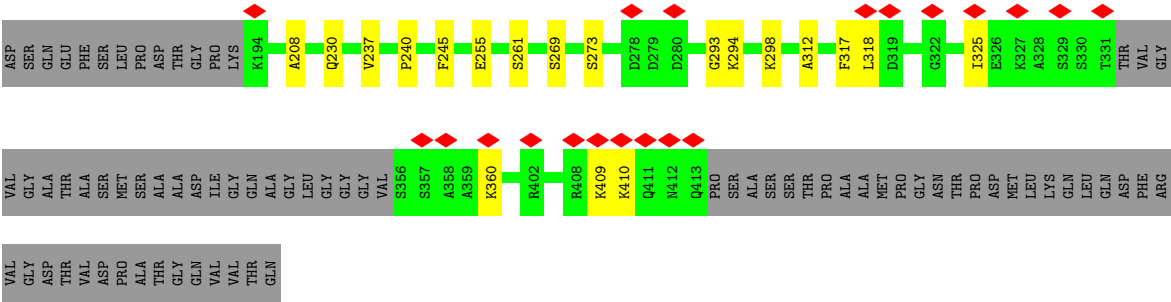


Response	Percentage
Yes	39%
No	57%

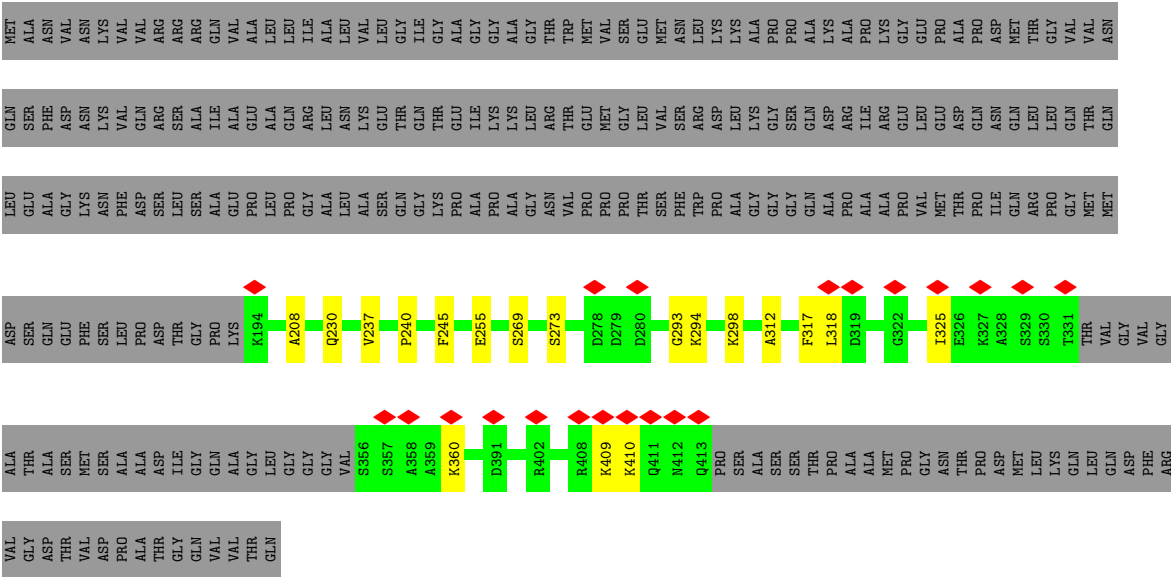


Response	Percentage
Yes	39%
No	57%

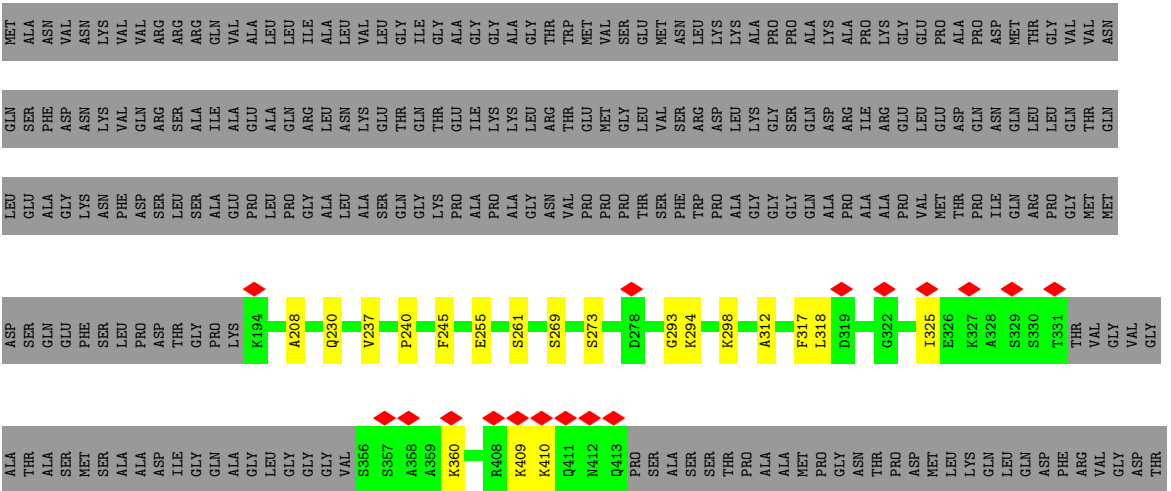




• Molecule 2: TraB



• Molecule 2: TraB





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C17	Depositor
Number of particles used	26000	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.908	Depositor
Minimum map value	-0.933	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.059	Depositor
Recommended contour level	0.38	Depositor
Map size (Å)	426.08, 426.08, 426.08	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0652, 1.0652, 1.0652	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	AB1	0.76	0/261	0.92	1/348 (0.3%)
1	AB10	0.76	0/261	0.92	1/348 (0.3%)
1	AB11	0.76	0/261	0.92	1/348 (0.3%)
1	AB12	0.76	0/261	0.92	1/348 (0.3%)
1	AB13	0.76	0/261	0.92	1/348 (0.3%)
1	AB14	0.76	0/261	0.92	1/348 (0.3%)
1	AB15	0.76	0/261	0.92	1/348 (0.3%)
1	AB16	0.76	0/261	0.92	1/348 (0.3%)
1	AB17	0.76	0/261	0.92	1/348 (0.3%)
1	AB2	0.76	0/261	0.92	1/348 (0.3%)
1	AB3	0.76	0/261	0.92	1/348 (0.3%)
1	AB4	0.76	0/261	0.92	1/348 (0.3%)
1	AB5	0.76	0/261	0.92	1/348 (0.3%)
1	AB6	0.76	0/261	0.92	1/348 (0.3%)
1	AB7	0.76	0/261	0.92	1/348 (0.3%)
1	AB8	0.76	0/261	0.92	1/348 (0.3%)
1	AB9	0.76	0/261	0.92	1/348 (0.3%)
2	EF1	0.72	1/1502 (0.1%)	0.97	5/2021 (0.2%)
2	EF10	0.72	1/1502 (0.1%)	0.97	5/2021 (0.2%)
2	EF11	0.72	1/1502 (0.1%)	0.97	5/2021 (0.2%)
2	EF12	0.72	1/1502 (0.1%)	0.97	5/2021 (0.2%)
2	EF13	0.72	1/1502 (0.1%)	0.97	5/2021 (0.2%)
2	EF14	0.72	1/1502 (0.1%)	0.97	5/2021 (0.2%)
2	EF15	0.72	1/1502 (0.1%)	0.97	5/2021 (0.2%)
2	EF16	0.72	1/1502 (0.1%)	0.97	5/2021 (0.2%)
2	EF17	0.73	1/1502 (0.1%)	0.97	5/2021 (0.2%)
2	EF2	0.72	1/1502 (0.1%)	0.97	5/2021 (0.2%)
2	EF3	0.72	1/1502 (0.1%)	0.97	5/2021 (0.2%)
2	EF4	0.72	1/1502 (0.1%)	0.97	5/2021 (0.2%)
2	EF5	0.72	1/1502 (0.1%)	0.97	5/2021 (0.2%)
2	EF6	0.72	1/1502 (0.1%)	0.97	5/2021 (0.2%)
2	EF7	0.72	1/1502 (0.1%)	0.97	5/2021 (0.2%)
2	EF8	0.72	1/1502 (0.1%)	0.97	5/2021 (0.2%)
2	EF9	0.72	1/1502 (0.1%)	0.97	5/2021 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.73	17/29971 (0.1%)	0.96	102/40273 (0.3%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	EF7	312	ALA	C-O	6.46	1.31	1.24
2	EF17	312	ALA	C-O	6.44	1.31	1.24
2	EF11	312	ALA	C-O	6.44	1.31	1.24
2	EF4	312	ALA	C-O	6.43	1.31	1.24
2	EF15	312	ALA	C-O	6.42	1.31	1.24
2	EF9	312	ALA	C-O	6.40	1.31	1.24
2	EF1	312	ALA	C-O	6.39	1.31	1.24
2	EF8	312	ALA	C-O	6.39	1.31	1.24
2	EF16	312	ALA	C-O	6.39	1.31	1.24
2	EF3	312	ALA	C-O	6.38	1.31	1.24
2	EF5	312	ALA	C-O	6.38	1.31	1.24
2	EF13	312	ALA	C-O	6.38	1.31	1.24
2	EF10	312	ALA	C-O	6.37	1.31	1.24
2	EF6	312	ALA	C-O	6.37	1.31	1.24
2	EF14	312	ALA	C-O	6.37	1.31	1.24
2	EF12	312	ALA	C-O	6.35	1.31	1.24
2	EF2	312	ALA	C-O	6.34	1.31	1.24

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	EF12	317	PHE	N-CA-C	-9.96	100.25	111.71
2	EF5	317	PHE	N-CA-C	-9.95	100.27	111.71
2	EF16	317	PHE	N-CA-C	-9.95	100.27	111.71
2	EF6	317	PHE	N-CA-C	-9.95	100.27	111.71
2	EF10	317	PHE	N-CA-C	-9.95	100.27	111.71
2	EF2	317	PHE	N-CA-C	-9.94	100.28	111.71
2	EF3	317	PHE	N-CA-C	-9.94	100.28	111.71
2	EF4	317	PHE	N-CA-C	-9.94	100.28	111.71
2	EF17	317	PHE	N-CA-C	-9.94	100.28	111.71
2	EF1	317	PHE	N-CA-C	-9.94	100.28	111.71
2	EF7	317	PHE	N-CA-C	-9.94	100.28	111.71
2	EF13	317	PHE	N-CA-C	-9.94	100.28	111.71
2	EF8	317	PHE	N-CA-C	-9.93	100.29	111.71
2	EF11	317	PHE	N-CA-C	-9.92	100.30	111.71
2	EF14	317	PHE	N-CA-C	-9.92	100.30	111.71
2	EF15	317	PHE	N-CA-C	-9.90	100.32	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	EF9	317	PHE	N-CA-C	-9.90	100.32	111.71
2	EF15	240	PRO	N-CA-C	5.93	121.94	113.47
2	EF12	240	PRO	N-CA-C	5.92	121.94	113.47
2	EF5	240	PRO	N-CA-C	5.92	121.93	113.47
2	EF6	240	PRO	N-CA-C	5.92	121.93	113.47
2	EF4	240	PRO	N-CA-C	5.91	121.92	113.47
2	EF3	240	PRO	N-CA-C	5.91	121.92	113.47
2	EF16	240	PRO	N-CA-C	5.91	121.92	113.47
2	EF10	240	PRO	N-CA-C	5.91	121.92	113.47
2	EF11	240	PRO	N-CA-C	5.91	121.92	113.47
2	EF1	240	PRO	N-CA-C	5.91	121.92	113.47
2	EF7	240	PRO	N-CA-C	5.91	121.91	113.47
2	EF9	240	PRO	N-CA-C	5.90	121.90	113.47
2	EF2	240	PRO	N-CA-C	5.89	121.90	113.47
2	EF14	240	PRO	N-CA-C	5.89	121.90	113.47
2	EF17	240	PRO	N-CA-C	5.89	121.89	113.47
2	EF8	240	PRO	N-CA-C	5.88	121.89	113.47
2	EF13	240	PRO	N-CA-C	5.88	121.88	113.47
2	EF12	208	ALA	N-CA-C	5.70	117.74	109.07
2	EF15	208	ALA	N-CA-C	5.70	117.74	109.07
2	EF7	208	ALA	N-CA-C	5.70	117.74	109.07
2	EF6	208	ALA	N-CA-C	5.70	117.73	109.07
2	EF11	208	ALA	N-CA-C	5.70	117.73	109.07
2	EF13	208	ALA	N-CA-C	5.70	117.73	109.07
2	EF1	208	ALA	N-CA-C	5.69	117.72	109.07
2	EF5	208	ALA	N-CA-C	5.69	117.72	109.07
2	EF8	208	ALA	N-CA-C	5.69	117.72	109.07
2	EF4	208	ALA	N-CA-C	5.69	117.72	109.07
2	EF3	208	ALA	N-CA-C	5.69	117.71	109.07
2	EF16	208	ALA	N-CA-C	5.69	117.72	109.07
2	EF2	208	ALA	N-CA-C	5.68	117.71	109.07
2	EF14	208	ALA	N-CA-C	5.68	117.71	109.07
2	EF17	208	ALA	N-CA-C	5.68	117.70	109.07
2	EF9	208	ALA	N-CA-C	5.68	117.70	109.07
2	EF10	208	ALA	N-CA-C	5.68	117.70	109.07
2	EF6	293	GLY	O-C-N	5.19	128.98	122.39
1	AB11	25	PHE	N-CA-C	-5.18	102.85	110.52
1	AB2	25	PHE	N-CA-C	-5.18	102.86	110.52
2	EF10	293	GLY	O-C-N	5.18	128.96	122.39
2	EF4	293	GLY	O-C-N	5.17	128.96	122.39
1	AB3	25	PHE	N-CA-C	-5.17	102.88	110.52
1	AB16	25	PHE	N-CA-C	-5.17	102.88	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AB1	25	PHE	N-CA-C	-5.16	102.88	110.52
1	AB10	25	PHE	N-CA-C	-5.16	102.88	110.52
1	AB15	25	PHE	N-CA-C	-5.16	102.88	110.52
1	AB17	25	PHE	N-CA-C	-5.16	102.88	110.52
1	AB13	25	PHE	N-CA-C	-5.16	102.88	110.52
1	AB4	25	PHE	N-CA-C	-5.16	102.88	110.52
1	AB9	25	PHE	N-CA-C	-5.16	102.88	110.52
2	EF16	293	GLY	O-C-N	5.16	128.94	122.39
2	EF17	293	GLY	O-C-N	5.16	128.94	122.39
1	AB5	25	PHE	N-CA-C	-5.16	102.89	110.52
1	AB7	25	PHE	N-CA-C	-5.16	102.89	110.52
1	AB12	25	PHE	N-CA-C	-5.16	102.89	110.52
2	EF2	293	GLY	O-C-N	5.16	128.94	122.39
2	EF9	293	GLY	O-C-N	5.16	128.94	122.39
1	AB6	25	PHE	N-CA-C	-5.15	102.89	110.52
1	AB14	25	PHE	N-CA-C	-5.15	102.89	110.52
2	EF8	293	GLY	O-C-N	5.15	128.93	122.39
2	EF12	293	GLY	O-C-N	5.15	128.93	122.39
1	AB8	25	PHE	N-CA-C	-5.15	102.90	110.52
2	EF13	293	GLY	O-C-N	5.15	128.93	122.39
2	EF1	293	GLY	O-C-N	5.14	128.92	122.39
2	EF5	293	GLY	O-C-N	5.13	128.91	122.39
2	EF15	293	GLY	O-C-N	5.13	128.91	122.39
2	EF3	293	GLY	O-C-N	5.13	128.90	122.39
2	EF11	293	GLY	O-C-N	5.12	128.89	122.39
2	EF14	293	GLY	O-C-N	5.12	128.89	122.39
2	EF7	293	GLY	O-C-N	5.11	128.88	122.39
2	EF13	318	LEU	N-CA-C	-5.08	105.40	111.03
2	EF7	318	LEU	N-CA-C	-5.07	105.40	111.03
2	EF3	318	LEU	N-CA-C	-5.06	105.41	111.03
2	EF11	318	LEU	N-CA-C	-5.06	105.41	111.03
2	EF5	318	LEU	N-CA-C	-5.05	105.42	111.03
2	EF12	318	LEU	N-CA-C	-5.05	105.42	111.03
2	EF17	318	LEU	N-CA-C	-5.05	105.42	111.03
2	EF6	318	LEU	N-CA-C	-5.04	105.43	111.03
2	EF1	318	LEU	N-CA-C	-5.04	105.44	111.03
2	EF16	318	LEU	N-CA-C	-5.03	105.45	111.03
2	EF15	318	LEU	N-CA-C	-5.03	105.45	111.03
2	EF9	318	LEU	N-CA-C	-5.02	105.45	111.03
2	EF14	318	LEU	N-CA-C	-5.02	105.45	111.03
2	EF8	318	LEU	N-CA-C	-5.02	105.46	111.03
2	EF2	318	LEU	N-CA-C	-5.01	105.47	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	EF4	318	LEU	N-CA-C	-5.01	105.47	111.03
2	EF10	318	LEU	N-CA-C	-5.01	105.47	111.03

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	AB1	35/204 (17%)	32 (91%)	3 (9%)	0	100	100
1	AB10	35/204 (17%)	32 (91%)	3 (9%)	0	100	100
1	AB11	35/204 (17%)	32 (91%)	3 (9%)	0	100	100
1	AB12	35/204 (17%)	32 (91%)	3 (9%)	0	100	100
1	AB13	35/204 (17%)	32 (91%)	3 (9%)	0	100	100
1	AB14	35/204 (17%)	32 (91%)	3 (9%)	0	100	100
1	AB15	35/204 (17%)	32 (91%)	3 (9%)	0	100	100
1	AB16	35/204 (17%)	32 (91%)	3 (9%)	0	100	100
1	AB17	35/204 (17%)	32 (91%)	3 (9%)	0	100	100
1	AB2	35/204 (17%)	32 (91%)	3 (9%)	0	100	100
1	AB3	35/204 (17%)	32 (91%)	3 (9%)	0	100	100
1	AB4	35/204 (17%)	32 (91%)	3 (9%)	0	100	100
1	AB5	35/204 (17%)	32 (91%)	3 (9%)	0	100	100
1	AB6	35/204 (17%)	32 (91%)	3 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AB7	35/204 (17%)	32 (91%)	3 (9%)	0	100	100
1	AB8	35/204 (17%)	32 (91%)	3 (9%)	0	100	100
1	AB9	35/204 (17%)	32 (91%)	3 (9%)	0	100	100
2	EF1	192/453 (42%)	186 (97%)	6 (3%)	0	100	100
2	EF10	192/453 (42%)	186 (97%)	6 (3%)	0	100	100
2	EF11	192/453 (42%)	186 (97%)	6 (3%)	0	100	100
2	EF12	192/453 (42%)	186 (97%)	6 (3%)	0	100	100
2	EF13	192/453 (42%)	186 (97%)	6 (3%)	0	100	100
2	EF14	192/453 (42%)	186 (97%)	6 (3%)	0	100	100
2	EF15	192/453 (42%)	186 (97%)	6 (3%)	0	100	100
2	EF16	192/453 (42%)	186 (97%)	6 (3%)	0	100	100
2	EF17	192/453 (42%)	186 (97%)	6 (3%)	0	100	100
2	EF2	192/453 (42%)	186 (97%)	6 (3%)	0	100	100
2	EF3	192/453 (42%)	186 (97%)	6 (3%)	0	100	100
2	EF4	192/453 (42%)	186 (97%)	6 (3%)	0	100	100
2	EF5	192/453 (42%)	186 (97%)	6 (3%)	0	100	100
2	EF6	192/453 (42%)	186 (97%)	6 (3%)	0	100	100
2	EF7	192/453 (42%)	186 (97%)	6 (3%)	0	100	100
2	EF8	192/453 (42%)	186 (97%)	6 (3%)	0	100	100
2	EF9	192/453 (42%)	186 (97%)	6 (3%)	0	100	100
All	All	3859/11169 (35%)	3706 (96%)	153 (4%)	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	AB1	28/168 (17%)	24 (86%)	4 (14%)	3	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AB10	28/168 (17%)	24 (86%)	4 (14%)	3	18
1	AB11	28/168 (17%)	24 (86%)	4 (14%)	3	18
1	AB12	28/168 (17%)	24 (86%)	4 (14%)	3	18
1	AB13	28/168 (17%)	24 (86%)	4 (14%)	3	18
1	AB14	28/168 (17%)	24 (86%)	4 (14%)	3	18
1	AB15	28/168 (17%)	24 (86%)	4 (14%)	3	18
1	AB16	28/168 (17%)	24 (86%)	4 (14%)	3	18
1	AB17	28/168 (17%)	24 (86%)	4 (14%)	3	18
1	AB2	28/168 (17%)	24 (86%)	4 (14%)	3	18
1	AB3	28/168 (17%)	24 (86%)	4 (14%)	3	18
1	AB4	28/168 (17%)	24 (86%)	4 (14%)	3	18
1	AB5	28/168 (17%)	24 (86%)	4 (14%)	3	18
1	AB6	28/168 (17%)	24 (86%)	4 (14%)	3	18
1	AB7	28/168 (17%)	24 (86%)	4 (14%)	3	18
1	AB8	28/168 (17%)	24 (86%)	4 (14%)	3	18
1	AB9	28/168 (17%)	24 (86%)	4 (14%)	3	18
2	EF1	155/353 (44%)	142 (92%)	13 (8%)	10	35
2	EF10	155/353 (44%)	142 (92%)	13 (8%)	10	35
2	EF11	155/353 (44%)	142 (92%)	13 (8%)	10	35
2	EF12	155/353 (44%)	142 (92%)	13 (8%)	10	35
2	EF13	155/353 (44%)	143 (92%)	12 (8%)	12	37
2	EF14	155/353 (44%)	142 (92%)	13 (8%)	10	35
2	EF15	155/353 (44%)	142 (92%)	13 (8%)	10	35
2	EF16	155/353 (44%)	142 (92%)	13 (8%)	10	35
2	EF17	155/353 (44%)	142 (92%)	13 (8%)	10	35
2	EF2	155/353 (44%)	142 (92%)	13 (8%)	10	35
2	EF3	155/353 (44%)	142 (92%)	13 (8%)	10	35
2	EF4	155/353 (44%)	142 (92%)	13 (8%)	10	35
2	EF5	155/353 (44%)	142 (92%)	13 (8%)	10	35
2	EF6	155/353 (44%)	142 (92%)	13 (8%)	10	35
2	EF7	155/353 (44%)	142 (92%)	13 (8%)	10	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	EF8	155/353 (44%)	142 (92%)	13 (8%)	10	35
2	EF9	155/353 (44%)	142 (92%)	13 (8%)	10	35
All	All	3111/8857 (35%)	2823 (91%)	288 (9%)	11	32

All (288) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AB1	32	SER
1	AB1	35	CYS
1	AB1	36	MET
1	AB1	39	THR
1	AB2	32	SER
1	AB2	35	CYS
1	AB2	36	MET
1	AB2	39	THR
1	AB3	32	SER
1	AB3	35	CYS
1	AB3	36	MET
1	AB3	39	THR
1	AB4	32	SER
1	AB4	35	CYS
1	AB4	36	MET
1	AB4	39	THR
1	AB5	32	SER
1	AB5	35	CYS
1	AB5	36	MET
1	AB5	39	THR
1	AB6	32	SER
1	AB6	35	CYS
1	AB6	36	MET
1	AB6	39	THR
1	AB7	32	SER
1	AB7	35	CYS
1	AB7	36	MET
1	AB7	39	THR
1	AB8	32	SER
1	AB8	35	CYS
1	AB8	36	MET
1	AB8	39	THR
1	AB9	32	SER
1	AB9	35	CYS

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Mol	Chain	Res	Type
1	AB9	36	MET
1	AB9	39	THR
1	AB10	32	SER
1	AB10	35	CYS
1	AB10	36	MET
1	AB10	39	THR
1	AB11	32	SER
1	AB11	35	CYS
1	AB11	36	MET
1	AB11	39	THR
1	AB12	32	SER
1	AB12	35	CYS
1	AB12	36	MET
1	AB12	39	THR
1	AB13	32	SER
1	AB13	35	CYS
1	AB13	36	MET
1	AB13	39	THR
1	AB14	32	SER
1	AB14	35	CYS
1	AB14	36	MET
1	AB14	39	THR
1	AB15	32	SER
1	AB15	35	CYS
1	AB15	36	MET
1	AB15	39	THR
1	AB16	32	SER
1	AB16	35	CYS
1	AB16	36	MET
1	AB16	39	THR
1	AB17	32	SER
1	AB17	35	CYS
1	AB17	36	MET
1	AB17	39	THR
2	EF1	230	GLN
2	EF1	237	VAL
2	EF1	245	PHE
2	EF1	255	GLU
2	EF1	261	SER
2	EF1	269	SER
2	EF1	273	SER
2	EF1	294	LYS

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Mol	Chain	Res	Type
2	EF1	298	LYS
2	EF1	325	ILE
2	EF1	360	LYS
2	EF1	409	LYS
2	EF1	410	LYS
2	EF2	230	GLN
2	EF2	237	VAL
2	EF2	245	PHE
2	EF2	255	GLU
2	EF2	261	SER
2	EF2	269	SER
2	EF2	273	SER
2	EF2	294	LYS
2	EF2	298	LYS
2	EF2	325	ILE
2	EF2	360	LYS
2	EF2	409	LYS
2	EF2	410	LYS
2	EF3	230	GLN
2	EF3	237	VAL
2	EF3	245	PHE
2	EF3	255	GLU
2	EF3	261	SER
2	EF3	269	SER
2	EF3	273	SER
2	EF3	294	LYS
2	EF3	298	LYS
2	EF3	325	ILE
2	EF3	360	LYS
2	EF3	409	LYS
2	EF3	410	LYS
2	EF4	230	GLN
2	EF4	237	VAL
2	EF4	245	PHE
2	EF4	255	GLU
2	EF4	261	SER
2	EF4	269	SER
2	EF4	273	SER
2	EF4	294	LYS
2	EF4	298	LYS
2	EF4	325	ILE
2	EF4	360	LYS

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Mol	Chain	Res	Type
2	EF4	409	LYS
2	EF4	410	LYS
2	EF5	230	GLN
2	EF5	237	VAL
2	EF5	245	PHE
2	EF5	255	GLU
2	EF5	261	SER
2	EF5	269	SER
2	EF5	273	SER
2	EF5	294	LYS
2	EF5	298	LYS
2	EF5	325	ILE
2	EF5	360	LYS
2	EF5	409	LYS
2	EF5	410	LYS
2	EF6	230	GLN
2	EF6	237	VAL
2	EF6	245	PHE
2	EF6	255	GLU
2	EF6	261	SER
2	EF6	269	SER
2	EF6	273	SER
2	EF6	294	LYS
2	EF6	298	LYS
2	EF6	325	ILE
2	EF6	360	LYS
2	EF6	409	LYS
2	EF6	410	LYS
2	EF7	230	GLN
2	EF7	237	VAL
2	EF7	245	PHE
2	EF7	255	GLU
2	EF7	261	SER
2	EF7	269	SER
2	EF7	273	SER
2	EF7	294	LYS
2	EF7	298	LYS
2	EF7	325	ILE
2	EF7	360	LYS
2	EF7	409	LYS
2	EF7	410	LYS
2	EF8	230	GLN

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Mol	Chain	Res	Type
2	EF8	237	VAL
2	EF8	245	PHE
2	EF8	255	GLU
2	EF8	261	SER
2	EF8	269	SER
2	EF8	273	SER
2	EF8	294	LYS
2	EF8	298	LYS
2	EF8	325	ILE
2	EF8	360	LYS
2	EF8	409	LYS
2	EF8	410	LYS
2	EF9	230	GLN
2	EF9	237	VAL
2	EF9	245	PHE
2	EF9	255	GLU
2	EF9	261	SER
2	EF9	269	SER
2	EF9	273	SER
2	EF9	294	LYS
2	EF9	298	LYS
2	EF9	325	ILE
2	EF9	360	LYS
2	EF9	409	LYS
2	EF9	410	LYS
2	EF10	230	GLN
2	EF10	237	VAL
2	EF10	245	PHE
2	EF10	255	GLU
2	EF10	261	SER
2	EF10	269	SER
2	EF10	273	SER
2	EF10	294	LYS
2	EF10	298	LYS
2	EF10	325	ILE
2	EF10	360	LYS
2	EF10	409	LYS
2	EF10	410	LYS
2	EF11	230	GLN
2	EF11	237	VAL
2	EF11	245	PHE
2	EF11	255	GLU

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Mol	Chain	Res	Type
2	EF11	261	SER
2	EF11	269	SER
2	EF11	273	SER
2	EF11	294	LYS
2	EF11	298	LYS
2	EF11	325	ILE
2	EF11	360	LYS
2	EF11	409	LYS
2	EF11	410	LYS
2	EF12	230	GLN
2	EF12	237	VAL
2	EF12	245	PHE
2	EF12	255	GLU
2	EF12	261	SER
2	EF12	269	SER
2	EF12	273	SER
2	EF12	294	LYS
2	EF12	298	LYS
2	EF12	325	ILE
2	EF12	360	LYS
2	EF12	409	LYS
2	EF12	410	LYS
2	EF13	230	GLN
2	EF13	237	VAL
2	EF13	245	PHE
2	EF13	255	GLU
2	EF13	269	SER
2	EF13	273	SER
2	EF13	294	LYS
2	EF13	298	LYS
2	EF13	325	ILE
2	EF13	360	LYS
2	EF13	409	LYS
2	EF13	410	LYS
2	EF14	230	GLN
2	EF14	237	VAL
2	EF14	245	PHE
2	EF14	255	GLU
2	EF14	261	SER
2	EF14	269	SER
2	EF14	273	SER
2	EF14	294	LYS

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Mol	Chain	Res	Type
2	EF14	298	LYS
2	EF14	325	ILE
2	EF14	360	LYS
2	EF14	409	LYS
2	EF14	410	LYS
2	EF15	230	GLN
2	EF15	237	VAL
2	EF15	245	PHE
2	EF15	255	GLU
2	EF15	261	SER
2	EF15	269	SER
2	EF15	273	SER
2	EF15	294	LYS
2	EF15	298	LYS
2	EF15	325	ILE
2	EF15	360	LYS
2	EF15	409	LYS
2	EF15	410	LYS
2	EF16	230	GLN
2	EF16	237	VAL
2	EF16	245	PHE
2	EF16	255	GLU
2	EF16	261	SER
2	EF16	269	SER
2	EF16	273	SER
2	EF16	294	LYS
2	EF16	298	LYS
2	EF16	325	ILE
2	EF16	360	LYS
2	EF16	409	LYS
2	EF16	410	LYS
2	EF17	230	GLN
2	EF17	237	VAL
2	EF17	245	PHE
2	EF17	255	GLU
2	EF17	261	SER
2	EF17	269	SER
2	EF17	273	SER
2	EF17	294	LYS
2	EF17	298	LYS
2	EF17	325	ILE
2	EF17	360	LYS

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Mol	Chain	Res	Type
2	EF17	409	LYS
2	EF17	410	LYS

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

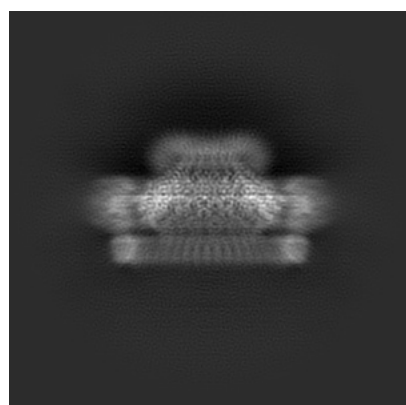
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24772. These allow visual inspection of the internal detail of the map and identification of artifacts.

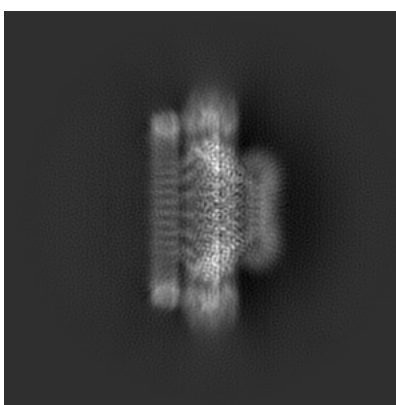
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

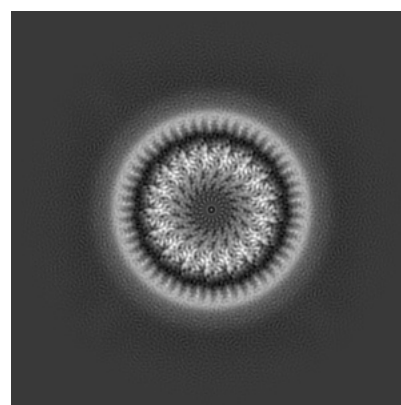
6.1.1 Primary map



X



Y

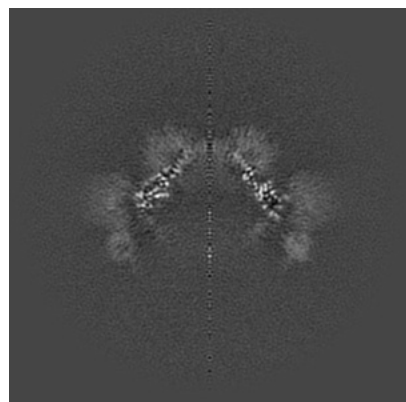


Z

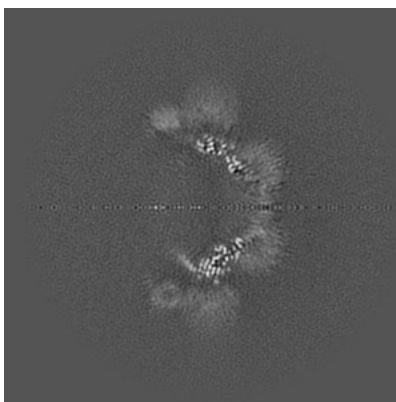
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

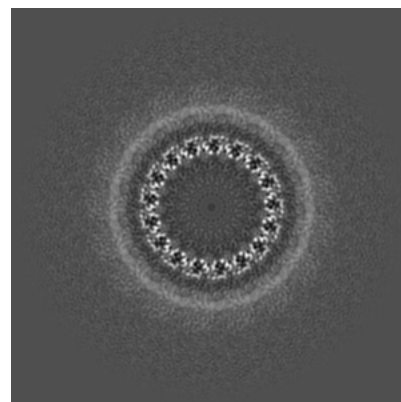
6.2.1 Primary map



X Index: 200



Y Index: 200

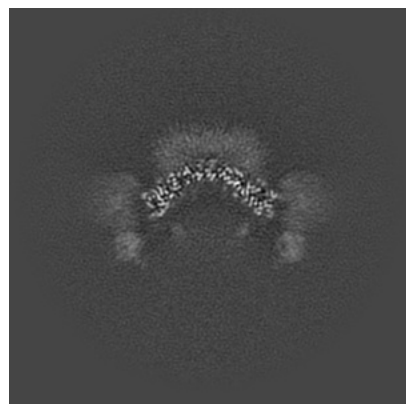


Z Index: 200

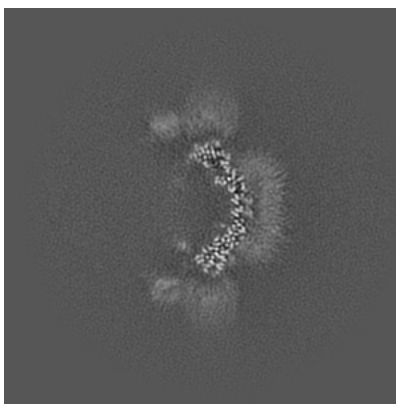
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

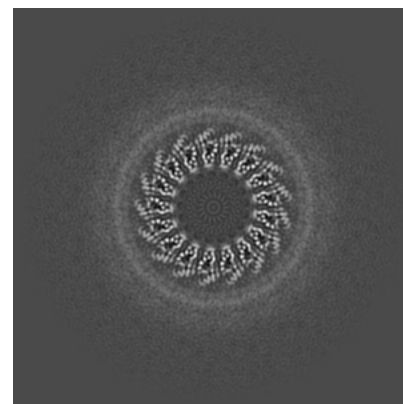
6.3.1 Primary map



X Index: 166



Y Index: 167

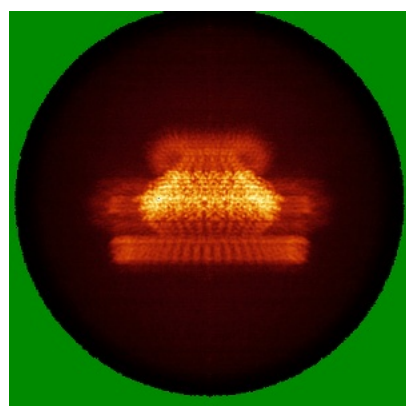


Z Index: 212

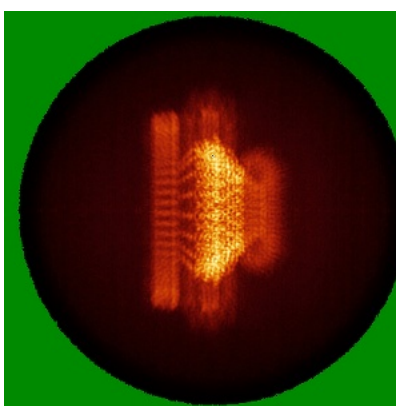
The images above show the largest variance slices of the map in three orthogonal directions.

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

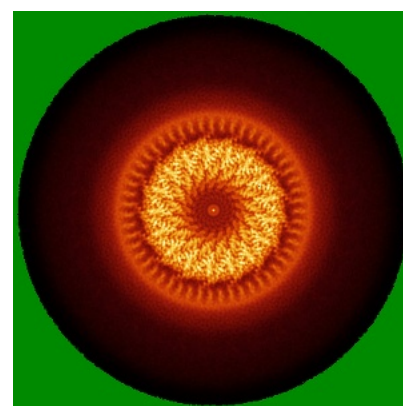
6.4.1 Primary map



X



Y

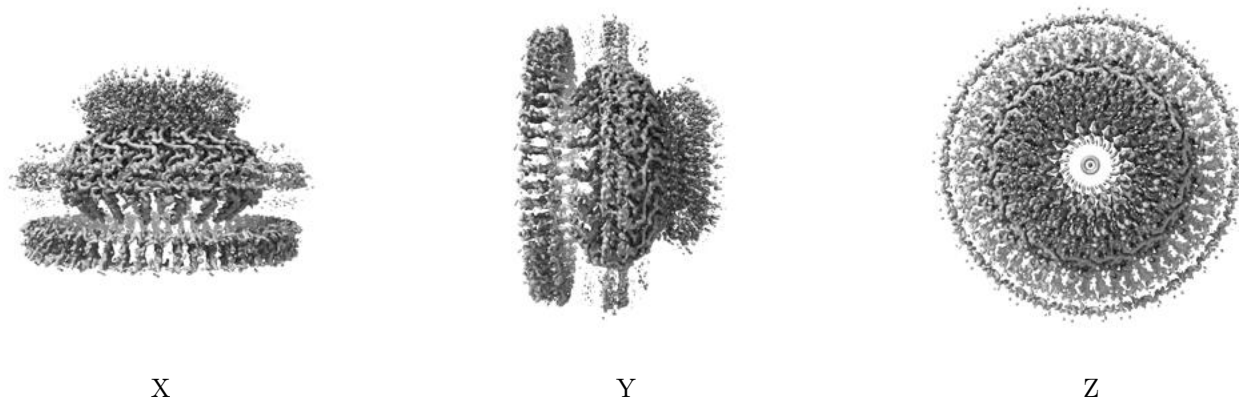


Z

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

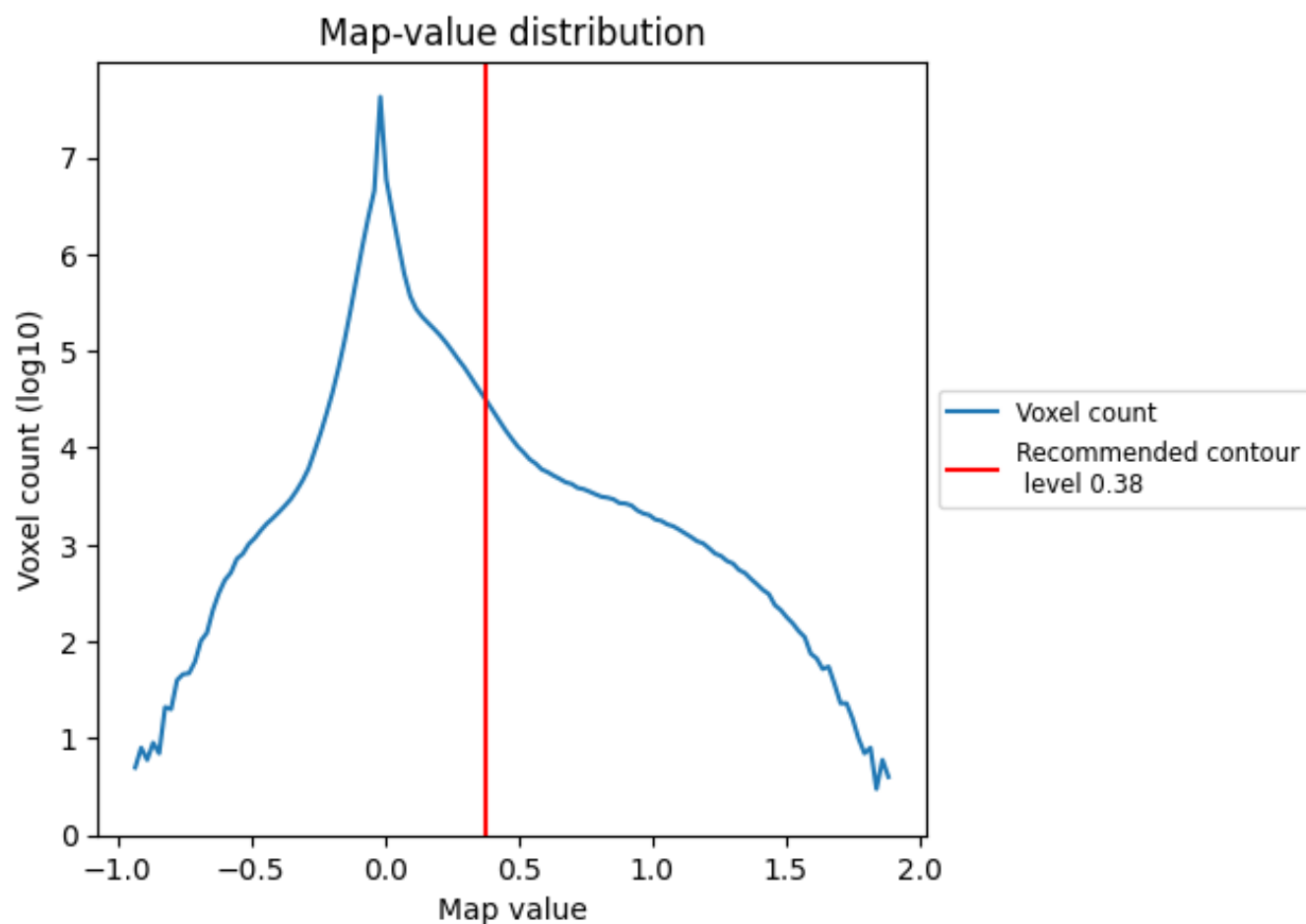
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

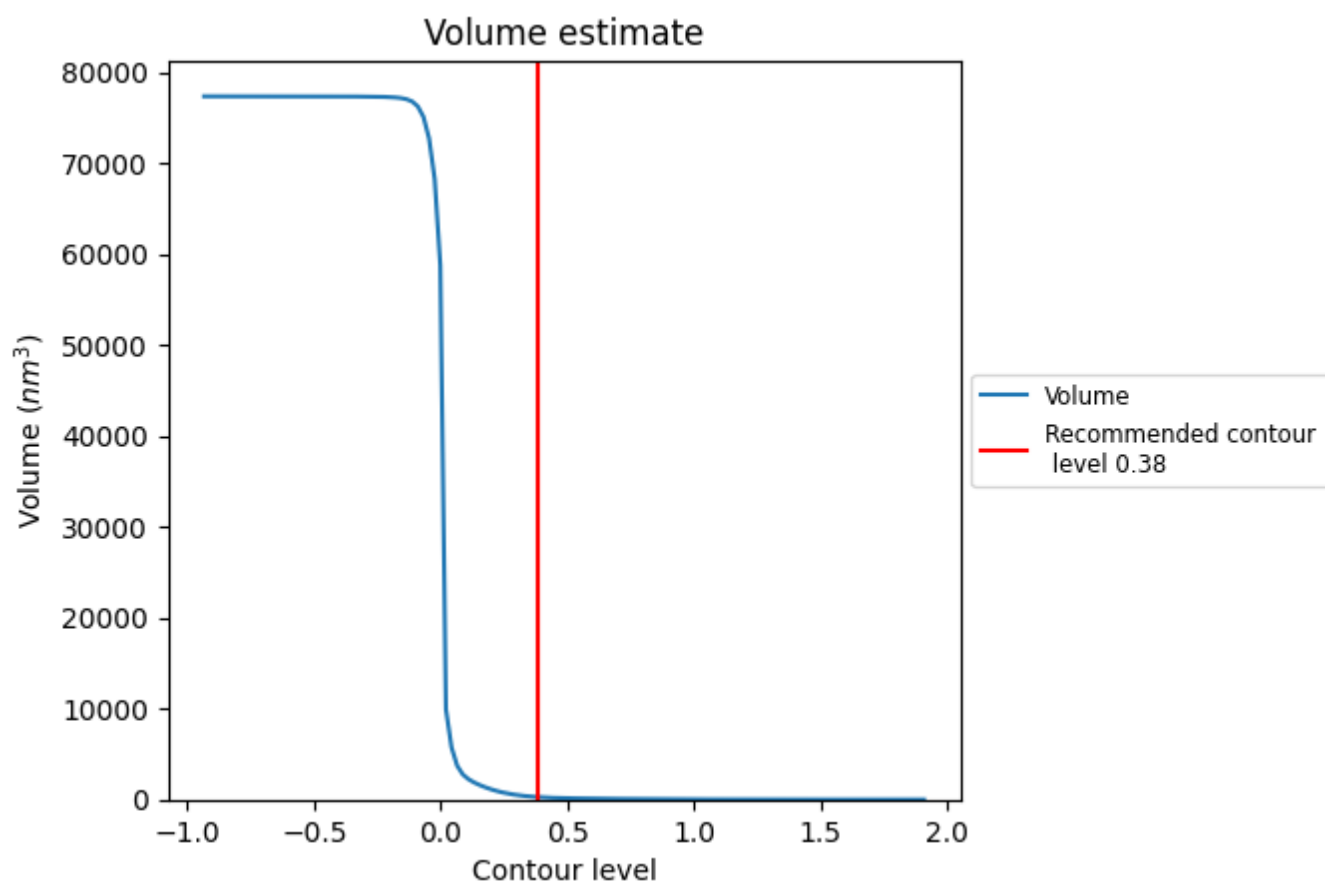
This section contains the results of statistical analysis of the map.

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.

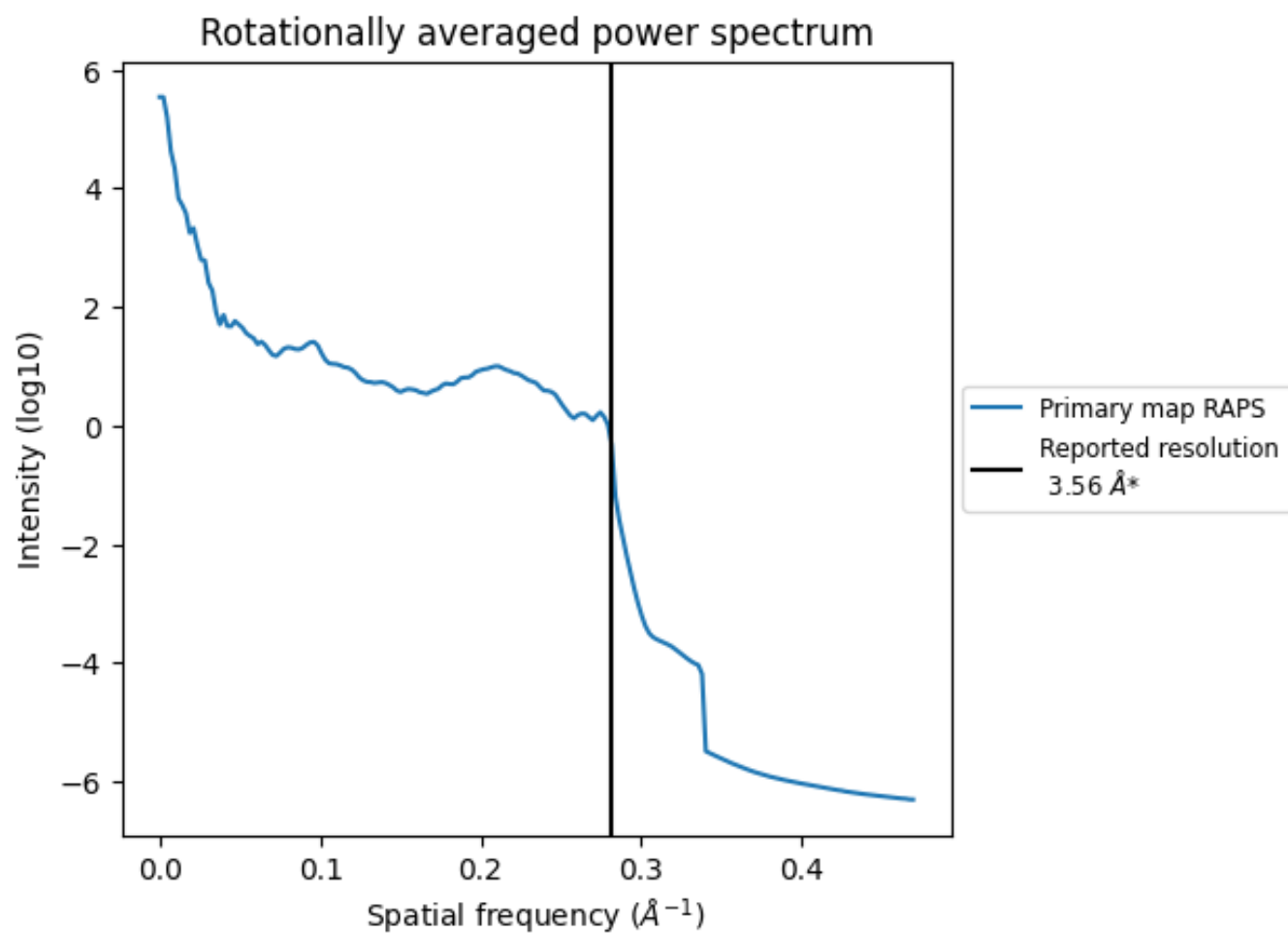
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 279 nm³; this corresponds to an approximate mass of 252 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 0.281 Å⁻¹

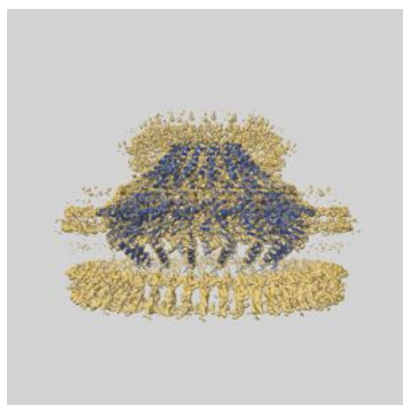
8 Fourier-Shell correlation ⓘ

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

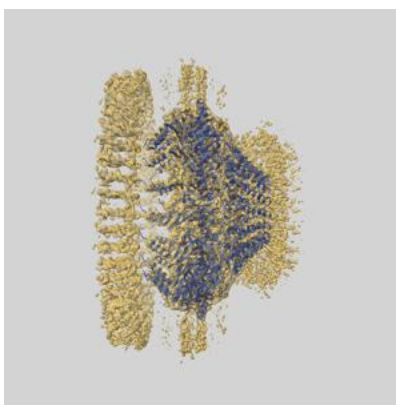
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-24772 and PDB model 7SPJ. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



X



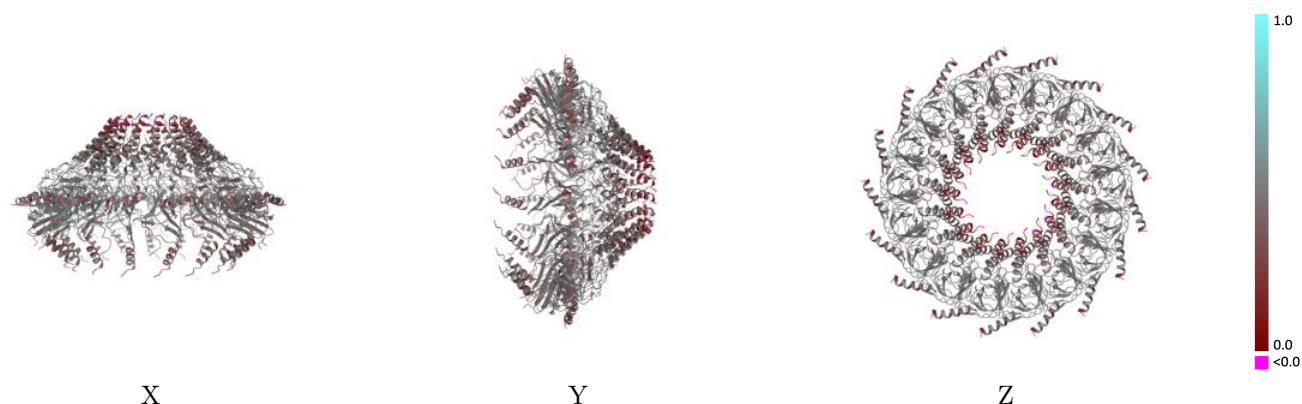
Y



Z

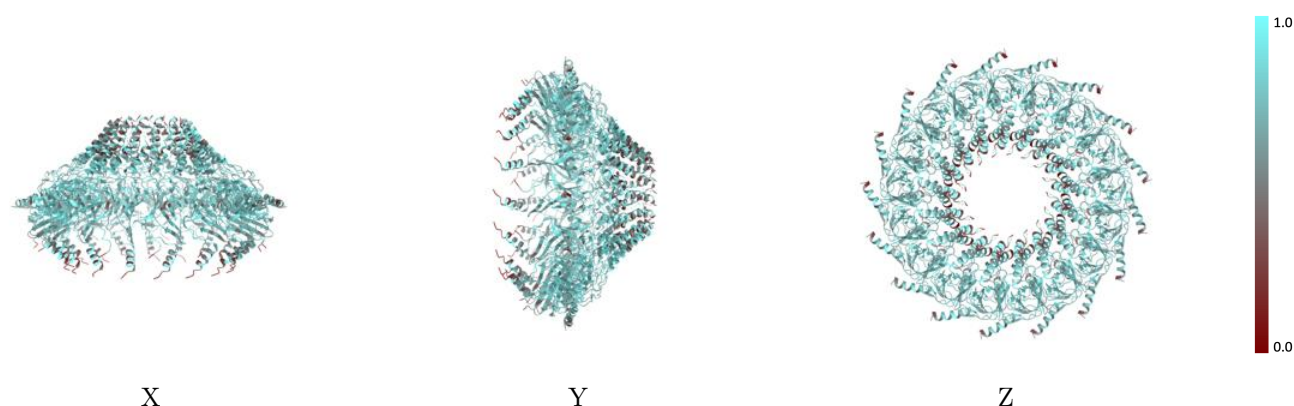
The images above show the 3D surface view of the map at the recommended contour level 0.38 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



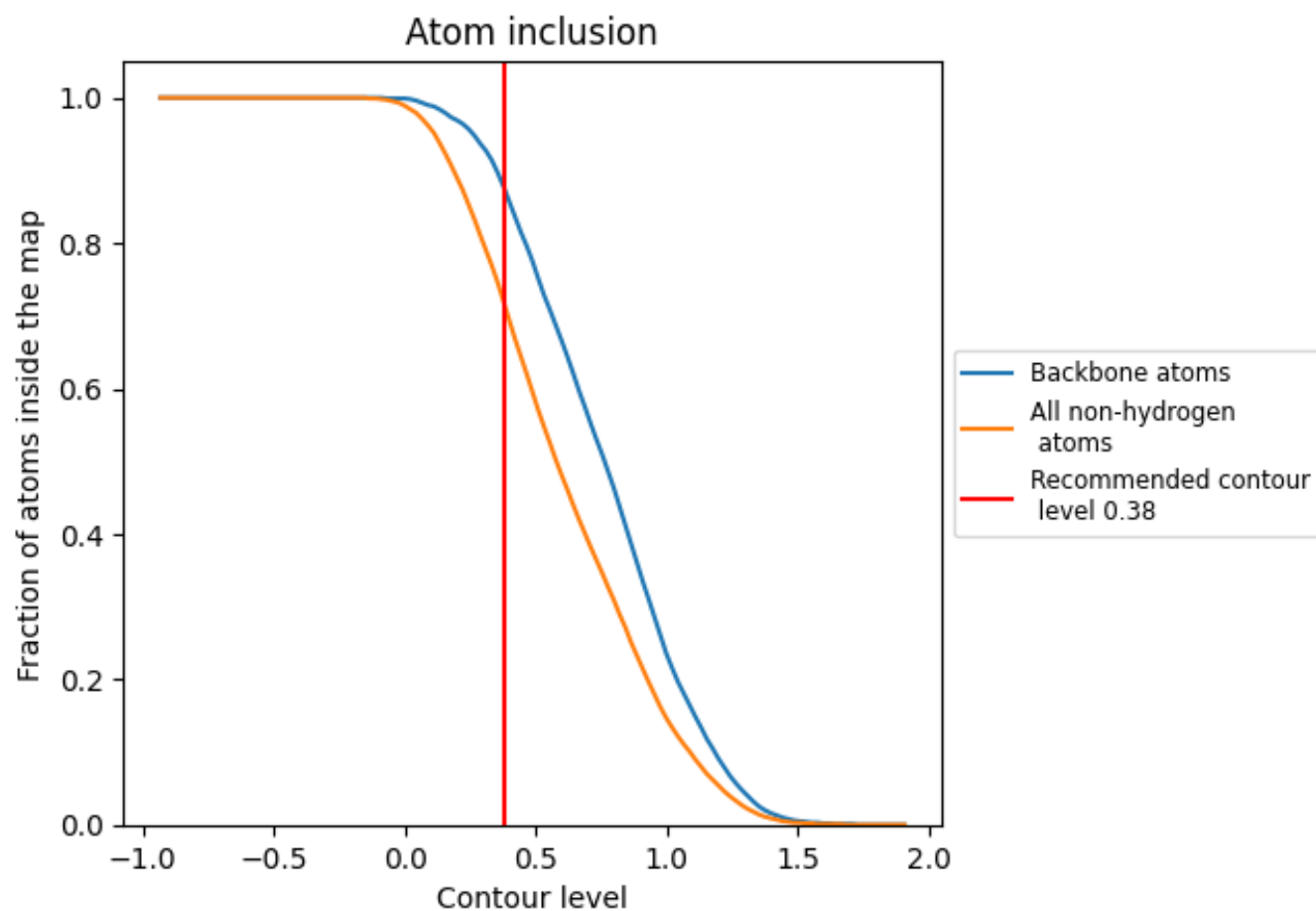
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.38).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.38) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7160	 0.4300
AB1	 0.7070	 0.4350
AB10	 0.6990	 0.4060
AB11	 0.7070	 0.4110
AB12	 0.6990	 0.4130
AB13	 0.7030	 0.4210
AB14	 0.7030	 0.4260
AB15	 0.7180	 0.4280
AB16	 0.7180	 0.4330
AB17	 0.7220	 0.4330
AB2	 0.6950	 0.4330
AB3	 0.6870	 0.4290
AB4	 0.6790	 0.4290
AB5	 0.6910	 0.4230
AB6	 0.6790	 0.4170
AB7	 0.6830	 0.4130
AB8	 0.6910	 0.4120
AB9	 0.6910	 0.4080
EF1	 0.7320	 0.4490
EF10	 0.7070	 0.4170
EF11	 0.7040	 0.4170
EF12	 0.7120	 0.4220
EF13	 0.7090	 0.4270
EF14	 0.7160	 0.4330
EF15	 0.7280	 0.4400
EF16	 0.7320	 0.4450
EF17	 0.7350	 0.4500
EF2	 0.7340	 0.4470
EF3	 0.7240	 0.4430
EF4	 0.7220	 0.4360
EF5	 0.7260	 0.4310
EF6	 0.7180	 0.4250
EF7	 0.7170	 0.4220
EF8	 0.7080	 0.4180
EF9	 0.7050	 0.4140

