



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:31 AM UTC

PDB ID : 8HIW / pdb_00008hiw
EMDB ID : EMD-34828
Title : AtALMT9 in the apo state
Authors : Gong, D.S.
Deposited on : 2022-11-22
Resolution : 3.34 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
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

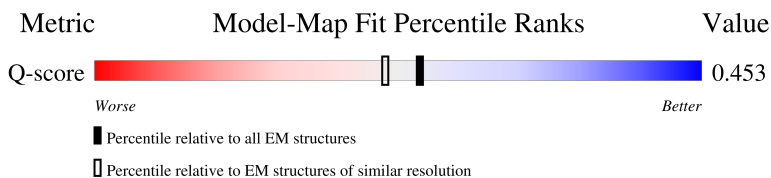
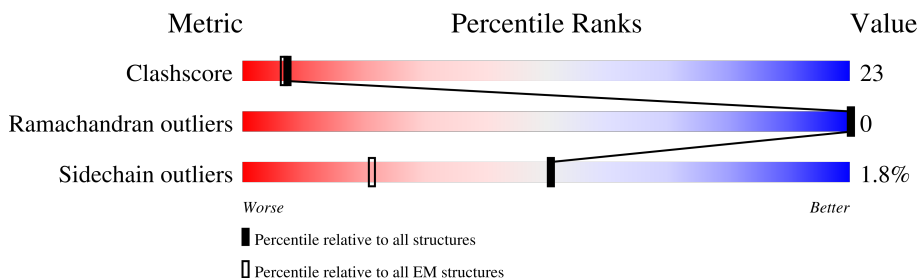
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

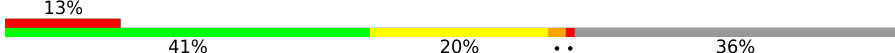
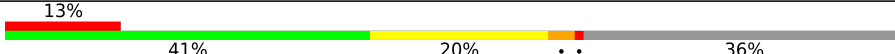
The reported resolution of this entry is 3.34 Å.

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	14446 (2.84 - 3.84)

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	598	
1	B	598	

2 Entry composition [i](#)

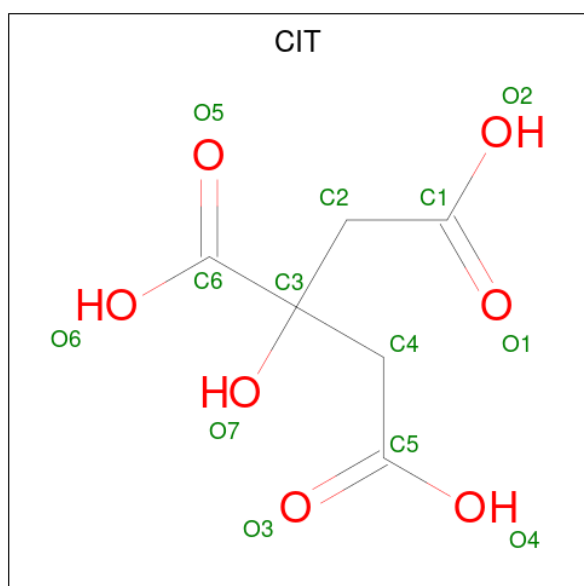
There are 2 unique types of molecules in this entry. The entry contains 5945 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

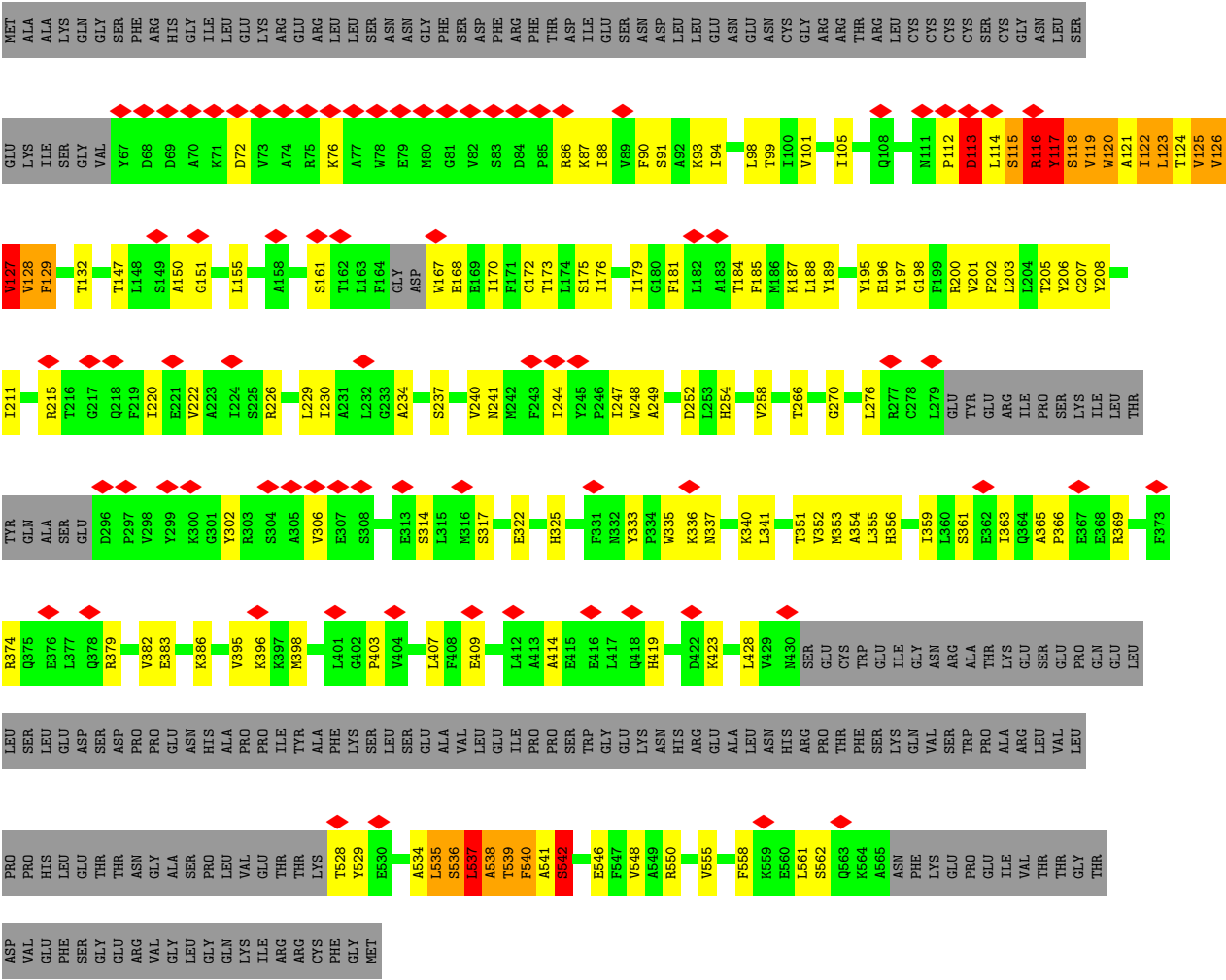
- Molecule 1 is a protein called Aluminum-activated malate transporter 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	384	Total	C	N	O	S	0	0
			2966	1941	479	531	15		
1	B	384	Total	C	N	O	S	0	0
			2966	1941	479	531	15		

- Molecule 2 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
2	B	1	Total	C	O	0
			13	6	7	



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	121436	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)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	8.141	Depositor
Minimum map value	-3.648	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.096	Depositor
Recommended contour level	0.82	Depositor
Map size (Å)	274.9952, 274.9952, 274.9952	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CIT

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	1.54	73/3031 (2.4%)	1.05	50/4106 (1.2%)
1	B	1.53	72/3031 (2.4%)	1.04	48/4106 (1.2%)
All	All	1.54	145/6062 (2.4%)	1.04	98/8212 (1.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
All	All	0	4

All (145) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	VAL	C-O	-17.66	1.03	1.24
1	B	125	VAL	C-O	-17.65	1.03	1.24
1	A	540	PHE	CA-C	-16.31	1.36	1.52
1	A	120	TRP	CA-C	-15.95	1.32	1.52
1	B	120	TRP	CA-C	-15.95	1.32	1.52
1	B	126	VAL	C-O	-15.93	1.05	1.24
1	A	126	VAL	C-O	-15.85	1.05	1.24
1	B	119	VAL	C-O	-14.68	1.04	1.24
1	B	125	VAL	CA-CB	-14.67	1.35	1.54
1	A	125	VAL	CA-CB	-14.64	1.35	1.54
1	A	119	VAL	C-O	-14.30	1.04	1.24
1	B	119	VAL	CA-CB	-14.22	1.36	1.54
1	A	119	VAL	CA-CB	-13.26	1.36	1.54
1	B	539	THR	C-O	-12.84	1.07	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	541	ALA	C-O	-12.72	1.08	1.24
1	A	126	VAL	CA-C	-12.70	1.36	1.52
1	B	126	VAL	CA-C	-12.66	1.36	1.52
1	A	540	PHE	C-O	-12.64	1.05	1.23
1	B	540	PHE	CA-C	-12.47	1.35	1.52
1	A	120	TRP	C-O	-12.19	1.10	1.24
1	B	120	TRP	C-O	-12.19	1.10	1.24
1	B	542	SER	C-O	-12.05	1.08	1.24
1	B	540	PHE	C-O	-12.01	1.08	1.24
1	A	542	SER	C-O	-11.99	1.07	1.24
1	A	541	ALA	C-O	-11.78	1.08	1.24
1	B	119	VAL	N-CA	-11.78	1.30	1.46
1	A	114	LEU	CA-C	11.71	1.70	1.52
1	B	114	LEU	CA-C	11.67	1.70	1.52
1	A	119	VAL	N-CA	-11.65	1.30	1.46
1	B	117	TYR	N-CA	-11.16	1.30	1.46
1	A	540	PHE	CA-CB	-11.14	1.35	1.54
1	B	123	LEU	CA-CB	-10.79	1.35	1.53
1	A	123	LEU	CA-CB	-10.79	1.35	1.53
1	B	124	THR	C-O	-10.61	1.10	1.24
1	A	124	THR	C-O	-10.54	1.10	1.24
1	B	127	VAL	C-O	-10.34	1.12	1.24
1	A	127	VAL	C-O	-10.31	1.12	1.24
1	A	123	LEU	CA-C	-10.23	1.38	1.52
1	B	123	LEU	CA-C	-10.17	1.38	1.52
1	B	116	ARG	N-CA	-10.12	1.33	1.46
1	A	114	LEU	N-CA	10.11	1.61	1.46
1	B	114	LEU	N-CA	10.08	1.61	1.46
1	A	123	LEU	C-O	-9.98	1.10	1.24
1	B	123	LEU	C-O	-9.98	1.10	1.24
1	A	125	VAL	CA-C	-9.80	1.40	1.52
1	B	125	VAL	CA-C	-9.80	1.40	1.52
1	B	128	VAL	CA-CB	-9.76	1.41	1.54
1	A	128	VAL	CA-CB	-9.62	1.41	1.54
1	A	536	SER	C-O	-9.55	1.11	1.24
1	B	540	PHE	CA-CB	-9.50	1.38	1.53
1	A	122	ILE	CA-CB	-9.48	1.40	1.54
1	B	122	ILE	CA-CB	-9.48	1.40	1.54
1	A	116	ARG	CA-C	-9.29	1.40	1.52
1	A	542	SER	CA-C	-9.09	1.41	1.52
1	B	538	ALA	C-O	-8.96	1.13	1.24
1	B	539	THR	CB-CG2	-8.91	1.23	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	117	TYR	N-CA	-8.73	1.33	1.46
1	A	116	ARG	N-CA	-8.63	1.35	1.46
1	A	122	ILE	C-O	-8.55	1.12	1.24
1	B	122	ILE	C-O	-8.55	1.12	1.24
1	A	542	SER	CA-CB	-8.52	1.41	1.53
1	B	536	SER	CA-C	-8.50	1.41	1.52
1	A	126	VAL	CA-CB	-8.39	1.43	1.54
1	B	126	VAL	CA-CB	-8.39	1.43	1.54
1	A	536	SER	CA-CB	-8.28	1.39	1.53
1	A	118	SER	CA-CB	-7.77	1.40	1.53
1	A	124	THR	CA-C	-7.71	1.42	1.52
1	B	124	THR	CA-C	-7.71	1.42	1.52
1	B	118	SER	CA-CB	-7.68	1.40	1.53
1	A	538	ALA	C-O	-7.67	1.14	1.24
1	A	114	LEU	C-O	7.64	1.32	1.24
1	B	114	LEU	C-O	7.63	1.32	1.24
1	B	119	VAL	CA-C	-7.61	1.42	1.52
1	A	536	SER	CA-C	-7.60	1.42	1.52
1	A	539	THR	CB-CG2	-7.56	1.27	1.52
1	A	115	SER	C-O	7.52	1.33	1.24
1	B	115	SER	C-O	7.52	1.33	1.24
1	A	538	ALA	N-CA	-7.50	1.36	1.46
1	B	541	ALA	CA-C	-7.44	1.42	1.52
1	B	542	SER	CA-CB	-7.43	1.43	1.53
1	B	127	VAL	CA-C	-7.42	1.44	1.52
1	A	538	ALA	CA-C	-7.39	1.42	1.52
1	B	534	ALA	CA-C	-7.35	1.43	1.52
1	A	127	VAL	CA-C	-7.33	1.44	1.52
1	B	115	SER	CA-C	7.31	1.63	1.52
1	A	115	SER	CA-C	7.29	1.62	1.52
1	B	128	VAL	CA-C	-7.24	1.43	1.52
1	A	128	VAL	CA-C	-7.02	1.43	1.52
1	A	129	PHE	CA-CB	-7.00	1.43	1.53
1	B	129	PHE	CA-CB	-6.99	1.43	1.53
1	A	128	VAL	C-O	-6.97	1.15	1.24
1	A	534	ALA	C-N	-6.97	1.25	1.33
1	B	541	ALA	N-CA	-6.92	1.37	1.46
1	B	128	VAL	C-O	-6.89	1.15	1.24
1	A	119	VAL	CA-C	-6.89	1.42	1.52
1	A	538	ALA	C-N	-6.86	1.24	1.33
1	B	116	ARG	CA-C	-6.82	1.44	1.52
1	B	535	LEU	C-O	-6.73	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	536	SER	C-O	-6.70	1.15	1.24
1	A	117	TYR	CA-CB	-6.68	1.43	1.53
1	B	539	THR	CA-C	-6.66	1.43	1.52
1	A	539	THR	N-CA	-6.54	1.37	1.46
1	A	541	ALA	N-CA	-6.47	1.37	1.46
1	B	538	ALA	CA-CB	-6.46	1.43	1.53
1	B	118	SER	CA-C	-6.42	1.43	1.52
1	A	535	LEU	CA-C	-6.40	1.43	1.52
1	A	118	SER	CA-C	-6.28	1.43	1.52
1	A	536	SER	N-CA	-6.24	1.38	1.46
1	A	120	TRP	CD2-CE2	-6.19	1.30	1.41
1	B	120	TRP	CD2-CE2	-6.19	1.30	1.41
1	A	129	PHE	CG-CD2	-6.05	1.26	1.38
1	B	129	PHE	CG-CD2	-6.05	1.26	1.38
1	B	117	TYR	CA-CB	-6.04	1.44	1.53
1	B	120	TRP	C-N	-5.96	1.26	1.33
1	A	538	ALA	CA-CB	-5.92	1.43	1.53
1	A	120	TRP	C-N	-5.91	1.26	1.33
1	B	537	LEU	CB-CG	-5.91	1.41	1.53
1	B	113	ASP	C-N	5.90	1.42	1.33
1	A	113	ASP	C-N	5.88	1.42	1.33
1	A	535	LEU	N-CA	-5.82	1.39	1.46
1	B	538	ALA	CA-C	-5.73	1.45	1.52
1	B	536	SER	CA-CB	-5.68	1.43	1.53
1	B	116	ARG	CA-CB	-5.61	1.44	1.53
1	B	120	TRP	CG-CD1	-5.61	1.23	1.36
1	A	120	TRP	CG-CD1	-5.57	1.23	1.36
1	B	542	SER	CA-C	-5.55	1.45	1.52
1	A	129	PHE	C-N	5.54	1.41	1.33
1	A	542	SER	CB-OG	-5.49	1.31	1.42
1	B	129	PHE	C-N	5.48	1.41	1.33
1	A	116	ARG	C-N	-5.46	1.24	1.33
1	B	116	ARG	C-N	-5.46	1.24	1.33
1	A	120	TRP	NE1-CE2	-5.41	1.31	1.37
1	A	123	LEU	N-CA	-5.40	1.39	1.46
1	B	123	LEU	N-CA	-5.40	1.39	1.46
1	A	121	ALA	CA-C	5.38	1.59	1.52
1	A	537	LEU	CB-CG	-5.34	1.42	1.53
1	B	121	ALA	CA-C	5.32	1.59	1.52
1	B	120	TRP	NE1-CE2	-5.29	1.31	1.37
1	B	120	TRP	CE2-CZ2	-5.26	1.28	1.39
1	B	124	THR	CB-OG1	-5.25	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	120	TRP	CE2-CZ2	-5.24	1.28	1.39
1	A	124	THR	CB-OG1	-5.19	1.35	1.43
1	A	120	TRP	CG-CD2	-5.09	1.34	1.43
1	B	120	TRP	CG-CD2	-5.06	1.34	1.43
1	B	129	PHE	C-O	-5.03	1.18	1.24

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	114	LEU	N-CA-C	19.14	134.53	110.61
1	A	114	LEU	N-CA-C	19.09	134.47	110.61
1	B	539	THR	OG1-CB-CG2	-9.65	90.00	109.30
1	B	539	THR	CA-C-O	-9.49	108.00	119.49
1	B	129	PHE	CA-C-O	-9.47	110.17	120.30
1	A	129	PHE	CA-C-O	-9.45	110.19	120.30
1	A	538	ALA	N-CA-C	-9.41	100.91	111.82
1	B	537	LEU	CB-CG-CD2	-9.39	82.54	110.70
1	B	113	ASP	CB-CA-C	9.20	125.53	110.81
1	A	113	ASP	CB-CA-C	9.19	125.51	110.81
1	B	116	ARG	CA-C-N	-9.03	104.21	122.55
1	B	116	ARG	C-N-CA	-9.03	104.21	122.55
1	A	116	ARG	CA-C-N	-9.02	104.24	122.55
1	A	116	ARG	C-N-CA	-9.02	104.24	122.55
1	B	115	SER	N-CA-C	8.73	123.99	113.16
1	A	115	SER	N-CA-C	8.70	123.95	113.16
1	A	540	PHE	N-CA-C	-8.64	101.43	112.93
1	B	118	SER	N-CA-C	8.46	123.41	113.18
1	A	539	THR	OG1-CB-CG2	-8.43	92.45	109.30
1	A	118	SER	N-CA-C	8.42	123.39	113.20
1	B	125	VAL	CA-C-O	-8.28	112.07	120.85
1	A	125	VAL	CA-C-O	-8.27	112.08	120.85
1	A	126	VAL	CA-C-O	-8.10	112.27	120.85
1	B	126	VAL	CA-C-O	-8.04	112.32	120.85
1	B	537	LEU	N-CA-C	-8.02	101.83	111.69
1	B	124	THR	CA-C-O	-7.95	110.41	119.79
1	A	124	THR	CA-C-O	-7.93	110.43	119.79
1	B	539	THR	N-CA-CB	7.45	122.98	110.32
1	A	541	ALA	CA-C-N	-7.22	111.16	122.49
1	A	541	ALA	C-N-CA	-7.22	111.16	122.49
1	A	540	PHE	CB-CA-C	-7.11	98.92	110.08
1	B	114	LEU	CA-C-O	7.09	128.58	121.20
1	A	538	ALA	CA-C-O	-7.08	111.83	119.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	LEU	CA-C-O	7.05	128.53	121.20
1	B	115	SER	CA-C-O	7.01	127.77	119.28
1	A	536	SER	N-CA-CB	7.01	121.09	110.30
1	A	115	SER	CA-C-O	7.01	127.76	119.28
1	A	113	ASP	N-CA-C	-6.87	102.87	111.11
1	B	113	ASP	N-CA-C	-6.86	102.88	111.11
1	B	122	ILE	CB-CA-C	-6.79	96.36	111.77
1	A	122	ILE	CB-CA-C	-6.79	96.36	111.77
1	A	119	VAL	CA-C-O	-6.72	112.99	120.25
1	A	536	SER	CA-C-O	-6.60	112.00	119.79
1	B	124	THR	N-CA-CB	6.56	120.41	110.30
1	A	124	THR	N-CA-CB	6.55	120.39	110.30
1	A	113	ASP	CA-C-N	6.38	134.15	122.54
1	A	113	ASP	C-N-CA	6.38	134.15	122.54
1	B	113	ASP	CA-C-N	6.38	134.15	122.54
1	B	113	ASP	C-N-CA	6.38	134.15	122.54
1	A	119	VAL	CB-CA-C	-6.34	101.82	112.16
1	A	125	VAL	N-CA-C	-6.20	104.46	110.72
1	B	125	VAL	N-CA-C	-6.20	104.46	110.72
1	B	119	VAL	N-CA-C	-6.17	103.93	112.50
1	B	540	PHE	CB-CA-C	-6.13	97.35	109.67
1	B	538	ALA	CA-C-O	-5.87	114.33	120.55
1	A	336	LYS	N-CA-C	-5.84	107.14	114.56
1	B	124	THR	OG1-CB-CG2	-5.83	97.63	109.30
1	A	116	ARG	NE-CZ-NH1	-5.83	115.67	121.50
1	A	117	TYR	CA-CB-CG	5.81	124.36	113.90
1	A	124	THR	OG1-CB-CG2	-5.81	97.68	109.30
1	B	336	LYS	N-CA-C	-5.81	107.18	114.56
1	B	116	ARG	NE-CZ-NH1	-5.80	115.70	121.50
1	A	120	TRP	CA-C-O	-5.78	114.75	120.82
1	B	120	TRP	CA-C-O	-5.78	114.75	120.82
1	B	535	LEU	N-CA-C	5.67	119.94	113.19
1	A	119	VAL	N-CA-C	-5.65	103.88	111.44
1	B	541	ALA	CA-C-O	-5.62	113.75	120.10
1	B	541	ALA	CA-C-N	-5.61	113.75	122.67
1	B	541	ALA	C-N-CA	-5.61	113.75	122.67
1	A	540	PHE	CA-C-O	-5.60	112.51	120.07
1	B	539	THR	O-C-N	-5.59	115.12	122.39
1	A	539	THR	N-CA-C	5.57	119.16	112.93
1	B	121	ALA	N-CA-C	5.54	117.77	111.02
1	A	121	ALA	N-CA-C	5.52	117.75	111.02
1	A	116	ARG	CG-CD-NE	5.47	124.04	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	116	ARG	CG-CD-NE	5.47	124.04	112.00
1	A	538	ALA	CA-C-N	-5.47	113.57	122.65
1	A	538	ALA	C-N-CA	-5.47	113.57	122.65
1	B	537	LEU	CA-C-O	-5.46	114.19	120.24
1	A	116	ARG	N-CA-CB	-5.44	102.11	110.16
1	A	541	ALA	O-C-N	-5.42	115.22	122.43
1	B	119	VAL	CA-C-O	-5.41	113.03	119.58
1	A	127	VAL	CG1-CB-CG2	-5.35	99.03	110.80
1	B	127	VAL	CG1-CB-CG2	-5.35	99.04	110.80
1	A	117	TYR	N-CA-C	-5.29	107.12	113.21
1	A	534	ALA	CA-C-N	-5.28	114.23	122.73
1	A	534	ALA	C-N-CA	-5.28	114.23	122.73
1	A	119	VAL	CA-CB-CG1	-5.25	101.47	110.40
1	B	119	VAL	CA-CB-CG1	-5.22	101.53	110.40
1	B	116	ARG	CA-CB-CG	-5.20	103.70	114.10
1	A	122	ILE	N-CA-C	5.20	119.31	112.04
1	B	122	ILE	N-CA-C	5.19	119.31	112.04
1	B	537	LEU	CA-C-N	-5.13	113.41	120.28
1	B	537	LEU	C-N-CA	-5.13	113.41	120.28
1	B	119	VAL	O-C-N	-5.07	115.13	122.12
1	B	117	TYR	CA-CB-CG	5.06	123.02	113.90
1	B	125	VAL	CB-CA-C	-5.05	105.26	112.22
1	A	125	VAL	CB-CA-C	-5.03	105.28	112.22

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	ASP	Mainchain
1	A	542	SER	Mainchain
1	B	113	ASP	Mainchain
1	B	542	SER	Mainchain

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	2966	0	2950	170	0
1	B	2966	0	2950	172	0
2	B	13	0	5	5	0
All	All	5945	0	5905	276	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 23.

All (276) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:LYS:HD3	1:B:189:TYR:OH	1.39	1.18
1:A:189:TYR:OH	1:B:76:LYS:HD3	1.41	1.17
1:A:116:ARG:HE	1:A:116:ARG:HA	1.20	1.06
1:B:116:ARG:HE	1:B:116:ARG:HA	1.19	1.02
1:A:188:LEU:HD11	1:B:90:PHE:HD1	1.25	0.98
1:A:90:PHE:HD1	1:B:188:LEU:HD11	1.27	0.97
1:B:428:LEU:HD12	1:B:538:ALA:HB2	1.45	0.95
1:A:185:PHE:CZ	1:B:88:ILE:HA	2.01	0.95
1:A:120:TRP:CZ2	2:B:601:CIT:H21	2.01	0.95
1:B:116:ARG:HA	1:B:116:ARG:NE	1.75	0.94
1:A:88:ILE:HA	1:B:185:PHE:CZ	2.04	0.92
1:A:354:ALA:HB2	1:B:354:ALA:HB2	1.50	0.92
1:A:185:PHE:HZ	1:B:88:ILE:HA	1.33	0.92
1:A:116:ARG:HA	1:A:116:ARG:NE	1.78	0.91
1:A:88:ILE:HA	1:B:185:PHE:HZ	1.35	0.90
1:A:117:TYR:HD1	1:A:226:ARG:NE	1.71	0.89
1:A:117:TYR:CD1	1:A:226:ARG:NE	2.41	0.88
1:A:90:PHE:CD1	1:B:188:LEU:HD11	2.10	0.87
1:A:188:LEU:HD11	1:B:90:PHE:CD1	2.08	0.86
1:B:117:TYR:CD1	1:B:226:ARG:NE	2.43	0.86
1:B:117:TYR:HD1	1:B:226:ARG:NE	1.72	0.86
1:B:355:LEU:CD1	1:B:540:PHE:CE1	2.62	0.83
1:B:355:LEU:HD11	1:B:540:PHE:CE1	2.14	0.82
1:B:120:TRP:CZ2	2:B:601:CIT:H41	2.14	0.82
1:A:215:ARG:CB	1:B:116:ARG:HH22	1.96	0.79
1:B:428:LEU:CD1	1:B:538:ALA:HB2	2.14	0.78
1:A:116:ARG:HH22	1:B:215:ARG:CB	1.97	0.78
1:A:355:LEU:HD11	1:A:540:PHE:CE1	2.19	0.77
1:A:537:LEU:HD22	1:A:537:LEU:H	1.49	0.77
1:A:215:ARG:CB	1:B:116:ARG:NH2	2.48	0.77
1:A:355:LEU:CD1	1:A:540:PHE:CE1	2.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:LEU:HD12	1:B:538:ALA:CB	2.14	0.76
1:A:116:ARG:NH2	1:B:215:ARG:CB	2.49	0.76
1:A:200:ARG:NH2	1:B:127:VAL:HG23	2.01	0.75
1:A:127:VAL:HG23	1:B:200:ARG:NH2	2.01	0.75
1:A:208:TYR:OH	1:A:226:ARG:NH1	2.20	0.75
1:B:208:TYR:OH	1:B:226:ARG:NH1	2.20	0.73
1:A:203:LEU:HD21	1:B:98:LEU:HD11	1.70	0.73
1:A:184:THR:HG21	1:B:91:SER:HA	1.71	0.72
1:B:129:PHE:CE2	1:B:241:ASN:HB2	2.25	0.72
1:A:91:SER:HA	1:B:184:THR:HG21	1.73	0.71
1:A:129:PHE:CE2	1:A:241:ASN:HB2	2.25	0.71
1:A:200:ARG:HH21	1:B:127:VAL:HG23	1.58	0.69
1:B:355:LEU:HD12	1:B:540:PHE:CE1	2.27	0.69
1:A:98:LEU:HD11	1:B:203:LEU:HD21	1.72	0.69
1:A:128:VAL:HG13	1:A:128:VAL:O	1.93	0.68
1:A:189:TYR:OH	1:B:76:LYS:CD	2.33	0.68
1:A:127:VAL:HG23	1:B:200:ARG:HH21	1.58	0.67
1:A:117:TYR:HB2	1:A:229:LEU:HD13	1.76	0.67
1:A:122:ILE:HG22	1:A:122:ILE:O	1.95	0.66
1:B:117:TYR:HB2	1:B:229:LEU:HD13	1.76	0.66
1:B:122:ILE:O	1:B:122:ILE:HG22	1.95	0.66
1:A:128:VAL:O	1:A:128:VAL:HG22	1.96	0.66
1:B:128:VAL:HG13	1:B:128:VAL:O	1.93	0.66
1:B:98:LEU:HD21	1:B:126:VAL:HG23	1.79	0.65
1:A:76:LYS:CD	1:B:189:TYR:OH	2.32	0.65
1:B:119:VAL:HG12	1:B:119:VAL:O	1.97	0.64
1:B:128:VAL:O	1:B:128:VAL:HG22	1.96	0.64
1:B:86:ARG:NH1	1:B:252:ASP:OD1	2.30	0.64
1:A:185:PHE:CE1	1:B:91:SER:OG	2.51	0.64
1:A:355:LEU:HD12	1:A:540:PHE:CE1	2.33	0.64
1:A:119:VAL:HG12	1:A:119:VAL:O	1.97	0.64
1:B:337:ASN:HB2	1:B:561:LEU:HD13	1.80	0.63
1:A:86:ARG:NH1	1:A:252:ASP:OD1	2.30	0.63
1:A:361:SER:HB2	1:B:546:GLU:CD	2.24	0.63
1:A:337:ASN:HB2	1:A:561:LEU:HD13	1.80	0.63
1:A:98:LEU:HD21	1:A:126:VAL:HG23	1.81	0.63
1:A:546:GLU:CD	1:B:361:SER:HB2	2.23	0.63
1:B:150:ALA:HB2	1:B:202:PHE:HD2	1.63	0.63
1:A:200:ARG:NH2	1:B:127:VAL:CG2	2.61	0.62
1:B:535:LEU:HD23	1:B:535:LEU:O	2.00	0.62
1:A:150:ALA:HB2	1:A:202:PHE:HD2	1.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:VAL:CG2	1:B:200:ARG:NH2	2.62	0.61
1:A:535:LEU:O	1:A:535:LEU:HD23	1.99	0.61
1:B:258:VAL:HG21	1:B:396:LYS:HB2	1.82	0.61
1:B:222:VAL:O	1:B:226:ARG:HG2	2.01	0.61
1:A:258:VAL:HG21	1:A:396:LYS:HB2	1.82	0.61
1:A:222:VAL:O	1:A:226:ARG:HG2	2.01	0.60
1:A:248:TRP:HE3	1:A:322:GLU:HG2	1.65	0.60
1:A:306:VAL:HG21	1:A:353:MET:HE1	1.83	0.60
1:B:98:LEU:CD2	1:B:122:ILE:HG22	2.31	0.60
1:B:127:VAL:HG22	1:B:127:VAL:O	2.01	0.60
1:B:248:TRP:HE3	1:B:322:GLU:HG2	1.65	0.60
1:A:98:LEU:CD2	1:A:122:ILE:HG22	2.32	0.59
1:A:537:LEU:HD22	1:A:537:LEU:N	2.17	0.59
1:B:306:VAL:HG21	1:B:353:MET:HE1	1.83	0.59
1:A:127:VAL:O	1:A:127:VAL:HG22	2.01	0.59
1:A:341:LEU:HD13	1:A:558:PHE:HB2	1.85	0.59
1:B:276:LEU:HD23	1:B:374:ARG:HG3	1.85	0.59
1:B:341:LEU:HD13	1:B:558:PHE:HB2	1.85	0.59
1:A:276:LEU:HD23	1:A:374:ARG:HG3	1.85	0.58
1:B:537:LEU:HD12	1:B:537:LEU:O	2.03	0.58
1:A:132:THR:HB	1:A:249:ALA:HB2	1.86	0.58
1:A:127:VAL:O	1:A:127:VAL:HG13	2.03	0.58
1:B:127:VAL:O	1:B:127:VAL:HG13	2.03	0.57
1:A:539:THR:O	1:A:539:THR:OG1	2.04	0.57
1:A:119:VAL:HG12	1:A:123:LEU:HD13	1.87	0.57
1:B:132:THR:HB	1:B:249:ALA:HB2	1.86	0.57
1:A:150:ALA:HB2	1:A:202:PHE:CD2	2.40	0.56
1:A:185:PHE:HE1	1:B:87:LYS:O	1.88	0.56
1:A:207:CYS:O	1:A:211:ILE:HG12	2.05	0.56
1:B:254:HIS:NE2	1:B:395:VAL:O	2.34	0.56
1:B:207:CYS:O	1:B:211:ILE:HG12	2.05	0.56
1:A:185:PHE:CE1	1:B:88:ILE:HA	2.41	0.56
1:B:93:LYS:NZ	1:B:244:ILE:O	2.35	0.56
1:A:211:ILE:HG13	1:B:122:ILE:HD12	1.88	0.56
1:A:254:HIS:NE2	1:A:395:VAL:O	2.34	0.56
1:A:120:TRP:HZ2	2:B:601:CIT:H21	1.62	0.56
1:B:119:VAL:HG12	1:B:123:LEU:HD13	1.87	0.56
1:B:179:ILE:HG21	1:B:206:TYR:CD2	2.41	0.55
1:B:539:THR:O	1:B:539:THR:OG1	2.22	0.55
1:A:116:ARG:NE	1:A:116:ARG:CA	2.62	0.55
1:B:428:LEU:HD11	1:B:538:ALA:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ILE:HG21	1:A:206:TYR:CD2	2.41	0.55
1:A:337:ASN:HA	1:A:340:LYS:HB3	1.88	0.55
1:B:528:THR:OG1	1:B:529:TYR:N	2.40	0.55
1:A:122:ILE:HD12	1:B:211:ILE:HG13	1.88	0.55
1:A:535:LEU:HD21	1:B:542:SER:HB3	1.89	0.55
1:A:184:THR:HG21	1:B:91:SER:CA	2.36	0.55
1:B:150:ALA:HB2	1:B:202:PHE:CD2	2.40	0.55
1:A:87:LYS:O	1:B:185:PHE:HE1	1.90	0.55
1:B:98:LEU:CD2	1:B:122:ILE:CG2	2.84	0.54
1:A:535:LEU:CD2	1:B:542:SER:HB3	2.37	0.54
1:A:98:LEU:CD2	1:A:122:ILE:CG2	2.85	0.54
1:B:337:ASN:HA	1:B:340:LYS:HB3	1.88	0.54
1:A:379:ARG:HG2	1:A:379:ARG:HH21	1.73	0.54
1:A:382:VAL:O	1:A:386:LYS:HG2	2.08	0.54
1:B:105:ILE:HD11	1:B:118:SER:O	2.08	0.54
1:A:354:ALA:CB	1:B:354:ALA:HB2	2.32	0.54
1:A:88:ILE:HA	1:B:185:PHE:CE1	2.43	0.53
1:A:116:ARG:C	1:A:118:SER:H	2.15	0.53
1:A:542:SER:HB3	1:B:535:LEU:CD2	2.39	0.53
1:B:382:VAL:O	1:B:386:LYS:HG2	2.08	0.53
1:B:379:ARG:HG2	1:B:379:ARG:HH21	1.72	0.53
1:B:428:LEU:CD1	1:B:538:ALA:N	2.71	0.53
1:A:91:SER:CA	1:B:184:THR:HG21	2.36	0.53
1:A:354:ALA:HB2	1:B:354:ALA:CB	2.32	0.52
1:B:72:ASP:O	1:B:76:LYS:HG3	2.09	0.52
1:B:116:ARG:C	1:B:118:SER:N	2.62	0.52
1:B:351:THR:O	1:B:355:LEU:N	2.34	0.52
1:A:72:ASP:O	1:A:76:LYS:HG3	2.09	0.52
1:B:116:ARG:C	1:B:118:SER:H	2.16	0.52
1:A:105:ILE:HD11	1:A:118:SER:O	2.10	0.52
1:A:116:ARG:C	1:A:118:SER:N	2.61	0.52
1:A:167:TRP:O	1:A:170:ILE:HG22	2.10	0.52
1:A:542:SER:HB3	1:B:535:LEU:HD21	1.92	0.52
1:B:355:LEU:HD12	1:B:540:PHE:HE1	1.75	0.51
1:A:361:SER:OG	1:A:363:ILE:O	2.29	0.51
1:A:407:LEU:HD11	1:A:555:VAL:HG21	1.93	0.51
1:B:167:TRP:O	1:B:170:ILE:HG22	2.10	0.51
1:A:351:THR:O	1:A:355:LEU:N	2.34	0.51
1:A:123:LEU:CD1	1:A:123:LEU:N	2.74	0.50
1:A:195:TYR:CE1	1:A:198:GLY:HA3	2.47	0.50
1:A:123:LEU:N	1:A:123:LEU:HD12	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:LEU:CD1	1:B:123:LEU:N	2.74	0.50
1:B:195:TYR:CE1	1:B:198:GLY:HA3	2.47	0.50
1:B:419:HIS:O	1:B:423:LYS:NZ	2.33	0.50
1:B:536:SER:O	1:B:536:SER:OG	2.30	0.50
1:A:187:LYS:HG3	1:A:196:GLU:HG2	1.94	0.49
1:B:361:SER:OG	1:B:363:ILE:O	2.29	0.49
1:B:355:LEU:CD1	1:B:540:PHE:HE1	2.20	0.49
1:B:407:LEU:HD11	1:B:555:VAL:HG21	1.93	0.49
1:A:539:THR:O	1:A:539:THR:HG23	2.12	0.49
1:A:528:THR:OG1	1:A:529:TYR:N	2.40	0.49
1:B:414:ALA:HB2	1:B:548:VAL:HG21	1.94	0.49
1:B:123:LEU:N	1:B:123:LEU:HD12	2.27	0.49
1:A:226:ARG:O	1:A:230:ILE:HG13	2.13	0.49
1:A:181:PHE:CE2	1:B:91:SER:OG	2.66	0.48
1:B:226:ARG:O	1:B:230:ILE:HG13	2.13	0.48
1:B:197:TYR:O	1:B:201:VAL:HG23	2.13	0.48
1:A:112:PRO:O	1:A:113:ASP:C	2.55	0.48
1:B:187:LYS:HG3	1:B:196:GLU:HG2	1.94	0.48
1:A:535:LEU:CD2	1:B:542:SER:CB	2.92	0.48
1:A:184:THR:OG1	1:B:94:ILE:HG21	2.14	0.48
1:A:414:ALA:HB2	1:A:548:VAL:HG21	1.94	0.48
1:A:91:SER:OG	1:B:181:PHE:CE2	2.67	0.48
1:A:176:ILE:HA	1:A:179:ILE:HG22	1.95	0.48
1:A:197:TYR:O	1:A:201:VAL:HG23	2.13	0.48
1:B:112:PRO:O	1:B:113:ASP:C	2.55	0.48
1:A:356:HIS:O	1:A:359:ILE:HG22	2.14	0.48
1:A:383:GLU:OE1	1:A:409:GLU:HB3	2.14	0.47
1:B:101:VAL:HG21	1:B:125:VAL:HG21	1.96	0.47
1:B:176:ILE:HA	1:B:179:ILE:HG22	1.95	0.47
1:B:398:MET:HE1	1:B:562:SER:HA	1.96	0.47
1:B:383:GLU:OE1	1:B:409:GLU:HB3	2.14	0.47
1:A:91:SER:OG	1:B:185:PHE:CE1	2.53	0.47
1:A:181:PHE:HE2	1:B:91:SER:OG	1.98	0.47
1:B:195:TYR:HE1	1:B:198:GLY:HA3	1.78	0.47
1:A:120:TRP:HZ2	2:B:601:CIT:C2	2.25	0.47
1:A:188:LEU:CD1	1:B:90:PHE:HD1	2.12	0.47
1:A:195:TYR:HE1	1:A:198:GLY:HA3	1.78	0.46
1:A:203:LEU:CD2	1:B:126:VAL:HG22	2.45	0.46
1:A:302:TYR:OH	1:A:356:HIS:CD2	2.69	0.46
1:A:398:MET:HE1	1:A:562:SER:HA	1.96	0.46
1:B:356:HIS:O	1:B:359:ILE:HG22	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:LEU:N	1:A:537:LEU:HD13	2.30	0.46
1:A:542:SER:CB	1:B:535:LEU:CD2	2.93	0.46
1:B:98:LEU:HD23	1:B:122:ILE:CG2	2.45	0.46
1:B:161:SER:HA	1:B:168:GLU:OE1	2.15	0.46
1:A:203:LEU:CD2	1:B:126:VAL:CG2	2.94	0.46
1:A:91:SER:OG	1:B:181:PHE:HE2	1.99	0.46
1:A:101:VAL:HG21	1:A:125:VAL:HG21	1.97	0.46
1:A:172:CYS:HA	1:A:175:SER:OG	2.16	0.45
1:A:419:HIS:O	1:A:423:LYS:NZ	2.33	0.45
1:B:302:TYR:OH	1:B:356:HIS:CD2	2.68	0.45
1:A:94:ILE:HG21	1:B:184:THR:OG1	2.16	0.45
1:A:98:LEU:HD23	1:A:122:ILE:CG2	2.46	0.45
1:A:210:LEU:HD12	1:A:210:LEU:HA	1.72	0.45
1:B:355:LEU:CD1	1:B:540:PHE:CD1	3.00	0.45
1:A:161:SER:HA	1:A:168:GLU:OE1	2.16	0.45
1:A:181:PHE:HE2	1:B:91:SER:HG	1.65	0.45
1:A:333:TYR:HB3	1:A:335:TRP:NE1	2.32	0.45
1:A:76:LYS:HD3	1:B:189:TYR:CZ	2.44	0.45
1:A:240:VAL:HG13	1:A:244:ILE:HD12	1.99	0.45
1:B:240:VAL:HG13	1:B:244:ILE:HD12	1.99	0.45
1:A:129:PHE:CZ	1:A:241:ASN:HB2	2.52	0.45
1:B:333:TYR:HB3	1:B:335:TRP:NE1	2.32	0.45
1:B:129:PHE:CZ	1:B:241:ASN:HB2	2.52	0.44
1:B:266:THR:O	1:B:270:GLY:N	2.42	0.44
1:A:355:LEU:HD12	1:A:540:PHE:HE1	1.79	0.44
1:B:151:GLY:O	1:B:155:LEU:HD23	2.18	0.44
1:B:172:CYS:HA	1:B:175:SER:OG	2.17	0.44
1:B:366:PRO:HG2	1:B:369:ARG:HB2	2.00	0.44
1:B:403:PRO:HG3	1:B:558:PHE:CE2	2.53	0.44
1:A:173:THR:CG2	1:B:99:THR:OG1	2.66	0.44
1:B:185:PHE:O	1:B:188:LEU:N	2.51	0.44
1:A:151:GLY:O	1:A:155:LEU:HD23	2.18	0.44
1:A:403:PRO:HG3	1:A:558:PHE:CE2	2.53	0.44
1:A:93:LYS:NZ	1:A:244:ILE:O	2.35	0.44
1:A:241:ASN:O	1:A:241:ASN:ND2	2.50	0.44
1:B:241:ASN:C	1:B:241:ASN:HD22	2.25	0.44
1:A:366:PRO:HG2	1:A:369:ARG:HB2	2.00	0.43
1:A:126:VAL:CG2	1:B:203:LEU:CD2	2.96	0.43
1:A:173:THR:HG23	1:B:99:THR:OG1	2.19	0.43
1:B:355:LEU:HD12	1:B:540:PHE:CD1	2.53	0.43
1:A:184:THR:CG2	1:B:91:SER:HB3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:HIS:CG	1:A:325:HIS:O	2.72	0.43
1:B:72:ASP:O	1:B:76:LYS:N	2.39	0.43
1:B:325:HIS:CG	1:B:325:HIS:O	2.72	0.43
1:A:91:SER:HB3	1:B:184:THR:CG2	2.49	0.43
1:A:99:THR:OG1	1:B:173:THR:CG2	2.66	0.43
1:B:234:ALA:HA	1:B:237:SER:HB3	2.00	0.43
1:A:185:PHE:O	1:A:188:LEU:N	2.51	0.43
1:A:536:SER:O	1:A:539:THR:HG22	2.19	0.43
1:A:126:VAL:HG22	1:B:203:LEU:CD2	2.48	0.43
1:B:241:ASN:O	1:B:241:ASN:ND2	2.50	0.43
1:A:179:ILE:HD11	1:A:202:PHE:CZ	2.54	0.42
1:B:147:THR:HG23	1:B:205:THR:HG21	2.01	0.42
1:A:147:THR:HG23	1:A:205:THR:HG21	2.01	0.42
1:B:314:SER:O	1:B:317:SER:OG	2.34	0.42
1:A:352:VAL:HA	1:A:355:LEU:HB3	2.02	0.42
1:A:359:ILE:HD12	1:A:359:ILE:HA	1.86	0.42
1:B:179:ILE:HD11	1:B:202:PHE:CZ	2.54	0.42
1:A:99:THR:OG1	1:B:173:THR:HG23	2.19	0.42
1:A:120:TRP:CZ2	2:B:601:CIT:C2	2.86	0.42
1:B:91:SER:HA	1:B:94:ILE:HG22	2.02	0.42
1:A:91:SER:HA	1:A:94:ILE:HG22	2.02	0.42
1:A:234:ALA:HA	1:A:237:SER:HB3	2.00	0.42
1:A:132:THR:HA	1:A:247:ILE:O	2.19	0.41
1:B:352:VAL:HA	1:B:355:LEU:HB3	2.02	0.41
1:A:100:ILE:HD13	1:A:100:ILE:HA	1.92	0.41
1:B:132:THR:HA	1:B:247:ILE:O	2.19	0.41
1:A:391:LEU:HD23	1:A:391:LEU:HA	1.90	0.41
1:A:178:CYS:SG	1:A:179:ILE:N	2.94	0.41
1:A:428:LEU:HD11	1:A:537:LEU:HB2	2.03	0.41
1:A:546:GLU:O	1:A:550:ARG:HG2	2.21	0.41
1:B:535:LEU:O	1:B:535:LEU:CG	2.69	0.41
1:B:546:GLU:O	1:B:550:ARG:HG2	2.21	0.41
1:A:325:HIS:O	1:A:325:HIS:ND1	2.54	0.40
1:B:365:ALA:CB	1:B:537:LEU:HB2	2.51	0.40
1:A:116:ARG:O	1:A:117:TYR:C	2.56	0.40
1:B:116:ARG:O	1:B:117:TYR:C	2.56	0.40
1:B:220:ILE:HD12	1:B:220:ILE:HA	1.86	0.40
1:A:128:VAL:O	1:A:128:VAL:CG1	2.63	0.40
1:B:119:VAL:CG1	1:B:123:LEU:HD13	2.50	0.40
1:B:379:ARG:HG2	1:B:379:ARG:NH2	2.37	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	376/598 (63%)	358 (95%)	18 (5%)	0	100	100
1	B	376/598 (63%)	358 (95%)	18 (5%)	0	100	100
All	All	752/1196 (63%)	716 (95%)	36 (5%)	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	305/512 (60%)	299 (98%)	6 (2%)	48	67
1	B	305/512 (60%)	300 (98%)	5 (2%)	55	71
All	All	610/1024 (60%)	599 (98%)	11 (2%)	51	69

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	SER
1	A	116	ARG
1	A	117	TYR
1	A	127	VAL
1	A	535	LEU
1	A	537	LEU
1	B	115	SER
1	B	116	ARG

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Mol	Chain	Res	Type
1	B	117	TYR
1	B	127	VAL
1	B	537	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	ASN
1	A	347	HIS
1	A	356	HIS
1	B	241	ASN
1	B	347	HIS
1	B	356	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CIT	B	601	-	12,12,12	1.17	1 (8%)	17,17,17	1.24	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CIT	B	601	-	-	6/16/16/16	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	CIT	C3-C6	-2.06	1.51	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	CIT	O6-C6-C3	2.93	118.75	113.14

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	CIT	O7-C3-C6-O6
2	B	601	CIT	C4-C3-C6-O6
2	B	601	CIT	C2-C3-C6-O6
2	B	601	CIT	C4-C3-C6-O5
2	B	601	CIT	C2-C3-C6-O5
2	B	601	CIT	O7-C3-C6-O5

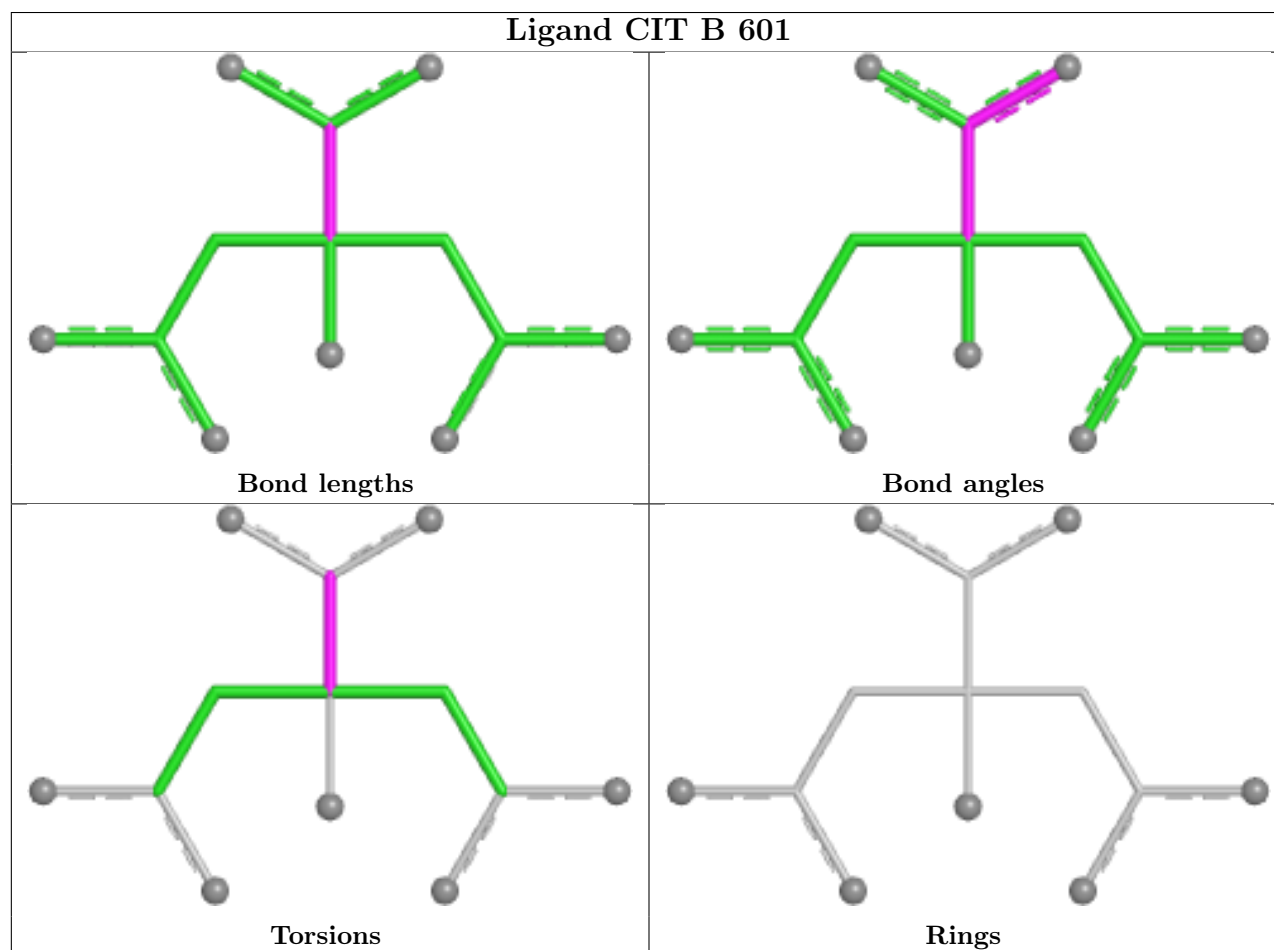
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	CIT	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

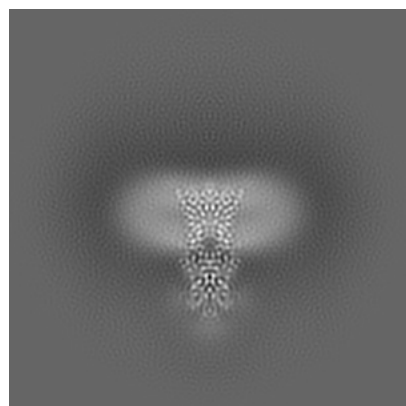
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34828. These allow visual inspection of the internal detail of the map and identification of artifacts.

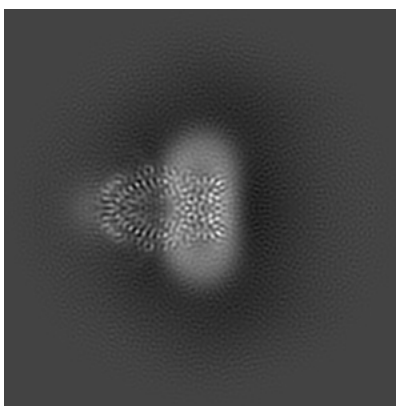
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

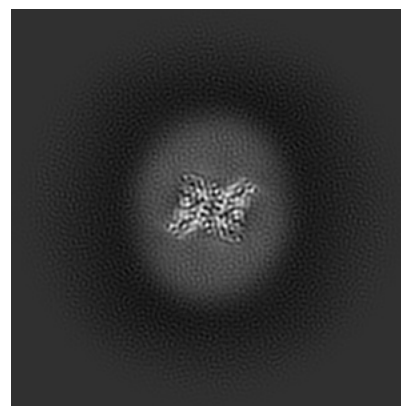
6.1.1 Primary map



X

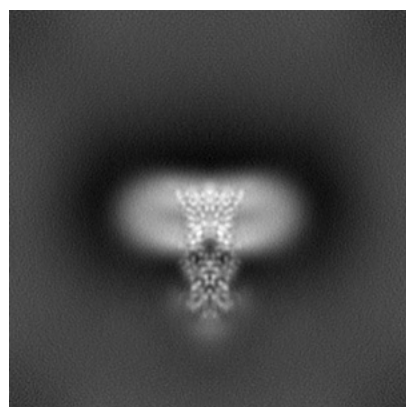


Y

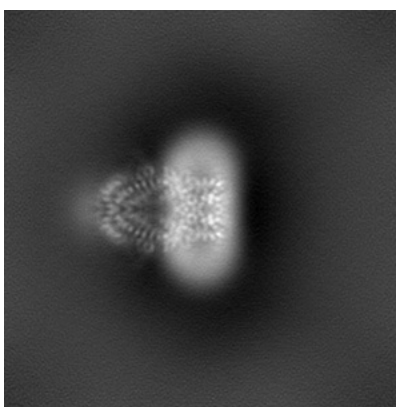


Z

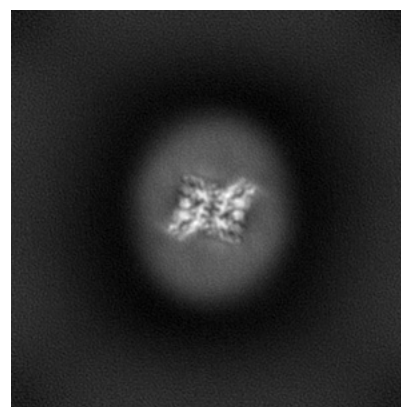
6.1.2 Raw map



X



Y

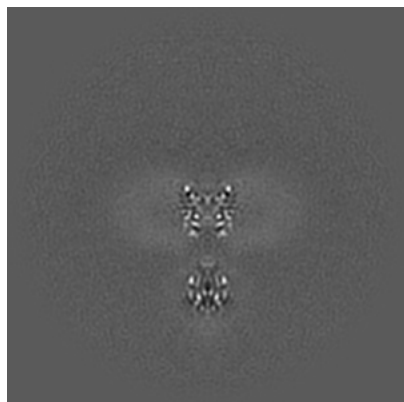


Z

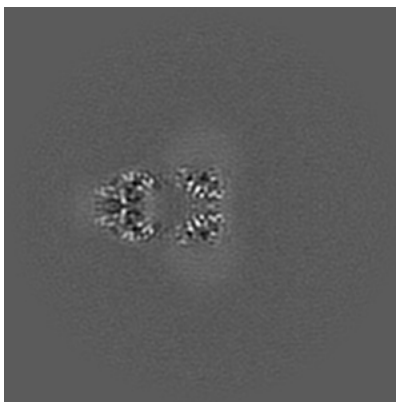
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

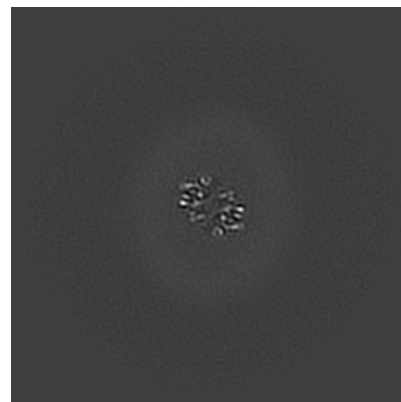
6.2.1 Primary map



X Index: 128

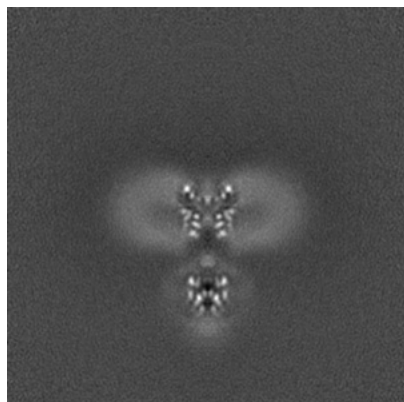


Y Index: 128

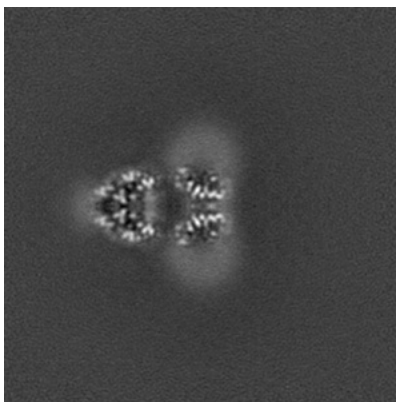


Z Index: 128

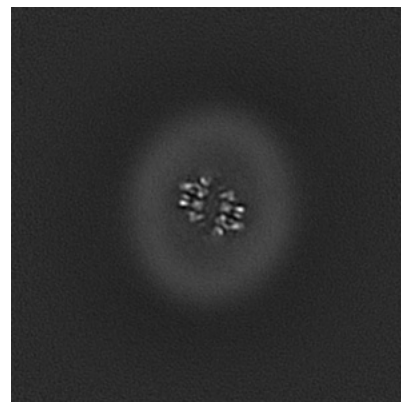
6.2.2 Raw map



X Index: 128



Y Index: 128

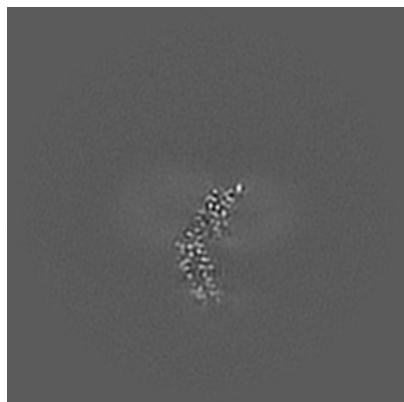


Z Index: 128

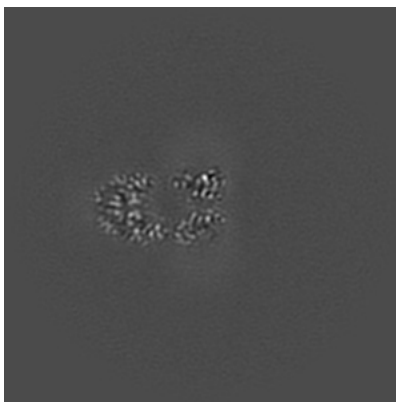
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

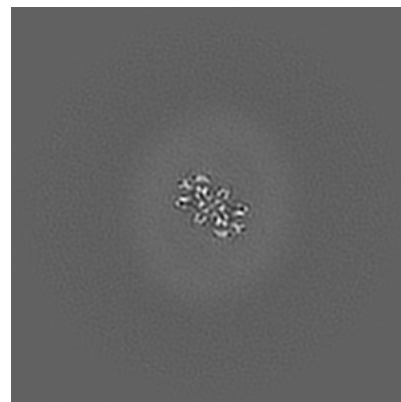
6.3.1 Primary map



X Index: 111

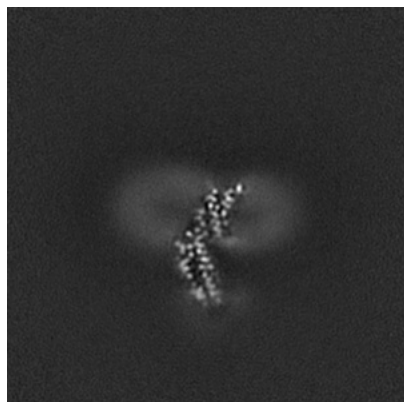


Y Index: 126

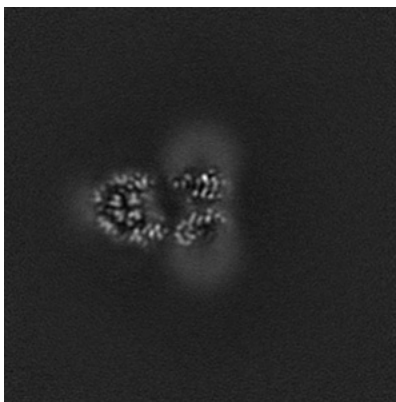


Z Index: 132

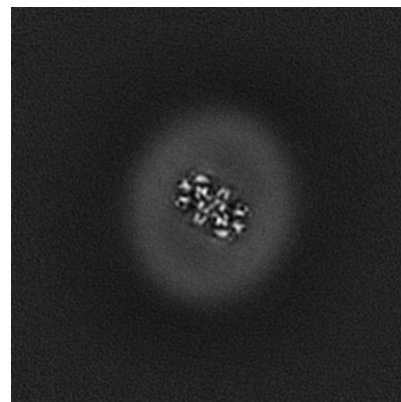
6.3.2 Raw map



X Index: 111



Y Index: 126

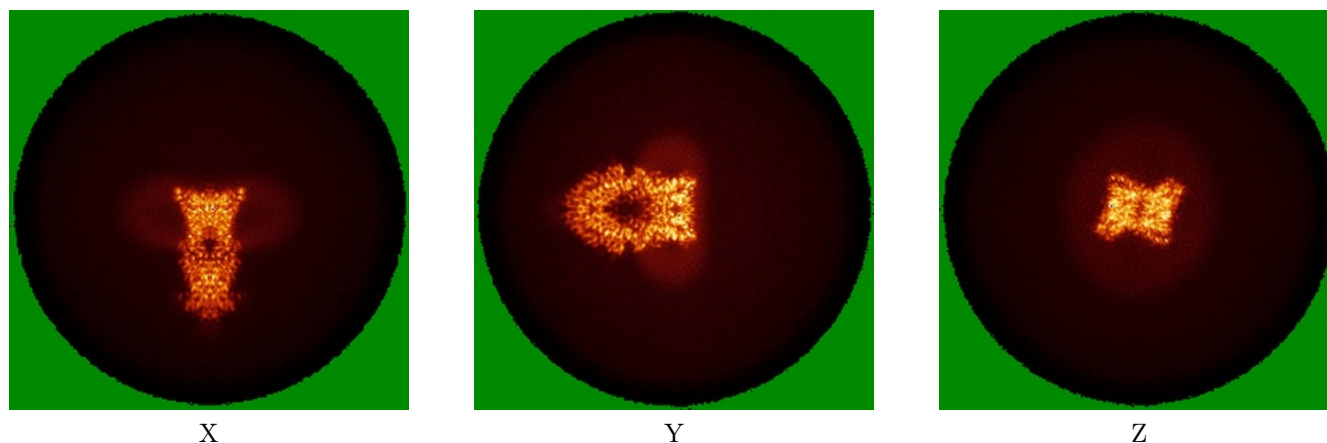


Z Index: 132

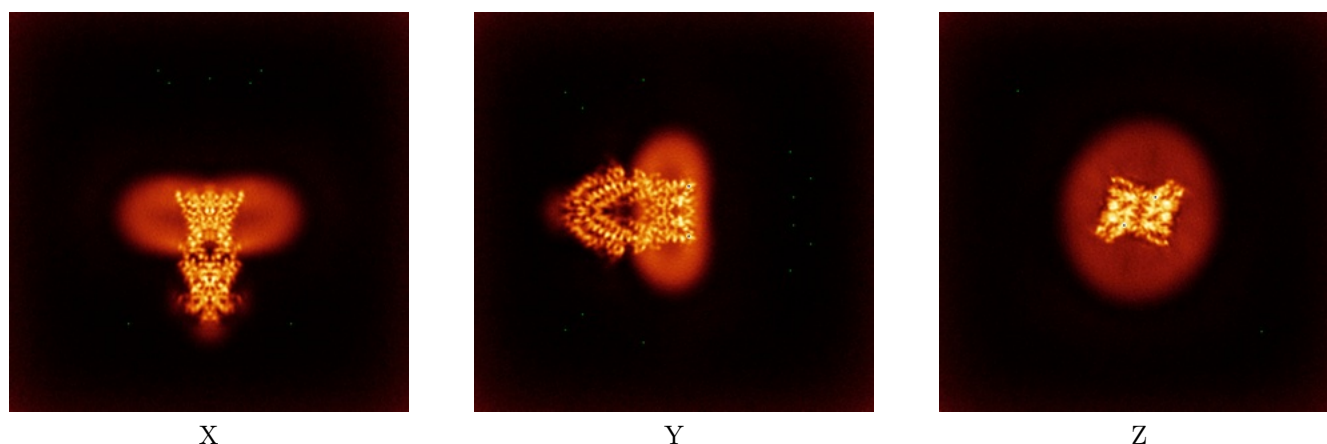
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

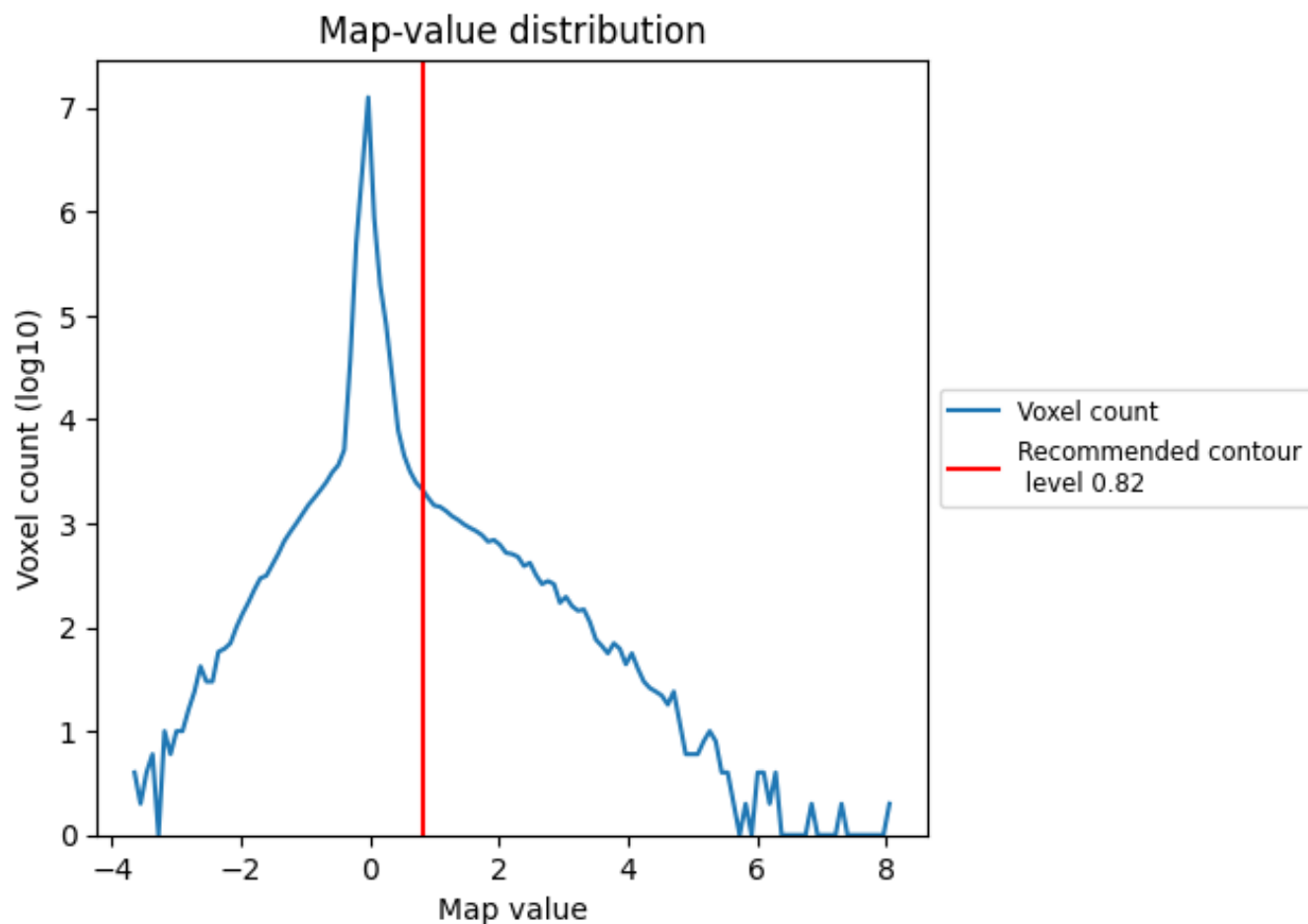
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

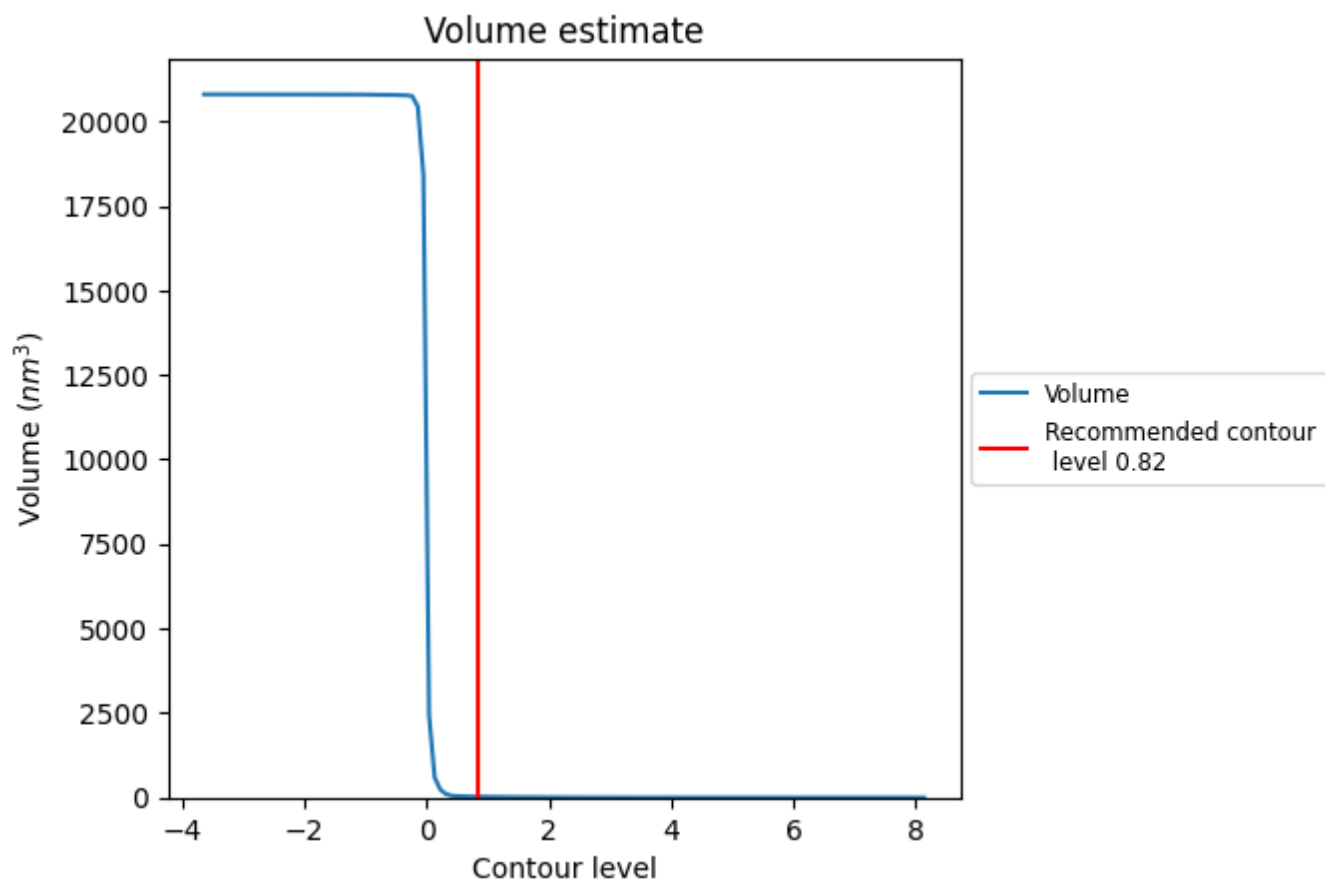
This section contains the results of statistical analysis of the map.

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.

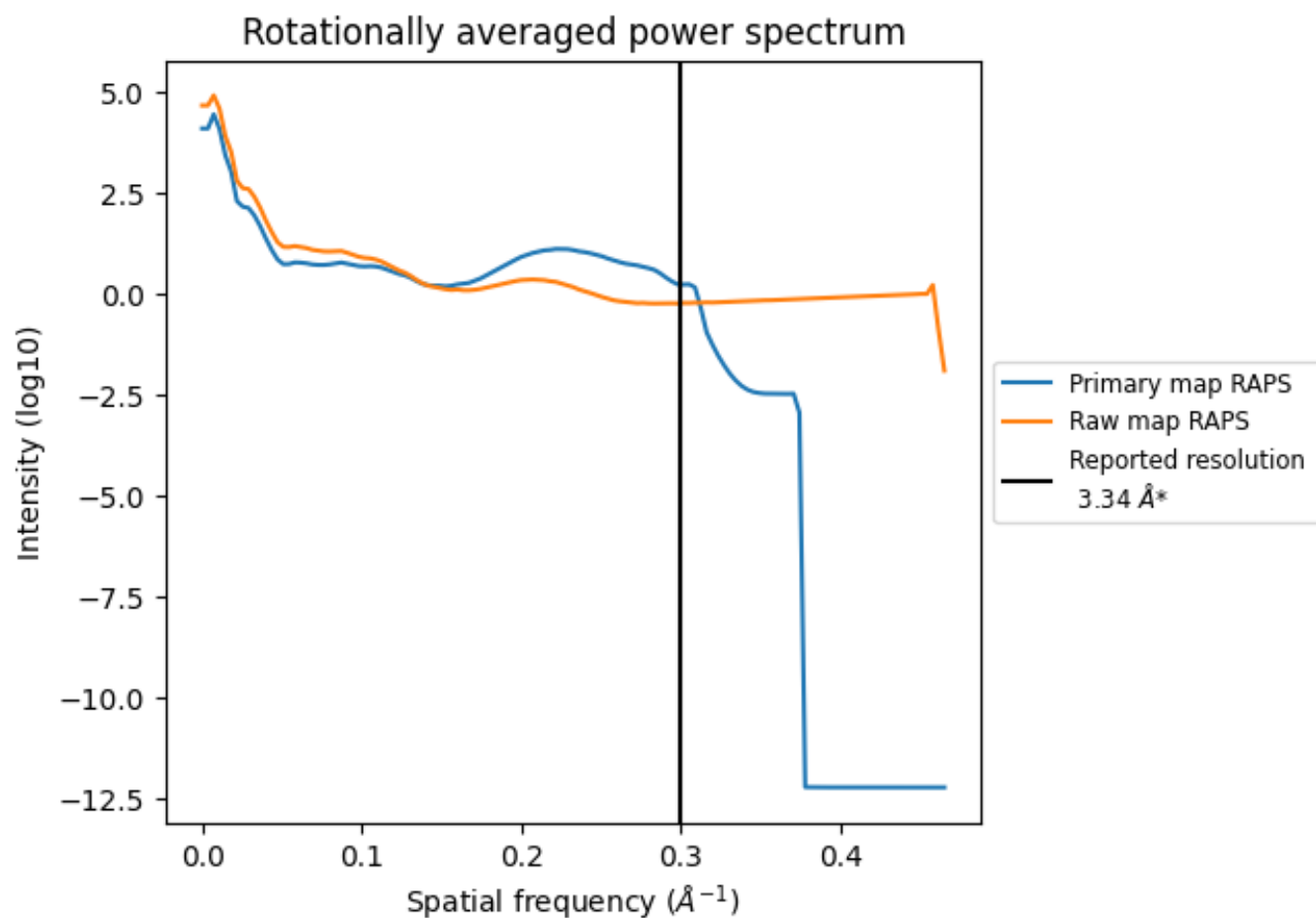
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 26 nm^3 ; this corresponds to an approximate mass of 23 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 ⓘ

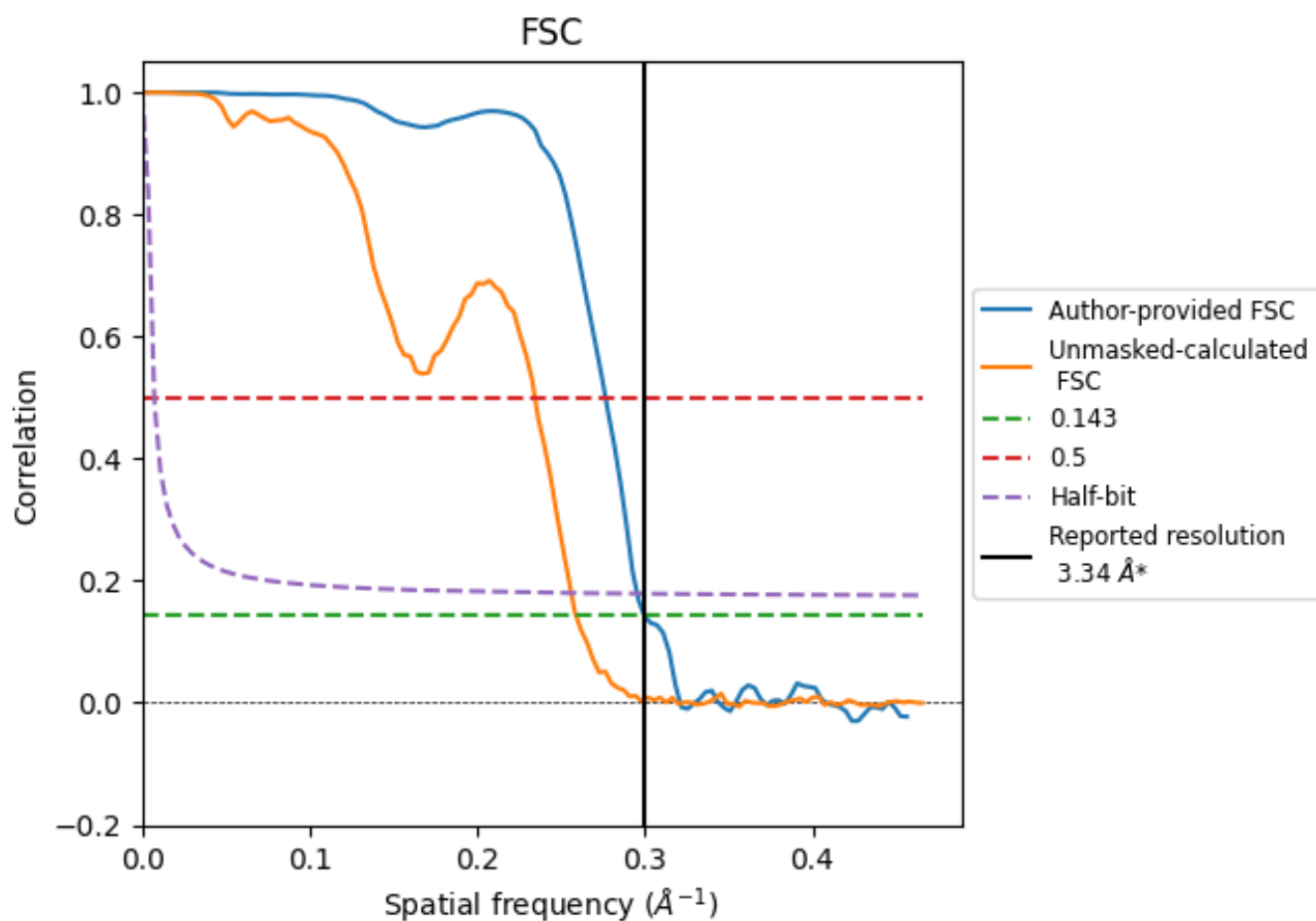


*Reported resolution corresponds to spatial frequency of 0.299 Å⁻¹

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 0.299 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

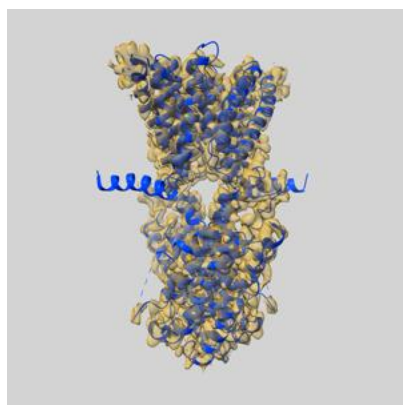
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.34	-	-
Author-provided FSC curve	3.34	3.62	3.39
Unmasked-calculated*	3.86	4.27	3.90

*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 3.86 differs from the reported value 3.34 by more than 10 %

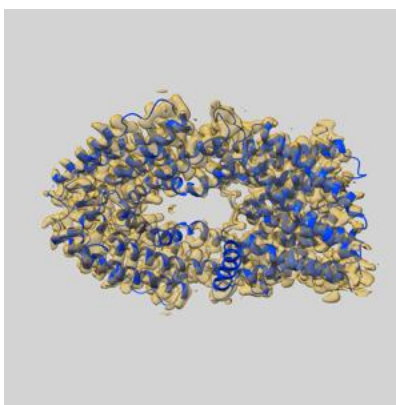
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-34828 and PDB model 8HIW. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

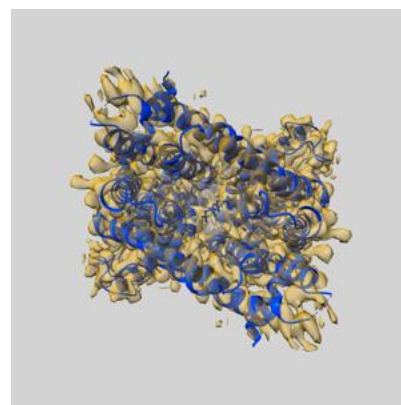
9.1 Map-model overlay [i](#)



X



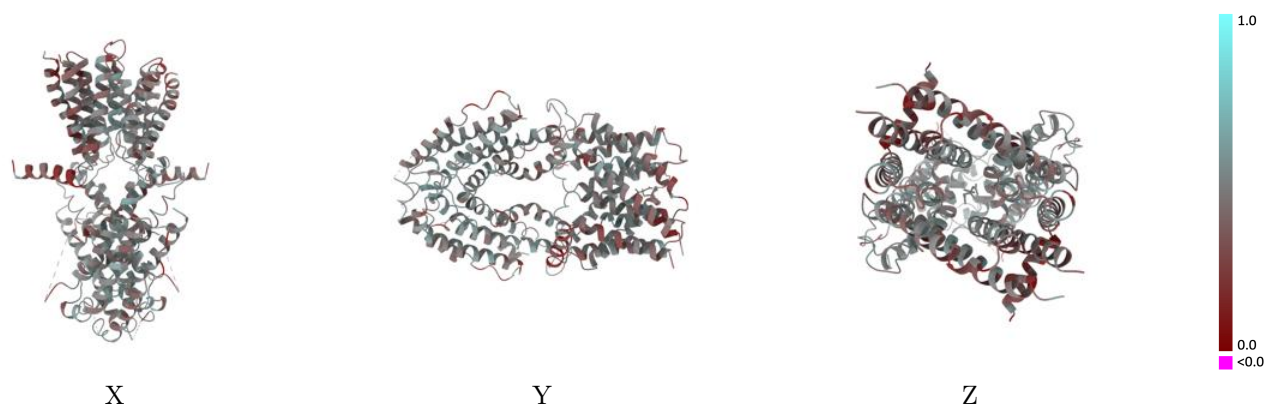
Y



Z

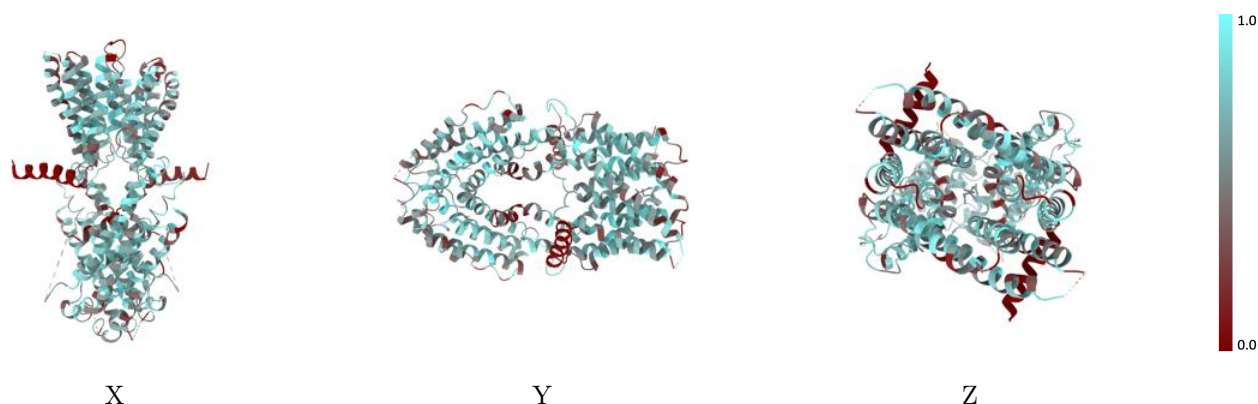
The images above show the 3D surface view of the map at the recommended contour level 0.82 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



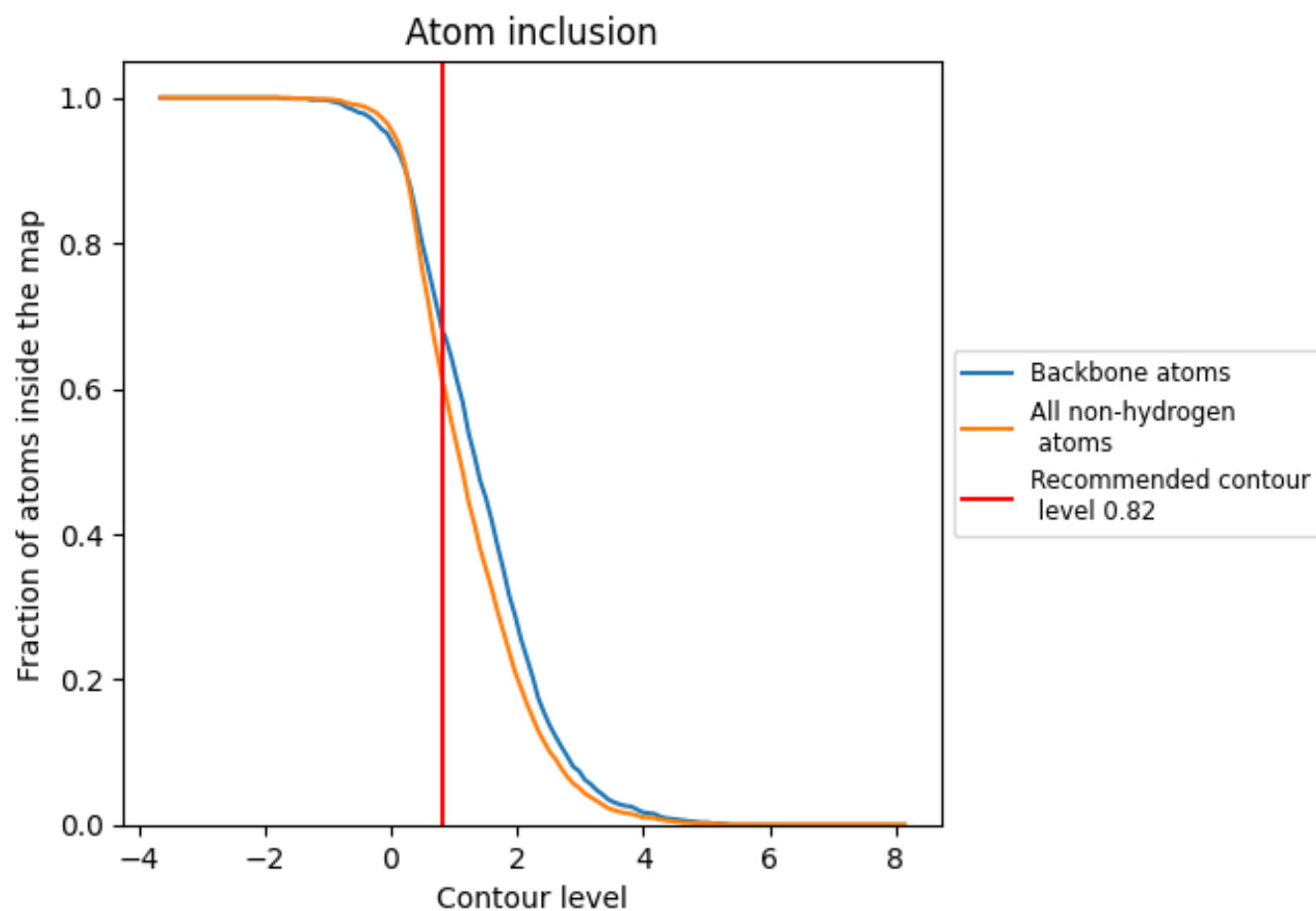
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.82).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 61% 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 (0.82) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6100	0.4530
A	0.6100	0.4530
B	0.6090	0.4530

