



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 12:57 AM UTC

PDB ID : 7TDD / pdb_00007tdd
EMDB ID : EMD-25825
Title : AtTPC1 D454N-EDTA state II
Authors : Dickinson, M.S.; Stroud, R.M.
Deposited on : 2021-12-30
Resolution : 3.50 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

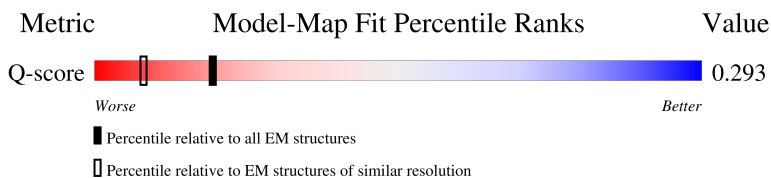
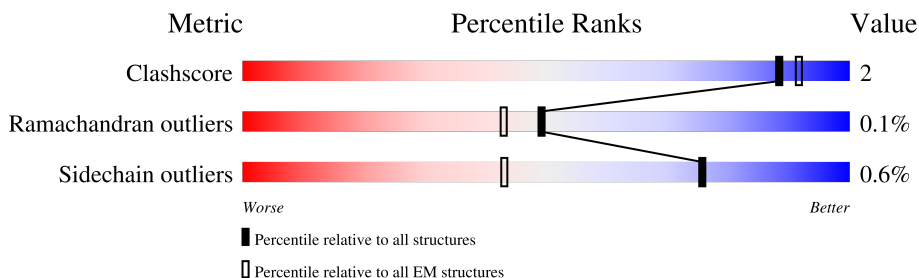
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	13950 (3.00 - 4.00)

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	675	18% 72% 17% • 10%
1	B	675	16% 72% 17% • 10%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 20031 atoms, of which 10025 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 Two pore calcium channel protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	605	Total	C	H	N	O	S	0	0
			10006	3342	5007	774	860	23		
1	B	606	Total	C	H	N	O	S	0	0
			10025	3348	5018	775	861	23		

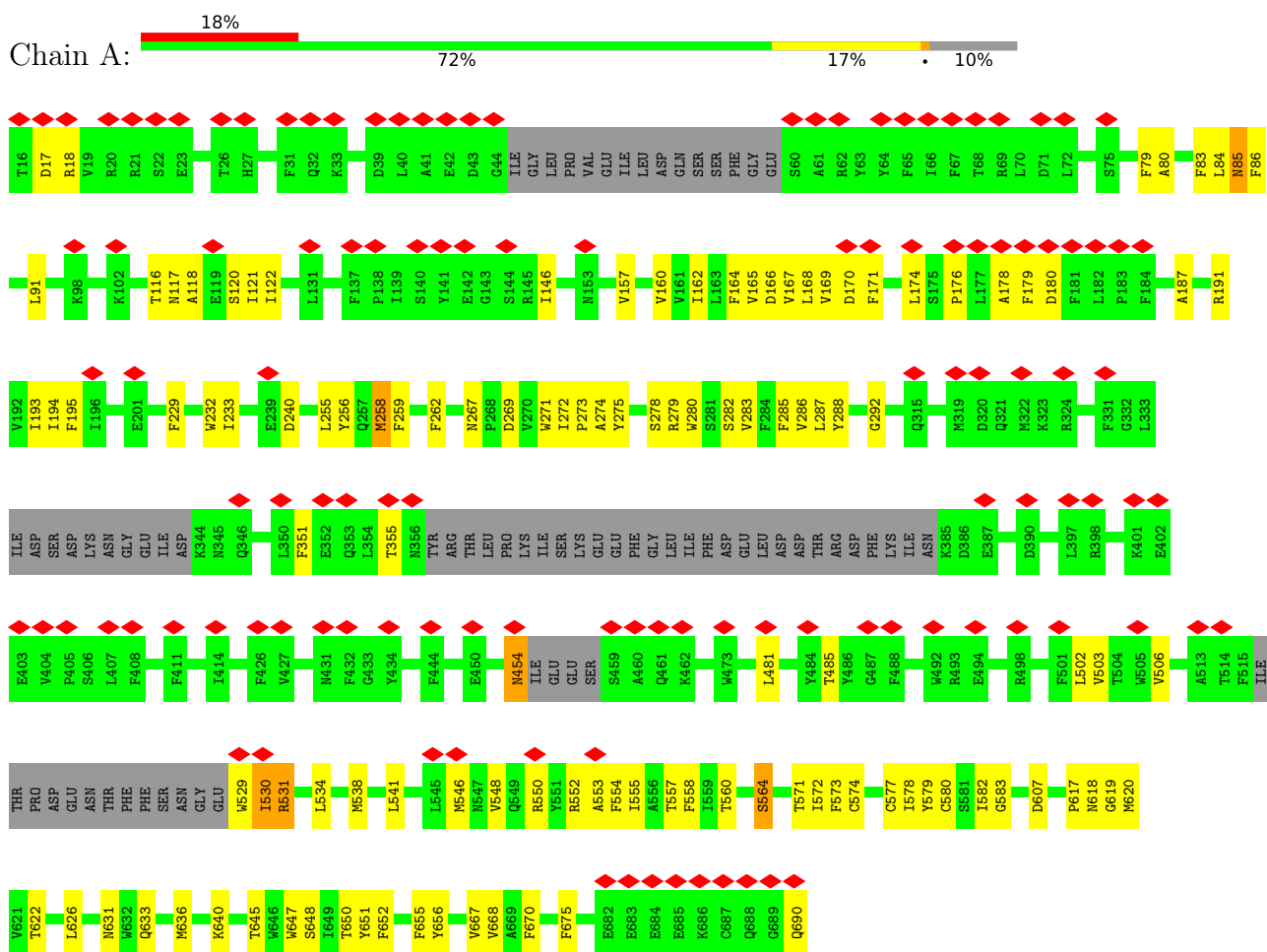
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	454	ASN	ASP	engineered mutation	UNP Q94KI8
B	454	ASN	ASP	engineered mutation	UNP Q94KI8

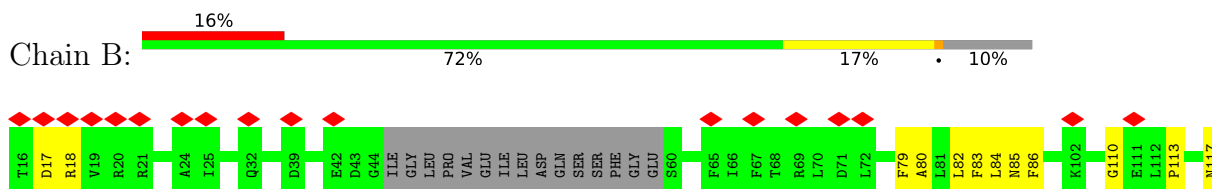
3 Residue-property plots

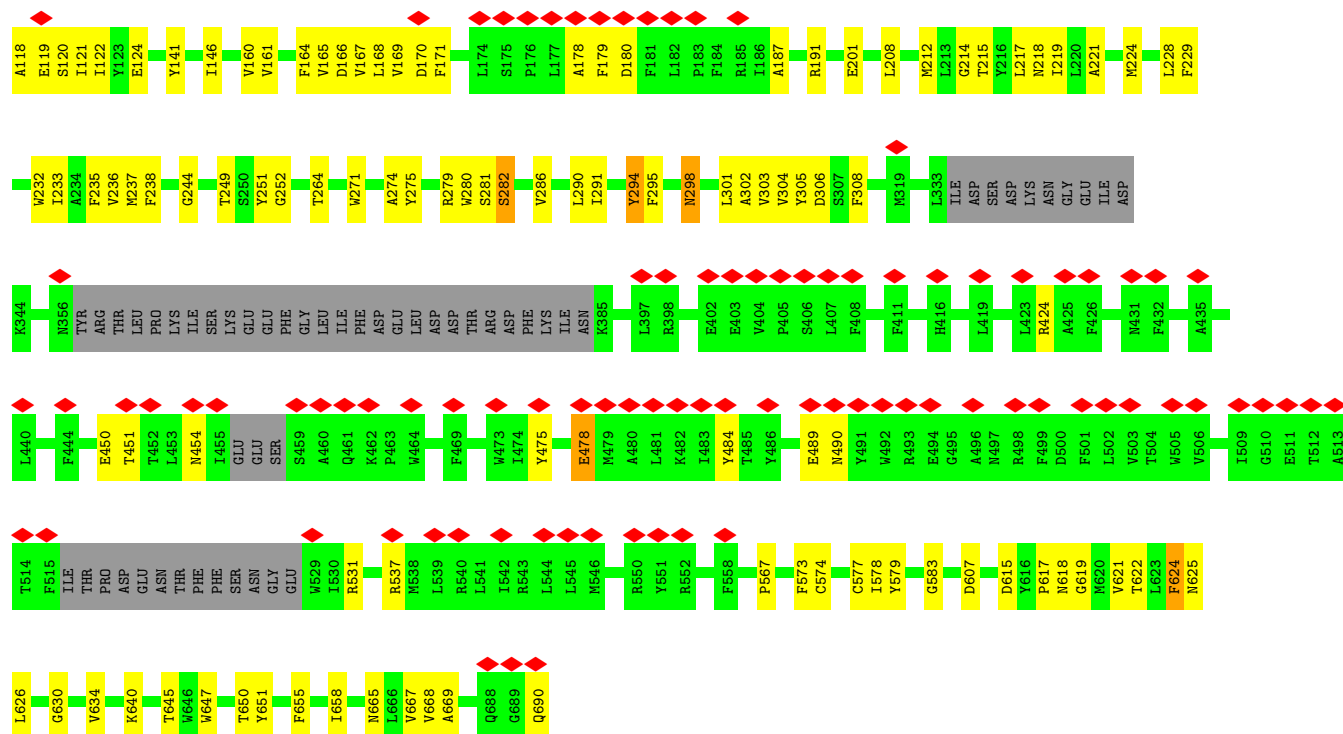
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Two pore calcium channel protein 1



- Molecule 1: Two pore calcium channel protein 1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	68456	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	66	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.175	Depositor
Minimum map value	-0.068	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.104	Depositor
Map size (Å)	360.72, 360.72, 360.72	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.835, 0.835, 0.835	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	1.38	18/5136 (0.4%)	1.52	167/6984 (2.4%)
1	B	1.45	23/5144 (0.4%)	1.58	167/6995 (2.4%)
All	All	1.42	41/10280 (0.4%)	1.55	334/13979 (2.4%)

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	264	THR	CB-OG1	-10.23	1.27	1.43
1	A	187	ALA	CA-CB	-9.11	1.43	1.53
1	B	187	ALA	CA-CB	-9.10	1.43	1.53
1	B	191	ARG	CZ-NH2	-7.89	1.23	1.33
1	A	191	ARG	CZ-NH2	-7.88	1.23	1.33
1	A	279	ARG	CZ-NH2	-7.79	1.23	1.33
1	B	279	ARG	CZ-NH2	-7.75	1.23	1.33
1	A	531	ARG	CZ-NH2	-7.31	1.24	1.33
1	B	191	ARG	CZ-NH1	-7.23	1.22	1.32
1	A	191	ARG	CZ-NH1	-7.20	1.22	1.32
1	B	279	ARG	CZ-NH1	-7.20	1.22	1.32
1	A	279	ARG	CZ-NH1	-7.11	1.22	1.32
1	A	118	ALA	CA-CB	-6.98	1.42	1.53
1	A	272	ILE	CA-CB	-6.94	1.50	1.54
1	A	80	ALA	CA-CB	-6.84	1.42	1.53
1	B	118	ALA	CA-CB	-6.82	1.42	1.53
1	A	531	ARG	CZ-NH1	-6.77	1.23	1.32
1	A	178	ALA	CA-CB	-6.75	1.42	1.53
1	B	302	ALA	CA-CB	-6.62	1.43	1.53
1	B	80	ALA	CA-CB	-6.61	1.43	1.53
1	B	669	ALA	CA-CB	-6.57	1.43	1.53
1	B	178	ALA	CA-CB	-6.56	1.42	1.53
1	B	221	ALA	CA-CB	-6.46	1.43	1.53
1	A	274	ALA	CA-CB	-6.42	1.43	1.53
1	A	619	GLY	N-CA	-6.30	1.37	1.45
1	B	244	GLY	N-CA	-6.28	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	619	GLY	N-CA	-6.22	1.37	1.45
1	A	583	GLY	N-CA	-6.17	1.38	1.45
1	B	583	GLY	N-CA	-5.96	1.38	1.45
1	B	252	GLY	N-CA	-5.70	1.38	1.45
1	B	110	GLY	N-CA	-5.66	1.37	1.44
1	B	279	ARG	CD-NE	-5.58	1.38	1.46
1	A	279	ARG	CD-NE	-5.57	1.38	1.46
1	B	191	ARG	CD-NE	-5.49	1.38	1.46
1	A	191	ARG	CD-NE	-5.37	1.38	1.46
1	B	618	ASN	CG-ND2	-5.20	1.22	1.33
1	B	113	PRO	CA-CB	-5.20	1.46	1.53
1	B	630	GLY	N-CA	-5.17	1.37	1.45
1	A	618	ASN	CG-ND2	-5.15	1.22	1.33
1	A	531	ARG	CD-NE	-5.10	1.39	1.46
1	B	625	ASN	CG-ND2	-5.07	1.22	1.33

All (334) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	272	ILE	N-CA-CB	7.87	115.79	110.52
1	A	86	PHE	CA-CB-CG	7.82	121.62	113.80
1	B	618	ASN	CA-CB-CG	7.54	120.14	112.60
1	A	85	ASN	CA-CB-CG	7.53	120.13	112.60
1	B	166	ASP	CA-CB-CG	7.42	120.02	112.60
1	A	271	TRP	CA-C-N	7.31	127.44	120.43
1	A	271	TRP	C-N-CA	7.31	127.44	120.43
1	A	618	ASN	CA-CB-CG	7.28	119.88	112.60
1	A	558	PHE	CA-CB-CG	7.18	120.98	113.80
1	B	86	PHE	CA-CB-CG	7.13	120.93	113.80
1	B	625	ASN	CA-CB-CG	7.11	119.71	112.60
1	B	85	ASN	CA-CB-CG	6.98	119.58	112.60
1	A	560	THR	CA-C-N	6.97	129.51	120.44
1	A	560	THR	C-N-CA	6.97	129.51	120.44
1	A	607	ASP	CA-CB-CG	6.96	119.56	112.60
1	A	166	ASP	CA-CB-CG	6.95	119.55	112.60
1	B	607	ASP	CA-CB-CG	6.92	119.52	112.60
1	B	170	ASP	CA-CB-CG	6.88	119.48	112.60
1	A	267	ASN	CA-CB-CG	6.87	119.47	112.60
1	B	229	PHE	CA-CB-CG	6.87	120.67	113.80
1	A	170	ASP	CA-CB-CG	6.87	119.47	112.60
1	B	665	ASN	CA-CB-CG	6.85	119.45	112.60
1	A	195	PHE	CA-CB-CG	6.80	120.60	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	117	ASN	CA-CB-CG	6.80	119.40	112.60
1	A	554	PHE	CA-CB-CG	6.77	120.57	113.80
1	A	117	ASN	CA-CB-CG	6.73	119.33	112.60
1	B	218	ASN	CA-CB-CG	6.67	119.27	112.60
1	A	255	LEU	CA-C-N	6.62	129.05	120.44
1	A	255	LEU	C-N-CA	6.62	129.05	120.44
1	B	180	ASP	CA-CB-CG	6.55	119.15	112.60
1	A	262	PHE	CA-CB-CG	6.50	120.30	113.80
1	A	180	ASP	CA-CB-CG	6.50	119.10	112.60
1	A	655	PHE	CA-CB-CG	6.43	120.23	113.80
1	A	83	PHE	CA-CB-CG	6.41	120.21	113.80
1	B	655	PHE	CA-CB-CG	6.41	120.21	113.80
1	B	298	ASN	CA-CB-CG	6.39	118.99	112.60
1	A	171	PHE	CA-CB-CG	6.38	120.18	113.80
1	B	79	PHE	CA-CB-CG	6.38	120.18	113.80
1	B	626	LEU	CA-C-N	6.34	128.78	120.28
1	B	626	LEU	C-N-CA	6.34	128.78	120.28
1	A	626	LEU	CA-C-N	6.33	129.05	120.44
1	A	626	LEU	C-N-CA	6.33	129.05	120.44
1	A	79	PHE	CA-CB-CG	6.31	120.11	113.80
1	B	573	PHE	CA-CB-CG	6.31	120.11	113.80
1	B	83	PHE	CA-CB-CG	6.30	120.10	113.80
1	A	557	THR	CA-C-N	6.27	129.01	120.54
1	A	557	THR	C-N-CA	6.27	129.01	120.54
1	A	84	LEU	CA-C-N	6.26	129.83	120.31
1	A	84	LEU	C-N-CA	6.26	129.83	120.31
1	A	573	PHE	CA-CB-CG	6.25	120.05	113.80
1	B	295	PHE	CA-CB-CG	6.23	120.03	113.80
1	A	164	PHE	CA-C-N	6.20	128.60	120.60
1	A	164	PHE	C-N-CA	6.20	128.60	120.60
1	B	179	PHE	CA-CB-CG	6.20	120.00	113.80
1	B	274	ALA	CA-C-N	6.19	128.58	120.28
1	B	274	ALA	C-N-CA	6.19	128.58	120.28
1	B	168	LEU	CA-C-N	6.16	128.32	120.56
1	B	168	LEU	C-N-CA	6.16	128.32	120.56
1	B	80	ALA	CA-C-N	6.16	128.53	120.28
1	B	80	ALA	C-N-CA	6.16	128.53	120.28
1	A	269	ASP	CA-CB-CG	6.16	118.76	112.60
1	A	550	ARG	CA-C-N	6.12	129.32	120.38
1	A	550	ARG	C-N-CA	6.12	129.32	120.38
1	B	279	ARG	CD-NE-CZ	6.11	132.95	124.40
1	A	645	THR	CA-C-N	6.08	129.04	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	645	THR	C-N-CA	6.08	129.04	120.28
1	A	179	PHE	CA-C-N	6.07	128.69	120.44
1	A	179	PHE	C-N-CA	6.07	128.69	120.44
1	A	179	PHE	CA-CB-CG	6.07	119.87	113.80
1	B	171	PHE	CA-CB-CG	6.06	119.86	113.80
1	A	80	ALA	CA-C-N	6.05	128.67	120.38
1	A	80	ALA	C-N-CA	6.05	128.67	120.38
1	A	650	THR	CA-C-N	6.04	128.62	120.65
1	A	650	THR	C-N-CA	6.04	128.62	120.65
1	A	193	ILE	CA-C-N	6.03	128.72	120.46
1	A	193	ILE	C-N-CA	6.03	128.72	120.46
1	A	636	MET	CA-C-N	6.02	128.60	120.65
1	A	636	MET	C-N-CA	6.02	128.60	120.65
1	B	622	THR	CA-C-N	6.01	128.34	120.28
1	B	622	THR	C-N-CA	6.01	128.34	120.28
1	A	564	SER	CA-C-N	6.00	129.44	120.31
1	A	564	SER	C-N-CA	6.00	129.44	120.31
1	B	238	PHE	CA-C-N	5.99	128.62	120.54
1	B	238	PHE	C-N-CA	5.99	128.62	120.54
1	A	274	ALA	CA-C-N	5.97	128.28	120.28
1	A	274	ALA	C-N-CA	5.97	128.28	120.28
1	A	652	PHE	CA-C-N	5.97	128.16	120.70
1	A	652	PHE	C-N-CA	5.97	128.16	120.70
1	B	306	ASP	CA-CB-CG	5.95	118.55	112.60
1	A	85	ASN	CA-C-N	5.95	129.36	120.31
1	A	85	ASN	C-N-CA	5.95	129.36	120.31
1	A	279	ARG	CD-NE-CZ	5.94	132.72	124.40
1	A	651	TYR	CA-C-N	5.94	128.73	120.29
1	A	651	TYR	C-N-CA	5.94	128.73	120.29
1	B	233	ILE	N-CA-CB	5.93	117.09	110.51
1	A	652	PHE	CA-CB-CG	5.90	119.70	113.80
1	B	251	TYR	N-CA-CB	5.86	118.51	110.01
1	A	531	ARG	CD-NE-CZ	5.86	132.60	124.40
1	A	191	ARG	CA-C-N	5.86	127.94	120.56
1	A	191	ARG	C-N-CA	5.86	127.94	120.56
1	A	191	ARG	CD-NE-CZ	5.84	132.57	124.40
1	A	553	ALA	CA-C-N	5.81	128.06	120.28
1	A	553	ALA	C-N-CA	5.81	128.06	120.28
1	B	238	PHE	CA-CB-CG	5.81	119.61	113.80
1	B	236	VAL	CA-C-N	5.80	128.05	120.28
1	B	236	VAL	C-N-CA	5.80	128.05	120.28
1	A	162	ILE	CA-C-N	5.79	127.97	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	ILE	C-N-CA	5.79	127.97	120.44
1	B	85	ASN	CA-C-N	5.79	128.51	120.29
1	B	85	ASN	C-N-CA	5.79	128.51	120.29
1	B	215	THR	CA-C-N	5.79	128.04	120.28
1	B	215	THR	C-N-CA	5.79	128.04	120.28
1	B	235	PHE	CA-CB-CG	5.78	119.58	113.80
1	A	120	SER	CA-C-N	5.78	127.84	120.56
1	A	120	SER	C-N-CA	5.78	127.84	120.56
1	A	168	LEU	CA-C-N	5.76	127.82	120.56
1	A	168	LEU	C-N-CA	5.76	127.82	120.56
1	A	534	LEU	CA-C-N	5.76	127.93	120.44
1	A	534	LEU	C-N-CA	5.76	127.93	120.44
1	A	622	THR	CA-C-N	5.75	127.98	120.28
1	A	622	THR	C-N-CA	5.75	127.98	120.28
1	A	656	TYR	CA-C-N	5.74	128.00	120.60
1	A	656	TYR	C-N-CA	5.74	128.00	120.60
1	B	665	ASN	CA-C-N	5.74	127.90	120.44
1	B	665	ASN	C-N-CA	5.74	127.90	120.44
1	B	191	ARG	CD-NE-CZ	5.73	132.42	124.40
1	A	675	PHE	CA-CB-CG	5.72	119.53	113.80
1	B	219	ILE	CA-C-N	5.71	127.93	120.28
1	B	219	ILE	C-N-CA	5.71	127.93	120.28
1	A	273	PRO	CA-C-N	5.69	128.37	120.63
1	A	273	PRO	C-N-CA	5.69	128.37	120.63
1	A	174	LEU	CA-C-N	5.68	130.70	121.83
1	A	174	LEU	C-N-CA	5.68	130.70	121.83
1	B	191	ARG	CA-C-N	5.65	127.79	120.56
1	B	191	ARG	C-N-CA	5.65	127.79	120.56
1	B	212	MET	CA-C-N	5.62	127.81	120.28
1	B	212	MET	C-N-CA	5.62	127.81	120.28
1	B	161	VAL	CA-C-N	5.61	127.63	120.56
1	B	161	VAL	C-N-CA	5.61	127.63	120.56
1	B	122	ILE	N-CA-CB	5.61	116.74	110.62
1	A	617	PRO	CA-C-N	5.61	127.73	120.44
1	A	617	PRO	C-N-CA	5.61	127.73	120.44
1	B	282	SER	CA-C-N	5.60	128.14	120.46
1	B	282	SER	C-N-CA	5.60	128.14	120.46
1	B	650	THR	CA-C-N	5.60	128.57	120.79
1	B	650	THR	C-N-CA	5.60	128.57	120.79
1	A	675	PHE	N-CA-CB	5.59	118.08	109.91
1	B	305	TYR	CA-CB-CG	5.59	123.97	113.90
1	B	302	ALA	CA-C-N	5.59	127.60	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	302	ALA	C-N-CA	5.59	127.60	120.56
1	B	634	VAL	CA-C-N	5.58	128.02	120.44
1	B	634	VAL	C-N-CA	5.58	128.02	120.44
1	A	176	PRO	CA-C-N	5.57	127.74	120.28
1	A	176	PRO	C-N-CA	5.57	127.74	120.28
1	B	164	PHE	CA-C-N	5.56	127.78	120.60
1	B	164	PHE	C-N-CA	5.56	127.78	120.60
1	A	258	MET	CA-C-N	5.56	127.67	120.44
1	A	258	MET	C-N-CA	5.56	127.67	120.44
1	A	578	ILE	CA-C-N	5.56	127.73	120.28
1	A	578	ILE	C-N-CA	5.56	127.73	120.28
1	B	578	ILE	CA-C-N	5.55	127.72	120.28
1	B	578	ILE	C-N-CA	5.55	127.72	120.28
1	A	531	ARG	N-CA-CB	5.54	118.27	110.12
1	A	122	ILE	N-CA-CB	5.54	116.66	110.62
1	B	84	LEU	CA-C-N	5.54	128.46	120.38
1	B	84	LEU	C-N-CA	5.54	128.46	120.38
1	A	288	TYR	CA-C-N	5.53	127.53	120.56
1	A	288	TYR	C-N-CA	5.53	127.53	120.56
1	A	571	THR	CA-C-N	5.52	127.72	120.60
1	A	571	THR	C-N-CA	5.52	127.72	120.60
1	B	574	CYS	CA-C-N	5.52	127.52	120.56
1	B	574	CYS	C-N-CA	5.52	127.52	120.56
1	B	658	ILE	CA-C-N	5.52	127.95	120.44
1	B	658	ILE	C-N-CA	5.52	127.95	120.44
1	B	244	GLY	CA-C-N	5.51	129.42	120.60
1	B	244	GLY	C-N-CA	5.51	129.42	120.60
1	B	208	LEU	CA-C-N	5.51	128.21	120.28
1	B	208	LEU	C-N-CA	5.51	128.21	120.28
1	A	259	PHE	CA-CB-CG	5.51	119.31	113.80
1	A	280	TRP	CA-C-N	5.49	127.90	120.38
1	A	280	TRP	C-N-CA	5.49	127.90	120.38
1	B	640	LYS	N-CA-CB	5.48	118.11	109.94
1	B	214	GLY	CA-C-N	5.48	127.89	120.44
1	B	214	GLY	C-N-CA	5.48	127.89	120.44
1	A	166	ASP	CA-C-N	5.48	127.47	120.56
1	A	166	ASP	C-N-CA	5.48	127.47	120.56
1	A	619	GLY	CA-C-N	5.45	127.53	120.44
1	A	619	GLY	C-N-CA	5.45	127.53	120.44
1	B	167	VAL	CA-C-N	5.45	127.52	120.44
1	B	167	VAL	C-N-CA	5.45	127.52	120.44
1	B	275	TYR	CA-C-N	5.44	127.58	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	275	TYR	C-N-CA	5.44	127.58	120.28
1	A	648	SER	CA-C-N	5.42	129.51	120.62
1	A	648	SER	C-N-CA	5.42	129.51	120.62
1	B	281	SER	CA-C-N	5.42	127.80	120.38
1	B	281	SER	C-N-CA	5.42	127.80	120.38
1	B	170	ASP	CA-C-N	5.41	127.47	120.44
1	B	170	ASP	C-N-CA	5.41	127.47	120.44
1	A	582	ILE	N-CA-CB	5.41	116.52	110.51
1	A	285	PHE	CA-CB-CG	5.41	119.21	113.80
1	B	271	TRP	CA-C-N	5.40	123.64	120.24
1	B	271	TRP	C-N-CA	5.40	123.64	120.24
1	A	580	CYS	N-CA-CB	5.40	117.84	110.01
1	A	194	ILE	CA-C-N	5.40	127.46	120.44
1	A	194	ILE	C-N-CA	5.40	127.46	120.44
1	A	292	GLY	CA-C-N	5.40	129.19	120.55
1	A	292	GLY	C-N-CA	5.40	129.19	120.55
1	A	633	GLN	CA-C-N	5.40	127.56	120.60
1	A	633	GLN	C-N-CA	5.40	127.56	120.60
1	B	624	PHE	N-CA-CB	5.39	117.98	109.94
1	B	165	VAL	N-CA-CB	5.38	116.48	110.51
1	A	631	ASN	CA-C-N	5.38	127.49	120.28
1	A	631	ASN	C-N-CA	5.38	127.49	120.28
1	A	256	TYR	CA-C-N	5.38	127.48	120.28
1	A	256	TYR	C-N-CA	5.38	127.48	120.28
1	A	116	THR	CA-C-N	5.37	127.79	120.54
1	A	116	THR	C-N-CA	5.37	127.79	120.54
1	B	617	PRO	CA-C-N	5.36	127.77	120.54
1	B	617	PRO	C-N-CA	5.36	127.77	120.54
1	A	278	SER	CA-C-N	5.36	127.72	120.38
1	A	278	SER	C-N-CA	5.36	127.72	120.38
1	A	541	LEU	CA-C-N	5.35	129.40	120.62
1	A	541	LEU	C-N-CA	5.35	129.40	120.62
1	A	121	ILE	CA-C-N	5.35	127.39	120.70
1	A	121	ILE	C-N-CA	5.35	127.39	120.70
1	A	651	TYR	CA-CB-CG	5.35	123.53	113.90
1	B	625	ASN	CA-C-N	5.35	127.45	120.28
1	B	625	ASN	C-N-CA	5.35	127.45	120.28
1	A	275	TYR	CA-CB-CG	5.35	123.53	113.90
1	B	651	TYR	CA-CB-CG	5.35	123.52	113.90
1	A	647	TRP	CA-C-N	5.34	127.69	120.38
1	A	647	TRP	C-N-CA	5.34	127.69	120.38
1	B	191	ARG	CG-CD-NE	5.34	123.74	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	624	PHE	CA-C-N	5.33	127.42	120.28
1	B	624	PHE	C-N-CA	5.33	127.42	120.28
1	B	171	PHE	CA-C-N	5.32	127.67	120.38
1	B	171	PHE	C-N-CA	5.32	127.67	120.38
1	A	167	VAL	CA-C-N	5.31	127.34	120.44
1	A	167	VAL	C-N-CA	5.31	127.34	120.44
1	A	171	PHE	CA-C-N	5.29	127.38	120.28
1	A	171	PHE	C-N-CA	5.29	127.38	120.28
1	B	624	PHE	CA-CB-CG	5.29	119.09	113.80
1	B	119	GLU	CA-C-N	5.29	127.31	120.44
1	B	119	GLU	C-N-CA	5.29	127.31	120.44
1	B	120	SER	CA-C-N	5.29	127.70	120.46
1	B	120	SER	C-N-CA	5.29	127.70	120.46
1	A	572	ILE	N-CA-CB	5.28	116.38	110.51
1	B	645	THR	CA-C-N	5.28	128.09	120.38
1	B	645	THR	C-N-CA	5.28	128.09	120.38
1	B	301	LEU	CA-C-N	5.27	127.30	120.44
1	B	301	LEU	C-N-CA	5.27	127.30	120.44
1	B	291	ILE	N-CA-CB	5.27	116.37	110.62
1	A	579	TYR	CA-C-N	5.27	127.29	120.44
1	A	579	TYR	C-N-CA	5.27	127.29	120.44
1	B	294	TYR	CA-C-N	5.27	127.80	120.63
1	B	294	TYR	C-N-CA	5.27	127.80	120.63
1	B	304	VAL	CA-C-N	5.26	128.11	120.79
1	B	304	VAL	C-N-CA	5.26	128.11	120.79
1	B	290	LEU	CA-C-N	5.25	127.26	120.70
1	B	290	LEU	C-N-CA	5.25	127.26	120.70
1	B	655	PHE	N-CA-CB	5.24	117.74	109.94
1	B	577	CYS	CA-C-N	5.23	127.15	120.56
1	B	577	CYS	C-N-CA	5.23	127.15	120.56
1	A	169	VAL	CA-C-N	5.22	127.28	120.28
1	A	169	VAL	C-N-CA	5.22	127.28	120.28
1	B	191	ARG	CA-CB-CG	5.22	124.54	114.10
1	A	279	ARG	CA-C-N	5.22	127.80	120.28
1	A	279	ARG	C-N-CA	5.22	127.80	120.28
1	B	579	TYR	CA-C-N	5.22	127.27	120.28
1	B	579	TYR	C-N-CA	5.22	127.27	120.28
1	B	280	TRP	CA-C-N	5.21	127.51	120.38
1	B	280	TRP	C-N-CA	5.21	127.51	120.38
1	B	249	THR	CA-C-N	5.20	130.69	121.80
1	B	249	THR	C-N-CA	5.20	130.69	121.80
1	A	655	PHE	N-CA-CB	5.20	117.69	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	640	LYS	N-CA-CB	5.19	117.68	109.94
1	B	82	LEU	CA-C-N	5.19	127.76	120.28
1	B	82	LEU	C-N-CA	5.19	127.76	120.28
1	B	169	VAL	CA-C-N	5.19	127.23	120.28
1	B	169	VAL	C-N-CA	5.19	127.23	120.28
1	B	647	TRP	CA-C-N	5.19	127.95	120.38
1	B	647	TRP	C-N-CA	5.19	127.95	120.38
1	A	656	TYR	N-CA-CB	5.18	117.67	109.94
1	B	303	VAL	CA-C-N	5.18	127.09	120.56
1	B	303	VAL	C-N-CA	5.18	127.09	120.56
1	B	110	GLY	CA-C-N	5.18	130.50	122.26
1	B	110	GLY	C-N-CA	5.18	130.50	122.26
1	B	619	GLY	CA-C-N	5.18	127.22	120.28
1	B	619	GLY	C-N-CA	5.18	127.22	120.28
1	A	174	LEU	N-CA-CB	5.17	117.72	110.12
1	A	578	ILE	N-CA-CB	5.17	116.26	110.62
1	B	615	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	667	VAL	CA-C-N	5.16	127.15	120.70
1	A	667	VAL	C-N-CA	5.16	127.15	120.70
1	A	538	MET	CA-C-N	5.16	127.44	120.38
1	A	538	MET	C-N-CA	5.16	127.44	120.38
1	A	577	CYS	CA-C-N	5.14	127.13	120.70
1	A	577	CYS	C-N-CA	5.14	127.13	120.70
1	B	308	PHE	N-CA-CB	5.14	117.64	109.82
1	B	232	TRP	N-CA-CB	5.14	117.52	110.07
1	B	621	VAL	CA-C-N	5.13	127.11	120.44
1	B	621	VAL	C-N-CA	5.13	127.11	120.44
1	A	572	ILE	CA-C-N	5.13	127.57	120.29
1	A	572	ILE	C-N-CA	5.13	127.57	120.29
1	A	117	ASN	CA-C-N	5.13	127.46	120.54
1	A	117	ASN	C-N-CA	5.13	127.46	120.54
1	B	121	ILE	CA-C-N	5.12	127.10	120.70
1	B	121	ILE	C-N-CA	5.12	127.10	120.70
1	A	191	ARG	CG-CD-NE	5.12	123.25	112.00
1	B	165	VAL	CA-C-N	5.12	127.14	120.28
1	B	165	VAL	C-N-CA	5.12	127.14	120.28
1	A	165	VAL	N-CA-CB	5.11	116.19	110.51
1	B	275	TYR	CA-CB-CG	5.11	123.11	113.90
1	B	308	PHE	CA-CB-CG	5.11	118.91	113.80
1	B	82	LEU	N-CA-CB	5.10	117.47	110.07
1	A	574	CYS	CA-C-N	5.09	126.98	120.56
1	A	574	CYS	C-N-CA	5.09	126.98	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	668	VAL	N-CA-CB	5.09	116.17	110.62
1	B	224	MET	CA-C-N	5.06	127.07	120.28
1	B	224	MET	C-N-CA	5.06	127.07	120.28
1	B	573	PHE	CA-C-N	5.06	127.06	120.28
1	B	573	PHE	C-N-CA	5.06	127.06	120.28
1	A	668	VAL	N-CA-CB	5.06	116.13	110.62
1	A	267	ASN	N-CA-CB	5.04	117.25	110.14
1	B	124	GLU	CA-CB-CG	5.04	124.18	114.10
1	B	237	MET	CA-CB-CG	5.03	124.17	114.10
1	B	217	LEU	CA-C-N	5.03	127.29	120.65
1	B	217	LEU	C-N-CA	5.03	127.29	120.65
1	B	118	ALA	CA-C-N	5.01	126.99	120.28
1	B	118	ALA	C-N-CA	5.01	126.99	120.28
1	A	620	MET	CA-C-N	5.01	126.87	120.56
1	A	620	MET	C-N-CA	5.01	126.87	120.56
1	B	667	VAL	CA-C-N	5.00	126.95	120.70
1	B	667	VAL	C-N-CA	5.00	126.95	120.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4999	5007	5011	24	0
1	B	5007	5018	5022	16	0
All	All	10006	10025	10033	37	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (37) 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:454:ASN:O	1:A:454:ASN:ND2	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:ASN:C	1:A:454:ASN:HD22	1.96	0.73
1:B:424:ARG:NE	1:B:484:TYR:O	2.24	0.69
1:A:454:ASN:ND2	1:A:454:ASN:C	2.58	0.60
1:A:91:LEU:HD12	1:A:91:LEU:H	1.67	0.57
1:B:17:ASP:OD1	1:B:18:ARG:N	2.34	0.57
1:A:240:ASP:OD2	1:B:531:ARG:NH2	2.39	0.55
1:B:450:GLU:OE1	1:B:537:ARG:NH1	2.40	0.54
1:B:450:GLU:O	1:B:454:ASN:ND2	2.41	0.54
1:A:17:ASP:OD1	1:A:18:ARG:N	2.40	0.53
1:B:450:GLU:HG2	1:B:454:ASN:ND2	2.27	0.50
1:A:530:ILE:HG23	1:A:531:ARG:H	1.76	0.50
1:A:503:VAL:HA	1:A:506:VAL:HG12	1.95	0.48
1:A:481:LEU:O	1:A:485:THR:HG23	2.15	0.47
1:A:564:SER:HG	1:A:670:PHE:HZ	1.62	0.46
1:A:146:ILE:HD12	1:A:146:ILE:N	2.31	0.46
1:A:282:SER:O	1:A:286:VAL:HG12	2.15	0.45
1:B:690:GLN:O	1:B:690:GLN:NE2	2.50	0.45
1:B:201:GLU:HG2	1:B:567:PRO:HB3	1.98	0.45
1:B:282:SER:O	1:B:286:VAL:HG12	2.16	0.44
1:A:351:PHE:O	1:A:355:THR:HG23	2.17	0.44
1:B:294:TYR:O	1:B:298:ASN:ND2	2.51	0.43
1:A:286:VAL:HG23	1:B:624:PHE:CE1	2.54	0.43
1:A:548:VAL:O	1:A:552:ARG:HB2	2.19	0.43
1:B:146:ILE:HD12	1:B:146:ILE:H	1.85	0.42
1:A:529:TRP:O	1:A:531:ARG:N	2.53	0.42
1:B:489:GLU:HG2	1:B:490:ASN:N	2.35	0.42
1:A:232:TRP:HZ2	1:B:451:THR:HG21	1.85	0.41
1:A:258:MET:HA	1:A:258:MET:HE2	2.02	0.41
1:A:283:VAL:HA	1:A:286:VAL:HG12	2.02	0.41
1:A:286:VAL:HG13	1:A:287:LEU:N	2.35	0.41
1:B:475:TYR:O	1:B:478:GLU:HG3	2.21	0.41
1:A:546:MET:HA	1:A:555:ILE:HD13	2.01	0.41
1:B:141:TYR:CD1	1:B:141:TYR:C	2.98	0.41
1:A:229:PHE:CE2	1:A:233:ILE:HD11	2.56	0.40
1:A:157:VAL:HA	1:A:160:VAL:HG12	2.02	0.40
1:A:502:LEU:C	1:A:502:LEU:HD23	2.46	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	593/675 (88%)	583 (98%)	9 (2%)	1 (0%)	43	74
1	B	594/675 (88%)	585 (98%)	9 (2%)	0	100	100
All	All	1187/1350 (88%)	1168 (98%)	18 (2%)	1 (0%)	49	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	530	ILE

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	541/606 (89%)	538 (99%)	3 (1%)	78	79
1	B	542/606 (89%)	539 (99%)	3 (1%)	78	79
All	All	1083/1212 (89%)	1077 (99%)	6 (1%)	76	79

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	454	ASN
1	A	690	GLN
1	B	160	VAL
1	B	228	LEU

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Mol	Chain	Res	Type
1	B	478	GLU

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	134	HIS
1	A	218	ASN
1	A	321	GLN
1	A	454	ASN
1	B	134	HIS
1	B	321	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.

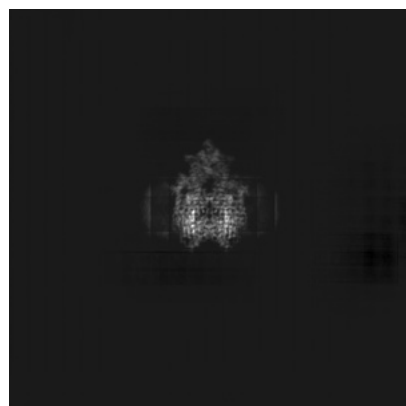
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25825. These allow visual inspection of the internal detail of the map and identification of artifacts.

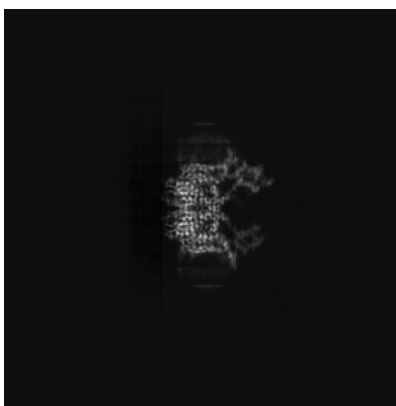
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

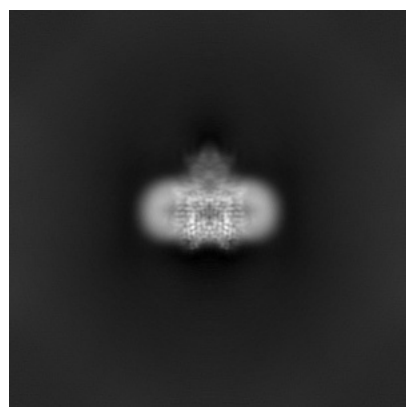


Y

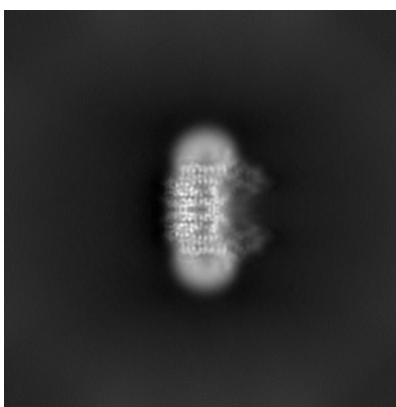


Z

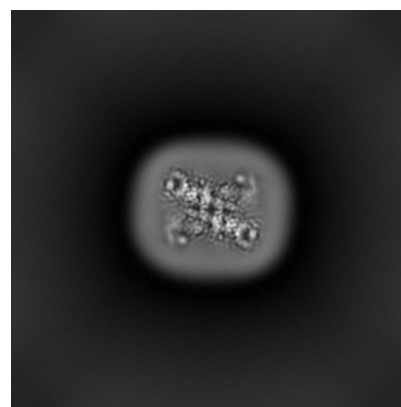
6.1.2 Raw map



X



Y



Z

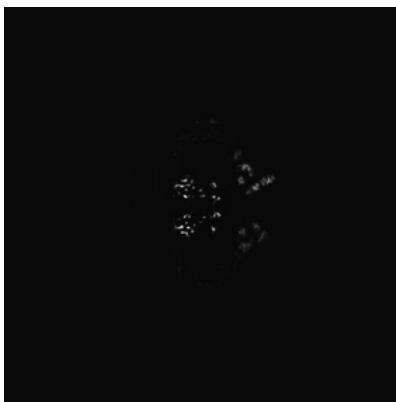
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 216

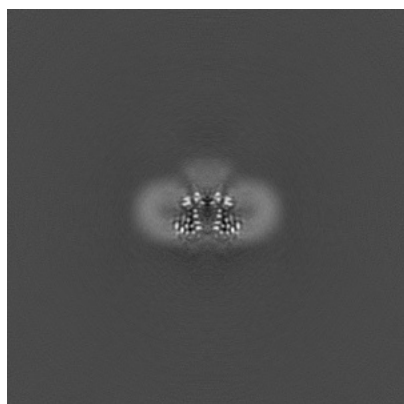


Y Index: 216

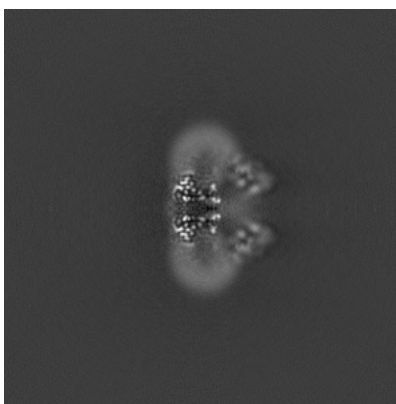


Z Index: 216

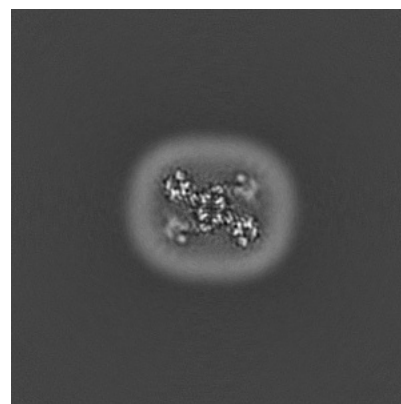
6.2.2 Raw map



X Index: 216



Y Index: 216



Z Index: 216

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: 206

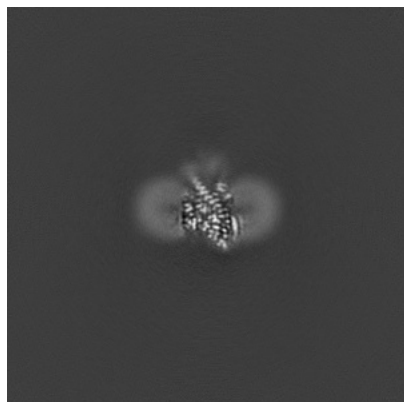


Y Index: 199

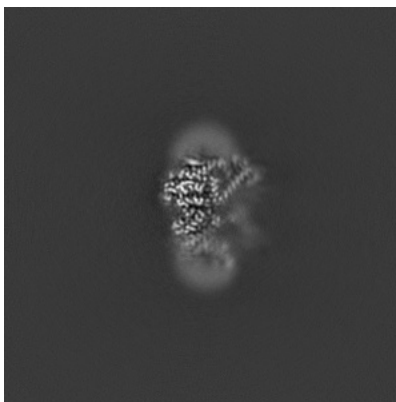


Z Index: 197

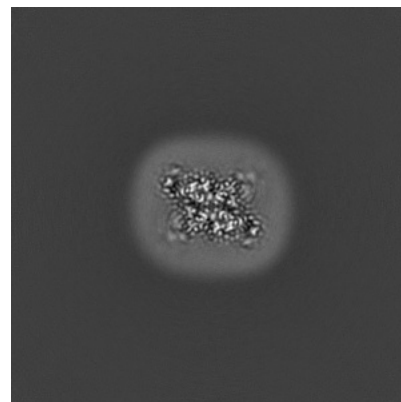
6.3.2 Raw map



X Index: 206



Y Index: 199

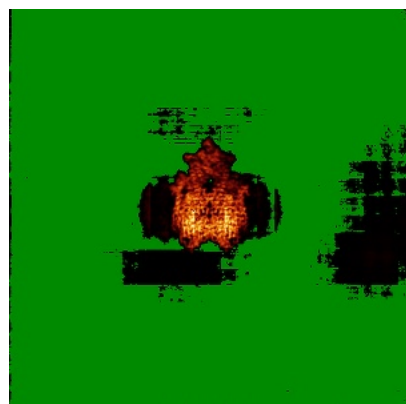


Z Index: 201

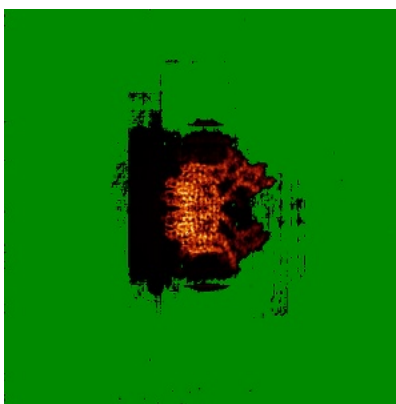
The images above show the largest variance slices of the map in three orthogonal directions.

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

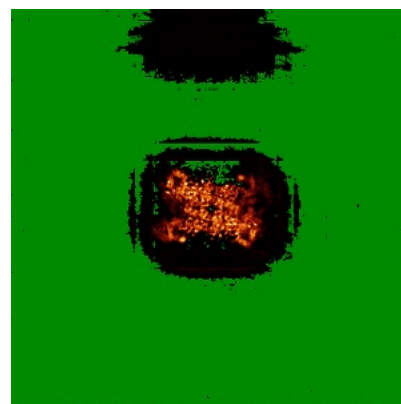
6.4.1 Primary map



X

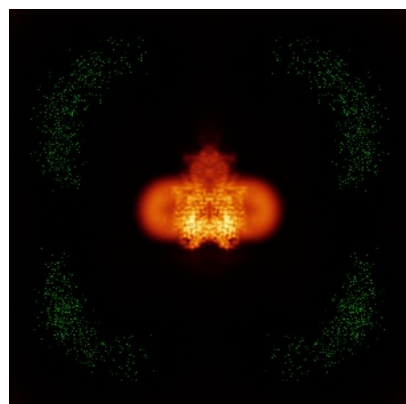


Y

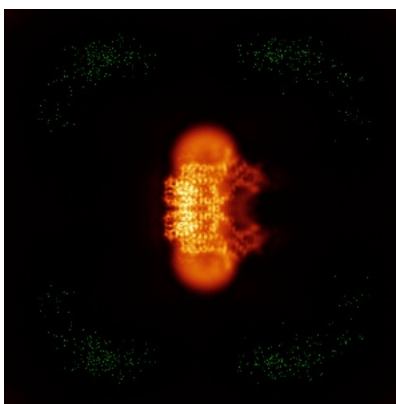


Z

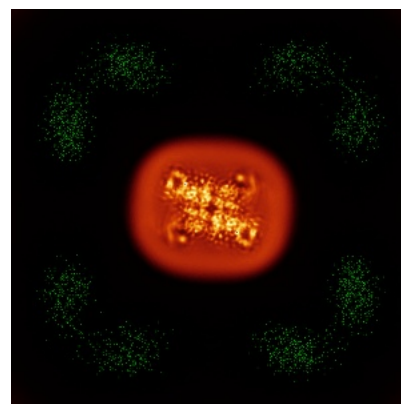
6.4.2 Raw map



X



Y

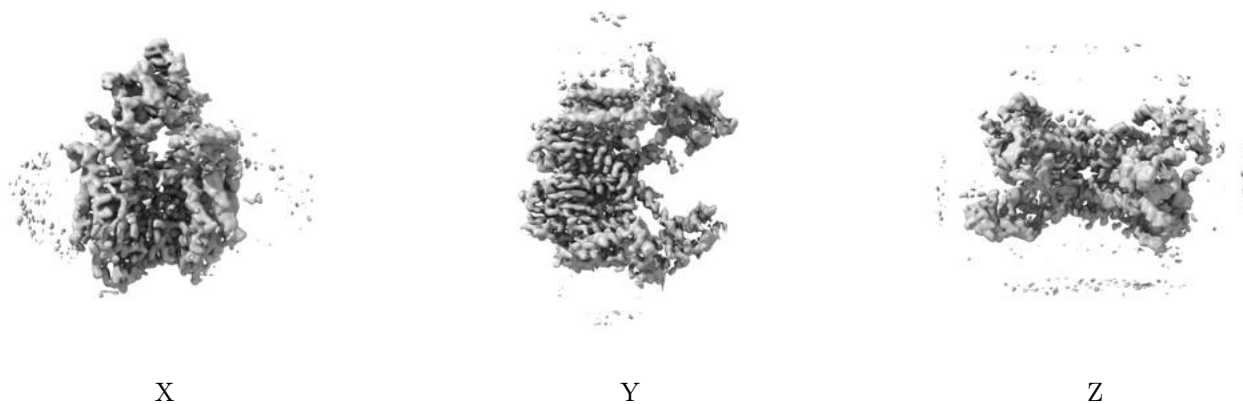


Z

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.

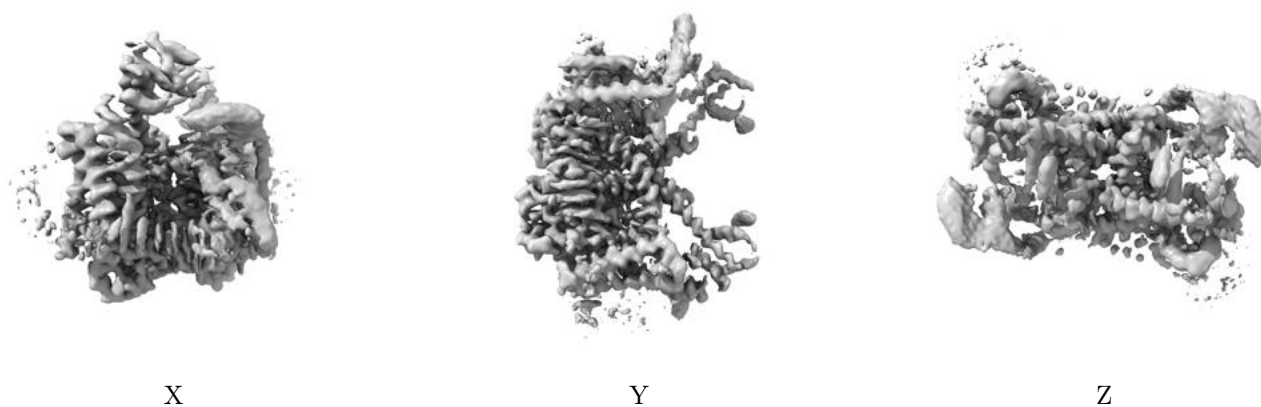
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.104. 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.

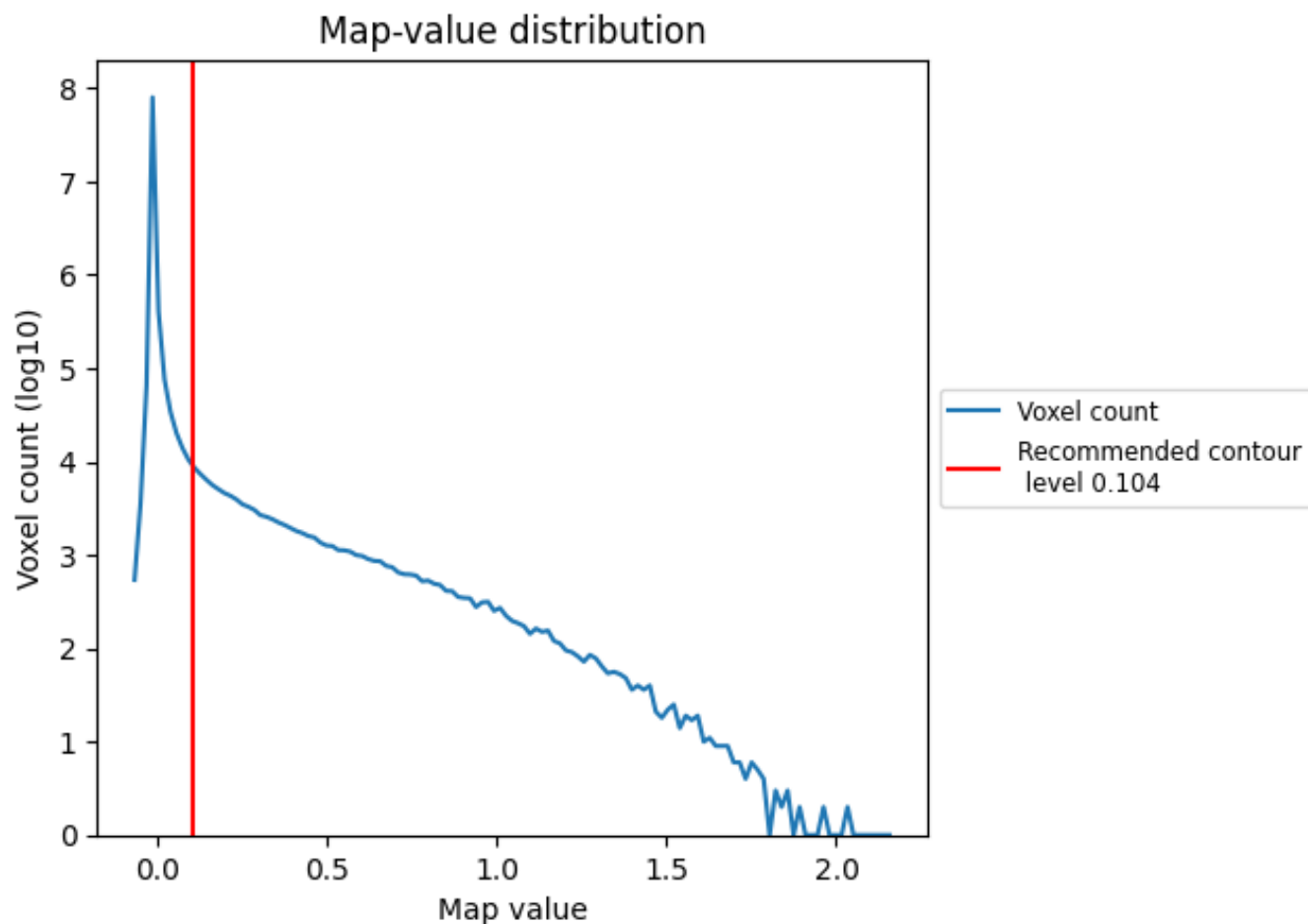
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

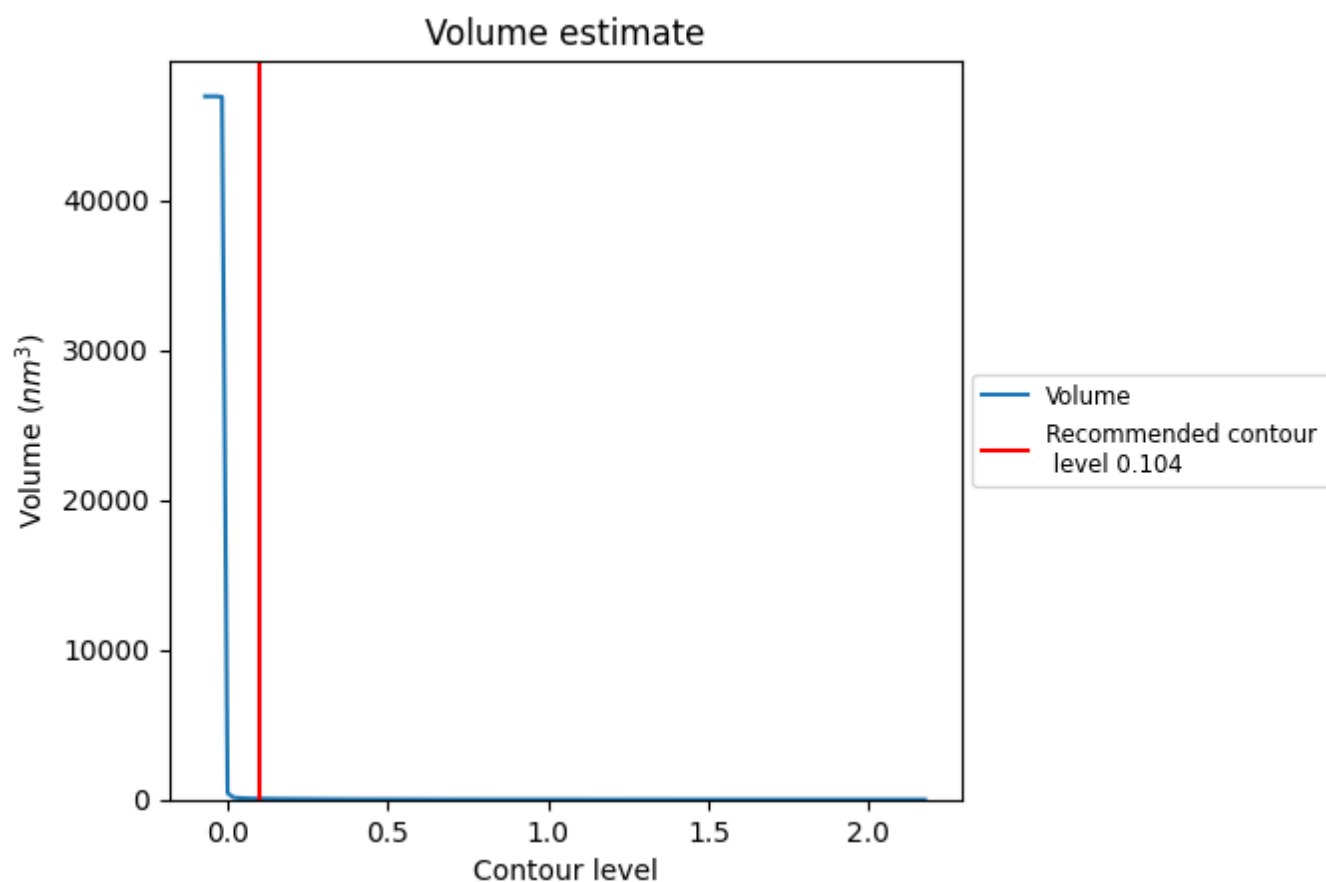
This section contains the results of statistical analysis of the map.

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.

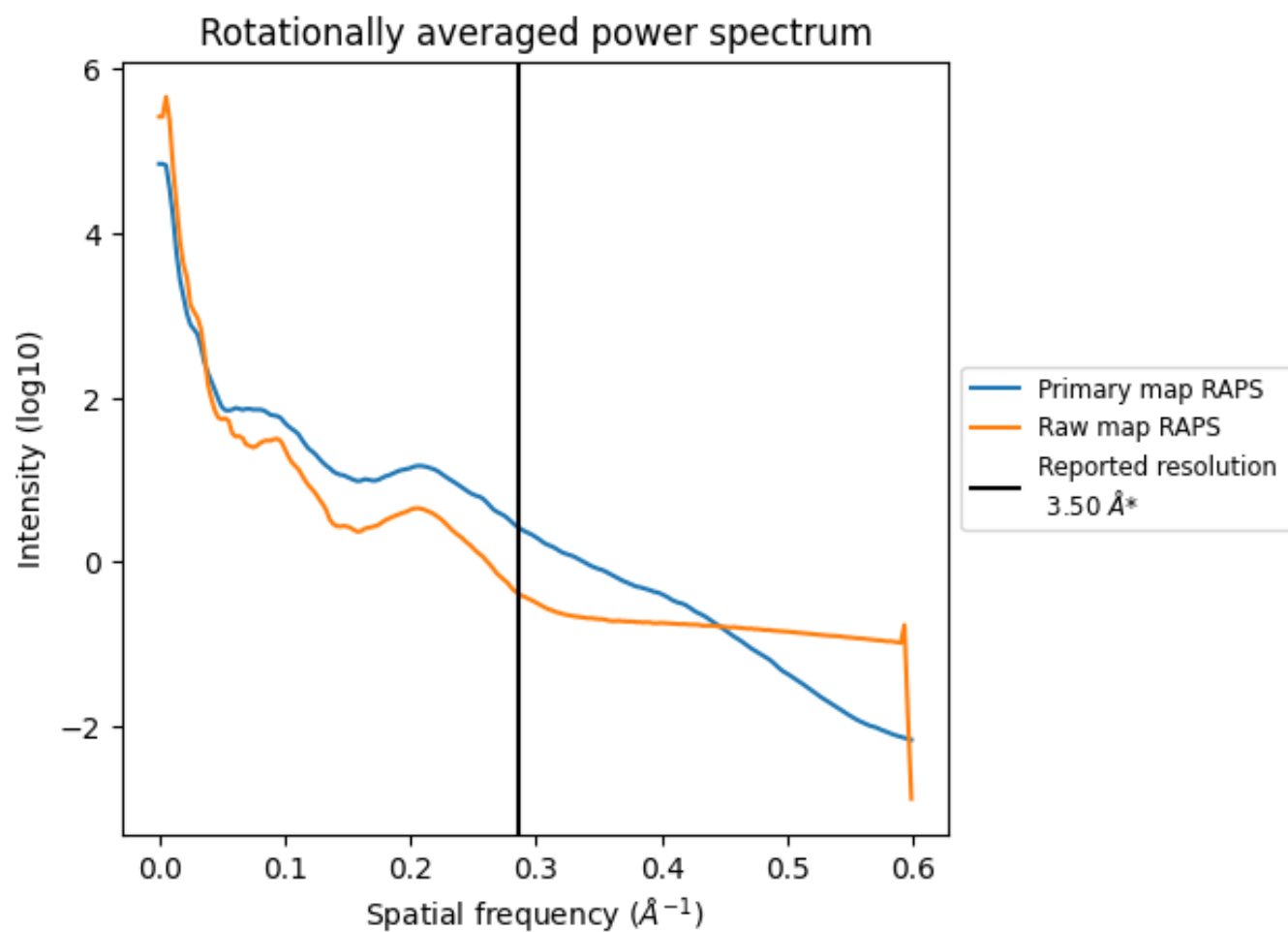
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 60 nm^3 ; this corresponds to an approximate mass of 54 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 ⓘ

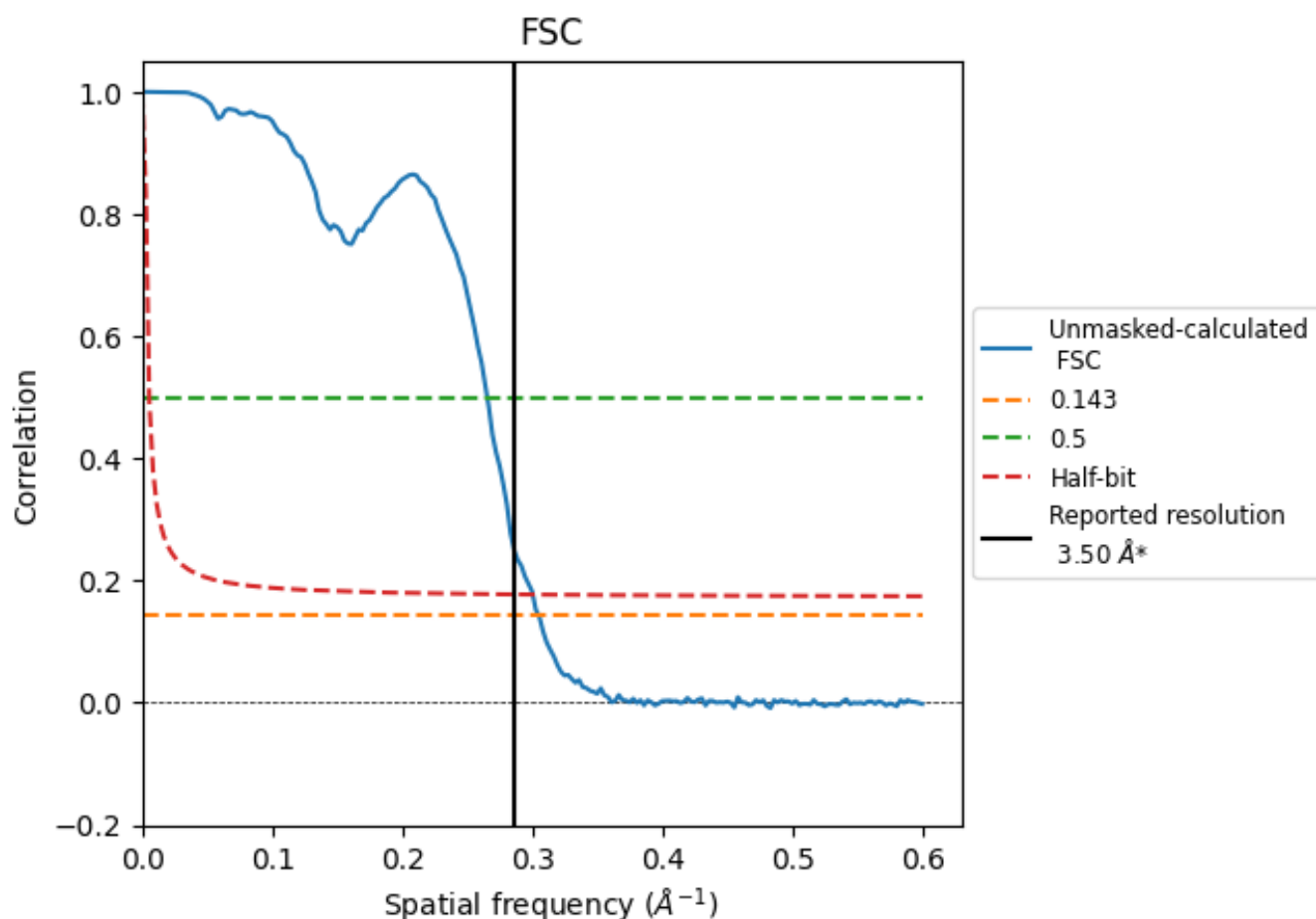


*Reported resolution corresponds to spatial frequency of $0.286 \text{ \AA}^{-1}$

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 0.286 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

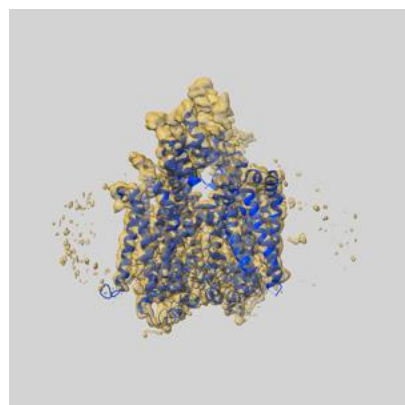
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.29	3.78	3.33

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

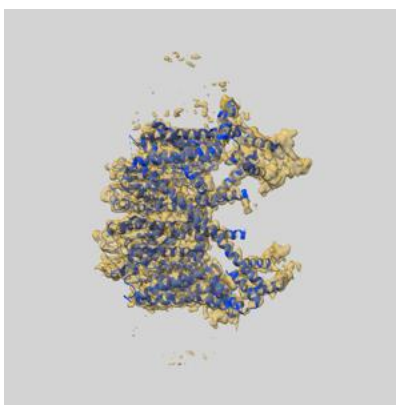
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25825 and PDB model 7TDD. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

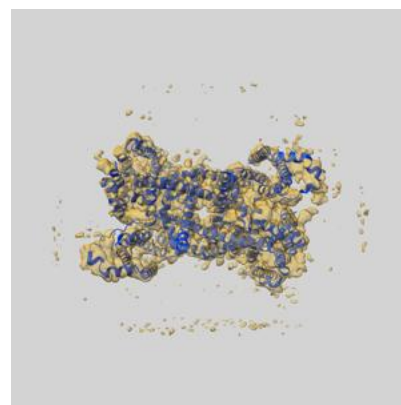
9.1 Map-model overlay [i](#)



X



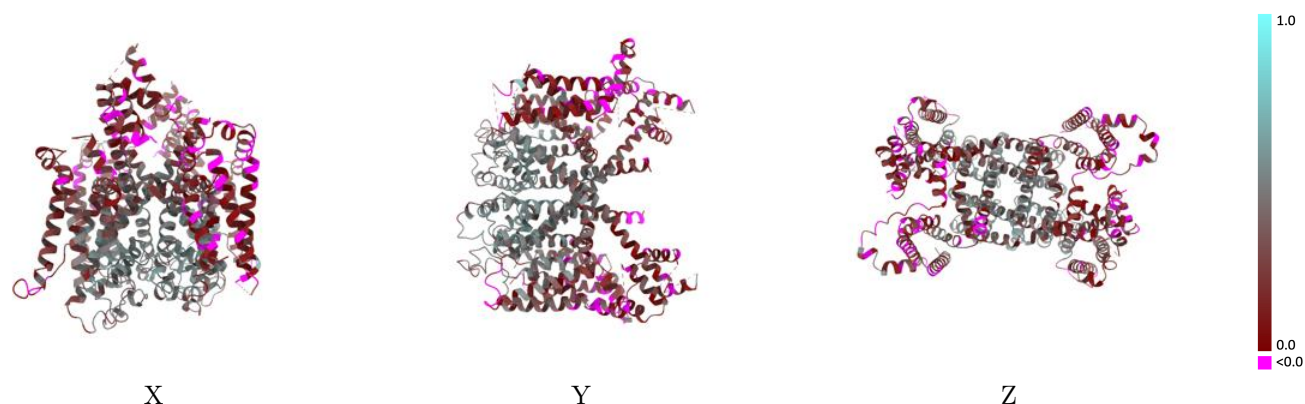
Y



Z

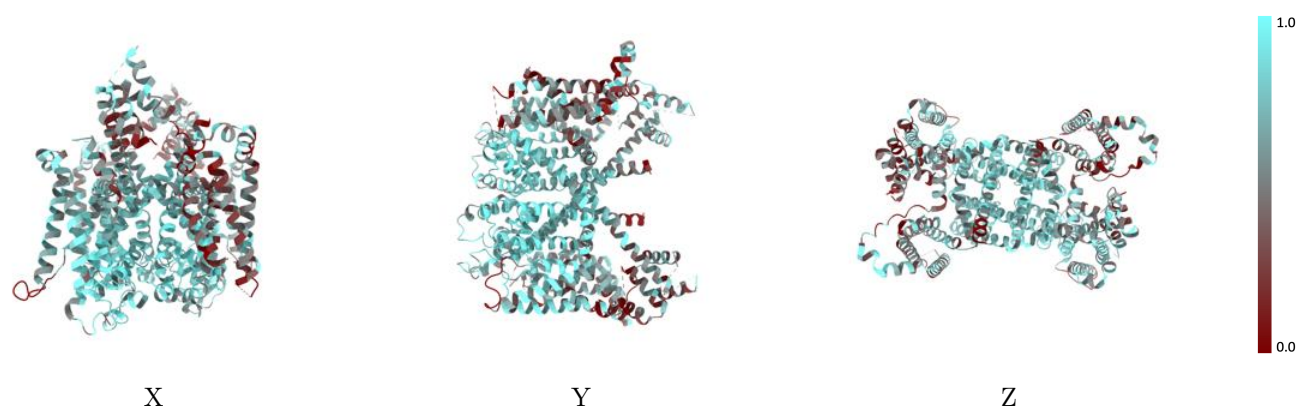
The images above show the 3D surface view of the map at the recommended contour level 0.104 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



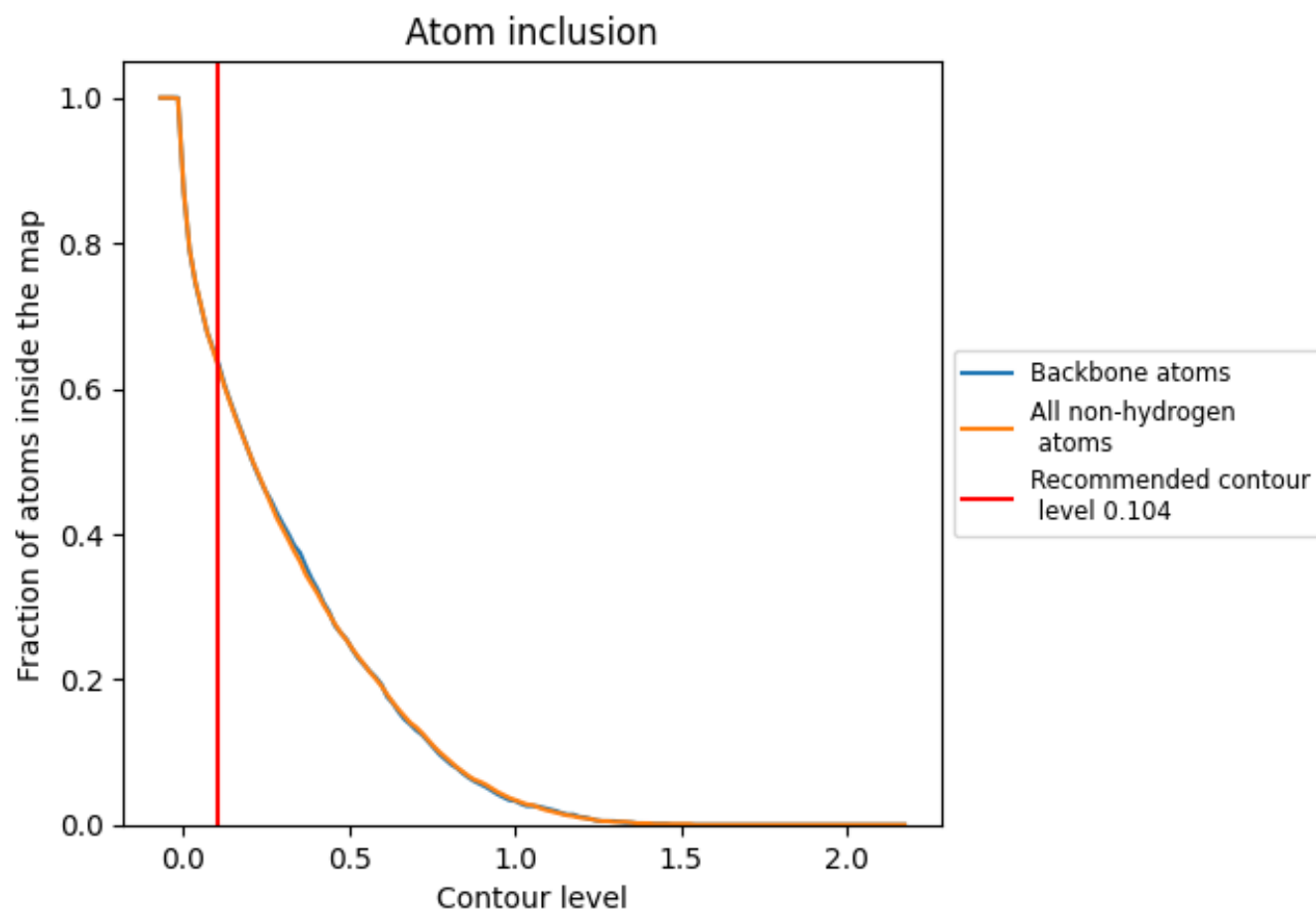
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.104).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 63% 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 (0.104) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6340	0.2930
A	0.6430	0.2910
B	0.6520	0.2940

