



Full wwPDB EM Validation Report ⓘ

May 18, 2026 – 01:17 pm BST

PDB ID : 9HLX / pdb_00009hlx
EMDB ID : EMD-52275
Title : Structure of Ba1Cas12a3 binary complex
Authors : Yuan, B.; Heinz, D.W.
Deposited on : 2024-12-05
Resolution : 3.80 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:

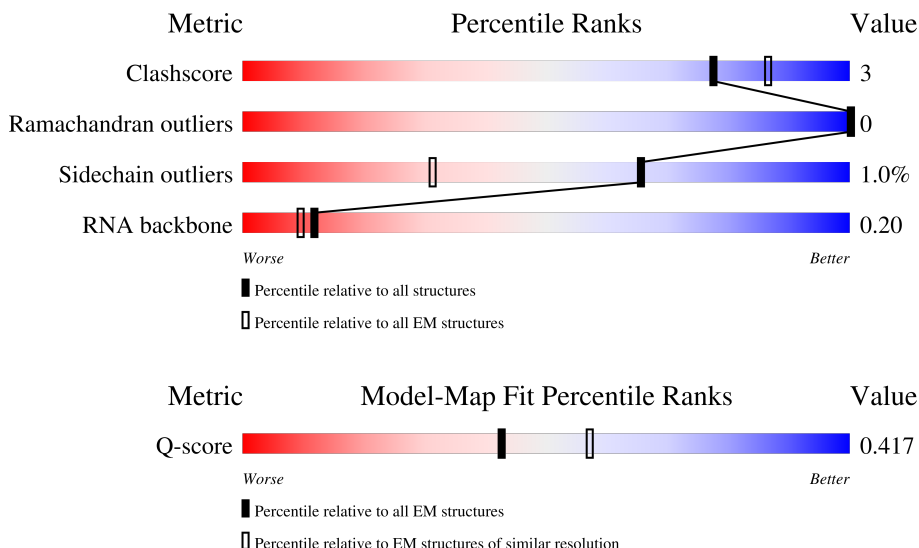
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.80 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	1168	 67% 30% ..
2	B	65	 17% 28% 12% 6% 37%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20252 atoms, of which 9966 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 Ba1Cas12a3.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1156	Total	C	H	N	O	S	0	0
			18950	5985	9528	1634	1781	22		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1161	LEU	-	expression tag	UNP A0A2N2ZXC5
A	1162	GLU	-	expression tag	UNP A0A2N2ZXC5
A	1163	HIS	-	expression tag	UNP A0A2N2ZXC5
A	1164	HIS	-	expression tag	UNP A0A2N2ZXC5
A	1165	HIS	-	expression tag	UNP A0A2N2ZXC5
A	1166	HIS	-	expression tag	UNP A0A2N2ZXC5
A	1167	HIS	-	expression tag	UNP A0A2N2ZXC5
A	1168	HIS	-	expression tag	UNP A0A2N2ZXC5

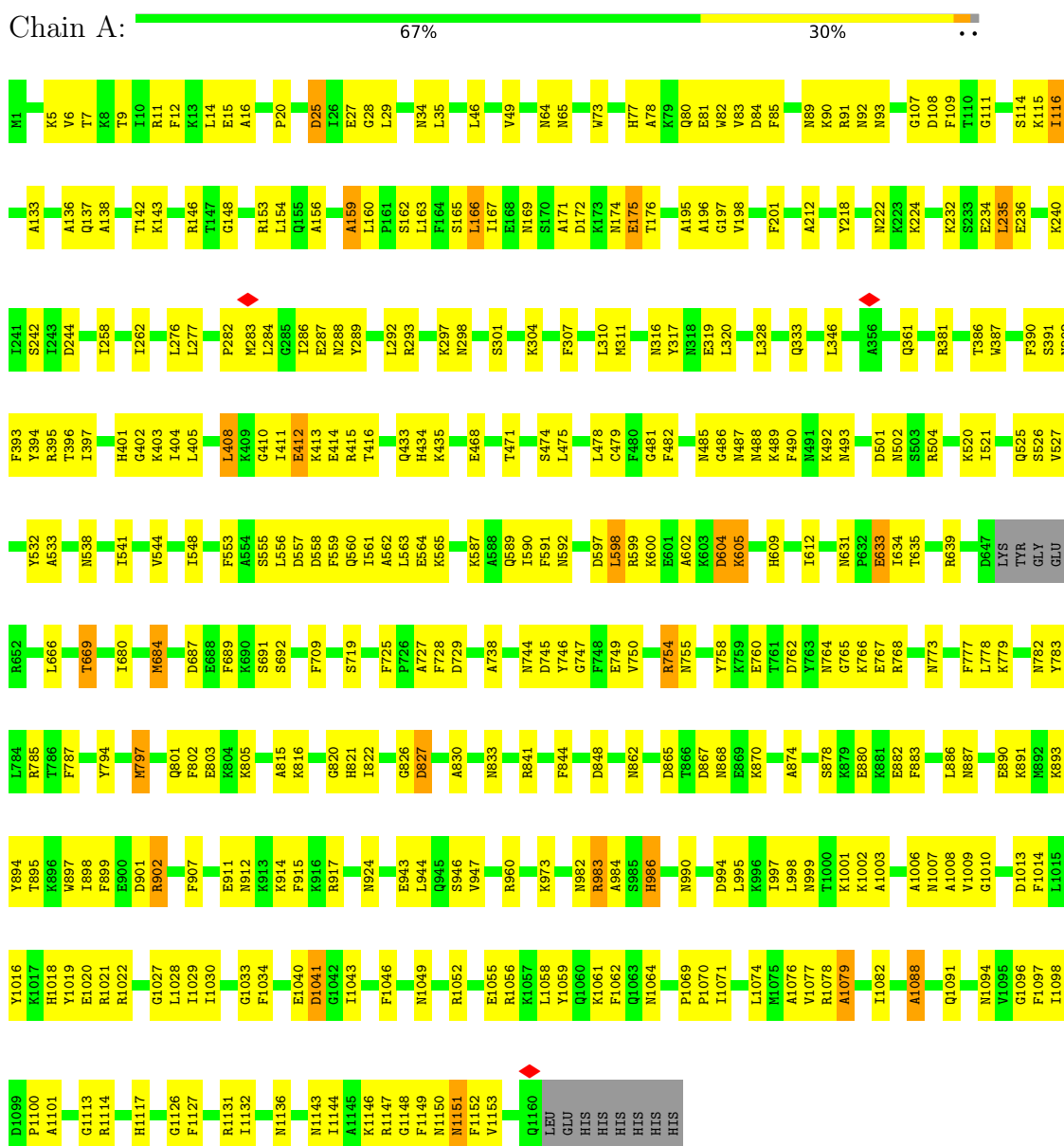
- Molecule 2 is a RNA chain called crRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	41	Total	C	H	N	O	P	0	0
			1302	387	438	146	290	41		

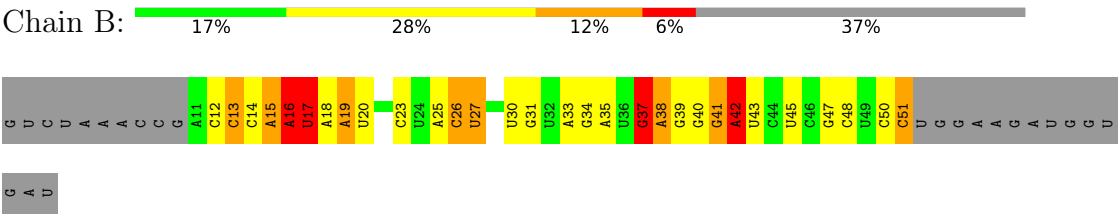
3 Residue-property plots

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: Ba1Cas12a3



• Molecule 2: crRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	99354	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.286	Depositor
Minimum map value	-0.211	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.009	Depositor
Map size ($\text{\AA}$)	232.96, 232.96, 232.96	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.91, 0.91, 0.91	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	1.99	132/9582 (1.4%)	1.99	434/12868 (3.4%)
2	B	1.25	4/963 (0.4%)	1.33	8/1496 (0.5%)
All	All	1.94	136/10545 (1.3%)	1.93	442/14364 (3.1%)

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	1
2	B	0	12
All	All	0	13

All (136) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	434	HIS	CE1-NE2	-8.94	1.23	1.32
1	A	401	HIS	CE1-NE2	-8.91	1.23	1.32
1	A	986	HIS	CE1-NE2	-8.88	1.23	1.32
1	A	77	HIS	CE1-NE2	-8.84	1.23	1.32
1	A	609	HIS	CE1-NE2	-8.81	1.23	1.32
1	A	159	ALA	CA-CB	-8.77	1.42	1.54
1	A	1018	HIS	ND1-CE1	-8.73	1.23	1.32
1	A	821	HIS	CE1-NE2	-8.71	1.23	1.32
1	A	1117	HIS	ND1-CE1	-8.70	1.23	1.32
1	A	983	ARG	CZ-NH2	-8.41	1.22	1.33
1	A	768	ARG	CZ-NH2	-8.38	1.22	1.33
1	A	504	ARG	CZ-NH2	-8.33	1.22	1.33
1	A	599	ARG	CZ-NH2	-8.29	1.22	1.33
1	A	754	ARG	CZ-NH2	-8.29	1.22	1.33
1	A	841	ARG	CZ-NH2	-8.29	1.22	1.33
1	A	415	ARG	CZ-NH2	-8.28	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	11	ARG	CZ-NH2	-8.27	1.22	1.33
1	A	146	ARG	CZ-NH2	-8.25	1.22	1.33
1	A	1078	ARG	CZ-NH2	-8.23	1.22	1.33
1	A	153	ARG	CZ-NH2	-8.21	1.22	1.33
1	A	293	ARG	CZ-NH2	-8.21	1.22	1.33
1	A	785	ARG	CZ-NH2	-8.19	1.22	1.33
1	A	1056	ARG	CZ-NH2	-8.18	1.22	1.33
1	A	1052	ARG	CZ-NH2	-8.15	1.22	1.33
1	A	434	HIS	CD2-NE2	-8.12	1.28	1.37
1	A	917	ARG	CZ-NH2	-8.10	1.23	1.33
1	A	609	HIS	CD2-NE2	-8.10	1.28	1.37
1	A	395	ARG	CZ-NH2	-8.09	1.23	1.33
1	A	77	HIS	CD2-NE2	-8.07	1.28	1.37
1	A	401	HIS	CD2-NE2	-8.04	1.29	1.37
1	A	986	HIS	CD2-NE2	-8.03	1.29	1.37
1	A	91	ARG	CZ-NH2	-8.02	1.23	1.33
1	A	381	ARG	CZ-NH2	-8.00	1.23	1.33
1	A	821	HIS	CD2-NE2	-8.00	1.29	1.37
1	A	1147	ARG	CZ-NH2	-7.94	1.23	1.33
1	A	902	ARG	CZ-NH2	-7.92	1.23	1.33
1	A	16	ALA	CA-CB	-7.90	1.42	1.53
1	A	1114	ARG	CZ-NH2	-7.89	1.23	1.33
1	A	1022	ARG	CZ-NH2	-7.88	1.23	1.33
1	A	1021	ARG	CZ-NH2	-7.83	1.23	1.33
1	A	1131	ARG	CZ-NH2	-7.83	1.23	1.33
1	A	78	ALA	CA-CB	-7.72	1.42	1.53
1	A	1069	PRO	CA-CB	-7.68	1.46	1.53
1	A	1096	GLY	N-CA	-7.24	1.38	1.45
1	A	830	ALA	CA-CB	-7.18	1.42	1.53
1	A	195	ALA	CA-CB	-7.10	1.42	1.53
1	A	533	ALA	CA-CB	-7.09	1.42	1.53
1	A	562	ALA	CA-CB	-7.08	1.42	1.53
1	A	1006	ALA	CA-CB	-7.08	1.42	1.53
1	A	984	ALA	CA-CB	-7.05	1.42	1.53
1	A	196	ALA	CA-CB	-7.04	1.42	1.53
1	A	133	ALA	CA-CB	-7.04	1.42	1.53
1	A	156	ALA	CA-CB	-7.04	1.42	1.53
1	A	138	ALA	CA-CB	-7.03	1.42	1.53
1	A	1003	ALA	CA-CB	-7.00	1.42	1.53
1	A	136	ALA	CA-CB	-6.96	1.42	1.53
1	A	602	ALA	CA-CB	-6.95	1.41	1.53
1	A	1100	PRO	CA-CB	-6.90	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	874	ALA	CA-CB	-6.82	1.42	1.53
1	A	1079	ALA	CA-CB	-6.81	1.42	1.53
1	A	212	ALA	CA-CB	-6.79	1.42	1.53
1	A	415	ARG	CZ-NH1	-6.78	1.23	1.32
1	A	504	ARG	CZ-NH1	-6.75	1.23	1.32
1	A	1078	ARG	CZ-NH1	-6.74	1.23	1.32
1	A	785	ARG	CZ-NH1	-6.74	1.23	1.32
1	A	768	ARG	CZ-NH1	-6.70	1.23	1.32
1	A	599	ARG	CZ-NH1	-6.69	1.23	1.32
1	A	754	ARG	CZ-NH1	-6.69	1.23	1.32
1	A	815	ALA	CA-CB	-6.69	1.42	1.53
1	A	1008	ALA	CA-CB	-6.69	1.43	1.53
1	A	1056	ARG	CZ-NH1	-6.69	1.23	1.32
1	A	11	ARG	CZ-NH1	-6.68	1.23	1.32
1	A	153	ARG	CZ-NH1	-6.67	1.23	1.32
1	A	146	ARG	CZ-NH1	-6.66	1.23	1.32
1	A	1052	ARG	CZ-NH1	-6.66	1.23	1.32
1	A	983	ARG	CZ-NH1	-6.65	1.23	1.32
1	A	293	ARG	CZ-NH1	-6.63	1.23	1.32
1	A	841	ARG	CZ-NH1	-6.61	1.23	1.32
1	A	917	ARG	CZ-NH1	-6.53	1.23	1.32
1	A	826	GLY	N-CA	-6.48	1.37	1.45
1	A	395	ARG	CZ-NH1	-6.45	1.23	1.32
1	A	91	ARG	CZ-NH1	-6.43	1.23	1.32
1	A	148	GLY	N-CA	-6.43	1.37	1.45
1	A	381	ARG	CZ-NH1	-6.42	1.23	1.32
1	A	1147	ARG	CZ-NH1	-6.41	1.23	1.32
1	A	1022	ARG	CZ-NH1	-6.38	1.23	1.32
1	A	1114	ARG	CZ-NH1	-6.37	1.23	1.32
1	A	1021	ARG	CZ-NH1	-6.37	1.23	1.32
1	A	1131	ARG	CZ-NH1	-6.36	1.23	1.32
1	A	902	ARG	CZ-NH1	-6.36	1.23	1.32
1	A	1076	ALA	CA-CB	-6.32	1.42	1.53
1	A	1148	GLY	N-CA	-6.30	1.38	1.45
1	A	1010	GLY	N-CA	-6.27	1.38	1.45
1	A	727	ALA	CA-CB	-6.19	1.43	1.53
1	A	410	GLY	N-CA	-6.16	1.37	1.45
1	A	402	GLY	N-CA	-6.04	1.38	1.45
1	A	1101	ALA	CA-CB	-5.97	1.43	1.53
1	A	197	GLY	N-CA	-5.97	1.38	1.45
1	A	171	ALA	CA-CB	-5.95	1.43	1.53
1	A	754	ARG	CD-NE	-5.64	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	11	ARG	CD-NE	-5.56	1.38	1.46
1	A	1078	ARG	CD-NE	-5.53	1.38	1.46
1	A	917	ARG	CD-NE	-5.51	1.38	1.46
1	A	504	ARG	CD-NE	-5.49	1.38	1.46
1	A	381	ARG	CD-NE	-5.43	1.38	1.46
1	A	1114	ARG	CD-NE	-5.40	1.38	1.46
1	A	983	ARG	CD-NE	-5.38	1.38	1.46
1	A	28	GLY	N-CA	-5.36	1.38	1.45
1	A	902	ARG	CD-NE	-5.35	1.38	1.46
1	A	153	ARG	CD-NE	-5.34	1.38	1.46
1	A	785	ARG	CD-NE	-5.33	1.38	1.46
1	A	1021	ARG	CD-NE	-5.32	1.38	1.46
1	A	293	ARG	CD-NE	-5.31	1.38	1.46
1	A	768	ARG	CD-NE	-5.31	1.38	1.46
1	A	841	ARG	CD-NE	-5.31	1.38	1.46
1	A	415	ARG	CD-NE	-5.30	1.38	1.46
1	A	1056	ARG	CD-NE	-5.30	1.38	1.46
1	A	1147	ARG	CD-NE	-5.29	1.38	1.46
1	A	747	GLY	N-CA	-5.29	1.37	1.45
2	B	33	A	C6-N6	-5.28	1.23	1.33
2	B	25	A	C6-N6	-5.26	1.23	1.33
1	A	146	ARG	CD-NE	-5.25	1.39	1.46
2	B	35	A	C6-N6	-5.21	1.23	1.33
1	A	91	ARG	CD-NE	-5.19	1.39	1.46
1	A	1131	ARG	CD-NE	-5.19	1.39	1.46
1	A	1022	ARG	CD-NE	-5.18	1.39	1.46
1	A	599	ARG	CD-NE	-5.18	1.39	1.46
1	A	1052	ARG	CD-NE	-5.16	1.39	1.46
1	A	1070	PRO	CA-CB	-5.16	1.46	1.53
1	A	395	ARG	CD-NE	-5.14	1.39	1.46
1	A	986	HIS	CA-CB	-5.14	1.46	1.53
1	A	107	GLY	N-CA	-5.11	1.37	1.45
2	B	34	G	C2-N2	-5.08	1.24	1.34
1	A	1033	GLY	N-CA	-5.08	1.38	1.45
1	A	481	GLY	N-CA	-5.08	1.38	1.45
1	A	486	GLY	N-CA	-5.05	1.37	1.45

All (442) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	844	PHE	CA-CB-CG	7.78	121.58	113.80
1	A	1131	ARG	CA-C-N	7.39	130.21	122.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1131	ARG	C-N-CA	7.39	130.21	122.97
1	A	833	ASN	CA-CB-CG	7.29	119.89	112.60
1	A	865	ASP	CA-CB-CG	7.22	119.82	112.60
1	A	901	ASP	CA-CB-CG	7.20	119.80	112.60
1	A	493	ASN	CA-CB-CG	7.19	119.79	112.60
1	A	93	ASN	CA-CB-CG	7.18	119.78	112.60
1	A	201	PHE	CA-CB-CG	7.16	120.96	113.80
1	A	1151	ASN	CA-CB-CG	7.15	119.75	112.60
1	A	591	PHE	CA-CB-CG	7.10	120.90	113.80
1	A	1150	ASN	CA-CB-CG	7.09	119.69	112.60
1	A	1062	PHE	CA-CB-CG	7.09	120.89	113.80
1	A	848	ASP	CA-CB-CG	7.06	119.66	112.60
1	A	65	ASN	CA-CB-CG	7.05	119.65	112.60
1	A	915	PHE	CA-CB-CG	7.04	120.84	113.80
2	B	37	G	C2'-C3'-O3'	7.03	120.04	109.50
1	A	725	PHE	CA-CB-CG	7.00	120.80	113.80
1	A	12	PHE	CA-CB-CG	6.98	120.78	113.80
1	A	1034	PHE	CA-CB-CG	6.91	120.71	113.80
1	A	994	ASP	CA-CB-CG	6.89	119.49	112.60
1	A	609	HIS	CA-CB-CG	6.88	120.68	113.80
1	A	777	PHE	CA-CB-CG	6.86	120.66	113.80
1	A	92	ASN	CA-CB-CG	6.86	119.46	112.60
1	A	689	PHE	CA-CB-CG	6.84	120.64	113.80
1	A	1136	ASN	CA-CB-CG	6.83	119.44	112.60
1	A	999	ASN	CA-CB-CG	6.83	119.43	112.60
1	A	592	ASN	CA-CB-CG	6.83	119.43	112.60
1	A	84	ASP	CA-CB-CG	6.81	119.41	112.60
1	A	298	ASN	CA-CB-CG	6.78	119.38	112.60
1	A	502	ASN	CA-CB-CG	6.78	119.38	112.60
1	A	1143	ASN	CA-CB-CG	6.78	119.38	112.60
1	A	744	ASN	CA-CB-CG	6.77	119.37	112.60
1	A	392	ASN	CA-CB-CG	6.74	119.34	112.60
1	A	802	PHE	CA-CB-CG	6.74	120.53	113.80
1	A	109	PHE	CA-CB-CG	6.71	120.51	113.80
1	A	25	ASP	CA-CB-CG	6.70	119.30	112.60
1	A	89	ASN	CA-CB-CG	6.69	119.29	112.60
1	A	782	ASN	CA-CB-CG	6.69	119.29	112.60
1	A	912	ASN	CA-CB-CG	6.68	119.28	112.60
1	A	488	ASN	CA-CB-CG	6.68	119.28	112.60
1	A	490	PHE	CA-CB-CG	6.66	120.46	113.80
1	A	557	ASP	CA-CB-CG	6.65	119.25	112.60
1	A	1064	ASN	CA-CB-CG	6.65	119.25	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	728	PHE	CA-CB-CG	6.65	120.45	113.80
1	A	827	ASP	CA-CB-CG	6.64	119.24	112.60
1	A	883	PHE	CA-CB-CG	6.64	120.44	113.80
1	A	1049	ASN	CA-CB-CG	6.62	119.22	112.60
1	A	401	HIS	CA-CB-CG	6.58	120.38	113.80
1	A	729	ASP	CA-CB-CG	6.56	119.16	112.60
1	A	64	ASN	CA-CB-CG	6.53	119.13	112.60
1	A	907	PHE	CA-CB-CG	6.52	120.32	113.80
1	A	390	PHE	CA-CB-CG	6.50	120.30	113.80
1	A	990	ASN	CA-CB-CG	6.46	119.06	112.60
1	A	773	ASN	CA-CB-CG	6.45	119.05	112.60
1	A	1013	ASP	CA-CB-CG	6.45	119.05	112.60
1	A	899	PHE	CA-CB-CG	6.44	120.24	113.80
1	A	867	ASP	CA-CB-CG	6.43	119.03	112.60
1	A	924	ASN	CA-CB-CG	6.41	119.01	112.60
1	A	986	HIS	CA-CB-CG	6.40	120.20	113.80
1	A	755	ASN	CA-CB-CG	6.40	119.00	112.60
1	A	172	ASP	CA-CB-CG	6.38	118.98	112.60
1	A	745	ASP	CA-CB-CG	6.36	118.96	112.60
1	A	1149	PHE	CA-CB-CG	6.34	120.14	113.80
1	A	1014	PHE	CA-CB-CG	6.30	120.10	113.80
1	A	434	HIS	CA-CB-CG	6.29	120.09	113.80
1	A	169	ASN	CA-CB-CG	6.29	118.89	112.60
1	A	1028	LEU	CA-C-N	6.28	130.93	122.90
1	A	1028	LEU	C-N-CA	6.28	130.93	122.90
1	A	485	ASN	CA-CB-CG	6.27	118.87	112.60
1	A	85	PHE	CA-CB-CG	6.26	120.06	113.80
1	A	1018	HIS	CA-CB-CG	6.26	120.06	113.80
1	A	870	LYS	CA-C-N	6.23	128.53	120.44
1	A	870	LYS	C-N-CA	6.23	128.53	120.44
1	A	1152	PHE	CA-CB-CG	6.22	120.02	113.80
1	A	1007	ASN	CA-CB-CG	6.21	118.81	112.60
1	A	174	ASN	CA-CB-CG	6.20	118.80	112.60
1	A	415	ARG	CD-NE-CZ	6.20	133.08	124.40
1	A	1046	PHE	CA-CB-CG	6.20	120.00	113.80
1	A	749	GLU	CA-C-N	6.18	130.61	122.51
1	A	749	GLU	C-N-CA	6.18	130.61	122.51
1	A	599	ARG	CD-NE-CZ	6.17	133.04	124.40
1	A	501	ASP	CA-C-N	6.17	128.83	120.38
1	A	501	ASP	C-N-CA	6.17	128.83	120.38
1	A	821	HIS	CA-CB-CG	6.17	119.97	113.80
1	A	768	ARG	CD-NE-CZ	6.16	133.03	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	HIS	CA-CB-CG	6.15	119.95	113.80
1	A	1127	PHE	CA-CB-CG	6.13	119.93	113.80
1	A	1131	ARG	CD-NE-CZ	6.12	132.97	124.40
1	A	821	HIS	CA-C-N	6.12	130.73	122.90
1	A	821	HIS	C-N-CA	6.12	130.73	122.90
1	A	395	ARG	CD-NE-CZ	6.11	132.95	124.40
1	A	393	PHE	CA-CB-CG	6.11	119.91	113.80
1	A	764	ASN	CA-CB-CG	6.10	118.70	112.60
1	A	553	PHE	CA-CB-CG	6.10	119.90	113.80
1	A	482	PHE	CA-CB-CG	6.08	119.88	113.80
1	A	1147	ARG	CD-NE-CZ	6.06	132.88	124.40
1	A	559	PHE	CA-CB-CG	6.06	119.86	113.80
1	A	1091	GLN	CA-C-N	6.03	131.64	122.95
1	A	1091	GLN	C-N-CA	6.03	131.64	122.95
1	A	293	ARG	CD-NE-CZ	6.03	132.84	124.40
1	A	91	ARG	CD-NE-CZ	6.02	132.83	124.40
1	A	635	THR	CA-C-N	6.02	131.02	123.14
1	A	635	THR	C-N-CA	6.02	131.02	123.14
1	A	1113	GLY	CA-C-N	6.01	131.47	122.99
1	A	1113	GLY	C-N-CA	6.01	131.47	122.99
1	A	487	ASN	CA-CB-CG	5.99	118.59	112.60
1	A	153	ARG	CD-NE-CZ	5.98	132.77	124.40
1	A	982	ASN	CA-CB-CG	5.98	118.58	112.60
1	A	1052	ARG	CD-NE-CZ	5.95	132.73	124.40
1	A	1029	ILE	CA-C-N	5.93	130.99	123.10
1	A	1029	ILE	C-N-CA	5.93	130.99	123.10
1	A	599	ARG	CA-C-N	5.93	129.90	121.42
1	A	599	ARG	C-N-CA	5.93	129.90	121.42
1	A	1022	ARG	CD-NE-CZ	5.88	132.63	124.40
1	A	893	LYS	CA-C-N	5.86	128.06	120.44
1	A	893	LYS	C-N-CA	5.86	128.06	120.44
1	A	1077	VAL	CA-C-N	5.84	130.69	122.05
1	A	1077	VAL	C-N-CA	5.84	130.69	122.05
1	A	1117	HIS	CA-CB-CG	5.83	119.64	113.80
1	A	1056	ARG	CD-NE-CZ	5.82	132.55	124.40
1	A	171	ALA	CA-C-N	5.82	131.20	122.99
1	A	171	ALA	C-N-CA	5.82	131.20	122.99
1	A	598	LEU	CA-C-N	5.82	128.55	120.29
1	A	598	LEU	C-N-CA	5.82	128.55	120.29
1	A	765	GLY	CA-C-N	5.80	131.01	123.00
1	A	765	GLY	C-N-CA	5.80	131.01	123.00
1	A	1043	ILE	CA-C-N	5.79	129.87	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1043	ILE	C-N-CA	5.79	129.87	120.60
1	A	146	ARG	CD-NE-CZ	5.79	132.50	124.40
1	A	816	LYS	CA-C-N	5.78	129.83	122.37
1	A	816	LYS	C-N-CA	5.78	129.83	122.37
1	A	924	ASN	N-CA-CB	5.78	118.46	109.97
1	A	1114	ARG	CA-C-N	5.76	130.32	122.84
1	A	1114	ARG	C-N-CA	5.76	130.32	122.84
1	A	767	GLU	CA-C-N	5.75	131.10	122.99
1	A	767	GLU	C-N-CA	5.75	131.10	122.99
1	A	787	PHE	CA-CB-CG	5.75	119.55	113.80
1	A	1027	GLY	CA-C-N	5.71	130.60	122.72
1	A	1027	GLY	C-N-CA	5.71	130.60	122.72
1	A	666	LEU	CA-C-N	5.70	130.92	122.99
1	A	666	LEU	C-N-CA	5.70	130.92	122.99
1	A	560	GLN	CA-C-N	5.67	127.70	120.56
1	A	560	GLN	C-N-CA	5.67	127.70	120.56
1	A	520	LYS	CA-C-N	5.67	127.78	120.70
1	A	520	LYS	C-N-CA	5.67	127.78	120.70
1	A	1097	PHE	CA-CB-CG	5.66	119.46	113.80
1	A	822	ILE	CA-C-N	5.65	130.71	123.13
1	A	822	ILE	C-N-CA	5.65	130.71	123.13
1	A	633	GLU	CA-C-N	5.65	130.72	122.69
1	A	633	GLU	C-N-CA	5.65	130.72	122.69
1	A	1094	ASN	CA-C-N	5.65	130.98	122.91
1	A	1094	ASN	C-N-CA	5.65	130.98	122.91
1	A	1076	ALA	CA-C-N	5.64	128.13	120.63
1	A	1076	ALA	C-N-CA	5.64	128.13	120.63
1	A	108	ASP	CA-CB-CG	5.64	118.24	112.60
1	A	868	ASN	CA-CB-CG	5.60	118.20	112.60
2	B	26	C	O4'-C1'-N1	5.59	116.58	108.20
1	A	1144	ILE	N-CA-CB	5.59	116.71	110.51
1	A	1055	GLU	CA-C-N	5.55	128.00	120.44
1	A	1055	GLU	C-N-CA	5.55	128.00	120.44
1	A	897	TRP	CA-C-N	5.55	127.55	120.56
1	A	897	TRP	C-N-CA	5.55	127.55	120.56
1	A	527	VAL	N-CA-CB	5.54	116.66	110.51
1	A	612	ILE	N-CA-CB	5.53	116.43	110.62
1	A	901	ASP	CA-C-N	5.52	128.23	120.28
1	A	901	ASP	C-N-CA	5.52	128.23	120.28
1	A	108	ASP	CA-C-N	5.51	130.75	122.99
1	A	108	ASP	C-N-CA	5.51	130.75	122.99
1	A	841	ARG	N-CA-CB	5.49	117.98	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	ASN	CA-C-N	5.47	127.55	120.44
1	A	64	ASN	C-N-CA	5.47	127.55	120.44
1	A	564	GLU	CA-C-N	5.46	127.86	120.44
1	A	564	GLU	C-N-CA	5.46	127.86	120.44
1	A	15	GLU	CA-C-N	5.45	129.62	121.72
1	A	15	GLU	C-N-CA	5.45	129.62	121.72
1	A	91	ARG	N-CA-CB	5.45	117.91	110.01
2	B	16	A	C4'-C3'-O3'	5.45	117.57	109.40
1	A	396	THR	CA-C-N	5.41	127.38	120.56
1	A	396	THR	C-N-CA	5.41	127.38	120.56
1	A	779	LYS	CA-C-N	5.39	127.45	120.44
1	A	779	LYS	C-N-CA	5.39	127.45	120.44
1	A	393	PHE	CA-C-N	5.39	127.45	120.44
1	A	393	PHE	C-N-CA	5.39	127.45	120.44
1	A	805	LYS	CA-C-N	5.39	130.37	122.39
1	A	805	LYS	C-N-CA	5.39	130.37	122.39
1	A	1018	HIS	CE1-NE2-CD2	-5.39	103.61	109.00
1	A	760	GLU	CA-C-N	5.38	130.74	122.93
1	A	760	GLU	C-N-CA	5.38	130.74	122.93
1	A	1052	ARG	CA-C-N	5.38	127.34	120.56
1	A	1052	ARG	C-N-CA	5.38	127.34	120.56
1	A	709	PHE	CA-CB-CG	5.38	119.18	113.80
2	B	17	U	C2'-C3'-O3'	5.36	117.55	109.50
1	A	521	ILE	N-CA-CB	5.36	116.46	110.62
1	A	1022	ARG	N-CA-CB	5.36	117.78	110.01
1	A	413	LYS	CA-C-N	5.34	127.38	120.44
1	A	413	LYS	C-N-CA	5.34	127.38	120.44
1	A	563	LEU	N-CA-CB	5.34	117.75	110.01
1	A	762	ASP	CA-C-N	5.34	127.97	120.28
1	A	762	ASP	C-N-CA	5.34	127.97	120.28
1	A	387	TRP	CA-C-N	5.34	127.38	120.44
1	A	387	TRP	C-N-CA	5.34	127.38	120.44
1	A	1002	LYS	CA-CB-CG	5.34	124.77	114.10
1	A	390	PHE	CA-C-N	5.33	127.37	120.44
1	A	390	PHE	C-N-CA	5.33	127.37	120.44
1	A	911	GLU	CA-C-N	5.32	127.36	120.44
1	A	911	GLU	C-N-CA	5.32	127.36	120.44
1	A	1061	LYS	N-CA-CB	5.32	117.87	109.94
1	A	198	VAL	N-CA-CB	5.32	116.77	110.55
2	B	37	G	P-O3'-C3'	5.31	128.17	120.20
1	A	1016	TYR	N-CA-CB	5.31	117.71	110.01
1	A	64	ASN	N-CA-CB	5.31	117.71	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	415	ARG	N-CA-CB	5.30	117.70	110.01
1	A	801	GLN	CA-C-N	5.30	130.54	122.65
1	A	801	GLN	C-N-CA	5.30	130.54	122.65
1	A	995	LEU	N-CA-CB	5.30	117.83	109.94
1	A	1097	PHE	CA-C-N	5.30	130.21	122.69
1	A	1097	PHE	C-N-CA	5.30	130.21	122.69
1	A	73	TRP	N-CA-CB	5.29	117.68	110.01
1	A	997	ILE	N-CA-CB	5.29	116.74	110.55
1	A	435	LYS	CA-C-N	5.29	129.65	122.19
1	A	435	LYS	C-N-CA	5.29	129.65	122.19
1	A	738	ALA	CA-C-N	5.29	127.31	120.44
1	A	738	ALA	C-N-CA	5.29	127.31	120.44
1	A	1070	PRO	CA-C-N	5.29	129.20	121.80
1	A	1070	PRO	C-N-CA	5.29	129.20	121.80
1	A	166	LEU	N-CA-CB	5.28	117.81	109.94
1	A	412	GLU	N-CA-CB	5.28	117.67	110.01
1	A	691	SER	CA-C-N	5.28	127.31	120.44
1	A	691	SER	C-N-CA	5.28	127.31	120.44
1	A	218	TYR	CA-C-N	5.28	127.31	120.44
1	A	218	TYR	C-N-CA	5.28	127.31	120.44
1	A	488	ASN	N-CA-CB	5.28	117.95	110.46
1	A	6	VAL	CA-C-N	5.27	130.43	122.99
1	A	6	VAL	C-N-CA	5.27	130.43	122.99
1	A	532	TYR	N-CA-CB	5.27	117.79	109.94
1	A	492	LYS	CA-C-N	5.26	127.28	120.44
1	A	492	LYS	C-N-CA	5.26	127.28	120.44
1	A	412	GLU	CA-C-N	5.26	127.28	120.44
1	A	412	GLU	C-N-CA	5.26	127.28	120.44
1	A	1117	HIS	CE1-NE2-CD2	-5.26	103.74	109.00
1	A	9	THR	CA-C-N	5.26	130.28	122.71
1	A	9	THR	C-N-CA	5.26	130.28	122.71
1	A	826	GLY	N-CA-C	5.25	118.59	112.50
1	A	605	LYS	CA-C-N	5.25	129.79	122.23
1	A	605	LYS	C-N-CA	5.25	129.79	122.23
1	A	1059	TYR	N-CA-CB	5.25	117.62	110.01
1	A	1030	ILE	CA-C-N	5.24	130.80	122.94
1	A	1030	ILE	C-N-CA	5.24	130.80	122.94
1	A	14	LEU	CA-C-N	5.24	130.37	122.99
1	A	14	LEU	C-N-CA	5.24	130.37	122.99
1	A	878	SER	CA-C-N	5.24	128.99	121.50
1	A	878	SER	C-N-CA	5.24	128.99	121.50
1	A	548	ILE	CA-C-N	5.24	127.24	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	548	ILE	C-N-CA	5.24	127.24	120.70
1	A	394	TYR	CA-C-N	5.23	127.24	120.44
1	A	394	TYR	C-N-CA	5.23	127.24	120.44
2	B	38	A	C4'-C3'-O3'	-5.23	101.55	109.40
1	A	282	PRO	CA-C-N	5.23	128.01	120.38
1	A	282	PRO	C-N-CA	5.23	128.01	120.38
1	A	433	GLN	CA-C-N	5.23	130.36	122.99
1	A	433	GLN	C-N-CA	5.23	130.36	122.99
1	A	411	ILE	N-CA-CB	5.22	116.66	110.55
1	A	687	ASP	CA-C-N	5.22	127.23	120.44
1	A	687	ASP	C-N-CA	5.22	127.23	120.44
1	A	80	GLN	N-CA-CB	5.22	117.58	110.01
1	A	297	LYS	CA-C-N	5.22	127.22	120.44
1	A	297	LYS	C-N-CA	5.22	127.22	120.44
1	A	1088	ALA	CA-C-N	5.21	129.93	121.95
1	A	1088	ALA	C-N-CA	5.21	129.93	121.95
1	A	526	SER	CA-C-N	5.21	127.32	120.60
1	A	526	SER	C-N-CA	5.21	127.32	120.60
1	A	410	GLY	CA-C-N	5.21	127.12	120.56
1	A	410	GLY	C-N-CA	5.21	127.12	120.56
1	A	1146	LYS	N-CA-CB	5.20	117.55	110.01
1	A	162	SER	N-CA-CB	5.20	117.54	110.01
1	A	405	LEU	N-CA-CB	5.20	117.54	110.01
1	A	758	TYR	N-CA-CB	5.20	117.67	109.83
1	A	1117	HIS	ND1-CG-CD2	-5.19	100.91	106.10
1	A	166	LEU	CA-C-N	5.19	127.09	120.56
1	A	166	LEU	C-N-CA	5.19	127.09	120.56
1	A	1071	ILE	N-CA-CB	5.17	116.74	110.95
1	A	1002	LYS	CA-C-N	5.17	127.16	120.44
1	A	1002	LYS	C-N-CA	5.17	127.16	120.44
1	A	165	SER	N-CA-CB	5.17	117.64	109.94
1	A	684	MET	CA-CB-CG	5.17	124.43	114.10
1	A	1018	HIS	ND1-CG-CD2	-5.17	100.94	106.10
1	A	862	ASN	CA-C-N	5.16	130.99	121.85
1	A	862	ASN	C-N-CA	5.16	130.99	121.85
1	A	1009	VAL	N-CA-CB	5.16	116.59	110.55
1	A	392	ASN	CA-C-N	5.16	127.15	120.44
1	A	392	ASN	C-N-CA	5.16	127.15	120.44
1	A	1001	LYS	CA-C-N	5.16	127.14	120.44
1	A	1001	LYS	C-N-CA	5.16	127.14	120.44
1	A	898	ILE	N-CA-CB	5.16	116.58	110.55
1	A	1153	VAL	N-CA-CB	5.16	116.58	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1018	HIS	CG-CD2-NE2	5.15	112.35	107.20
1	A	590	ILE	CA-C-N	5.15	131.07	122.73
1	A	590	ILE	C-N-CA	5.15	131.07	122.73
1	A	20	PRO	CA-C-N	5.15	128.61	120.89
1	A	20	PRO	C-N-CA	5.15	128.61	120.89
1	A	489	LYS	N-CA-CB	5.15	117.61	109.94
1	A	114	SER	CA-C-N	5.15	127.13	120.44
1	A	114	SER	C-N-CA	5.15	127.13	120.44
1	A	301	SER	N-CA-CB	5.15	117.47	110.01
1	A	692	SER	N-CA-CB	5.14	117.47	110.01
1	A	783	TYR	N-CA-CB	5.14	117.47	110.01
1	A	175	GLU	N-CA-CB	5.14	117.59	109.83
1	A	90	LYS	N-CA-CB	5.14	117.41	109.91
1	A	914	LYS	CA-C-N	5.13	127.11	120.44
1	A	914	LYS	C-N-CA	5.13	127.11	120.44
1	A	1040	GLU	CA-CB-CG	5.13	124.37	114.10
1	A	669	THR	CA-C-N	5.13	130.85	122.69
1	A	669	THR	C-N-CA	5.13	130.85	122.69
1	A	894	TYR	CA-C-N	5.13	127.11	120.44
1	A	894	TYR	C-N-CA	5.13	127.11	120.44
1	A	555	SER	CA-C-N	5.13	127.41	120.38
1	A	555	SER	C-N-CA	5.13	127.41	120.38
1	A	84	ASP	CA-C-N	5.13	127.11	120.44
1	A	84	ASP	C-N-CA	5.13	127.11	120.44
1	A	1052	ARG	CG-CD-NE	5.13	123.28	112.00
1	A	1077	VAL	N-CA-CB	5.13	117.00	110.13
1	A	1127	PHE	N-CA-CB	5.13	117.51	109.97
1	A	973	LYS	CA-C-N	5.12	127.10	120.44
1	A	973	LYS	C-N-CA	5.12	127.10	120.44
1	A	998	LEU	N-CA-CB	5.12	117.57	109.94
1	A	167	ILE	N-CA-CB	5.12	116.54	110.55
1	A	397	ILE	CA-C-N	5.12	127.10	120.44
1	A	397	ILE	C-N-CA	5.12	127.10	120.44
1	A	390	PHE	N-CA-CB	5.12	117.43	110.01
1	A	391	SER	N-CA-CB	5.12	117.43	110.01
1	A	403	LYS	CA-C-N	5.12	127.68	120.42
1	A	403	LYS	C-N-CA	5.12	127.68	120.42
1	A	559	PHE	N-CA-CB	5.12	117.43	110.01
1	A	234	GLU	CA-C-N	5.11	127.13	120.28
1	A	234	GLU	C-N-CA	5.11	127.13	120.28
1	A	1001	LYS	CA-CB-CG	5.11	124.33	114.10
1	A	83	VAL	CA-C-N	5.11	127.08	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	VAL	C-N-CA	5.11	127.08	120.44
1	A	1146	LYS	CA-C-N	5.11	127.08	120.44
1	A	1146	LYS	C-N-CA	5.11	127.08	120.44
1	A	1152	PHE	N-CA-CB	5.11	117.56	109.94
2	B	38	A	C2'-C3'-O3'	5.11	117.17	109.50
1	A	414	GLU	N-CA-CB	5.11	117.42	110.01
1	A	1002	LYS	CG-CD-CE	5.11	123.05	111.30
1	A	504	ARG	CA-CB-CG	5.11	124.31	114.10
1	A	558	ASP	CA-C-N	5.10	127.07	120.44
1	A	558	ASP	C-N-CA	5.10	127.07	120.44
1	A	153	ARG	CA-C-N	5.10	127.12	120.28
1	A	153	ARG	C-N-CA	5.10	127.12	120.28
1	A	115	LYS	N-CA-CB	5.10	117.40	110.01
1	A	1058	LEU	N-CA-CB	5.10	117.41	110.01
1	A	1126	GLY	CA-C-N	5.10	128.11	120.87
1	A	1126	GLY	C-N-CA	5.10	128.11	120.87
1	A	7	THR	CA-C-N	5.09	130.17	122.99
1	A	7	THR	C-N-CA	5.09	130.17	122.99
2	B	42	A	O4'-C4'-C3'	5.09	109.09	104.00
1	A	293	ARG	CG-CD-NE	5.09	123.20	112.00
1	A	413	LYS	CA-CB-CG	5.09	124.28	114.10
1	A	1052	ARG	N-CA-CB	5.09	117.39	110.01
1	A	162	SER	CA-C-N	5.09	127.06	120.44
1	A	162	SER	C-N-CA	5.09	127.06	120.44
1	A	882	GLU	CA-C-N	5.09	127.10	120.28
1	A	882	GLU	C-N-CA	5.09	127.10	120.28
1	A	1117	HIS	CG-CD2-NE2	5.08	112.28	107.20
1	A	82	TRP	N-CA-CB	5.08	117.38	110.01
1	A	1013	ASP	N-CA-CB	5.08	117.38	110.01
1	A	1149	PHE	N-CA-CB	5.08	117.38	110.01
1	A	766	LYS	CA-CB-CG	5.08	124.26	114.10
1	A	479	CYS	N-CA-CB	5.08	117.43	110.07
1	A	386	THR	CA-C-N	5.08	127.04	120.44
1	A	386	THR	C-N-CA	5.08	127.04	120.44
1	A	634	ILE	CA-C-N	5.08	130.54	122.62
1	A	634	ILE	C-N-CA	5.08	130.54	122.62
1	A	521	ILE	CA-C-N	5.07	127.08	120.28
1	A	521	ILE	C-N-CA	5.07	127.08	120.28
1	A	397	ILE	N-CA-CB	5.07	116.48	110.55
1	A	146	ARG	CG-CD-NE	5.07	123.15	112.00
1	A	304	LYS	N-CA-CB	5.07	117.36	110.01
1	A	142	THR	CA-C-N	5.07	127.02	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	142	THR	C-N-CA	5.07	127.02	120.44
1	A	5	LYS	CA-C-N	5.06	129.98	122.94
1	A	5	LYS	C-N-CA	5.06	129.98	122.94
1	A	82	TRP	CA-C-N	5.06	126.94	120.56
1	A	82	TRP	C-N-CA	5.06	126.94	120.56
1	A	34	ASN	CA-C-N	5.06	127.33	120.65
1	A	34	ASN	C-N-CA	5.06	127.33	120.65
1	A	163	LEU	N-CA-CB	5.06	117.34	110.01
1	A	415	ARG	CG-CD-NE	5.06	123.13	112.00
1	A	111	GLY	CA-C-N	5.06	127.06	120.28
1	A	111	GLY	C-N-CA	5.06	127.06	120.28
1	A	143	LYS	N-CA-CB	5.05	117.34	110.01
1	A	235	LEU	N-CA-CB	5.05	117.55	110.12
1	A	395	ARG	CG-CD-NE	5.05	123.12	112.00
1	A	556	LEU	CA-C-N	5.05	127.00	120.44
1	A	556	LEU	C-N-CA	5.05	127.00	120.44
1	A	490	PHE	N-CA-CB	5.05	117.46	109.94
1	A	778	LEU	CA-C-N	5.04	128.50	121.24
1	A	778	LEU	C-N-CA	5.04	128.50	121.24
1	A	387	TRP	N-CA-CB	5.04	117.32	110.01
1	A	794	TYR	N-CA-CB	5.04	117.45	109.94
1	A	767	GLU	CA-CB-CG	5.04	124.18	114.10
1	A	474	SER	CA-C-N	5.04	127.03	120.28
1	A	474	SER	C-N-CA	5.04	127.03	120.28
1	A	81	GLU	CA-C-N	5.04	126.99	120.44
1	A	81	GLU	C-N-CA	5.04	126.99	120.44
1	A	719	SER	N-CA-C	5.04	114.80	108.45
1	A	750	VAL	CA-C-N	5.03	130.71	122.81
1	A	750	VAL	C-N-CA	5.03	130.71	122.81
1	A	292	LEU	CA-C-N	5.03	127.33	120.54
1	A	292	LEU	C-N-CA	5.03	127.33	120.54
1	A	943	GLU	CA-C-N	5.03	127.72	120.38
1	A	943	GLU	C-N-CA	5.03	127.72	120.38
1	A	982	ASN	CA-C-N	5.03	127.33	120.54
1	A	982	ASN	C-N-CA	5.03	127.33	120.54
1	A	1020	GLU	N-CA-CB	5.03	117.30	110.01
1	A	805	LYS	CA-CB-CG	5.02	124.14	114.10
1	A	820	GLY	CA-C-N	5.02	130.45	122.62
1	A	820	GLY	C-N-CA	5.02	130.45	122.62
1	A	27	GLU	N-CA-CB	5.02	117.28	110.01
1	A	565	LYS	CA-CB-CG	5.02	124.14	114.10
1	A	600	LYS	CG-CD-CE	5.02	122.84	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	766	LYS	CA-C-N	5.02	128.00	120.87
1	A	766	LYS	C-N-CA	5.02	128.00	120.87
1	A	478	LEU	CA-C-N	5.02	127.26	120.44
1	A	478	LEU	C-N-CA	5.02	127.26	120.44
1	A	492	LYS	N-CA-CB	5.01	117.28	110.01
1	A	561	ILE	N-CA-CB	5.01	116.42	110.55
1	A	232	LYS	CA-CB-CG	5.01	124.12	114.10
1	A	283	MET	CA-CB-CG	5.01	124.12	114.10
1	A	525	GLN	CA-C-N	5.01	126.95	120.44
1	A	525	GLN	C-N-CA	5.01	126.95	120.44
1	A	154	LEU	N-CA-CB	5.01	117.48	110.12
1	A	475	LEU	N-CA-CB	5.01	117.48	110.12
1	A	560	GLN	CA-CB-CG	5.01	124.11	114.10
1	A	35	LEU	N-CA-CB	5.00	117.22	109.91
1	A	680	ILE	N-CA-CB	5.00	116.37	110.82
1	A	779	LYS	N-CA-CB	5.00	117.42	109.71
1	A	1007	ASN	CA-C-N	5.00	126.94	120.44
1	A	1007	ASN	C-N-CA	5.00	126.94	120.44
1	A	1132	ILE	CA-C-N	5.00	130.18	122.93
1	A	1132	ILE	C-N-CA	5.00	130.18	122.93

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	639	ARG	Sidechain
2	B	13	C	Sidechain
2	B	15	A	Sidechain
2	B	16	A	Sidechain
2	B	17	U	Sidechain
2	B	19	A	Sidechain
2	B	20	U	Sidechain
2	B	23	C	Sidechain
2	B	26	C	Sidechain
2	B	27	U	Sidechain
2	B	37	G	Sidechain
2	B	41	G	Sidechain
2	B	42	A	Sidechain

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	9422	9528	9526	57	0
2	B	864	438	423	1	0
All	All	10286	9966	9949	58	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 3.

All (58) 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:633:GLU:N	1:A:633:GLU:OE1	2.13	0.81
1:A:604:ASP:OD1	1:A:605:LYS:N	2.15	0.79
1:A:310:LEU:HD22	1:A:320:LEU:HD21	1.67	0.76
1:A:587:LYS:O	1:A:589:GLN:NE2	2.23	0.71
1:A:361:GLN:N	1:A:361:GLN:OE1	2.23	0.70
1:A:891:LYS:O	1:A:895:THR:HG23	1.93	0.68
1:A:287:GLU:O	1:A:288:ASN:ND2	2.27	0.68
1:A:983:ARG:NH2	1:A:986:HIS:O	2.31	0.64
1:A:242:SER:OG	1:A:244:ASP:OD1	2.10	0.63
1:A:222:ASN:OD1	1:A:224:LYS:NZ	2.30	0.61
1:A:1074:LEU:HD12	1:A:1074:LEU:O	2.01	0.60
1:A:944:LEU:HD12	1:A:944:LEU:O	2.02	0.59
1:A:311:MET:SD	1:A:311:MET:N	2.76	0.57
1:A:284:LEU:CD2	1:A:286:ILE:HD11	2.35	0.57
1:A:902:ARG:O	1:A:902:ARG:NH2	2.38	0.57
1:A:222:ASN:O	1:A:224:LYS:NZ	2.36	0.56
1:A:317:TYR:HA	1:A:320:LEU:HD12	1.86	0.55
1:A:468:GLU:OE2	1:A:538:ASN:N	2.36	0.54
1:A:175:GLU:OE1	1:A:176:THR:N	2.41	0.54
1:A:1041:ASP:OD1	1:A:1041:ASP:C	2.50	0.54
1:A:604:ASP:OD1	1:A:604:ASP:C	2.52	0.53
1:A:597:ASP:OD1	1:A:598:LEU:N	2.43	0.52
1:A:310:LEU:HD22	1:A:320:LEU:CD2	2.39	0.51
1:A:754:ARG:NH2	1:A:803:GLU:OE2	2.44	0.51
1:A:827:ASP:OD1	1:A:827:ASP:C	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1088:ALA:O	1:A:1151:ASN:ND2	2.45	0.50
1:A:1079:ALA:O	1:A:1082:ILE:HG22	2.13	0.49
1:A:258:ILE:O	1:A:262:ILE:HG12	2.13	0.49
2:B:50:C:H2'	2:B:51:C:H5'	1.95	0.48
1:A:333:GLN:OE1	1:A:333:GLN:N	2.43	0.48
1:A:276:LEU:HD12	1:A:277:LEU:N	2.28	0.47
1:A:412:GLU:O	1:A:416:THR:HG23	2.15	0.47
1:A:25:ASP:O	1:A:29:LEU:HD23	2.14	0.47
1:A:284:LEU:HD21	1:A:286:ILE:HD11	1.96	0.46
1:A:46:LEU:O	1:A:49:VAL:HG12	2.17	0.45
1:A:286:ILE:HG23	1:A:289:TYR:CD2	2.51	0.45
1:A:983:ARG:NH2	1:A:983:ARG:O	2.40	0.45
1:A:316:ASN:OD1	1:A:319:GLU:N	2.44	0.45
1:A:631:ASN:CG	1:A:669:THR:HG1	2.10	0.44
1:A:604:ASP:OD1	1:A:605:LYS:HG2	2.18	0.44
1:A:287:GLU:O	1:A:288:ASN:CG	2.60	0.44
1:A:886:LEU:HD12	1:A:886:LEU:N	2.34	0.43
1:A:541:ILE:HA	1:A:544:VAL:HG12	1.99	0.43
1:A:346:LEU:HD23	1:A:346:LEU:O	2.18	0.43
1:A:262:ILE:N	1:A:262:ILE:HD13	2.34	0.43
1:A:137:GLN:N	1:A:137:GLN:OE1	2.52	0.42
1:A:346:LEU:HD23	1:A:346:LEU:C	2.44	0.42
1:A:159:ALA:O	1:A:160:LEU:C	2.62	0.42
1:A:236:GLU:OE2	1:A:240:LYS:NZ	2.51	0.42
1:A:307:PHE:CD2	1:A:328:LEU:HD13	2.54	0.42
1:A:286:ILE:HD12	1:A:289:TYR:CE2	2.55	0.42
1:A:746:TYR:O	1:A:1019:TYR:OH	2.35	0.41
1:A:235:LEU:HD11	1:A:404:ILE:HG23	2.02	0.41
1:A:235:LEU:HD23	1:A:408:LEU:CD1	2.51	0.41
1:A:116:ILE:HD11	1:A:166:LEU:HD22	2.02	0.41
1:A:946:SER:O	1:A:947:VAL:C	2.63	0.41
1:A:887:ASN:N	1:A:890:GLU:OE1	2.43	0.40
1:A:797:MET:SD	1:A:797:MET:C	3.04	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	1152/1168 (99%)	1088 (94%)	64 (6%)	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	1038/1049 (99%)	1028 (99%)	10 (1%)	68	74

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	ILE
1	A	408	LEU
1	A	471	THR
1	A	604	ASP
1	A	684	MET
1	A	797	MET
1	A	880	GLU
1	A	960	ARG
1	A	1041	ASP
1	A	1098	ILE

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

Mol	Chain	Res	Type
1	A	44	ASN
1	A	174	ASN
1	A	205	GLN
1	A	335	GLN
1	A	589	GLN
1	A	713	ASN
1	A	847	ASN
1	A	862	ASN
1	A	945	GLN
1	A	980	ASN
1	A	982	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	40/65 (61%)	21 (52%)	6 (15%)

All (21) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	12	C
2	B	13	C
2	B	14	C
2	B	15	A
2	B	16	A
2	B	17	U
2	B	18	A
2	B	19	A
2	B	27	U
2	B	31	G
2	B	37	G
2	B	38	A
2	B	39	G
2	B	40	G
2	B	41	G
2	B	42	A
2	B	43	U
2	B	45	U
2	B	47	G
2	B	48	C
2	B	51	C

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	15	A
2	B	16	A
2	B	30	U
2	B	37	G
2	B	42	A
2	B	45	U

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.

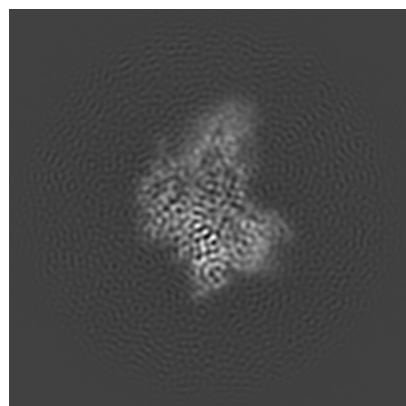
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52275. These allow visual inspection of the internal detail of the map and identification of artifacts.

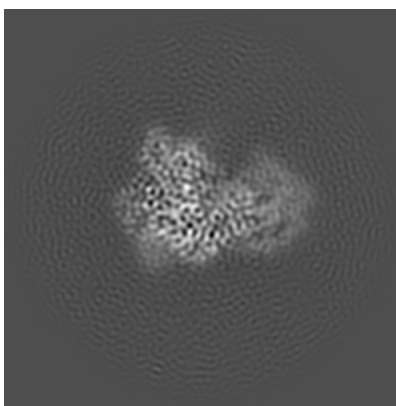
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

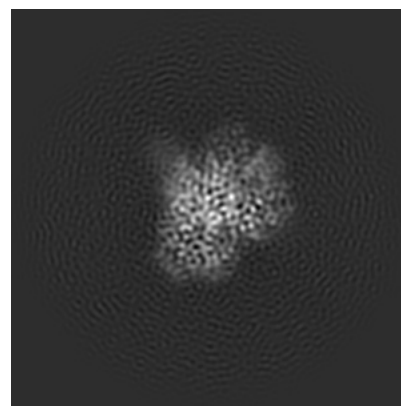
6.1.1 Primary map



X

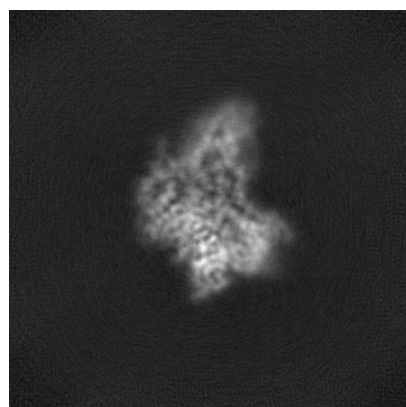


Y

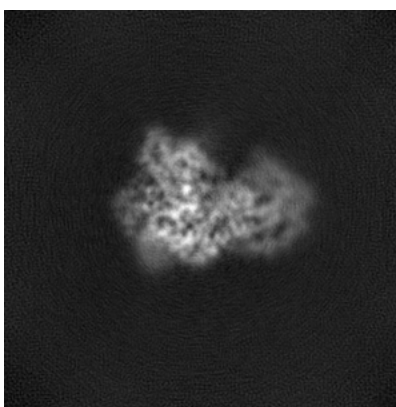


Z

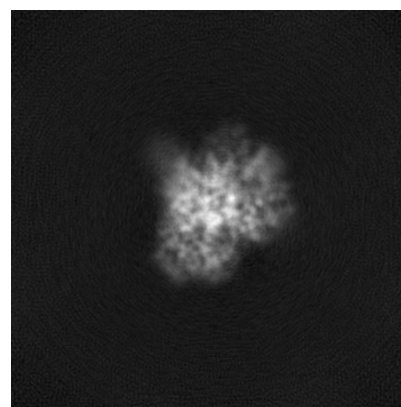
6.1.2 Raw map



X



Y

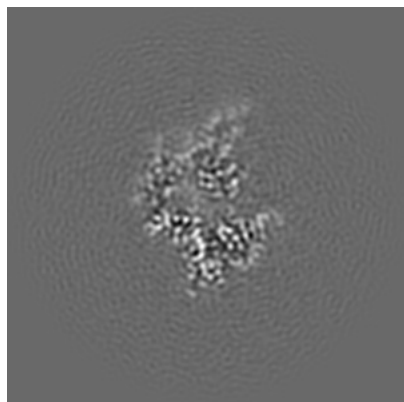


Z

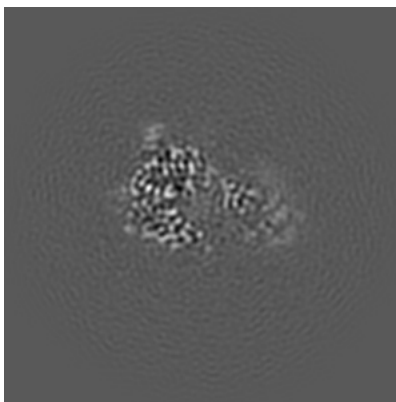
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

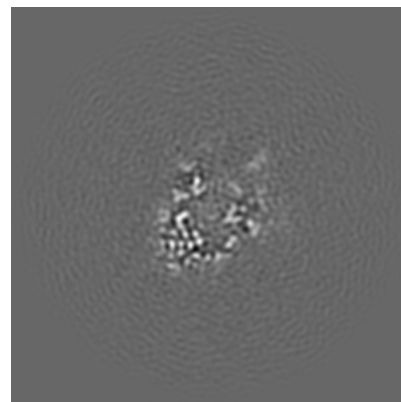
6.2.1 Primary map



X Index: 128

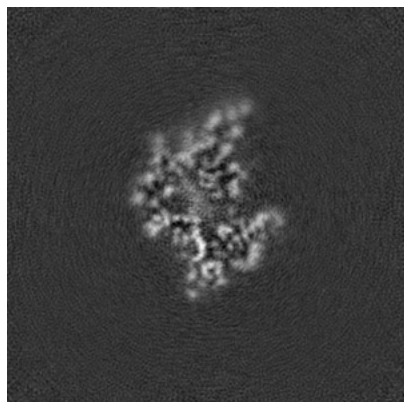


Y Index: 128

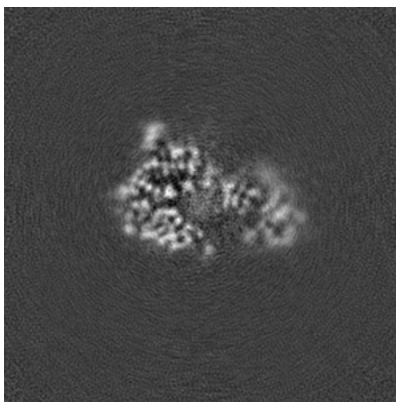


Z Index: 128

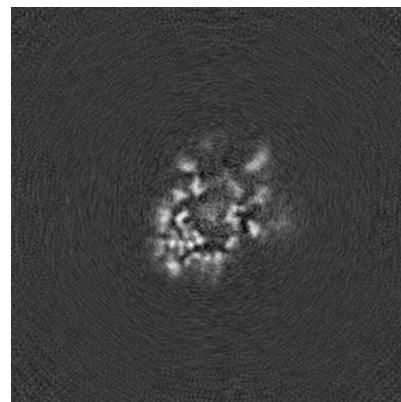
6.2.2 Raw map



X Index: 128



Y Index: 128

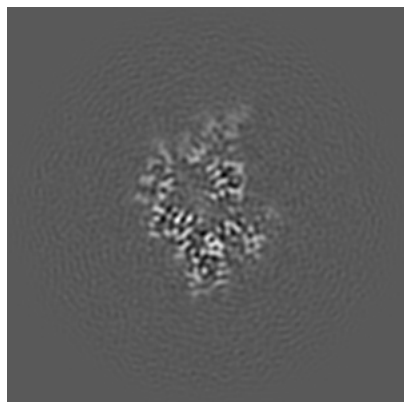


Z Index: 128

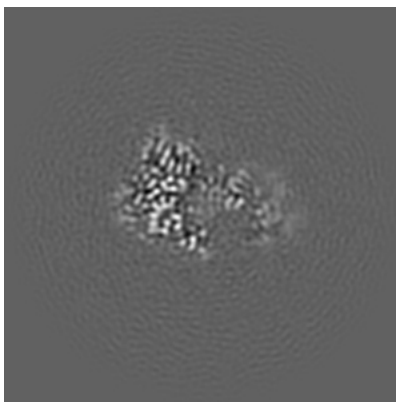
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

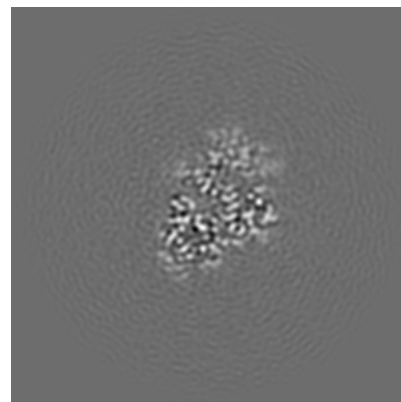
6.3.1 Primary map



X Index: 125

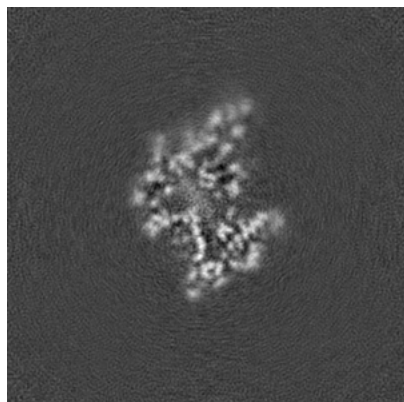


Y Index: 124

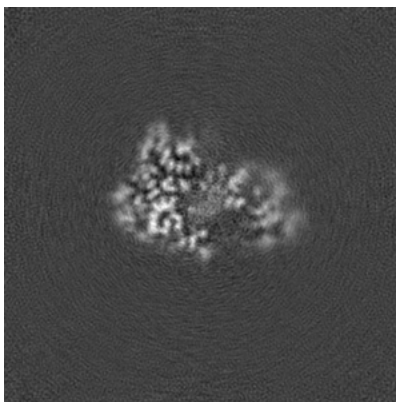


Z Index: 117

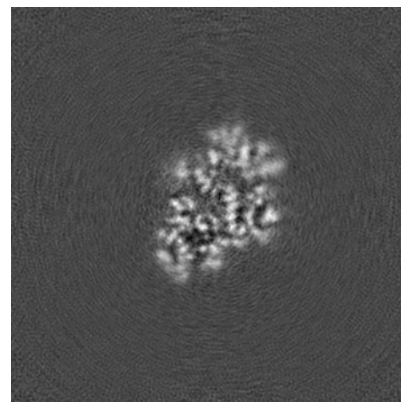
6.3.2 Raw map



X Index: 129



Y Index: 124

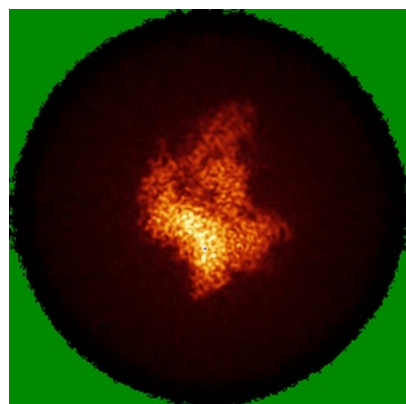


Z Index: 117

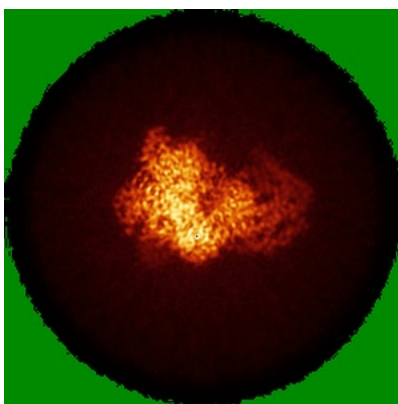
The images above show the largest variance slices of the map in three orthogonal directions.

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

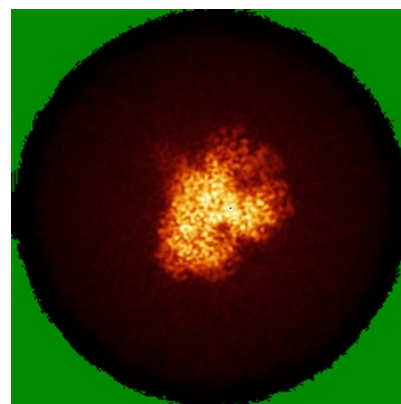
6.4.1 Primary map



X

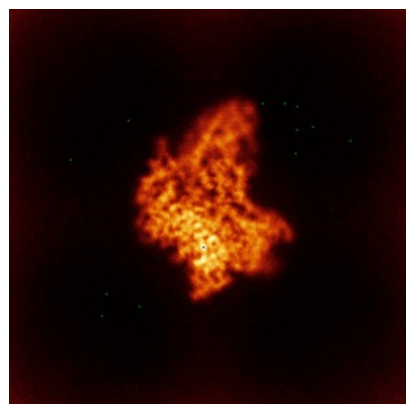


Y

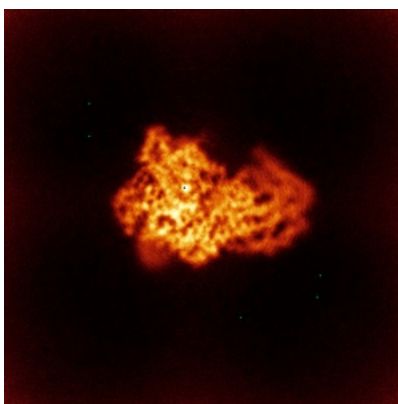


Z

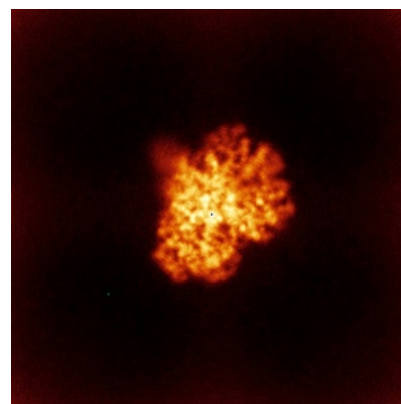
6.4.2 Raw map



X



Y

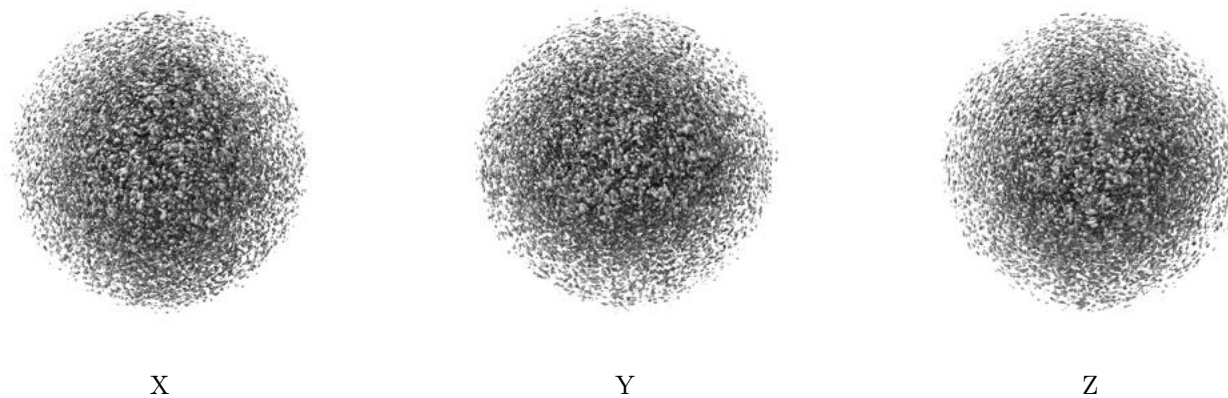


Z

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.

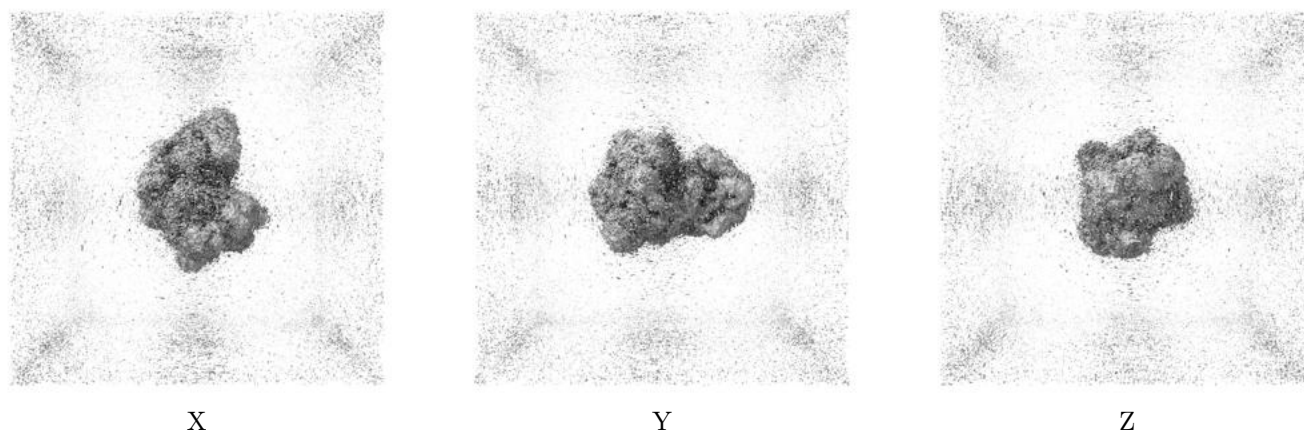
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.009. 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.

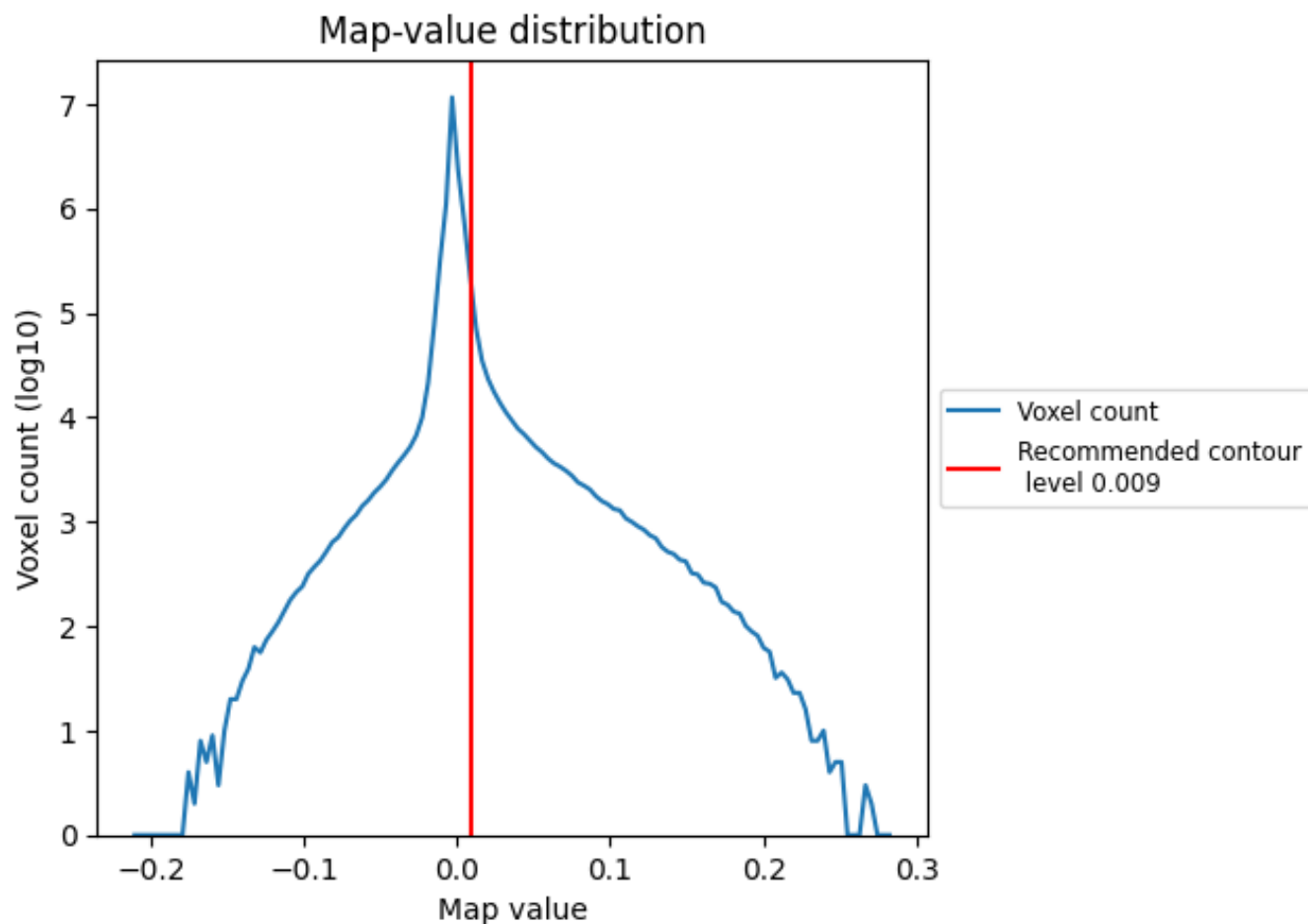
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

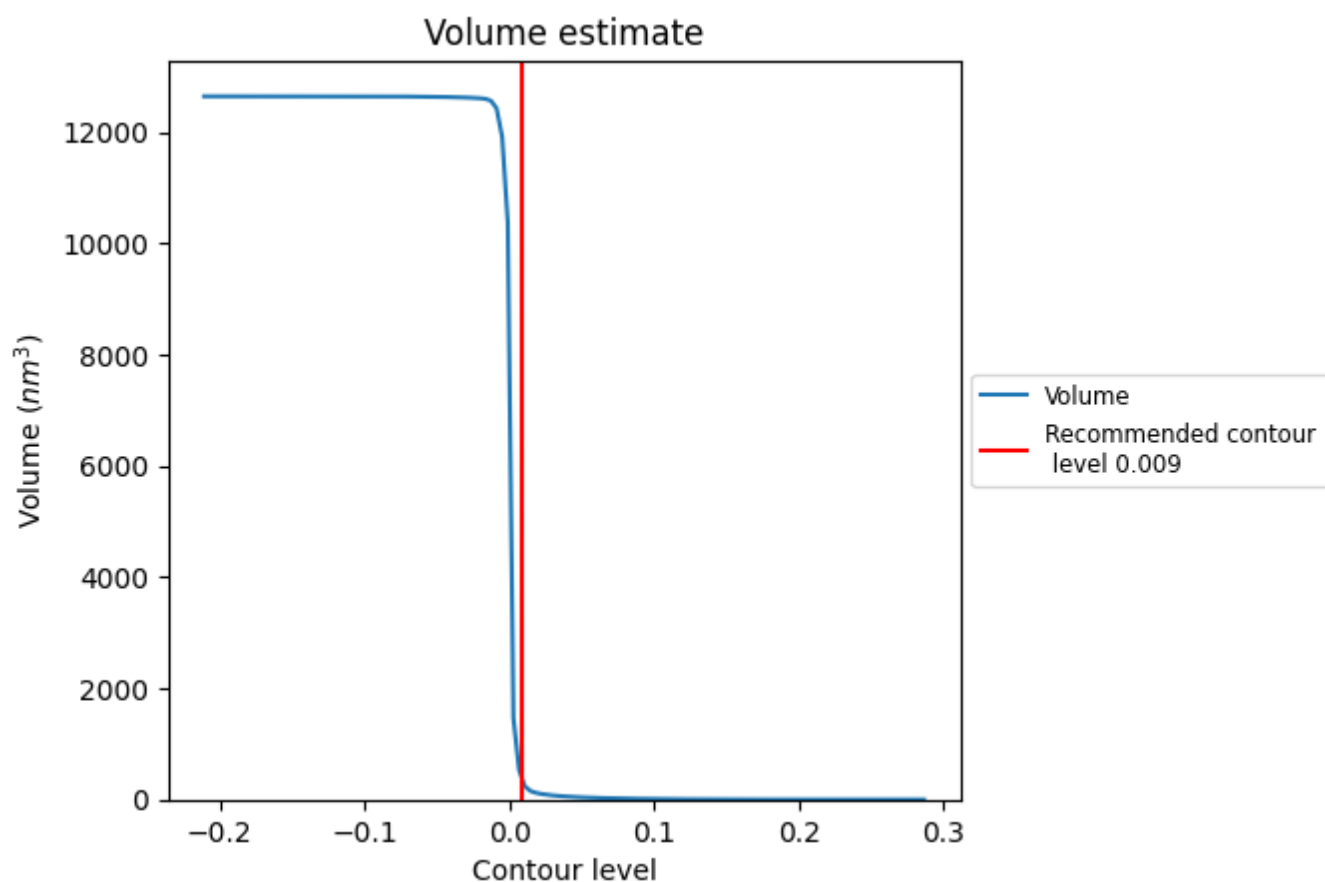
This section contains the results of statistical analysis of the map.

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.

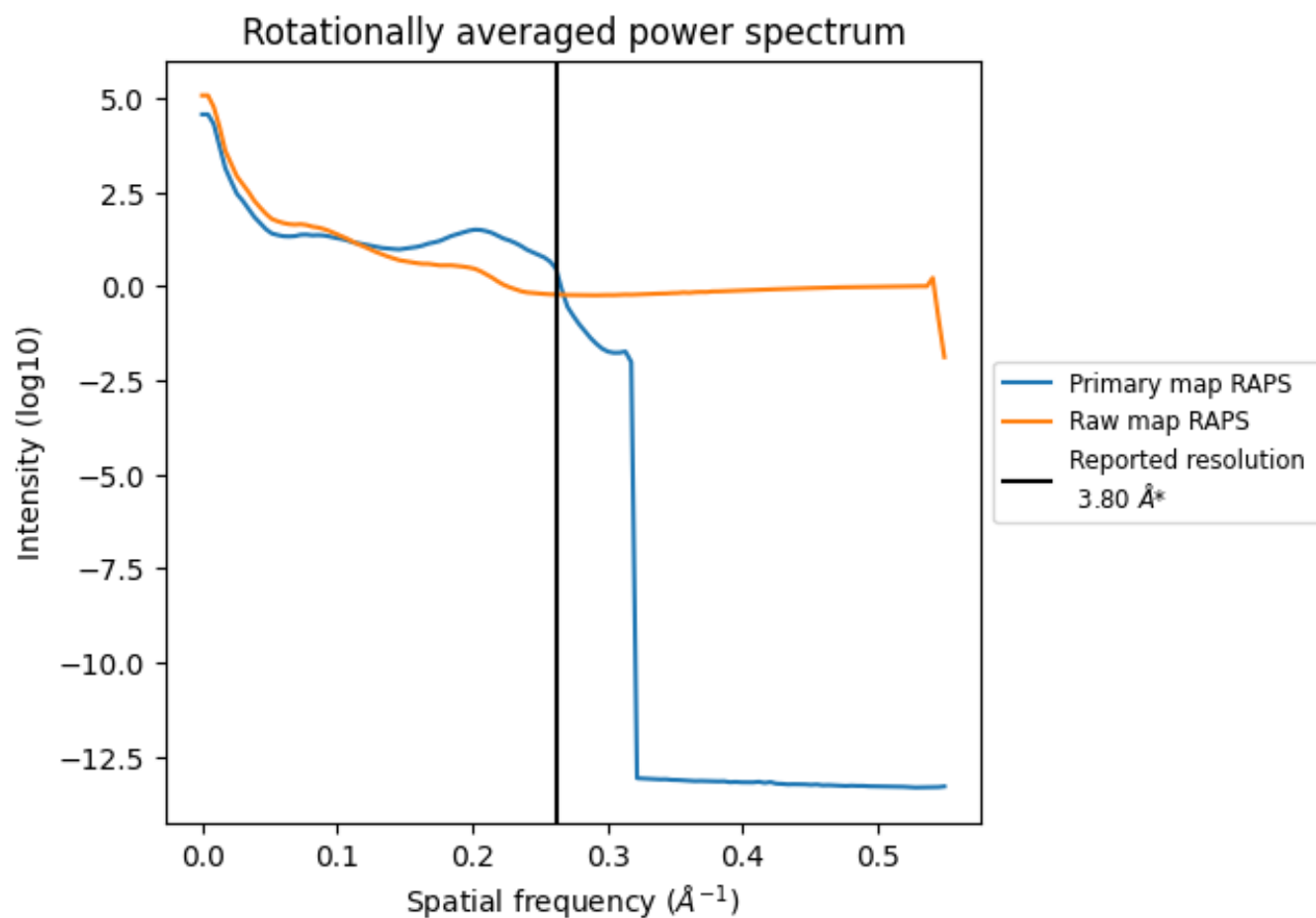
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 365 nm³; this corresponds to an approximate mass of 330 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 ⓘ

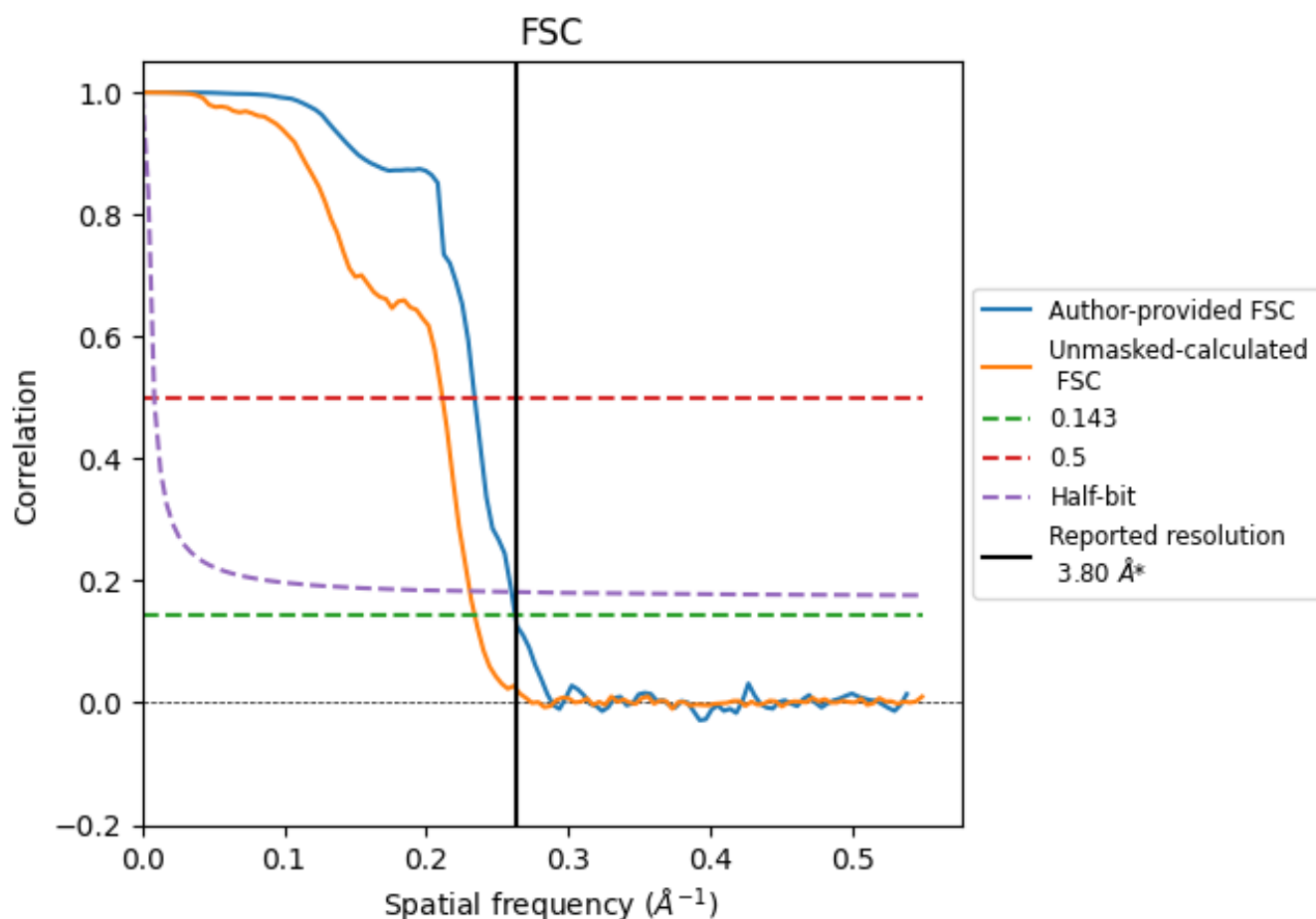


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

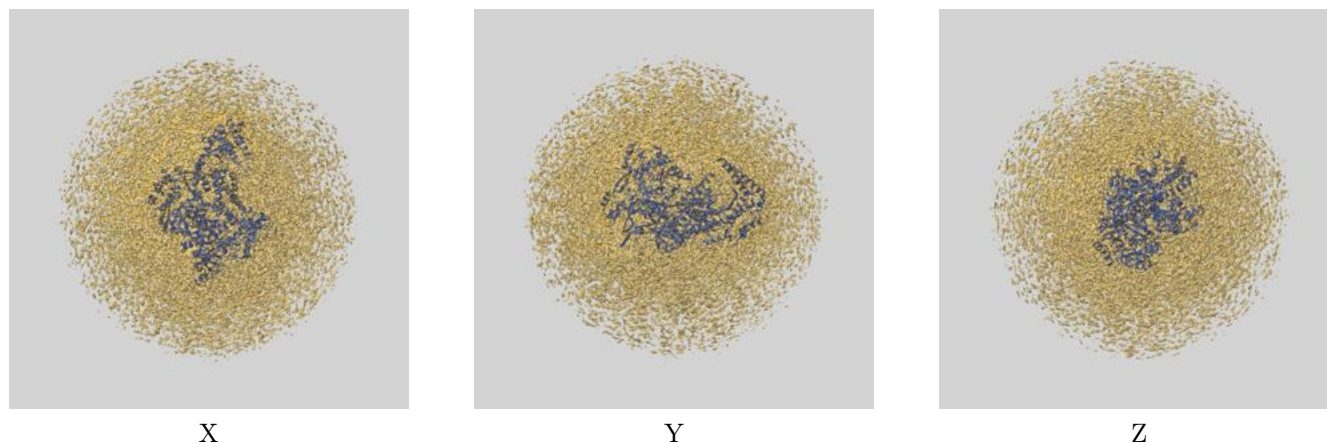
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.81	4.27	3.84
Unmasked-calculated*	4.27	4.73	4.33

*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 4.27 differs from the reported value 3.8 by more than 10 %

9 Map-model fit [i](#)

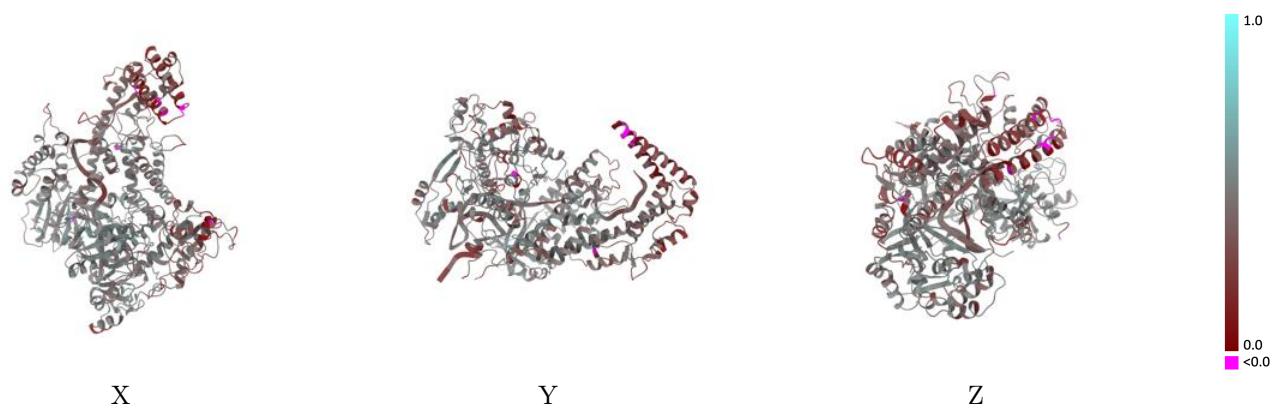
This section contains information regarding the fit between EMDB map EMD-52275 and PDB model 9HLX. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



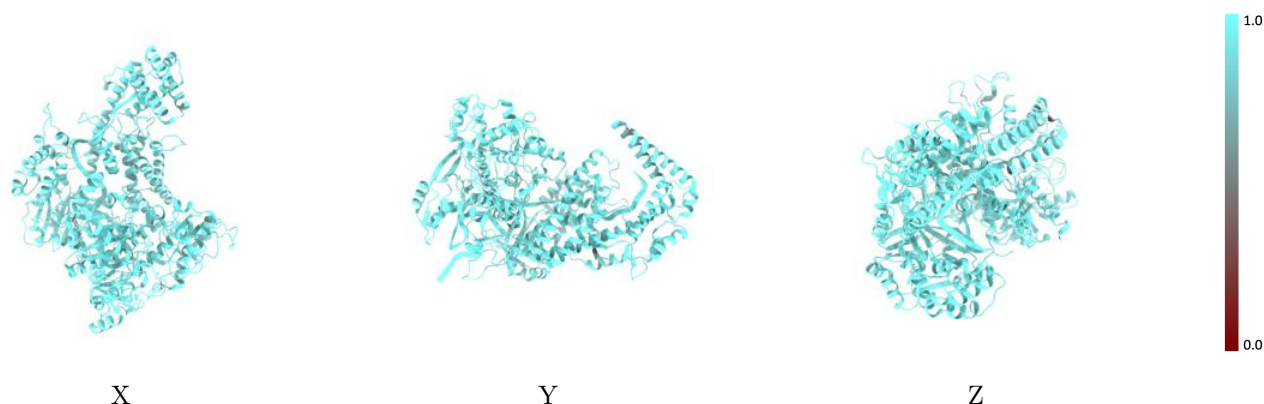
The images above show the 3D surface view of the map at the recommended contour level 0.009 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



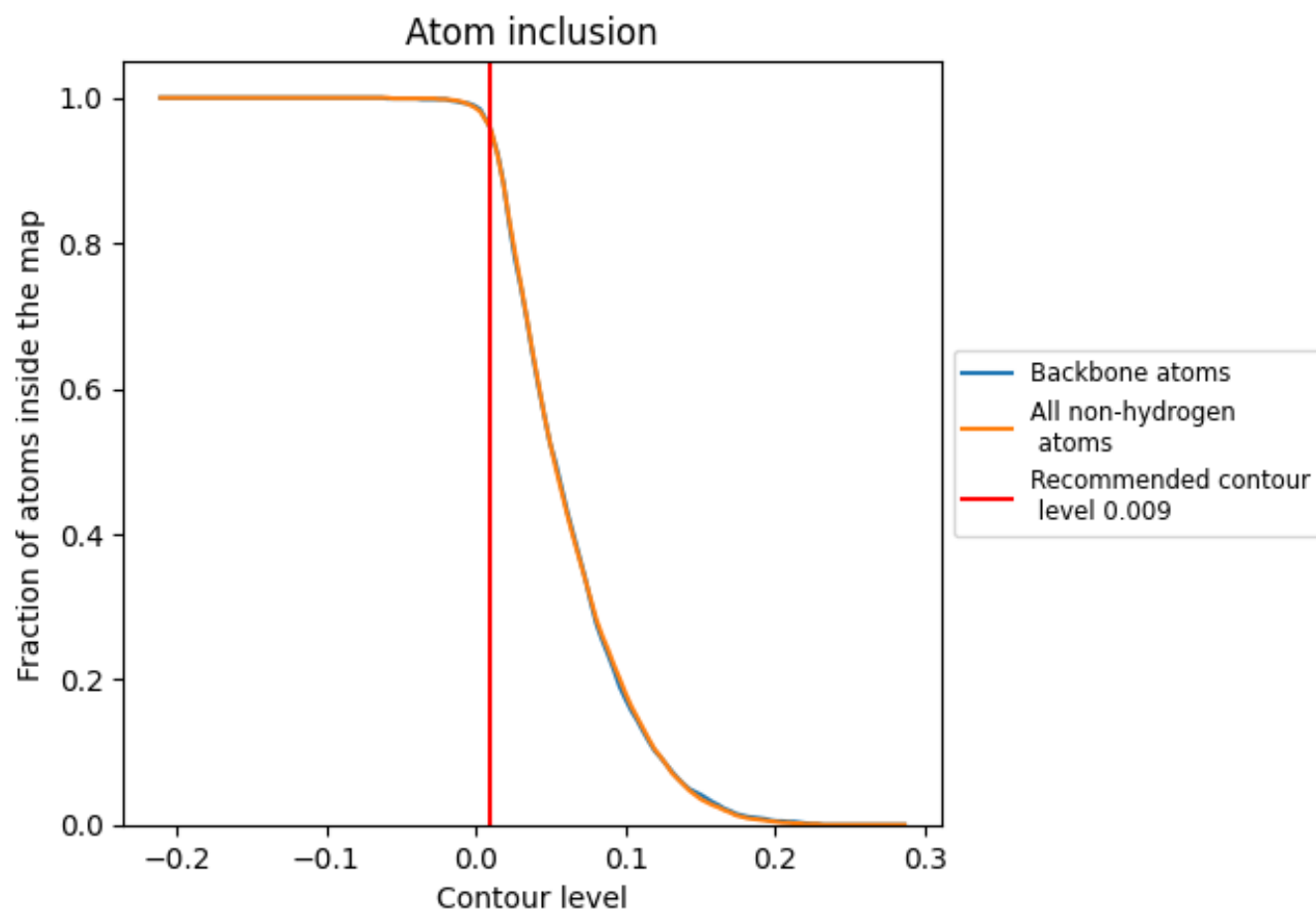
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.009).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 96% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9610	0.4170
A	0.9610	0.4200
B	0.9690	0.3870

