



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 06:10 PM UTC

PDB ID : 9HM6 / pdb_00009hm6
EMDB ID : EMD-52287
Title : Structure of Ba1Cas12a3 ternary complex
Authors : Yuan, B.; Heinz, D.W.
Deposited on : 2024-12-06
Resolution : 4.00 Å(reported)

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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

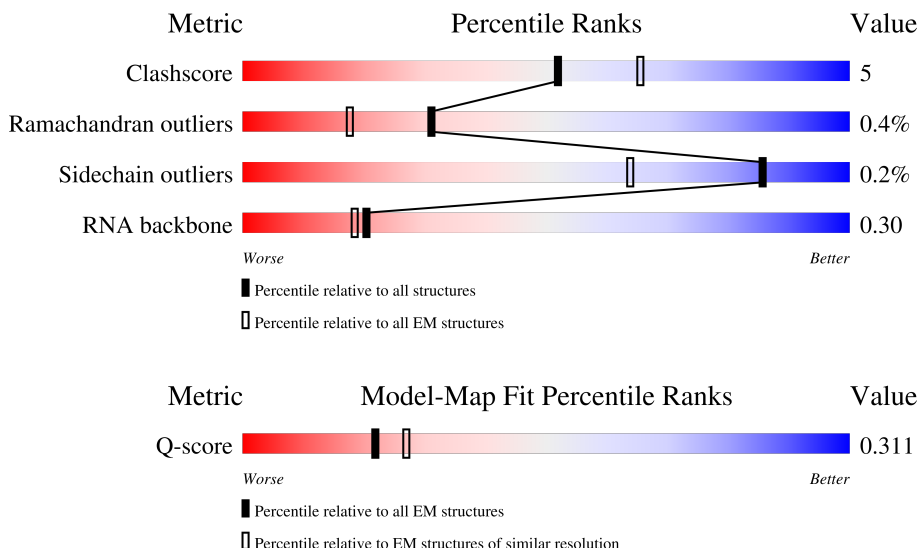
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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	7587 (3.50 - 4.50)

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	
2	B	65	
3	C	42	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18351 atoms, of which 8795 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	960	Total	C	H	N	O	S	0	0
			15793	5007	7936	1346	1484	20		

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	47	Total	C	H	N	O	P	0	0
			1506	448	502	176	333	47		

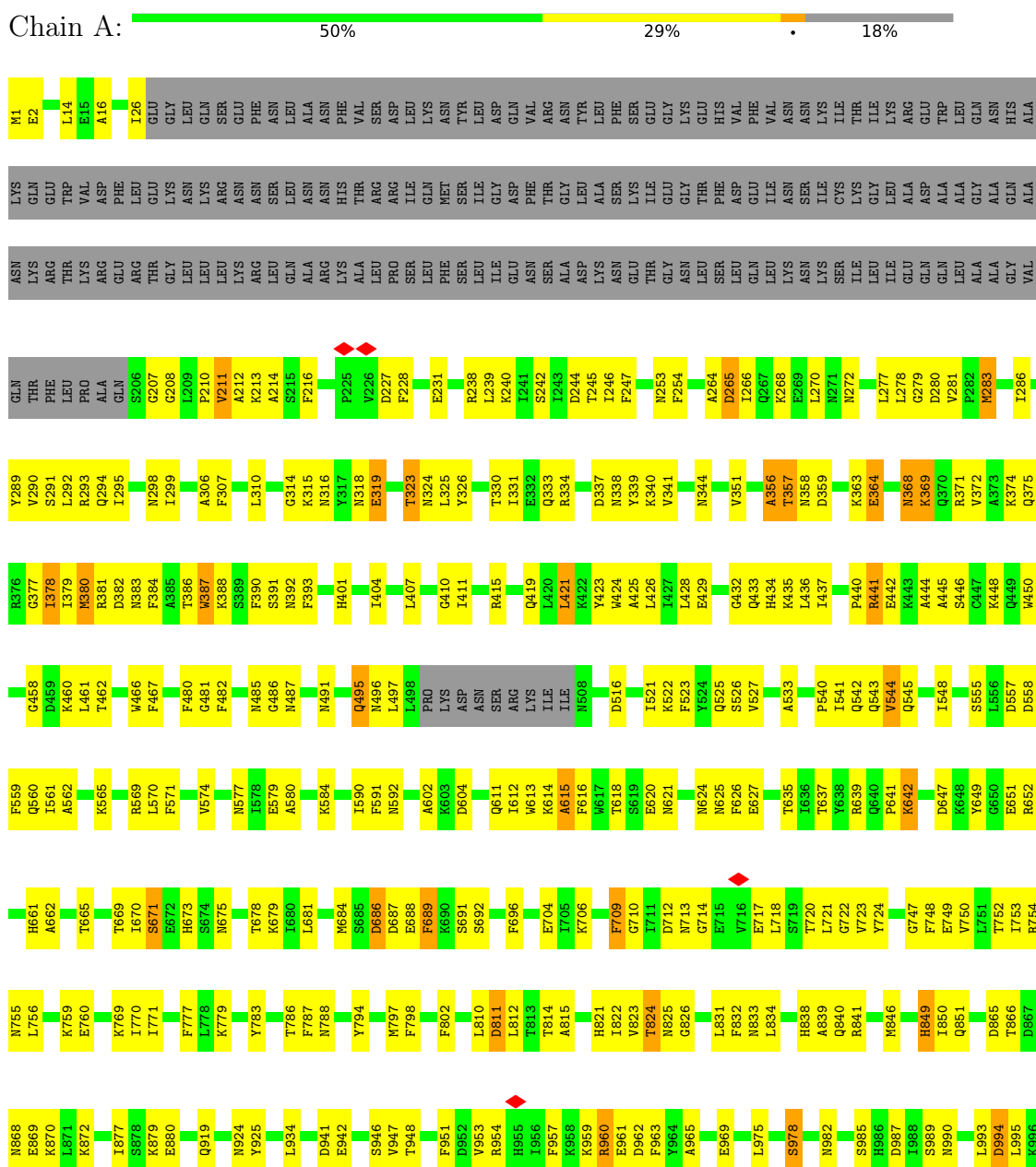
- Molecule 3 is a RNA chain called target RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	33	Total	C	H	N	O	P	0	0
			1052	312	357	123	227	33		

3 Residue-property plots

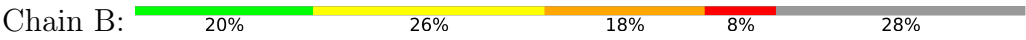
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

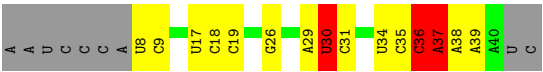




• Molecule 2: crRNA



• Molecule 3: target RNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	119647	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	0.369	Depositor
Minimum map value	-0.171	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.024	Depositor
Map size (\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 (\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	1.97	92/7994 (1.2%)	1.98	395/10733 (3.7%)
2	B	0.81	0/1122	1.42	18/1747 (1.0%)
3	C	0.80	0/775	1.23	3/1203 (0.2%)
All	All	1.81	92/9891 (0.9%)	1.86	416/13683 (3.0%)

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
2	B	0	12
3	C	0	11
All	All	0	23

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	661	HIS	CE1-NE2	-8.88	1.23	1.32
1	A	401	HIS	CE1-NE2	-8.87	1.23	1.32
1	A	838	HIS	CE1-NE2	-8.86	1.23	1.32
1	A	673	HIS	CE1-NE2	-8.83	1.23	1.32
1	A	849	HIS	ND1-CE1	-8.79	1.23	1.32
1	A	821	HIS	CE1-NE2	-8.77	1.23	1.32
1	A	1018	HIS	CE1-NE2	-8.74	1.23	1.32
1	A	434	HIS	CE1-NE2	-8.67	1.23	1.32
1	A	1078	ARG	CZ-NH2	-8.40	1.22	1.33
1	A	569	ARG	CZ-NH2	-8.32	1.22	1.33
1	A	841	ARG	CZ-NH2	-8.29	1.22	1.33
1	A	1021	ARG	CZ-NH2	-8.28	1.22	1.33
1	A	441	ARG	CZ-NH2	-8.27	1.22	1.33
1	A	1079	ALA	CA-CB	-8.27	1.43	1.54
1	A	238	ARG	CZ-NH2	-8.27	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	960	ARG	CZ-NH2	-8.27	1.22	1.33
1	A	371	ARG	CZ-NH2	-8.26	1.22	1.33
1	A	1056	ARG	CZ-NH2	-8.25	1.22	1.33
1	A	415	ARG	CZ-NH2	-8.24	1.22	1.33
1	A	334	ARG	CZ-NH2	-8.24	1.22	1.33
1	A	821	HIS	CD2-NE2	-8.23	1.28	1.37
1	A	652	ARG	CZ-NH2	-8.20	1.22	1.33
1	A	381	ARG	CZ-NH2	-8.20	1.22	1.33
1	A	838	HIS	CD2-NE2	-8.17	1.28	1.37
1	A	434	HIS	CD2-NE2	-8.14	1.28	1.37
1	A	661	HIS	CD2-NE2	-8.06	1.28	1.37
1	A	1018	HIS	CD2-NE2	-8.06	1.28	1.37
1	A	673	HIS	CD2-NE2	-8.00	1.29	1.37
1	A	401	HIS	CD2-NE2	-7.98	1.29	1.37
1	A	16	ALA	CA-CB	-7.95	1.42	1.53
1	A	425	ALA	CA-CB	-7.61	1.42	1.53
1	A	839	ALA	CA-CB	-7.15	1.42	1.53
1	A	212	ALA	CA-CB	-7.08	1.42	1.53
1	A	1008	ALA	CA-CB	-7.08	1.42	1.53
1	A	562	ALA	CA-CB	-7.07	1.42	1.53
1	A	306	ALA	CA-CB	-6.99	1.42	1.53
1	A	533	ALA	CA-CB	-6.96	1.42	1.53
1	A	602	ALA	CA-CB	-6.87	1.41	1.53
1	A	1078	ARG	CZ-NH1	-6.84	1.23	1.32
1	A	444	ALA	CA-CB	-6.84	1.42	1.53
1	A	569	ARG	CZ-NH1	-6.79	1.23	1.32
1	A	238	ARG	CZ-NH1	-6.75	1.23	1.32
1	A	381	ARG	CZ-NH1	-6.72	1.23	1.32
1	A	841	ARG	CZ-NH1	-6.71	1.23	1.32
1	A	1021	ARG	CZ-NH1	-6.70	1.23	1.32
1	A	441	ARG	CZ-NH1	-6.69	1.23	1.32
1	A	1056	ARG	CZ-NH1	-6.69	1.23	1.32
1	A	334	ARG	CZ-NH1	-6.68	1.23	1.32
1	A	371	ARG	CZ-NH1	-6.68	1.23	1.32
1	A	415	ARG	CZ-NH1	-6.66	1.23	1.32
1	A	652	ARG	CZ-NH1	-6.64	1.23	1.32
1	A	815	ALA	CA-CB	-6.64	1.42	1.53
1	A	960	ARG	CZ-NH1	-6.63	1.23	1.32
1	A	615	ALA	CA-CB	-6.62	1.42	1.53
1	A	965	ALA	CA-CB	-6.52	1.42	1.53
1	A	662	ALA	CA-CB	-6.50	1.42	1.53
1	A	445	ALA	CA-CB	-6.42	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	356	ALA	CA-CB	-6.36	1.42	1.53
1	A	826	GLY	N-CA	-6.16	1.37	1.45
1	A	377	GLY	N-CA	-6.08	1.38	1.45
1	A	1037	GLY	N-CA	-5.96	1.38	1.45
1	A	214	ALA	CA-CB	-5.87	1.42	1.54
1	A	207	GLY	N-CA	-5.74	1.37	1.45
1	A	1066	GLY	N-CA	-5.59	1.37	1.45
1	A	334	ARG	CD-NE	-5.57	1.38	1.46
1	A	486	GLY	N-CA	-5.57	1.37	1.45
1	A	841	ARG	CD-NE	-5.57	1.38	1.46
1	A	960	ARG	CD-NE	-5.52	1.38	1.46
1	A	569	ARG	CD-NE	-5.50	1.38	1.46
1	A	211	VAL	N-CA	-5.49	1.41	1.46
1	A	1070	PRO	CA-CB	-5.45	1.46	1.53
1	A	415	ARG	CD-NE	-5.44	1.38	1.46
1	A	1035	GLY	N-CA	-5.41	1.37	1.45
1	A	238	ARG	CD-NE	-5.38	1.38	1.46
1	A	1056	ARG	CD-NE	-5.36	1.38	1.46
1	A	1078	ARG	CD-NE	-5.36	1.38	1.46
1	A	1	MET	N-CA	-5.29	1.38	1.49
1	A	441	ARG	CD-NE	-5.28	1.38	1.46
1	A	1021	ARG	CD-NE	-5.28	1.38	1.46
1	A	481	GLY	N-CA	-5.28	1.37	1.45
1	A	652	ARG	CD-NE	-5.24	1.39	1.46
1	A	371	ARG	CD-NE	-5.24	1.39	1.46
1	A	641	PRO	CA-CB	-5.22	1.46	1.53
1	A	1033	GLY	N-CA	-5.21	1.37	1.45
1	A	381	ARG	CD-NE	-5.19	1.39	1.46
1	A	210	PRO	CA-CB	-5.17	1.46	1.53
1	A	432	GLY	N-CA	-5.16	1.37	1.45
1	A	208	GLY	N-CA	-5.16	1.37	1.45
1	A	279	GLY	N-CA	-5.16	1.37	1.45
1	A	314	GLY	N-CA	-5.16	1.38	1.45
1	A	1067	LEU	C-N	-5.07	1.29	1.33
1	A	540	PRO	CA-CB	-5.02	1.46	1.53

All (416) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	294	GLN	CA-C-N	8.02	130.94	120.60
1	A	294	GLN	C-N-CA	8.02	130.94	120.60
1	A	838	HIS	CA-CB-CG	7.48	121.28	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	788	ASN	CA-CB-CG	7.40	120.00	112.60
1	A	401	HIS	CA-CB-CG	7.38	121.18	113.80
1	A	591	PHE	CA-CB-CG	7.35	121.15	113.80
1	A	265	ASP	CA-CB-CG	7.34	119.94	112.60
1	A	254	PHE	CA-CB-CG	7.24	121.04	113.80
1	A	280	ASP	CA-CB-CG	7.23	119.83	112.60
1	A	675	ASN	CA-CB-CG	7.21	119.81	112.60
1	A	709	PHE	CA-CB-CG	7.15	120.95	113.80
1	A	482	PHE	CA-CB-CG	7.14	120.94	113.80
1	A	339	TYR	CA-C-N	7.12	129.70	120.44
1	A	339	TYR	C-N-CA	7.12	129.70	120.44
1	A	368	ASN	CA-CB-CG	7.11	119.71	112.60
1	A	467	PHE	CA-CB-CG	7.06	120.86	113.80
1	A	624	ASN	CA-CB-CG	7.05	119.65	112.60
1	A	571	PHE	CA-CB-CG	7.02	120.82	113.80
1	A	324	ASN	CA-CB-CG	6.99	119.59	112.60
1	A	849	HIS	CA-CB-CG	6.98	120.78	113.80
1	A	1034	PHE	CA-CB-CG	6.96	120.76	113.80
1	A	1062	PHE	CA-CB-CG	6.95	120.75	113.80
1	A	228	PHE	CA-CB-CG	6.94	120.74	113.80
1	A	390	PHE	CA-CB-CG	6.93	120.73	113.80
1	A	832	PHE	CA-CB-CG	6.92	120.72	113.80
1	A	227	ASP	CA-CB-CG	6.92	119.52	112.60
2	B	38	A	O4'-C1'-N9	6.87	118.80	108.50
1	A	423	TYR	CA-C-N	6.84	131.54	122.30
1	A	423	TYR	C-N-CA	6.84	131.54	122.30
1	A	383	ASN	CA-CB-CG	6.84	119.44	112.60
1	A	298	ASN	CA-CB-CG	6.79	119.39	112.60
1	A	821	HIS	CA-CB-CG	6.76	120.56	113.80
1	A	621	ASN	CA-CB-CG	6.76	119.36	112.60
1	A	384	PHE	CA-CB-CG	6.74	120.54	113.80
1	A	216	PHE	CA-CB-CG	6.74	120.54	113.80
1	A	344	ASN	CA-CB-CG	6.73	119.33	112.60
1	A	647	ASP	CA-CB-CG	6.72	119.32	112.60
1	A	661	HIS	CA-CB-CG	6.72	120.52	113.80
1	A	338	ASN	CA-CB-CG	6.69	119.29	112.60
1	A	962	ASP	CA-CB-CG	6.68	119.28	112.60
1	A	626	PHE	CA-CB-CG	6.67	120.47	113.80
1	A	487	ASN	CA-CB-CG	6.62	119.22	112.60
1	A	686	ASP	CA-CB-CG	6.62	119.22	112.60
1	A	811	ASP	CA-CB-CG	6.60	119.20	112.60
1	A	616	PHE	CA-CB-CG	6.59	120.39	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	755	ASN	CA-CB-CG	6.58	119.19	112.60
1	A	696	PHE	CA-CB-CG	6.58	120.38	113.80
1	A	382	ASP	CA-CB-CG	6.57	119.17	112.60
1	A	1097	PHE	CA-CB-CG	6.56	120.36	113.80
1	A	592	ASN	CA-CB-CG	6.56	119.16	112.60
1	A	957	PHE	CA-CB-CG	6.54	120.34	113.80
1	A	963	PHE	CA-CB-CG	6.54	120.34	113.80
1	A	307	PHE	CA-CB-CG	6.54	120.33	113.80
1	A	358	ASN	CA-CB-CG	6.51	119.11	112.60
1	A	604	ASP	CA-CB-CG	6.50	119.11	112.60
1	A	1018	HIS	CA-CB-CG	6.48	120.28	113.80
1	A	777	PHE	CA-CB-CG	6.44	120.24	113.80
1	A	337	ASP	CA-CB-CG	6.43	119.03	112.60
1	A	987	ASP	CA-C-N	6.43	131.16	123.19
1	A	987	ASP	C-N-CA	6.43	131.16	123.19
1	A	359	ASP	CA-CB-CG	6.41	119.01	112.60
1	A	592	ASN	CA-C-N	6.38	130.97	122.93
1	A	592	ASN	C-N-CA	6.38	130.97	122.93
1	A	1014	PHE	CA-CB-CG	6.38	120.18	113.80
1	A	1049	ASN	CA-C-N	6.38	128.83	120.60
1	A	1049	ASN	C-N-CA	6.38	128.83	120.60
1	A	637	THR	CA-C-N	6.33	132.10	122.93
1	A	637	THR	C-N-CA	6.33	132.10	122.93
1	A	392	ASN	CA-CB-CG	6.31	118.91	112.60
1	A	485	ASN	CA-CB-CG	6.31	118.91	112.60
1	A	371	ARG	CD-NE-CZ	6.28	133.19	124.40
1	A	1028	LEU	CA-C-N	6.27	130.32	122.48
1	A	1028	LEU	C-N-CA	6.27	130.32	122.48
1	A	434	HIS	CA-CB-CG	6.27	120.07	113.80
2	B	22	U	C2'-C3'-O3'	-6.27	104.30	113.70
2	B	38	A	C5'-C4'-O4'	6.26	119.18	109.80
1	A	635	THR	CA-C-N	6.25	131.42	123.10
1	A	635	THR	C-N-CA	6.25	131.42	123.10
2	B	37	G	C1'-O4'-C4'	-6.24	103.46	109.70
1	A	1067	LEU	CA-C-N	6.22	130.45	121.68
1	A	1067	LEU	C-N-CA	6.22	130.45	121.68
1	A	802	PHE	CA-CB-CG	6.20	120.00	113.80
1	A	441	ARG	CD-NE-CZ	6.17	133.04	124.40
1	A	612	ILE	N-CA-CB	6.16	117.09	110.62
1	A	381	ARG	CD-NE-CZ	6.15	133.01	124.40
1	A	523	PHE	CA-CB-CG	6.14	119.94	113.80
1	A	558	ASP	CA-CB-CG	6.14	118.74	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	LEU	CA-C-N	6.14	131.65	122.99
1	A	14	LEU	C-N-CA	6.14	131.65	122.99
1	A	491	ASN	CA-CB-CG	6.10	118.70	112.60
1	A	798	PHE	CA-CB-CG	6.08	119.89	113.80
1	A	480	PHE	CA-CB-CG	6.04	119.84	113.80
1	A	990	ASN	CA-CB-CG	6.04	118.64	112.60
2	B	36	U	C4'-C3'-O3'	6.03	118.44	109.40
2	B	37	G	C4'-C3'-O3'	6.01	118.41	109.40
1	A	673	HIS	CA-CB-CG	6.01	119.81	113.80
1	A	1049	ASN	CA-CB-CG	6.00	118.60	112.60
1	A	821	HIS	CA-C-N	5.99	130.57	122.90
1	A	821	HIS	C-N-CA	5.99	130.57	122.90
2	B	36	U	C1'-O4'-C4'	-5.99	103.71	109.70
1	A	440	PRO	CA-C-N	5.97	128.21	120.44
1	A	440	PRO	C-N-CA	5.97	128.21	120.44
1	A	569	ARG	CA-C-N	5.96	131.41	123.00
1	A	569	ARG	C-N-CA	5.96	131.41	123.00
1	A	652	ARG	CD-NE-CZ	5.96	132.75	124.40
1	A	426	LEU	CA-C-N	5.95	130.94	123.14
1	A	426	LEU	C-N-CA	5.95	130.94	123.14
1	A	689	PHE	N-CA-CB	5.95	118.64	110.01
1	A	559	PHE	CA-CB-CG	5.94	119.74	113.80
1	A	769	LYS	CA-C-N	5.93	128.25	120.60
1	A	769	LYS	C-N-CA	5.93	128.25	120.60
1	A	1078	ARG	CD-NE-CZ	5.93	132.70	124.40
1	A	625	ASN	CA-CB-CG	5.91	118.51	112.60
1	A	760	GLU	CA-C-N	5.91	131.32	122.99
1	A	760	GLU	C-N-CA	5.91	131.32	122.99
1	A	541	ILE	N-CA-CB	5.88	117.04	110.51
1	A	611	GLN	CA-C-N	5.88	128.48	120.77
1	A	611	GLN	C-N-CA	5.88	128.48	120.77
3	C	30	U	O4'-C1'-N1	5.86	117.29	108.50
1	A	750	VAL	CA-C-N	5.84	131.07	123.00
1	A	750	VAL	C-N-CA	5.84	131.07	123.00
1	A	1029	ILE	N-CA-CB	5.82	118.29	111.66
1	A	1056	ARG	CD-NE-CZ	5.81	132.53	124.40
1	A	642	LYS	CA-C-N	5.80	128.05	120.28
1	A	642	LYS	C-N-CA	5.80	128.05	120.28
1	A	1096	GLY	CA-C-N	5.79	131.63	122.94
1	A	1096	GLY	C-N-CA	5.79	131.63	122.94
1	A	410	GLY	CA-C-N	5.79	127.94	120.70
1	A	410	GLY	C-N-CA	5.79	127.94	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	450	TRP	CA-C-N	5.79	127.85	120.56
1	A	450	TRP	C-N-CA	5.79	127.85	120.56
1	A	393	PHE	CA-CB-CG	5.77	119.57	113.80
1	A	681	LEU	CA-C-N	5.77	127.94	120.44
1	A	681	LEU	C-N-CA	5.77	127.94	120.44
1	A	959	LYS	CA-C-N	5.76	131.61	122.62
1	A	959	LYS	C-N-CA	5.76	131.61	122.62
1	A	424	TRP	CA-C-N	5.75	130.30	122.19
1	A	424	TRP	C-N-CA	5.75	130.30	122.19
1	A	436	LEU	CA-C-N	5.75	130.98	122.99
1	A	436	LEU	C-N-CA	5.75	130.98	122.99
1	A	283	MET	CA-C-N	5.74	128.24	120.44
1	A	283	MET	C-N-CA	5.74	128.24	120.44
1	A	437	ILE	CA-C-N	5.72	131.06	123.00
1	A	437	ILE	C-N-CA	5.72	131.06	123.00
1	A	351	VAL	CA-C-N	5.71	127.93	120.28
1	A	351	VAL	C-N-CA	5.71	127.93	120.28
1	A	289	TYR	CA-C-N	5.71	130.92	122.99
1	A	289	TYR	C-N-CA	5.71	130.92	122.99
1	A	710	GLY	CA-C-N	5.68	130.50	123.12
1	A	710	GLY	C-N-CA	5.68	130.50	123.12
1	A	238	ARG	CD-NE-CZ	5.66	132.33	124.40
1	A	590	ILE	CA-C-N	5.66	131.45	122.62
1	A	590	ILE	C-N-CA	5.66	131.45	122.62
1	A	787	PHE	CA-CB-CG	5.66	119.46	113.80
2	B	26	C	C5'-C4'-C3'	-5.66	107.50	116.00
1	A	1021	ARG	CD-NE-CZ	5.66	132.33	124.40
1	A	747	GLY	CA-C-N	5.64	131.39	122.94
1	A	747	GLY	C-N-CA	5.64	131.39	122.94
1	A	419	GLN	CB-CG-CD	5.63	122.17	112.60
1	A	748	PHE	CA-C-N	5.62	129.77	120.94
1	A	748	PHE	C-N-CA	5.62	129.77	120.94
1	A	325	LEU	CA-C-N	5.59	128.04	120.38
1	A	325	LEU	C-N-CA	5.59	128.04	120.38
1	A	688	GLU	CB-CG-CD	5.55	122.04	112.60
1	A	1032	GLU	N-CA-CB	5.55	118.08	109.48
3	C	36	C	N1-C1'-C2'	5.53	120.30	112.00
1	A	277	LEU	CA-C-N	5.52	127.67	120.28
1	A	277	LEU	C-N-CA	5.52	127.67	120.28
1	A	1034	PHE	N-CA-CB	5.52	118.03	109.48
1	A	495	GLN	CA-C-N	5.51	127.67	120.28
1	A	495	GLN	C-N-CA	5.51	127.67	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	570	LEU	CA-C-N	5.50	130.91	122.93
1	A	570	LEU	C-N-CA	5.50	130.91	122.93
1	A	823	VAL	CA-C-N	5.50	127.60	120.44
1	A	823	VAL	C-N-CA	5.50	127.60	120.44
2	B	35	A	C4'-C3'-C2'	-5.48	97.12	102.60
1	A	540	PRO	CA-C-N	5.48	127.67	120.60
1	A	540	PRO	C-N-CA	5.48	127.67	120.60
1	A	357	THR	CA-C-N	5.48	130.06	122.77
1	A	357	THR	C-N-CA	5.48	130.06	122.77
1	A	1056	ARG	CG-CD-NE	5.47	124.04	112.00
1	A	665	THR	CA-C-N	5.47	129.32	121.50
1	A	665	THR	C-N-CA	5.47	129.32	121.50
1	A	380	MET	CA-C-N	5.46	127.54	120.44
1	A	380	MET	C-N-CA	5.46	127.54	120.44
1	A	1056	ARG	CA-CB-CG	5.46	125.02	114.10
1	A	441	ARG	CG-CD-NE	5.44	123.96	112.00
1	A	687	ASP	CA-C-N	5.43	127.50	120.44
1	A	687	ASP	C-N-CA	5.43	127.50	120.44
1	A	378	ILE	N-CA-CB	5.42	116.52	110.51
1	A	613	TRP	CA-C-N	5.41	127.47	120.44
1	A	613	TRP	C-N-CA	5.41	127.47	120.44
1	A	446	SER	CA-C-N	5.41	127.47	120.44
1	A	446	SER	C-N-CA	5.41	127.47	120.44
1	A	379	ILE	N-CA-CB	5.41	116.51	110.62
1	A	627	GLU	CA-C-N	5.41	129.60	122.30
1	A	627	GLU	C-N-CA	5.41	129.60	122.30
1	A	527	VAL	N-CA-CB	5.40	116.51	110.51
1	A	330	THR	CA-C-N	5.40	127.74	120.50
1	A	330	THR	C-N-CA	5.40	127.74	120.50
1	A	679	LYS	CA-C-N	5.39	130.55	123.11
1	A	679	LYS	C-N-CA	5.39	130.55	123.11
1	A	341	VAL	N-CA-CB	5.39	116.49	110.51
1	A	669	THR	CA-C-N	5.39	131.47	122.57
1	A	669	THR	C-N-CA	5.39	131.47	122.57
1	A	544	VAL	N-CA-CB	5.39	116.49	110.51
1	A	849	HIS	CE1-NE2-CD2	-5.38	103.62	109.00
1	A	779	LYS	CA-C-N	5.36	128.86	120.82
1	A	779	LYS	C-N-CA	5.36	128.86	120.82
1	A	2	GLU	CA-C-N	5.36	130.89	122.21
1	A	2	GLU	C-N-CA	5.36	130.89	122.21
1	A	994	ASP	O-C-N	-5.35	116.52	122.09
1	A	212	ALA	CA-C-N	5.35	130.98	122.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	ALA	C-N-CA	5.35	130.98	122.74
1	A	378	ILE	CA-C-N	5.35	127.39	120.70
1	A	378	ILE	C-N-CA	5.35	127.39	120.70
1	A	833	ASN	CA-C-N	5.35	127.71	120.65
1	A	833	ASN	C-N-CA	5.35	127.71	120.65
1	A	684	MET	CA-C-N	5.34	130.67	121.86
1	A	684	MET	C-N-CA	5.34	130.67	121.86
2	B	37	G	O5'-C5'-C4'	-5.32	103.72	111.70
1	A	1054	LEU	N-CA-CB	5.32	117.87	109.94
2	B	20	U	C2'-C3'-O3'	5.32	117.48	109.50
1	A	253	ASN	CA-C-N	5.31	130.91	122.94
1	A	253	ASN	C-N-CA	5.31	130.91	122.94
2	B	40	G	O4'-C1'-N9	5.31	116.46	108.50
1	A	559	PHE	CA-C-N	5.30	127.33	120.44
1	A	559	PHE	C-N-CA	5.30	127.33	120.44
1	A	1068	VAL	CB-CA-C	5.30	114.52	109.33
1	A	448	LYS	N-CA-CB	5.29	117.69	110.01
1	A	1001	LYS	CA-C-N	5.29	127.63	120.38
1	A	1001	LYS	C-N-CA	5.29	127.63	120.38
1	A	372	VAL	N-CA-CB	5.29	116.39	110.51
1	A	639	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	A	210	PRO	CA-C-N	5.28	128.92	121.53
1	A	210	PRO	C-N-CA	5.28	128.92	121.53
1	A	755	ASN	CA-C-N	5.28	127.79	120.29
1	A	755	ASN	C-N-CA	5.28	127.79	120.29
1	A	337	ASP	CA-C-N	5.28	127.30	120.44
1	A	337	ASP	C-N-CA	5.28	127.30	120.44
2	B	40	G	C4'-C3'-C2'	-5.28	97.32	102.60
1	A	822	ILE	CA-C-N	5.28	130.47	122.98
1	A	822	ILE	C-N-CA	5.28	130.47	122.98
1	A	671	SER	CA-C-N	5.27	130.85	122.94
1	A	671	SER	C-N-CA	5.27	130.85	122.94
1	A	293	ARG	NE-CZ-NH2	5.27	123.94	119.20
1	A	613	TRP	N-CA-CB	5.27	117.79	109.94
1	A	849	HIS	ND1-CG-CD2	-5.26	100.84	106.10
1	A	363	LYS	N-CA-CB	5.26	117.64	110.01
1	A	358	ASN	CA-C-N	5.25	127.58	120.65
1	A	358	ASN	C-N-CA	5.25	127.58	120.65
1	A	374	LYS	N-CA-CB	5.24	117.56	109.91
1	A	411	ILE	N-CA-CB	5.24	116.33	110.62
1	A	1081	GLY	CA-C-N	5.24	131.40	121.97
1	A	1081	GLY	C-N-CA	5.24	131.40	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	310	LEU	N-CA-CB	5.23	117.60	110.01
1	A	299	ILE	N-CA-CB	5.23	116.32	110.51
1	A	231	GLU	CA-C-N	5.23	127.59	120.54
1	A	231	GLU	C-N-CA	5.23	127.59	120.54
1	A	849	HIS	CG-CD2-NE2	5.22	112.42	107.20
1	A	1071	ILE	N-CA-C	5.22	115.09	107.88
1	A	783	TYR	CA-C-N	5.22	127.22	120.44
1	A	783	TYR	C-N-CA	5.22	127.22	120.44
1	A	387	TRP	CA-C-N	5.21	127.22	120.44
1	A	387	TRP	C-N-CA	5.21	127.22	120.44
1	A	989	SER	CA-C-N	5.21	127.69	120.29
1	A	989	SER	C-N-CA	5.21	127.69	120.29
1	A	1020	GLU	CA-C-N	5.21	127.22	120.44
1	A	1020	GLU	C-N-CA	5.21	127.22	120.44
1	A	1091	GLN	CA-C-N	5.21	131.26	123.23
1	A	1091	GLN	C-N-CA	5.21	131.26	123.23
1	A	340	LYS	N-CA-CB	5.21	117.56	110.01
1	A	749	GLU	CA-C-N	5.21	129.73	122.23
1	A	749	GLU	C-N-CA	5.21	129.73	122.23
1	A	364	GLU	CA-C-N	5.20	127.20	120.44
1	A	364	GLU	C-N-CA	5.20	127.20	120.44
1	A	295	ILE	N-CA-CB	5.20	116.28	110.51
1	A	407	LEU	CA-C-N	5.20	127.19	120.44
1	A	407	LEU	C-N-CA	5.20	127.19	120.44
1	A	839	ALA	CA-C-N	5.19	127.19	120.44
1	A	839	ALA	C-N-CA	5.19	127.19	120.44
1	A	565	LYS	CA-C-N	5.19	128.86	120.55
1	A	565	LYS	C-N-CA	5.19	128.86	120.55
1	A	544	VAL	CA-C-N	5.19	127.19	120.44
1	A	544	VAL	C-N-CA	5.19	127.19	120.44
2	B	50	C	C2'-C3'-O3'	5.19	121.49	113.70
1	A	434	HIS	CA-C-N	5.19	130.72	122.94
1	A	434	HIS	C-N-CA	5.19	130.72	122.94
1	A	621	ASN	N-CA-CB	5.19	117.53	110.01
1	A	419	GLN	CA-C-N	5.18	128.90	120.60
1	A	419	GLN	C-N-CA	5.18	128.90	120.60
1	A	377	GLY	CA-C-N	5.18	127.28	120.60
1	A	377	GLY	C-N-CA	5.18	127.28	120.60
1	A	421	LEU	CA-C-N	5.18	129.67	121.18
1	A	421	LEU	C-N-CA	5.18	129.67	121.18
1	A	1014	PHE	N-CA-CB	5.17	117.51	110.01
1	A	298	ASN	CA-C-N	5.17	127.27	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	ASN	C-N-CA	5.17	127.27	120.60
1	A	323	THR	CA-C-N	5.17	130.92	122.65
1	A	323	THR	C-N-CA	5.17	130.92	122.65
1	A	433	GLN	CA-C-N	5.17	130.35	122.65
1	A	433	GLN	C-N-CA	5.17	130.35	122.65
1	A	523	PHE	CA-C-N	5.17	127.16	120.44
1	A	523	PHE	C-N-CA	5.17	127.16	120.44
1	A	558	ASP	CA-C-N	5.17	127.16	120.44
1	A	558	ASP	C-N-CA	5.17	127.16	120.44
1	A	834	LEU	N-CA-CB	5.17	117.45	109.91
1	A	1053	ILE	N-CA-CB	5.16	116.25	110.62
1	A	838	HIS	CA-C-N	5.16	127.15	120.44
1	A	838	HIS	C-N-CA	5.16	127.15	120.44
1	A	525	GLN	CA-C-N	5.16	127.14	120.44
1	A	525	GLN	C-N-CA	5.16	127.14	120.44
1	A	391	SER	CA-C-N	5.15	127.14	120.44
1	A	391	SER	C-N-CA	5.15	127.14	120.44
1	A	749	GLU	N-CA-CB	5.15	117.59	110.17
1	A	369	LYS	CA-C-N	5.14	127.48	120.54
1	A	369	LYS	C-N-CA	5.14	127.48	120.54
1	A	1058	LEU	N-CA-CB	5.14	117.60	109.94
1	A	997	ILE	N-CA-CB	5.14	116.22	110.62
1	A	291	SER	CA-C-N	5.13	127.11	120.44
1	A	291	SER	C-N-CA	5.13	127.11	120.44
1	A	371	ARG	N-CA-CB	5.13	117.58	109.94
1	A	466	TRP	CA-C-N	5.13	130.37	122.93
1	A	466	TRP	C-N-CA	5.13	130.37	122.93
1	A	770	ILE	N-CA-CB	5.13	116.20	110.51
1	A	383	ASN	CA-C-N	5.12	129.97	122.85
1	A	383	ASN	C-N-CA	5.12	129.97	122.85
1	A	379	ILE	CA-C-N	5.12	127.10	120.44
1	A	379	ILE	C-N-CA	5.12	127.10	120.44
1	A	1058	LEU	CA-C-N	5.12	127.10	120.44
1	A	1058	LEU	C-N-CA	5.12	127.10	120.44
1	A	542	GLN	CA-C-N	5.12	127.41	120.44
1	A	542	GLN	C-N-CA	5.12	127.41	120.44
1	A	691	SER	CA-C-N	5.12	127.10	120.44
1	A	691	SER	C-N-CA	5.12	127.10	120.44
1	A	797	MET	N-CA-CB	5.12	117.60	109.82
1	A	268	LYS	N-CA-CB	5.12	117.56	109.94
1	A	435	LYS	CA-C-N	5.12	130.28	122.65
1	A	435	LYS	C-N-CA	5.12	130.28	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	752	THR	CA-C-N	5.12	127.94	120.98
1	A	752	THR	C-N-CA	5.12	127.94	120.98
1	A	333	GLN	CA-C-N	5.11	127.40	120.65
1	A	333	GLN	C-N-CA	5.11	127.40	120.65
1	A	543	GLN	CB-CG-CD	5.11	121.29	112.60
1	A	696	PHE	N-CA-CB	5.10	117.41	110.01
2	B	45	U	C4'-C3'-C2'	-5.10	97.50	102.60
1	A	292	LEU	N-CA-CB	5.10	117.40	110.01
1	A	565	LYS	N-CA-CB	5.10	117.54	109.94
1	A	978	SER	CA-C-N	5.10	127.07	120.44
1	A	978	SER	C-N-CA	5.10	127.07	120.44
1	A	824	THR	CA-C-N	5.10	130.68	122.83
1	A	824	THR	C-N-CA	5.10	130.68	122.83
1	A	240	LYS	CA-C-N	5.09	127.42	120.35
1	A	240	LYS	C-N-CA	5.09	127.42	120.35
1	A	386	THR	CA-C-N	5.09	127.36	120.65
1	A	386	THR	C-N-CA	5.09	127.36	120.65
1	A	387	TRP	N-CA-CB	5.09	117.34	109.91
1	A	561	ILE	CA-C-N	5.09	127.05	120.44
1	A	561	ILE	C-N-CA	5.09	127.05	120.44
1	A	526	SER	CA-C-N	5.08	127.15	120.60
1	A	526	SER	C-N-CA	5.08	127.15	120.60
1	A	616	PHE	N-CA-CB	5.08	117.37	110.01
1	A	1020	GLU	N-CA-CB	5.07	117.53	109.82
2	B	45	U	C2'-C3'-O3'	5.07	121.31	113.70
1	A	840	GLN	N-CA-CB	5.07	117.36	110.01
1	A	392	ASN	CA-C-N	5.07	127.38	120.54
1	A	392	ASN	C-N-CA	5.07	127.38	120.54
1	A	620	GLU	CA-C-N	5.07	127.03	120.44
1	A	620	GLU	C-N-CA	5.07	127.03	120.44
1	A	754	ARG	CA-C-N	5.06	130.46	123.07
1	A	754	ARG	C-N-CA	5.06	130.46	123.07
1	A	614	LYS	N-CA-CB	5.06	117.35	110.01
1	A	264	ALA	CA-C-N	5.06	127.02	120.44
1	A	264	ALA	C-N-CA	5.06	127.02	120.44
2	B	51	C	C2'-C3'-O3'	5.06	121.29	113.70
1	A	615	ALA	CA-C-N	5.06	127.02	120.44
1	A	615	ALA	C-N-CA	5.06	127.02	120.44
1	A	315	LYS	CB-CG-CD	5.05	122.92	111.30
1	A	331	ILE	CA-C-N	5.05	128.38	120.75
1	A	331	ILE	C-N-CA	5.05	128.38	120.75
2	B	49	U	C2'-C3'-O3'	5.05	121.28	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	759	LYS	CA-C-N	5.05	130.44	122.36
1	A	759	LYS	C-N-CA	5.05	130.44	122.36
1	A	1059	TYR	N-CA-CB	5.04	117.33	110.01
1	A	307	PHE	N-CA-CB	5.04	117.32	110.01
1	A	523	PHE	N-CA-CB	5.04	117.45	109.94
1	A	290	VAL	CA-C-N	5.04	129.02	121.72
1	A	290	VAL	C-N-CA	5.04	129.02	121.72
1	A	559	PHE	N-CA-CB	5.03	117.30	110.01
3	C	37	A	C2'-C3'-O3'	5.03	121.25	113.70
1	A	651	GLU	N-CA-CB	5.03	117.24	110.10
1	A	213	LYS	CG-CD-CE	5.03	122.86	111.30
1	A	319	GLU	CA-C-N	5.02	127.32	120.54
1	A	319	GLU	C-N-CA	5.02	127.32	120.54
1	A	560	GLN	N-CA-CB	5.02	117.29	110.01
1	A	1017	LYS	CA-CB-CG	5.02	124.14	114.10
1	A	786	THR	CA-C-N	5.02	130.27	122.49
1	A	786	THR	C-N-CA	5.02	130.27	122.49
1	A	621	ASN	CA-C-N	5.02	127.01	120.28
1	A	621	ASN	C-N-CA	5.02	127.01	120.28
1	A	390	PHE	N-CA-CB	5.02	117.50	110.12
1	A	388	LYS	N-CA-CB	5.01	117.28	110.01
1	A	545	GLN	N-CA-CB	5.01	117.28	110.01
1	A	1014	PHE	CA-C-N	5.01	126.95	120.44
1	A	1014	PHE	C-N-CA	5.01	126.95	120.44
1	A	1016	TYR	N-CA-CB	5.01	117.41	109.94
1	A	692	SER	N-CA-CB	5.01	117.28	110.01
1	A	388	LYS	CA-C-N	5.01	126.95	120.44
1	A	388	LYS	C-N-CA	5.01	126.95	120.44
1	A	684	MET	CA-CB-CG	5.01	124.11	114.10
1	A	993	LEU	N-CA-CB	5.01	117.43	109.82
1	A	794	TYR	N-CA-CB	5.00	117.40	109.94
1	A	961	GLU	CA-C-N	5.00	126.98	120.28
1	A	961	GLU	C-N-CA	5.00	126.98	120.28
1	A	541	ILE	CA-C-N	5.00	126.94	120.44
1	A	541	ILE	C-N-CA	5.00	126.94	120.44

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	22	U	Sidechain
2	B	25	A	Sidechain

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Mol	Chain	Res	Type	Group
2	B	29	U	Sidechain
2	B	31	G	Sidechain
2	B	37	G	Sidechain
2	B	42	A	Sidechain
2	B	45	U	Sidechain
2	B	52	U	Sidechain
2	B	53	G	Sidechain
2	B	58	A	Sidechain
2	B	59	U	Sidechain
2	B	62	U	Sidechain
3	C	17	U	Sidechain
3	C	18	C	Sidechain
3	C	19	C	Sidechain
3	C	26	G	Sidechain
3	C	30	U	Sidechain
3	C	31	C	Sidechain
3	C	34	U	Sidechain
3	C	35	C	Sidechain
3	C	36	C	Sidechain
3	C	37	A	Sidechain
3	C	39	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	7857	7936	7933	97	0
2	B	1004	502	503	2	0
3	C	695	357	358	0	0
All	All	9556	8795	8794	99	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 5.

All (99) 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:555:SER:OG	1:A:557:ASP:OD1	1.91	0.88
1:A:872:LYS:NZ	1:A:948:THR:O	2.16	0.78
1:A:712:ASP:OD1	1:A:713:ASN:N	2.17	0.78
1:A:717:GLU:OE2	1:A:960:ARG:NH2	2.19	0.76
1:A:814:THR:OG1	1:A:824:THR:O	2.04	0.74
1:A:925:TYR:OH	1:A:954:ARG:NE	2.24	0.71
1:A:866:THR:OG1	1:A:869:GLU:OE2	2.06	0.71
1:A:880:GLU:N	1:A:880:GLU:OE1	2.26	0.69
1:A:720:THR:HG21	1:A:1137:ASP:HB3	1.75	0.69
1:A:721:LEU:HD23	1:A:722:GLY:N	2.08	0.68
1:A:1001:LYS:NZ	1:A:1049:ASN:OD1	2.28	0.67
1:A:720:THR:HG21	1:A:1137:ASP:CB	2.25	0.66
1:A:364:GLU:OE2	1:A:368:ASN:ND2	2.30	0.65
1:A:316:ASN:OD1	1:A:318:ASN:N	2.29	0.65
1:A:969:GLU:N	1:A:969:GLU:OE1	2.28	0.64
1:A:706:LYS:NZ	1:A:1023:LEU:O	2.25	0.63
1:A:244:ASP:OD1	1:A:245:THR:HG23	1.99	0.61
1:A:319:GLU:O	1:A:323:THR:HG23	2.00	0.61
1:A:496:ASN:OD1	1:A:497:LEU:N	2.34	0.61
1:A:850:ILE:O	1:A:850:ILE:HG22	2.00	0.60
1:A:1082:ILE:HG22	1:A:1082:ILE:O	2.01	0.60
1:A:615:ALA:O	1:A:618:THR:HG22	2.02	0.60
1:A:242:SER:OG	1:A:244:ASP:OD1	2.19	0.59
1:A:495:GLN:N	1:A:495:GLN:OE1	2.36	0.59
1:A:975:LEU:O	1:A:978:SER:OG	2.21	0.58
1:A:709:PHE:O	1:A:1030:ILE:HG22	2.04	0.58
1:A:879:LYS:NZ	1:A:919:GLN:O	2.37	0.58
1:A:1030:ILE:HD12	1:A:1096:GLY:C	2.30	0.57
1:A:756:LEU:HD12	1:A:771:ILE:HD12	1.88	0.56
1:A:714:GLY:O	1:A:1051:TYR:OH	2.24	0.56
1:A:1030:ILE:HD12	1:A:1096:GLY:O	2.06	0.56
1:A:265:ASP:OD2	1:A:326:TYR:OH	2.16	0.54
1:A:428:LEU:HD23	1:A:429:GLU:N	2.23	0.54
1:A:810:LEU:HD23	1:A:811:ASP:C	2.33	0.54
1:A:1029:ILE:O	1:A:1029:ILE:HG23	2.07	0.53
1:A:460:LYS:O	1:A:462:THR:N	2.42	0.52
1:A:496:ASN:OD1	1:A:497:LEU:HD22	2.09	0.52
1:A:865:ASP:O	1:A:870:LYS:NZ	2.33	0.52
1:A:544:VAL:HG23	1:A:548:ILE:HD12	1.92	0.52
1:A:868:ASN:ND2	1:A:946:SER:O	2.43	0.51
1:A:1115:LEU:HD11	1:A:1119:THR:O	2.11	0.51
1:A:380:MET:SD	1:A:387:TRP:NE1	2.84	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1103:THR:O	1:A:1106:GLU:OE1	2.30	0.50
1:A:458:GLY:N	1:A:574:VAL:HG21	2.27	0.50
1:A:1020:GLU:O	1:A:1024:GLY:N	2.43	0.50
1:A:686:ASP:O	1:A:689:PHE:CD1	2.65	0.50
1:A:849:HIS:O	1:A:851:GLN:NE2	2.37	0.48
1:A:941:ASP:O	1:A:942:GLU:HG2	2.13	0.48
1:A:1117:HIS:CB	1:A:1136:ASN:HA	2.44	0.47
1:A:947:VAL:O	1:A:948:THR:HG23	2.14	0.47
1:A:1101:ALA:O	1:A:1147:ARG:NH2	2.42	0.47
2:B:28:G:H2'	2:B:29:U:H5''	1.95	0.47
2:B:37:G:C2	2:B:38:A:C8	3.02	0.47
1:A:1117:HIS:HB2	1:A:1136:ASN:HA	1.97	0.46
1:A:982:ASN:O	1:A:985:SER:OG	2.29	0.46
1:A:1117:HIS:CD2	1:A:1118:THR:HG23	2.50	0.46
1:A:1030:ILE:HD11	1:A:1098:ILE:HG23	1.97	0.46
1:A:380:MET:SD	1:A:380:MET:C	2.99	0.46
1:A:266:ILE:O	1:A:270:LEU:N	2.49	0.46
1:A:1085:ASN:HB3	1:A:1088:ALA:HB2	1.97	0.46
1:A:1117:HIS:O	1:A:1118:THR:OG1	2.29	0.46
1:A:239:LEU:HD22	1:A:278:LEU:HD13	1.98	0.46
1:A:580:ALA:O	1:A:584:LYS:N	2.37	0.46
1:A:1110:CYS:O	1:A:1112:GLU:N	2.47	0.45
1:A:678:THR:HG22	1:A:678:THR:O	2.16	0.45
1:A:1029:ILE:O	1:A:1029:ILE:CG2	2.64	0.45
1:A:281:VAL:HB	1:A:283:MET:HE2	1.99	0.45
1:A:1115:LEU:HD13	1:A:1121:CYS:HA	1.99	0.45
1:A:723:VAL:HG22	1:A:724:TYR:N	2.32	0.44
1:A:26:ILE:HD11	1:A:211:VAL:HG11	1.99	0.44
1:A:239:LEU:HD21	1:A:404:ILE:HD13	1.99	0.44
1:A:356:ALA:O	1:A:357:THR:C	2.60	0.44
1:A:877:ILE:HG22	1:A:877:ILE:O	2.17	0.44
1:A:704:GLU:OE2	1:A:1026:GLU:N	2.46	0.43
1:A:812:LEU:HD23	1:A:812:LEU:O	2.19	0.43
1:A:1120:THR:HG22	1:A:1121:CYS:N	2.34	0.43
1:A:670:ILE:HG22	1:A:671:SER:N	2.34	0.43
1:A:753:ILE:HD12	1:A:825:ASN:OD1	2.19	0.43
1:A:441:ARG:NE	1:A:442:GLU:OE2	2.52	0.43
1:A:239:LEU:CD2	1:A:278:LEU:HD13	2.48	0.43
1:A:718:LEU:CD1	1:A:1050:ILE:HD12	2.48	0.42
1:A:934:LEU:HB2	1:A:953:VAL:HG11	2.00	0.42
1:A:1033:GLY:O	1:A:1078:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1038:LYS:NZ	1:A:1083:GLU:OE2	2.51	0.42
1:A:375:GLN:HA	1:A:378:ILE:HD12	2.01	0.42
1:A:516:ASP:N	1:A:516:ASP:OD1	2.51	0.42
1:A:934:LEU:CB	1:A:953:VAL:HG11	2.50	0.42
1:A:577:ASN:OD1	1:A:577:ASN:O	2.38	0.42
1:A:924:ASN:OD1	1:A:925:TYR:N	2.53	0.41
1:A:831:LEU:HD22	1:A:1004:LEU:HD21	2.02	0.41
1:A:239:LEU:HD22	1:A:278:LEU:HD22	2.02	0.41
1:A:521:ILE:HG23	1:A:522:LYS:N	2.35	0.41
1:A:953:VAL:O	1:A:953:VAL:CG1	2.68	0.41
1:A:244:ASP:OD1	1:A:245:THR:N	2.53	0.41
1:A:642:LYS:HE3	1:A:642:LYS:HA	2.03	0.41
1:A:246:ILE:HG13	1:A:247:PHE:N	2.36	0.40
1:A:846:MET:HE2	1:A:951:PHE:CD2	2.56	0.40
1:A:994:ASP:OD1	1:A:995:LEU:N	2.54	0.40
1:A:579:GLU:HG2	1:A:580:ALA:N	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	952/1168 (82%)	880 (92%)	68 (7%)	4 (0%)	<div>30</div> <div>65</div>

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	286	ILE
1	A	461	LEU
1	A	421	LEU
1	A	272	ASN

5.3.2 Protein sidechains [i](#)

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	867/1049 (83%)	865 (100%)	2 (0%)	87	87

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	369	LYS
1	A	649	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	358	ASN
1	A	361	GLN
1	A	401	HIS
1	A	419	GLN
1	A	431	ASN
1	A	656	ASN
1	A	663	GLN
1	A	764	ASN
1	A	955	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	47/65 (72%)	24 (51%)	14 (29%)
3	C	33/42 (78%)	4 (12%)	3 (9%)
All	All	80/107 (74%)	28 (35%)	17 (21%)

All (28) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	19	A

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Mol	Chain	Res	Type
2	B	20	U
2	B	21	U
2	B	22	U
2	B	23	C
2	B	24	U
2	B	26	C
2	B	27	U
2	B	28	G
2	B	29	U
2	B	30	U
2	B	31	G
2	B	37	G
2	B	38	A
2	B	40	G
2	B	41	G
2	B	46	C
2	B	48	C
2	B	50	C
2	B	51	C
2	B	52	U
2	B	59	U
2	B	62	U
2	B	63	G
3	C	9	C
3	C	30	U
3	C	36	C
3	C	38	A

All (17) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	18	A
2	B	20	U
2	B	23	C
2	B	27	U
2	B	36	U
2	B	37	G
2	B	38	A
2	B	40	G
2	B	45	U
2	B	47	G
2	B	49	U

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Mol	Chain	Res	Type
2	B	50	C
2	B	51	C
2	B	62	U
3	C	8	U
3	C	29	A
3	C	37	A

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.

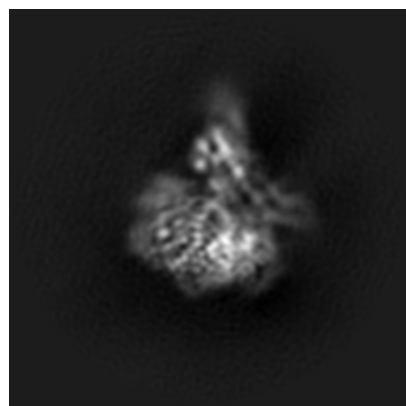
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52287. These allow visual inspection of the internal detail of the map and identification of artifacts.

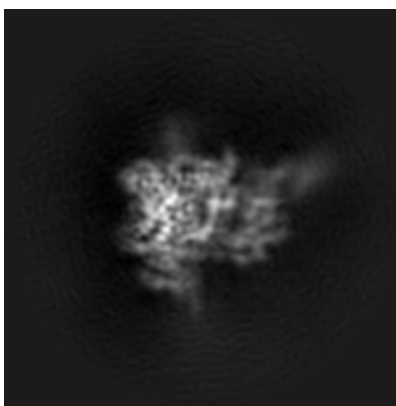
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

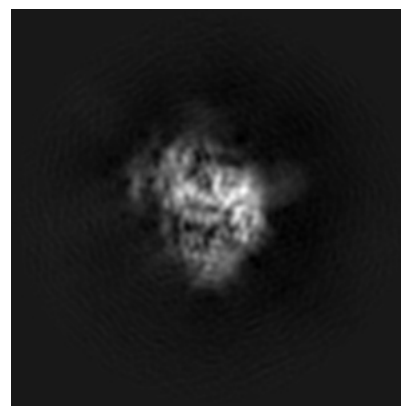
6.1.1 Primary map



X

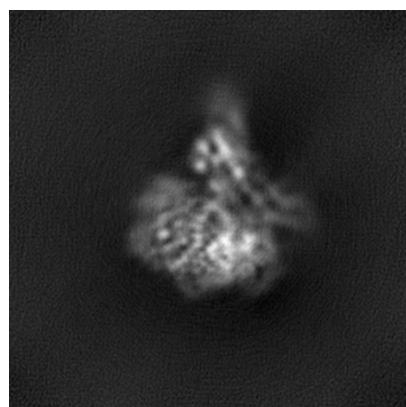


Y

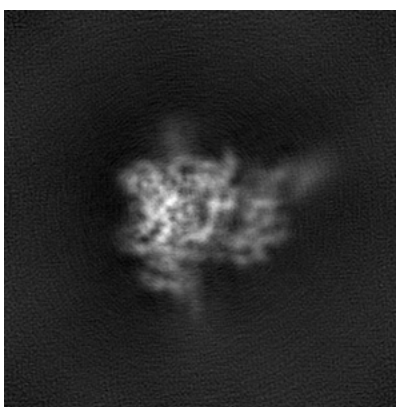


Z

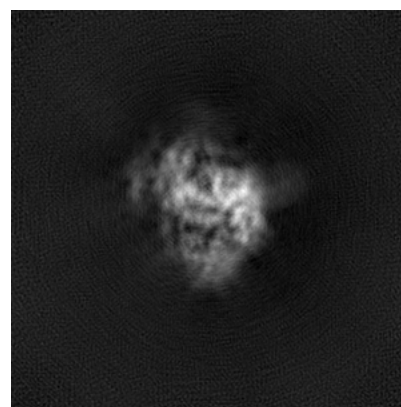
6.1.2 Raw map



X



Y

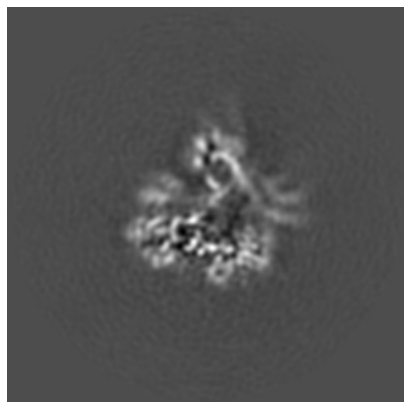


Z

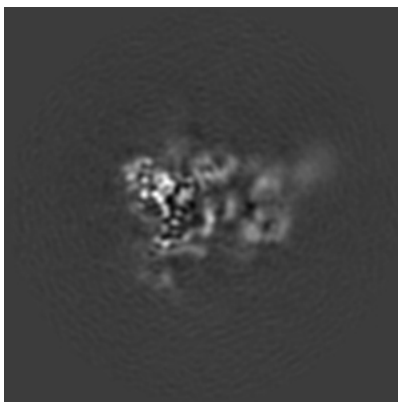
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

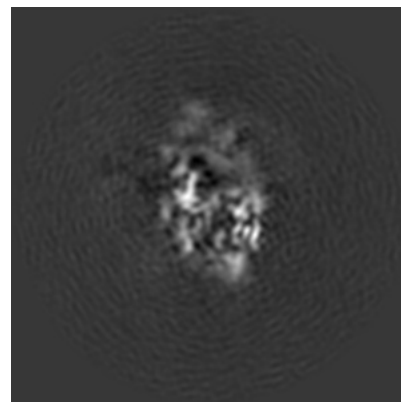
6.2.1 Primary map



X Index: 128

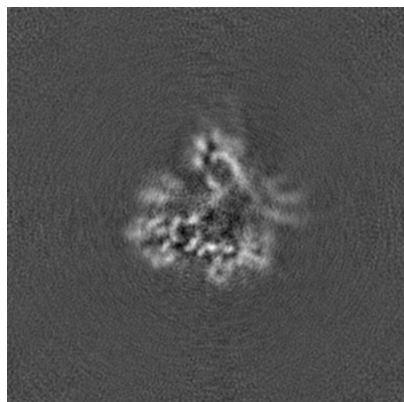


Y Index: 128

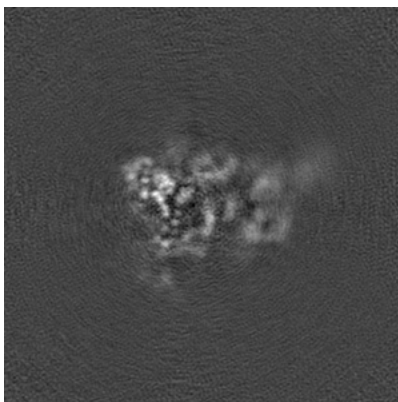


Z Index: 128

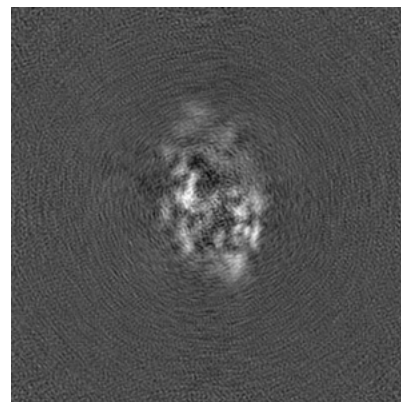
6.2.2 Raw map



X Index: 128



Y Index: 128

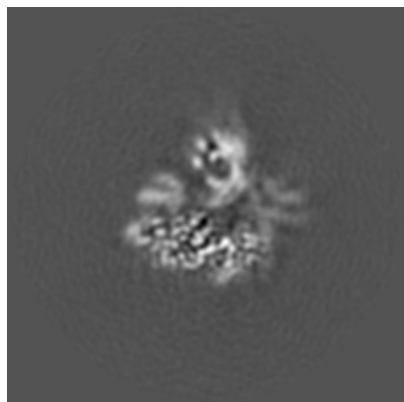


Z Index: 128

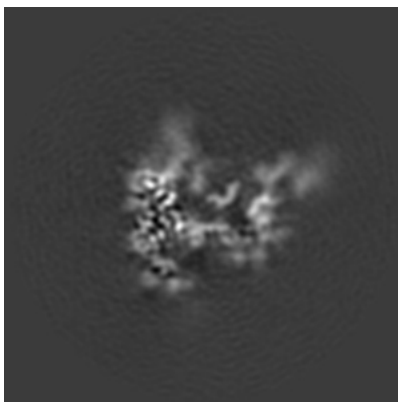
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

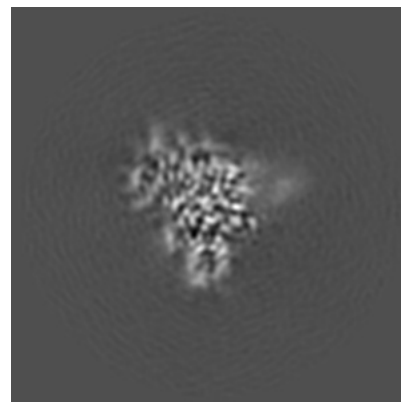
6.3.1 Primary map



X Index: 131

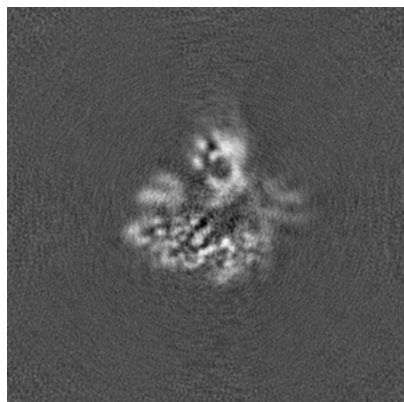


Y Index: 139

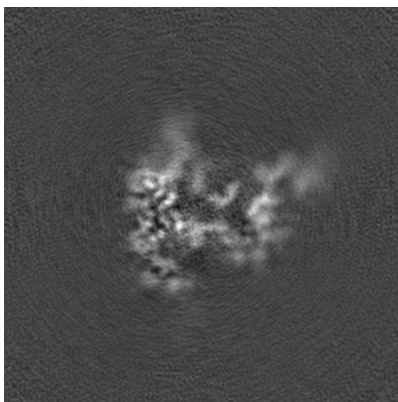


Z Index: 104

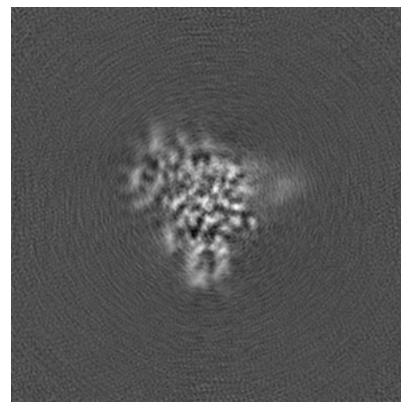
6.3.2 Raw map



X Index: 131



Y Index: 139

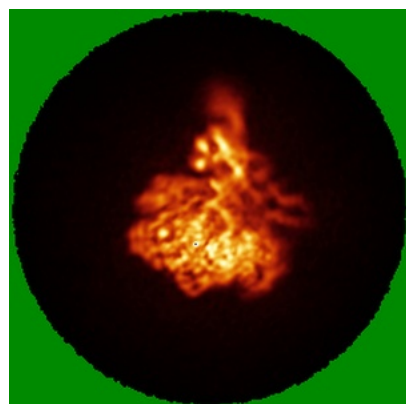


Z Index: 104

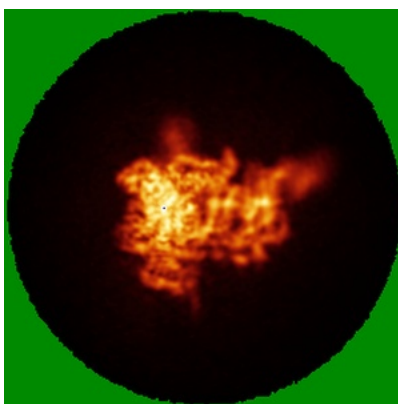
The images above show the largest variance slices of the map in three orthogonal directions.

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

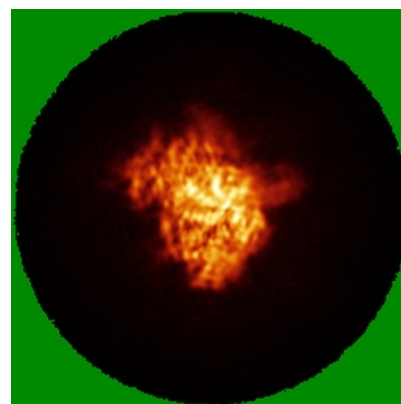
6.4.1 Primary map



X

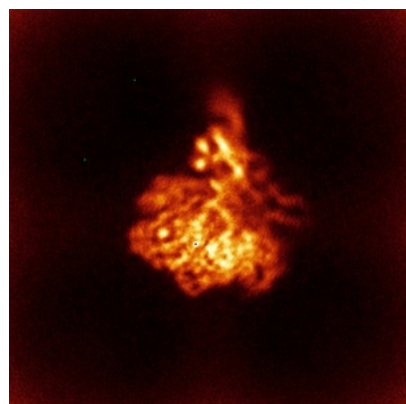


Y

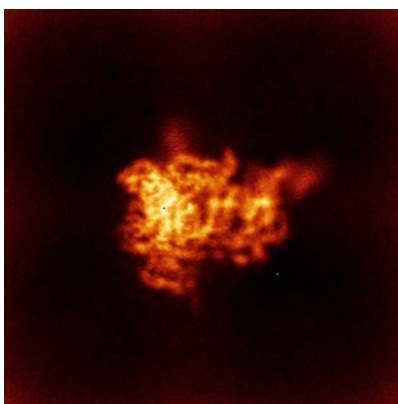


Z

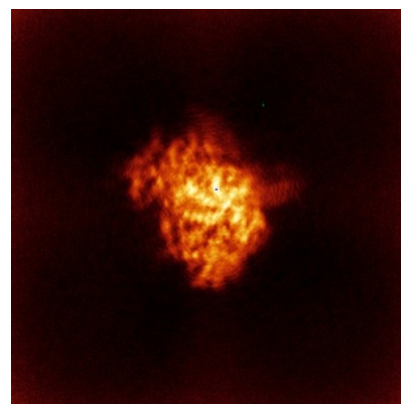
6.4.2 Raw map



X



Y

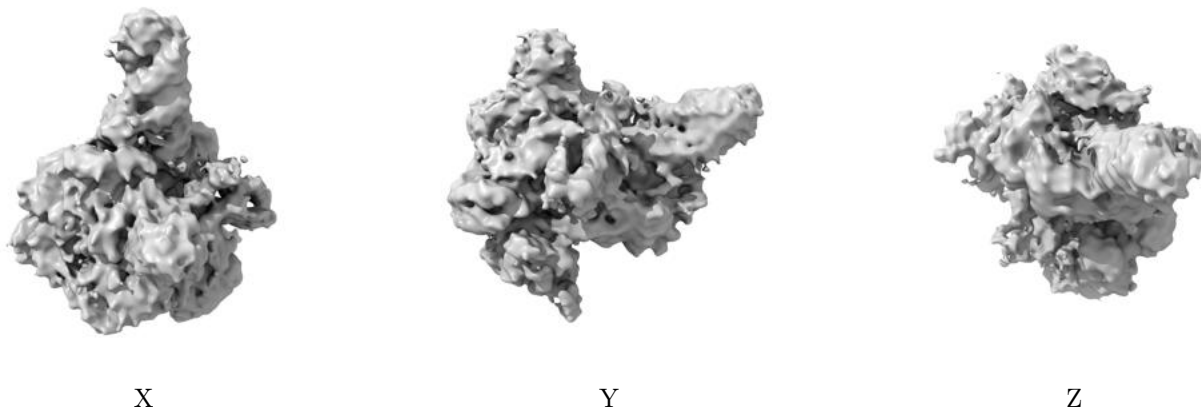


Z

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.

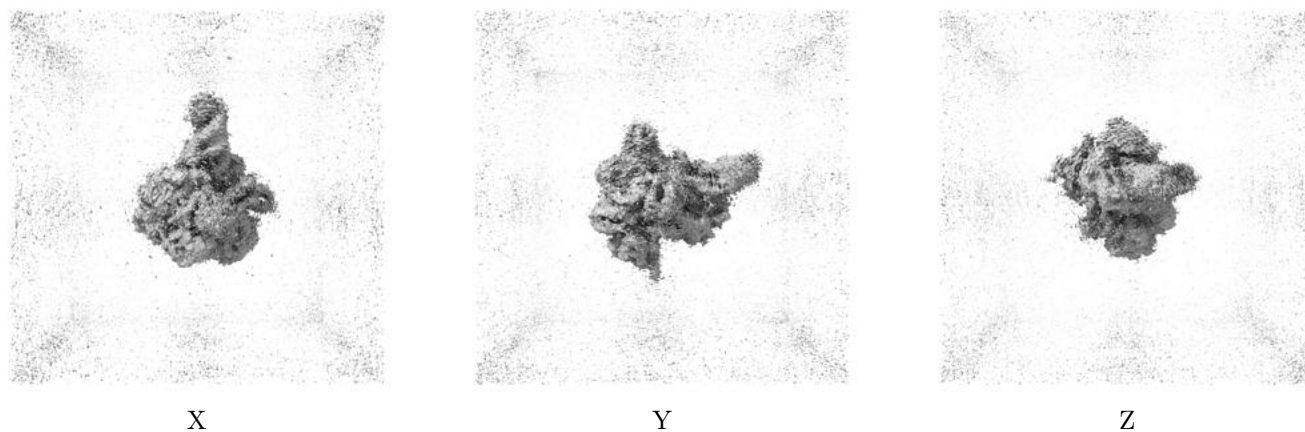
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.024. 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.

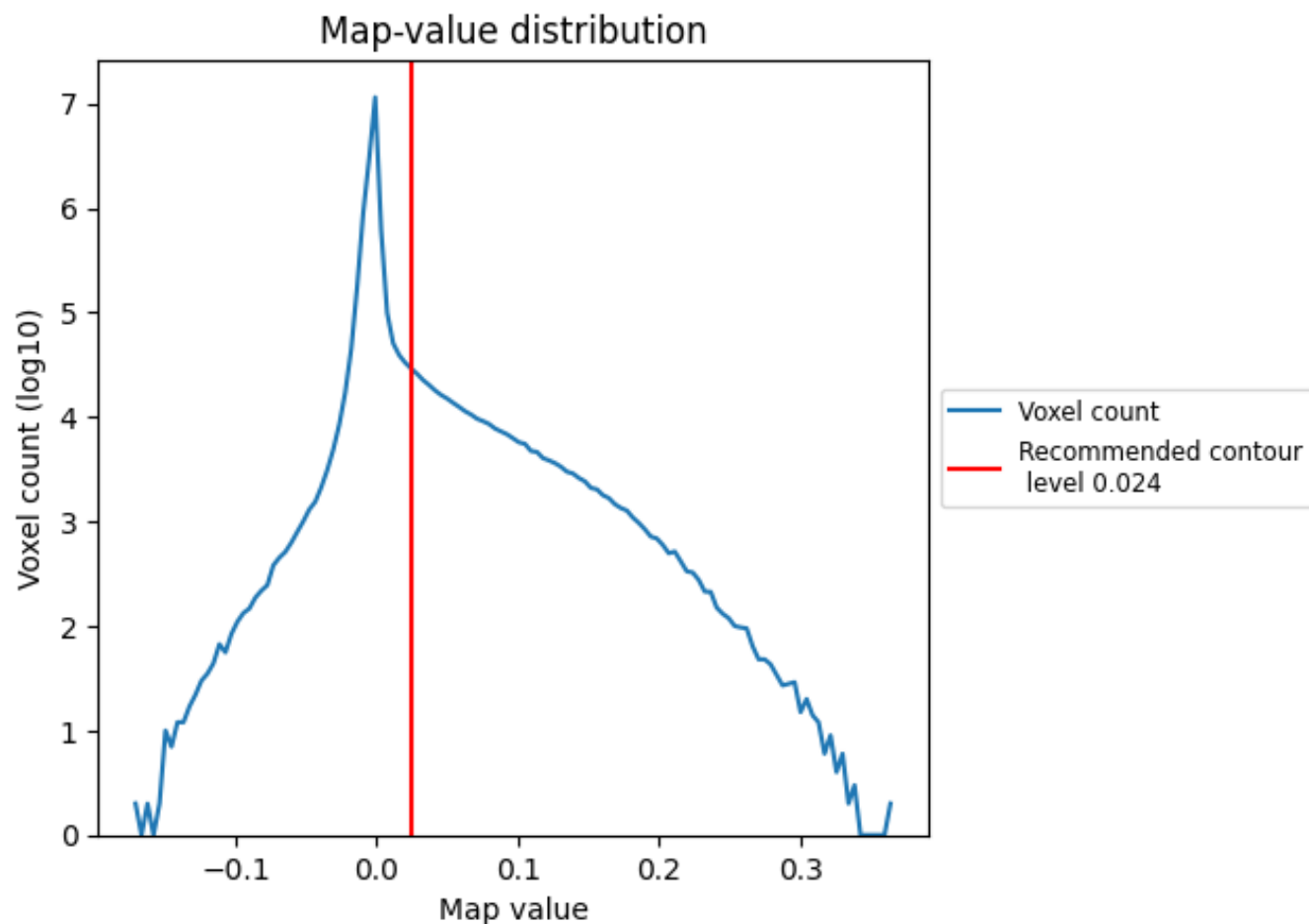
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

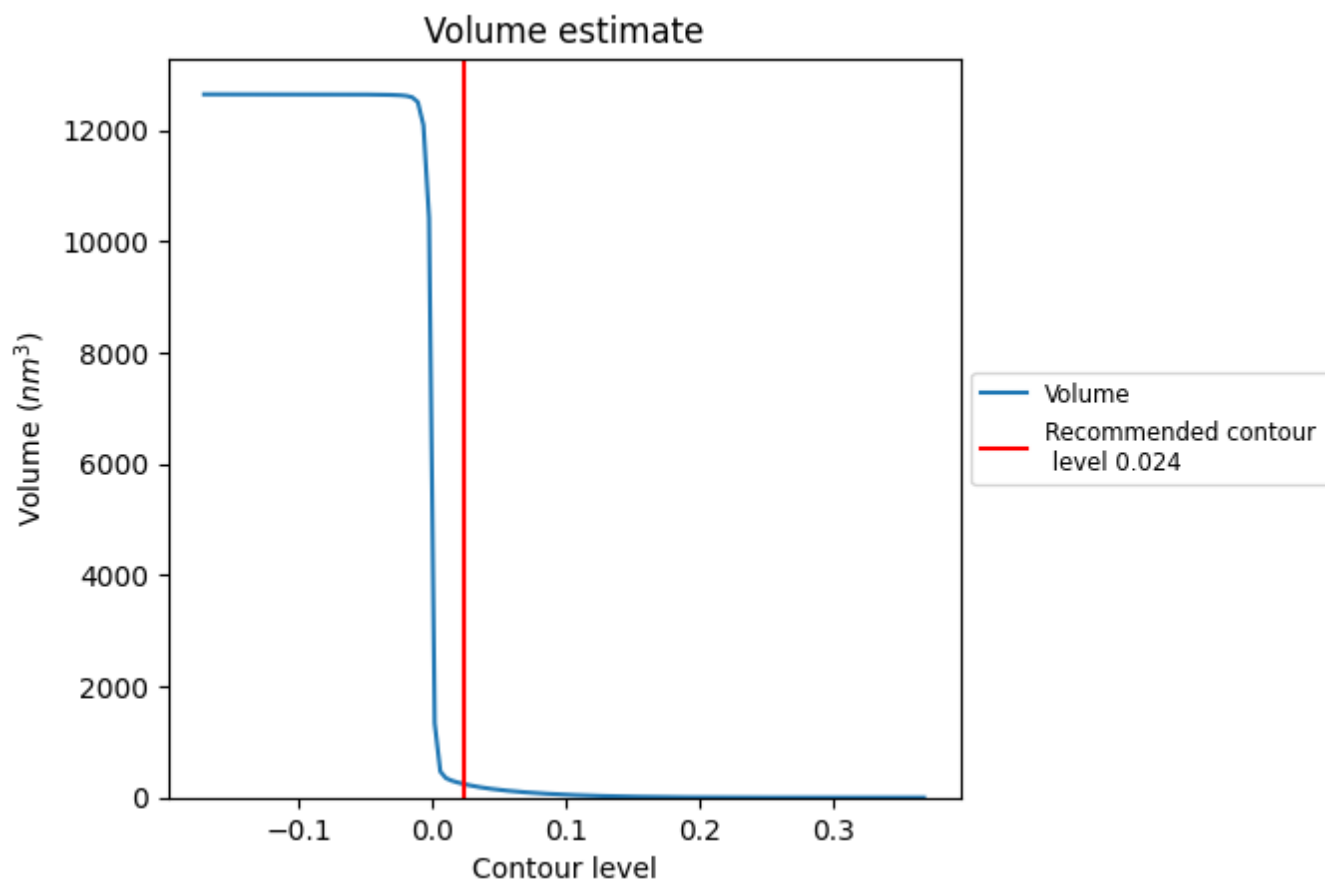
This section contains the results of statistical analysis of the map.

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.

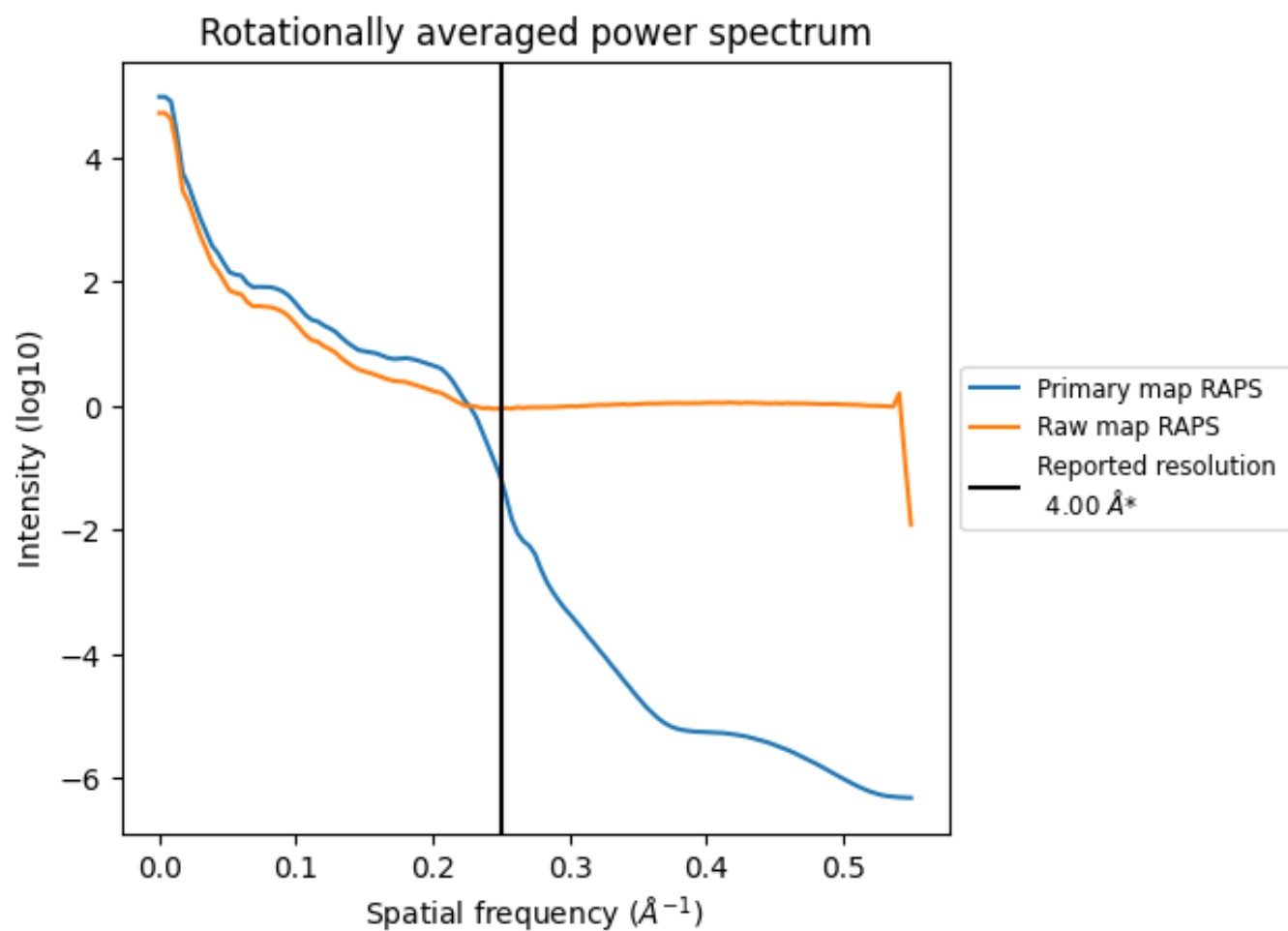
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 242 nm³; this corresponds to an approximate mass of 219 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 ⓘ

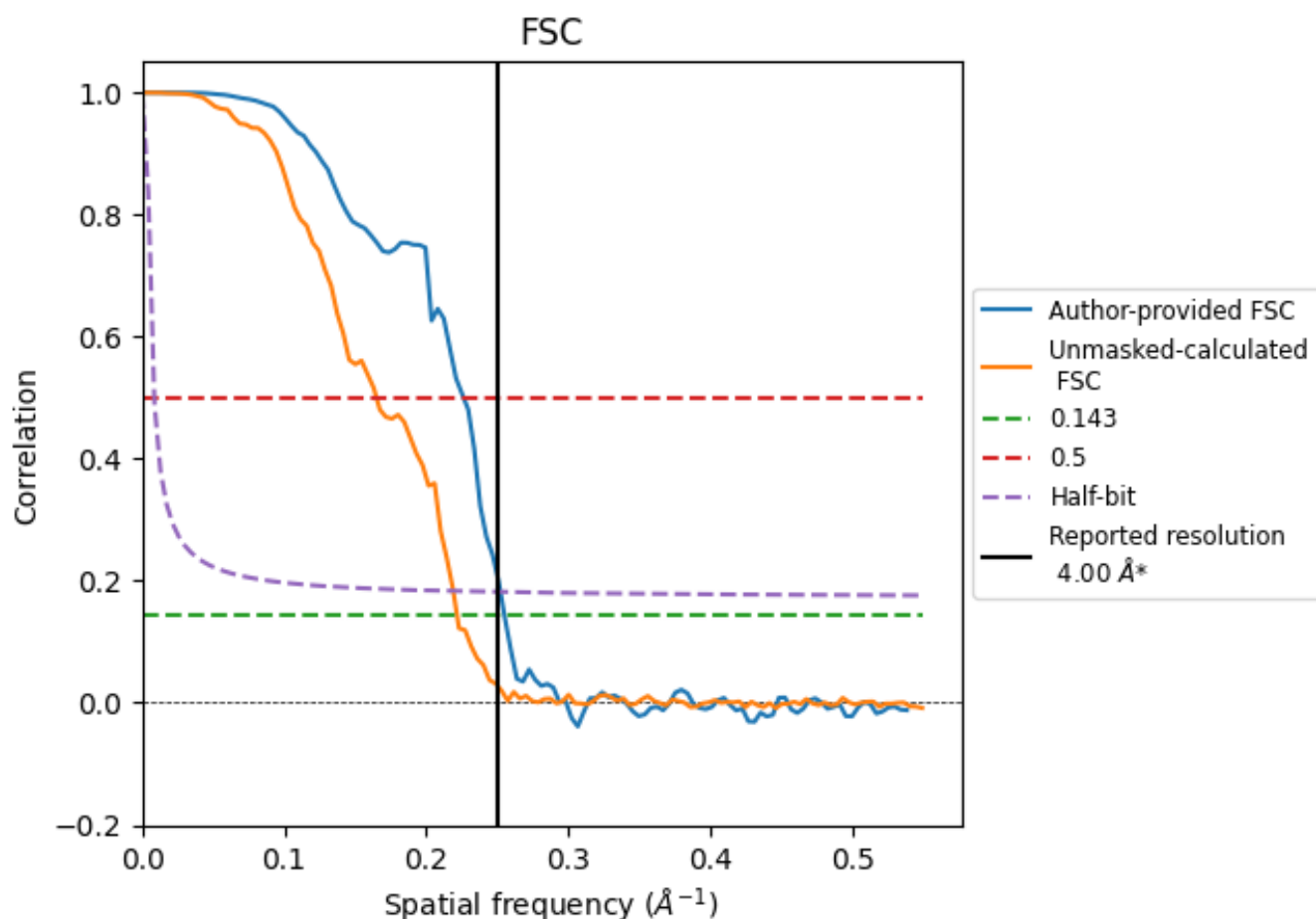


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

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 0.250 \AA^{-1}

8.2 Resolution estimates [i](#)

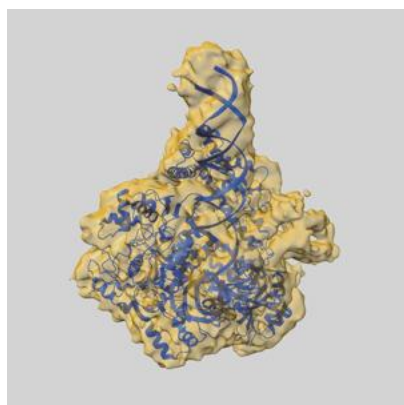
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.92	4.42	3.96
Unmasked-calculated*	4.51	6.06	4.56

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.51 differs from the reported value 4.0 by more than 10 %

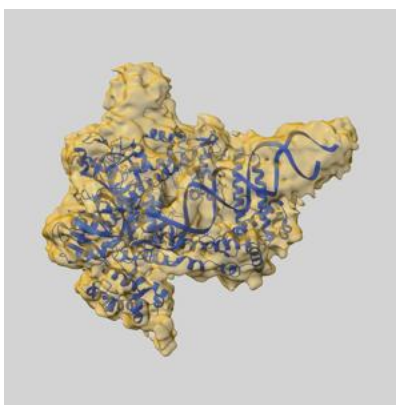
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52287 and PDB model 9HM6. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

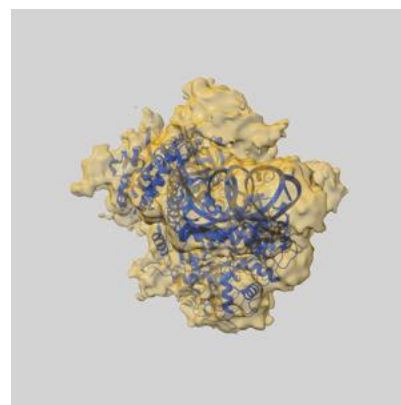
9.1 Map-model overlay [i](#)



X



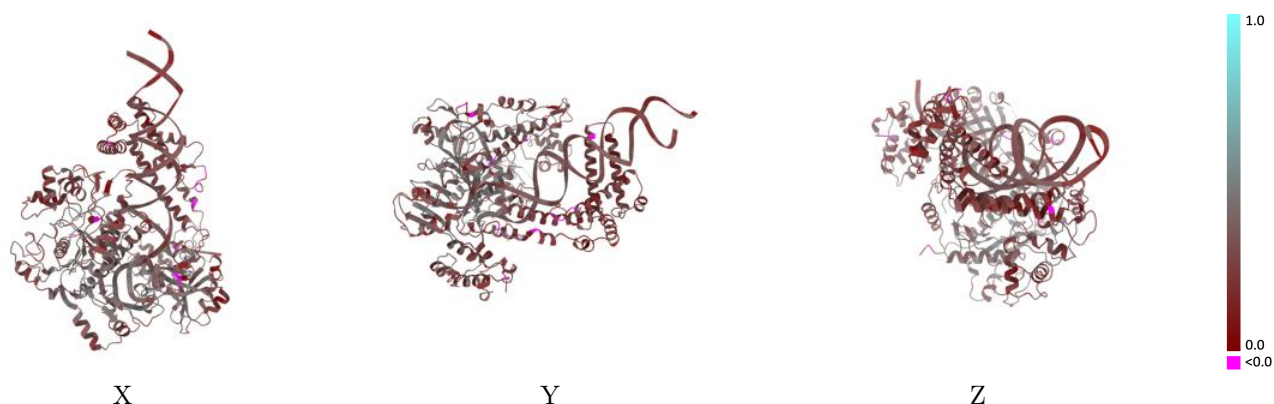
Y



Z

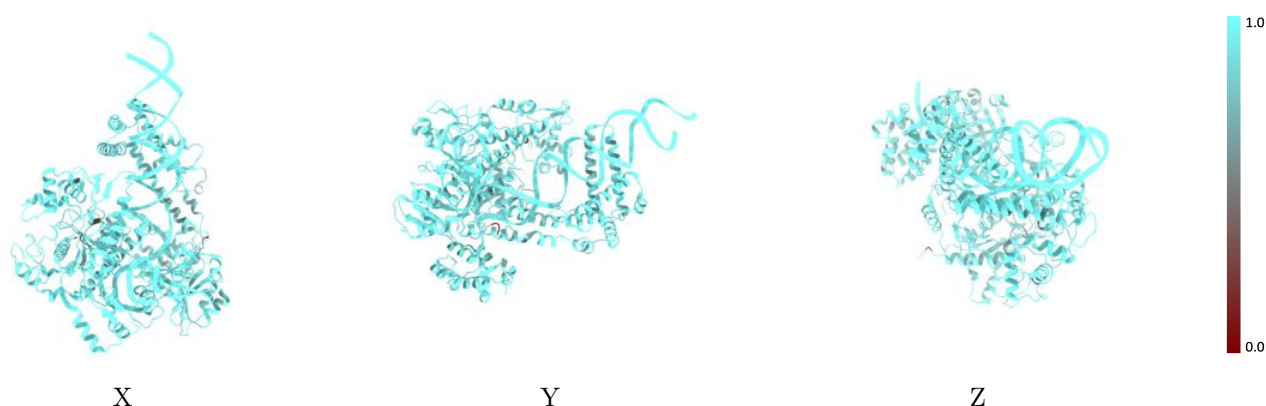
The images above show the 3D surface view of the map at the recommended contour level 0.024 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



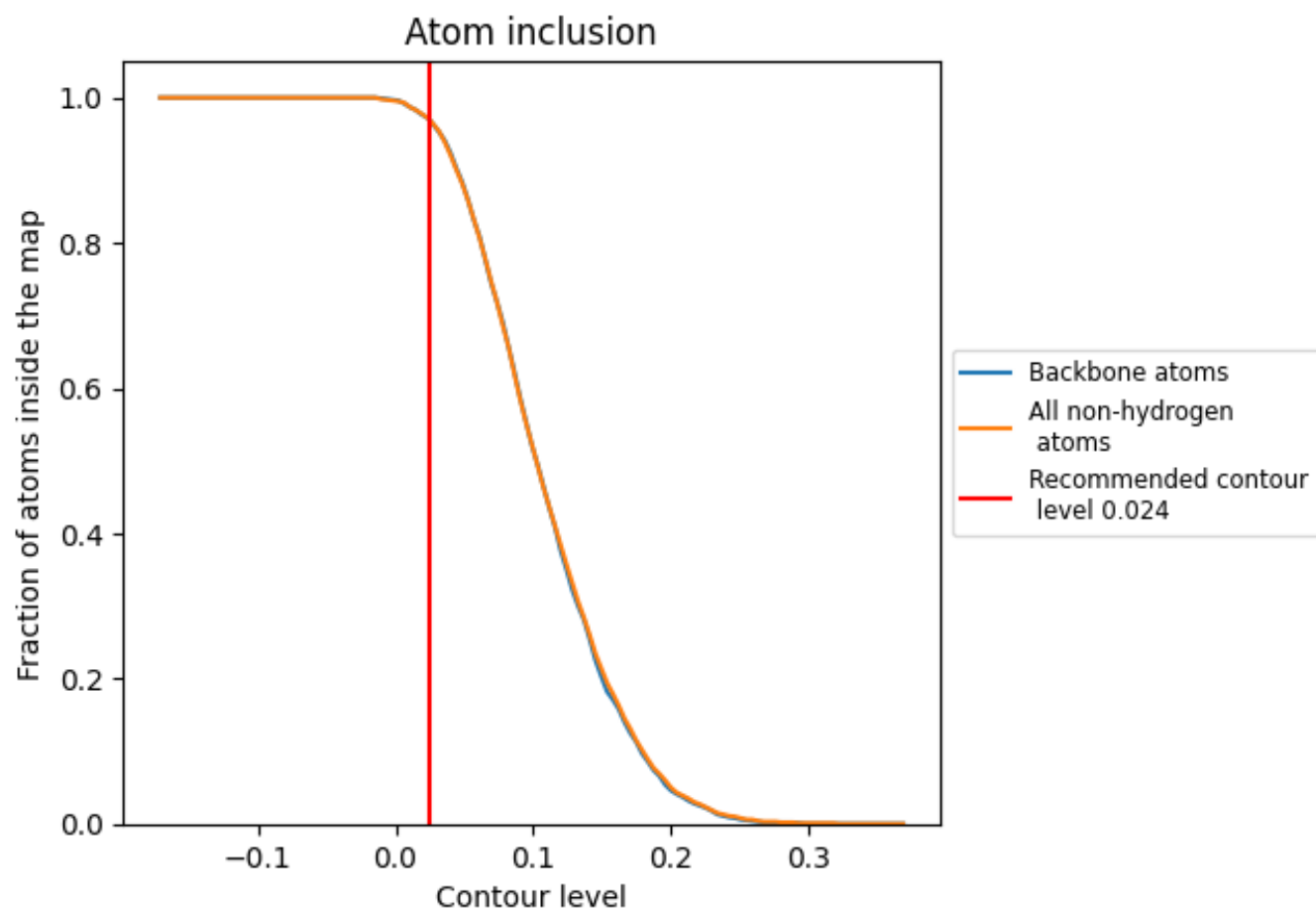
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.024).

9.4 Atom inclusion ⓘ



At the recommended contour level, 97% of all backbone atoms, 97% 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 (0.024) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9710	<div></div> 0.3110
A	<div></div> 0.9690	<div></div> 0.3080
B	<div></div> 0.9970	<div></div> 0.3330
C	<div></div> 0.9970	<div></div> 0.3130

