



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 12:11 PM UTC

PDB ID : 9R7Q / pdb_00009r7q
EMDB ID : EMD-53787
Title : Paranemic crossover triangle (PXT) with 2'-Fluoro-modified pyrimidines (FY RNA)
Authors : Kristoffersen, E.L.; Andersen, E.S.; Zwergius, N.H.
Deposited on : 2025-05-15
Resolution : 4.41 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
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

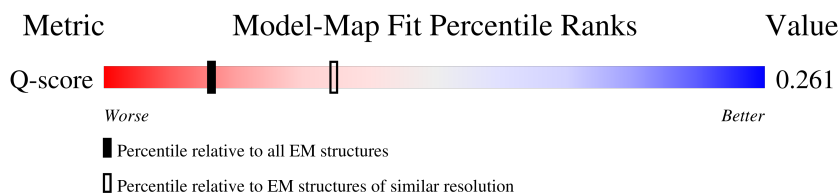
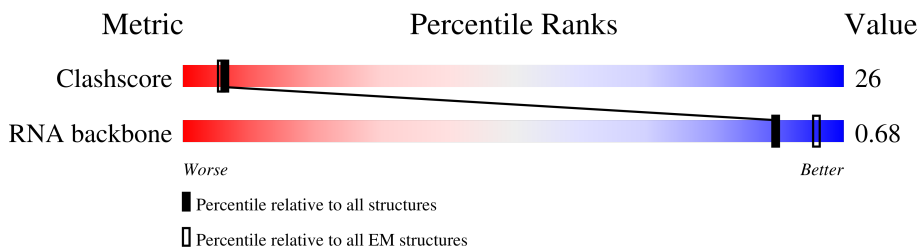
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

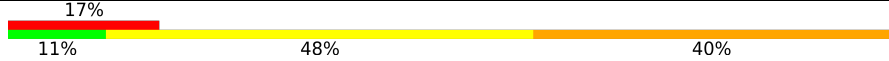
The reported resolution of this entry is 4.41 Å.

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	-
RNA backbone	8273	3508	-
Q-score	-	25397	3133 (3.91 - 4.91)

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	238	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5050 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

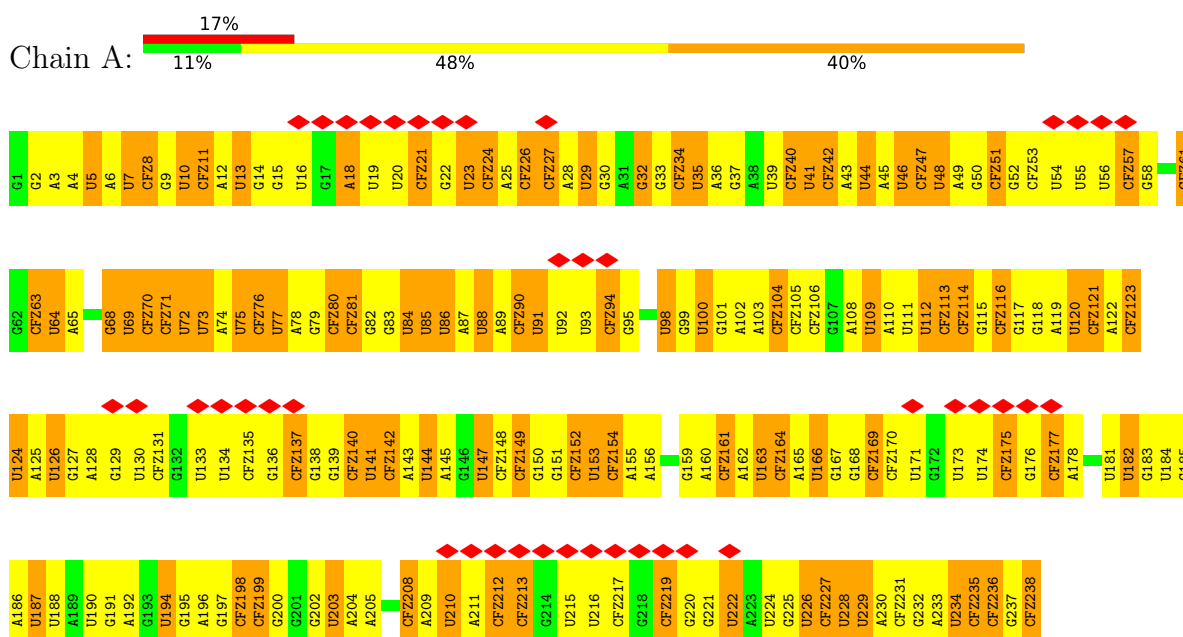
- Molecule 1 is a RNA chain called DNA/RNA (238-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	F	N	O	P		
1	A	238	5050	2255	125	872	1560	238	0	0

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: DNA/RNA (238-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	434756	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.248	Depositor
Minimum map value	-0.101	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0655	Depositor
Map size (Å)	258.80002, 258.80002, 258.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.6470001, 0.6470001, 0.6470001	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.54	17/2856 (0.6%)	0.29	0/4403

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	16	UFT	O3'-P	5.93	1.62	1.56
1	A	184	UFT	O3'-P	5.87	1.62	1.56
1	A	203	UFT	O3'-P	5.74	1.61	1.56
1	A	109	UFT	O3'-P	5.68	1.61	1.56
1	A	86	UFT	O3'-P	5.66	1.61	1.56

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	5050	0	2426	191	0
All	All	5050	0	2426	191	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 26.

The worst 5 of 191 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:89:A:H61	1:A:98:UFT:HN3	1.33	0.76
1:A:75:UFT:H2'	1:A:76:CFZ:H6	1.66	0.76
1:A:123:CFZ:H2'	1:A:124:UFT:H6	1.68	0.74
1:A:112:UFT:H2'	1:A:113:CFZ:H6	1.70	0.73
1:A:225:G:H3'	1:A:226:UFT:H6	1.71	0.73

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	50/238 (21%)	4 (8%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	18	A
1	A	32	G
1	A	68	G
1	A	156	A

There are no RNA pucker outliers to report.

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

125 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	UFT	A	181	1	18,21,22	2.71	10 (55%)	25,30,33	2.07	7 (28%)
1	CFZ	A	123	1	18,21,22	2.54	7 (38%)	25,30,33	1.25	1 (4%)
1	CFZ	A	238	1	18,21,22	2.51	7 (38%)	25,30,33	1.38	3 (12%)
1	CFZ	A	106	1	18,21,22	2.55	7 (38%)	25,30,33	1.19	2 (8%)
1	UFT	A	124	1	18,21,22	2.64	9 (50%)	25,30,33	1.94	6 (24%)
1	UFT	A	194	1	18,21,22	2.67	10 (55%)	25,30,33	2.05	7 (28%)
1	UFT	A	73	1	18,21,22	2.67	10 (55%)	25,30,33	1.99	6 (24%)
1	UFT	A	229	1	18,21,22	2.69	10 (55%)	25,30,33	2.06	7 (28%)
1	UFT	A	111	1	18,21,22	2.62	10 (55%)	25,30,33	1.85	7 (28%)
1	UFT	A	190	1	18,21,22	2.64	10 (55%)	25,30,33	2.05	8 (32%)
1	UFT	A	84	1	18,21,22	2.67	10 (55%)	25,30,33	2.07	7 (28%)
1	CFZ	A	199	1	18,21,22	2.54	7 (38%)	25,30,33	1.24	3 (12%)
1	UFT	A	54	1	18,21,22	2.64	10 (55%)	25,30,33	2.15	7 (28%)
1	UFT	A	153	1	18,21,22	2.68	9 (50%)	25,30,33	2.01	7 (28%)
1	CFZ	A	114	1	18,21,22	2.54	6 (33%)	25,30,33	1.57	3 (12%)
1	CFZ	A	213	1	18,21,22	2.56	7 (38%)	25,30,33	1.42	4 (16%)
1	CFZ	A	104	1	18,21,22	2.54	7 (38%)	25,30,33	1.20	2 (8%)
1	CFZ	A	169	1	18,21,22	2.53	7 (38%)	25,30,33	1.35	2 (8%)
1	CFZ	A	137	1	18,21,22	2.53	6 (33%)	25,30,33	1.32	4 (16%)
1	UFT	A	228	1	18,21,22	2.68	10 (55%)	25,30,33	2.22	7 (28%)
1	CFZ	A	231	1	18,21,22	2.46	7 (38%)	25,30,33	1.38	4 (16%)
1	UFT	A	23	1	18,21,22	2.64	10 (55%)	25,30,33	1.95	7 (28%)
1	CFZ	A	140	1	18,21,22	2.46	7 (38%)	25,30,33	1.37	4 (16%)
1	CFZ	A	61	1	18,21,22	2.51	7 (38%)	25,30,33	1.39	3 (12%)
1	UFT	A	222	1	18,21,22	2.67	10 (55%)	25,30,33	2.10	7 (28%)
1	UFT	A	171	1	18,21,22	2.69	10 (55%)	25,30,33	2.10	6 (24%)
1	CFZ	A	227	1	18,21,22	2.56	6 (33%)	25,30,33	1.20	1 (4%)
1	CFZ	A	51	1	18,21,22	2.56	7 (38%)	25,30,33	1.44	2 (8%)
1	UFT	A	133	1	18,21,22	2.62	10 (55%)	25,30,33	2.07	8 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	UFT	A	224	1	18,21,22	2.64	10 (55%)	25,30,33	2.18	8 (32%)
1	UFT	A	19	1	18,21,22	2.63	10 (55%)	25,30,33	2.11	8 (32%)
1	UFT	A	166	1	18,21,22	2.64	10 (55%)	25,30,33	2.01	6 (24%)
1	UFT	A	163	1	18,21,22	2.73	10 (55%)	25,30,33	2.18	8 (32%)
1	UFT	A	92	1	18,21,22	2.60	10 (55%)	25,30,33	2.05	7 (28%)
1	UFT	A	72	1	18,21,22	2.67	10 (55%)	25,30,33	2.01	6 (24%)
1	CFZ	A	27	1	18,21,22	2.53	7 (38%)	25,30,33	1.23	2 (8%)
1	UFT	A	20	1	18,21,22	2.58	10 (55%)	25,30,33	2.20	8 (32%)
1	UFT	A	91	1	18,21,22	2.68	10 (55%)	25,30,33	2.12	8 (32%)
1	UFT	A	55	1	18,21,22	2.63	10 (55%)	25,30,33	2.05	8 (32%)
1	CFZ	A	217	1	18,21,22	2.49	7 (38%)	25,30,33	1.30	2 (8%)
1	UFT	A	234	1	18,21,22	2.64	10 (55%)	25,30,33	2.16	8 (32%)
1	UFT	A	86	1	18,21,22	2.69	10 (55%)	25,30,33	1.97	7 (28%)
1	CFZ	A	149	1	18,21,22	2.51	7 (38%)	25,30,33	1.34	3 (12%)
1	UFT	A	144	1	18,21,22	2.66	10 (55%)	25,30,33	2.05	7 (28%)
1	UFT	A	7	1	18,21,22	2.67	9 (50%)	25,30,33	2.04	5 (20%)
1	CFZ	A	154	1	18,21,22	2.52	7 (38%)	25,30,33	1.25	3 (12%)
1	UFT	A	46	1	18,21,22	2.68	9 (50%)	25,30,33	2.03	7 (28%)
1	UFT	A	88	1	18,21,22	2.66	10 (55%)	25,30,33	1.97	8 (32%)
1	UFT	A	216	1	18,21,22	2.62	10 (55%)	25,30,33	2.09	6 (24%)
1	CFZ	A	152	1	18,21,22	2.53	7 (38%)	25,30,33	1.21	2 (8%)
1	CFZ	A	76	1	18,21,22	2.52	6 (33%)	25,30,33	1.33	3 (12%)
1	CFZ	A	80	1	18,21,22	2.58	7 (38%)	25,30,33	1.25	2 (8%)
1	CFZ	A	70	1	18,21,22	2.56	7 (38%)	25,30,33	1.27	3 (12%)
1	UFT	A	44	1	18,21,22	2.68	10 (55%)	25,30,33	1.99	6 (24%)
1	UFT	A	56	1	18,21,22	2.59	10 (55%)	25,30,33	2.20	8 (32%)
1	CFZ	A	24	1	18,21,22	2.52	7 (38%)	25,30,33	1.44	2 (8%)
1	CFZ	A	105	1	18,21,22	2.49	7 (38%)	25,30,33	1.16	1 (4%)
1	UFT	A	141	1	18,21,22	2.63	10 (55%)	25,30,33	2.09	7 (28%)
1	UFT	A	215	1	18,21,22	2.63	10 (55%)	25,30,33	2.03	7 (28%)
1	CFZ	A	236	1	18,21,22	2.49	7 (38%)	25,30,33	1.29	3 (12%)
1	CFZ	A	90	1	18,21,22	2.55	7 (38%)	25,30,33	1.38	3 (12%)
1	CFZ	A	175	1	18,21,22	2.42	7 (38%)	25,30,33	1.56	4 (16%)
1	UFT	A	48	1	18,21,22	2.63	10 (55%)	25,30,33	2.10	7 (28%)
1	UFT	A	174	1	18,21,22	2.62	10 (55%)	25,30,33	2.14	7 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CFZ	A	40	1	18,21,22	2.53	7 (38%)	25,30,33	1.25	3 (12%)
1	CFZ	A	94	1	18,21,22	2.40	7 (38%)	25,30,33	1.51	3 (12%)
1	UFT	A	93	1	18,21,22	2.59	10 (55%)	25,30,33	2.08	7 (28%)
1	UFT	A	173	1	18,21,22	2.63	10 (55%)	25,30,33	2.00	6 (24%)
1	UFT	A	109	1	18,21,22	2.69	10 (55%)	25,30,33	2.28	8 (32%)
1	CFZ	A	135	1	18,21,22	2.50	7 (38%)	25,30,33	1.18	1 (4%)
1	UFT	A	226	1	18,21,22	2.63	10 (55%)	25,30,33	2.18	7 (28%)
1	UFT	A	112	1	18,21,22	2.60	10 (55%)	25,30,33	1.98	7 (28%)
1	CFZ	A	42	1	18,21,22	2.55	7 (38%)	25,30,33	1.27	2 (8%)
1	CFZ	A	170	1	18,21,22	2.51	7 (38%)	25,30,33	1.53	2 (8%)
1	CFZ	A	235	1	18,21,22	2.51	7 (38%)	25,30,33	1.37	3 (12%)
1	UFT	A	39	1	18,21,22	2.64	10 (55%)	25,30,33	2.27	8 (32%)
1	UFT	A	85	1	18,21,22	2.63	10 (55%)	25,30,33	2.16	7 (28%)
1	CFZ	A	113	1	18,21,22	2.55	6 (33%)	25,30,33	1.35	3 (12%)
1	UFT	A	29	1	18,21,22	2.67	10 (55%)	25,30,33	2.07	7 (28%)
1	UFT	A	184	1	18,21,22	2.65	10 (55%)	25,30,33	2.24	8 (32%)
1	UFT	A	188	1	18,21,22	2.61	9 (50%)	25,30,33	2.11	8 (32%)
1	UFT	A	13	1	18,21,22	2.66	10 (55%)	25,30,33	2.02	6 (24%)
1	CFZ	A	161	1	18,21,22	2.56	7 (38%)	25,30,33	1.24	2 (8%)
1	UFT	A	120	1	18,21,22	2.67	9 (50%)	25,30,33	2.06	6 (24%)
1	UFT	A	41	1	18,21,22	2.67	10 (55%)	25,30,33	1.99	6 (24%)
1	UFT	A	16	1	18,21,22	2.62	9 (50%)	25,30,33	1.84	5 (20%)
1	CFZ	A	208	1	18,21,22	2.51	7 (38%)	25,30,33	1.34	2 (8%)
1	CFZ	A	8	1	18,21,22	2.52	7 (38%)	25,30,33	1.27	2 (8%)
1	UFT	A	35	1	18,21,22	2.65	9 (50%)	25,30,33	1.95	6 (24%)
1	CFZ	A	142	1	18,21,22	2.53	6 (33%)	25,30,33	1.21	2 (8%)
1	CFZ	A	26	1	18,21,22	2.53	7 (38%)	25,30,33	1.32	2 (8%)
1	CFZ	A	198	1	18,21,22	2.54	7 (38%)	25,30,33	1.22	2 (8%)
1	UFT	A	75	1	18,21,22	2.68	10 (55%)	25,30,33	2.11	7 (28%)
1	CFZ	A	116	1	18,21,22	2.54	7 (38%)	25,30,33	1.30	2 (8%)
1	CFZ	A	212	1	18,21,22	2.49	7 (38%)	25,30,33	1.38	2 (8%)
1	CFZ	A	81	1	18,21,22	2.54	7 (38%)	25,30,33	1.31	3 (12%)
1	CFZ	A	47	1	18,21,22	2.57	7 (38%)	25,30,33	1.25	3 (12%)
1	CFZ	A	164	1	18,21,22	2.54	7 (38%)	25,30,33	1.50	3 (12%)
1	UFT	A	130	1	18,21,22	2.62	10 (55%)	25,30,33	2.07	7 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	UFT	A	10	1	18,21,22	2.71	10 (55%)	25,30,33	2.11	8 (32%)
1	CFZ	A	21	1	18,21,22	2.49	7 (38%)	25,30,33	1.49	3 (12%)
1	CFZ	A	219	1	18,21,22	2.52	7 (38%)	25,30,33	1.52	3 (12%)
1	CFZ	A	53	1	18,21,22	2.46	7 (38%)	25,30,33	1.49	3 (12%)
1	UFT	A	126	1	18,21,22	2.64	10 (55%)	25,30,33	2.19	7 (28%)
1	UFT	A	203	1	18,21,22	2.63	10 (55%)	25,30,33	1.95	6 (24%)
1	CFZ	A	63	1	18,21,22	2.54	7 (38%)	25,30,33	1.22	2 (8%)
1	UFT	A	187	1	18,21,22	2.61	10 (55%)	25,30,33	2.12	7 (28%)
1	CFZ	A	34	1	18,21,22	2.57	7 (38%)	25,30,33	1.24	2 (8%)
1	UFT	A	64	1	18,21,22	2.66	10 (55%)	25,30,33	2.07	7 (28%)
1	UFT	A	98	1	18,21,22	2.64	10 (55%)	25,30,33	2.01	8 (32%)
1	CFZ	A	121	1	18,21,22	2.55	7 (38%)	25,30,33	1.38	2 (8%)
1	UFT	A	210	1	18,21,22	2.65	9 (50%)	25,30,33	1.96	6 (24%)
1	CFZ	A	71	1	18,21,22	2.56	7 (38%)	25,30,33	1.19	2 (8%)
1	UFT	A	147	1	18,21,22	2.63	10 (55%)	25,30,33	2.32	8 (32%)
1	UFT	A	77	1	18,21,22	2.68	9 (50%)	25,30,33	1.95	7 (28%)
1	CFZ	A	57	1	18,21,22	2.43	7 (38%)	25,30,33	1.40	3 (12%)
1	CFZ	A	177	1	18,21,22	2.55	7 (38%)	25,30,33	1.33	3 (12%)
1	CFZ	A	11	1	18,21,22	2.48	7 (38%)	25,30,33	1.35	3 (12%)
1	UFT	A	69	1	18,21,22	2.69	10 (55%)	25,30,33	2.05	7 (28%)
1	UFT	A	100	1	18,21,22	2.66	10 (55%)	25,30,33	2.05	7 (28%)
1	CFZ	A	148	1	18,21,22	2.55	7 (38%)	25,30,33	1.17	2 (8%)
1	UFT	A	134	1	18,21,22	2.58	10 (55%)	25,30,33	2.18	8 (32%)
1	UFT	A	5	1	18,21,22	2.69	10 (55%)	25,30,33	2.24	7 (28%)
1	UFT	A	182	1	18,21,22	2.61	10 (55%)	25,30,33	2.15	6 (24%)
1	CFZ	A	131	1	18,21,22	2.48	7 (38%)	25,30,33	1.51	4 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UFT	A	181	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	123	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	238	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	106	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UFT	A	124	1	-	0/7/25/26	0/2/2/2
1	UFT	A	194	1	-	0/7/25/26	0/2/2/2
1	UFT	A	73	1	-	0/7/25/26	0/2/2/2
1	UFT	A	229	1	-	0/7/25/26	0/2/2/2
1	UFT	A	111	1	-	0/7/25/26	0/2/2/2
1	UFT	A	190	1	-	0/7/25/26	0/2/2/2
1	UFT	A	84	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	199	1	-	0/7/25/26	0/2/2/2
1	UFT	A	54	1	-	2/7/25/26	0/2/2/2
1	UFT	A	153	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	114	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	213	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	104	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	169	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	137	1	-	0/7/25/26	0/2/2/2
1	UFT	A	228	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	231	1	-	0/7/25/26	0/2/2/2
1	UFT	A	23	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	140	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	61	1	-	0/7/25/26	0/2/2/2
1	UFT	A	222	1	-	0/7/25/26	0/2/2/2
1	UFT	A	171	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	227	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	51	1	-	2/7/25/26	0/2/2/2
1	UFT	A	133	1	-	0/7/25/26	0/2/2/2
1	UFT	A	224	1	-	0/7/25/26	0/2/2/2
1	UFT	A	19	1	-	2/7/25/26	0/2/2/2
1	UFT	A	166	1	-	0/7/25/26	0/2/2/2
1	UFT	A	163	1	-	0/7/25/26	0/2/2/2
1	UFT	A	92	1	-	0/7/25/26	0/2/2/2
1	UFT	A	72	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	27	1	-	0/7/25/26	0/2/2/2
1	UFT	A	20	1	-	2/7/25/26	0/2/2/2
1	UFT	A	91	1	-	2/7/25/26	0/2/2/2
1	UFT	A	55	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	217	1	-	3/7/25/26	0/2/2/2
1	UFT	A	234	1	-	3/7/25/26	0/2/2/2
1	UFT	A	86	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	149	1	-	0/7/25/26	0/2/2/2
1	UFT	A	144	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UFT	A	7	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	154	1	-	0/7/25/26	0/2/2/2
1	UFT	A	46	1	-	0/7/25/26	0/2/2/2
1	UFT	A	88	1	-	0/7/25/26	0/2/2/2
1	UFT	A	216	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	152	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	76	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	80	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	70	1	-	0/7/25/26	0/2/2/2
1	UFT	A	44	1	-	0/7/25/26	0/2/2/2
1	UFT	A	56	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	24	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	105	1	-	0/7/25/26	0/2/2/2
1	UFT	A	141	1	-	0/7/25/26	0/2/2/2
1	UFT	A	215	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	236	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	90	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	175	1	-	2/7/25/26	0/2/2/2
1	UFT	A	48	1	-	0/7/25/26	0/2/2/2
1	UFT	A	174	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	40	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	94	1	-	2/7/25/26	0/2/2/2
1	UFT	A	93	1	-	2/7/25/26	0/2/2/2
1	UFT	A	173	1	-	0/7/25/26	0/2/2/2
1	UFT	A	109	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	135	1	-	2/7/25/26	0/2/2/2
1	UFT	A	226	1	-	3/7/25/26	0/2/2/2
1	UFT	A	112	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	42	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	170	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	235	1	-	3/7/25/26	0/2/2/2
1	UFT	A	39	1	-	0/7/25/26	0/2/2/2
1	UFT	A	85	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	113	1	-	0/7/25/26	0/2/2/2
1	UFT	A	29	1	-	0/7/25/26	0/2/2/2
1	UFT	A	184	1	-	3/7/25/26	0/2/2/2
1	UFT	A	188	1	-	0/7/25/26	0/2/2/2
1	UFT	A	13	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	161	1	-	0/7/25/26	0/2/2/2
1	UFT	A	120	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UFT	A	41	1	-	0/7/25/26	0/2/2/2
1	UFT	A	16	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	208	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	8	1	-	0/7/25/26	0/2/2/2
1	UFT	A	35	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	142	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	26	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	198	1	-	0/7/25/26	0/2/2/2
1	UFT	A	75	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	116	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	212	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	81	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	47	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	164	1	-	0/7/25/26	0/2/2/2
1	UFT	A	130	1	-	0/7/25/26	0/2/2/2
1	UFT	A	10	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	21	1	-	5/7/25/26	0/2/2/2
1	CFZ	A	219	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	53	1	-	0/7/25/26	0/2/2/2
1	UFT	A	126	1	-	0/7/25/26	0/2/2/2
1	UFT	A	203	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	63	1	-	0/7/25/26	0/2/2/2
1	UFT	A	187	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	34	1	-	0/7/25/26	0/2/2/2
1	UFT	A	64	1	-	0/7/25/26	0/2/2/2
1	UFT	A	98	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	121	1	-	0/7/25/26	0/2/2/2
1	UFT	A	210	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	71	1	-	0/7/25/26	0/2/2/2
1	UFT	A	147	1	-	2/7/25/26	0/2/2/2
1	UFT	A	77	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	57	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	177	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	11	1	-	0/7/25/26	0/2/2/2
1	UFT	A	69	1	-	0/7/25/26	0/2/2/2
1	UFT	A	100	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	148	1	-	2/7/25/26	0/2/2/2
1	UFT	A	134	1	-	2/7/25/26	0/2/2/2
1	UFT	A	5	1	-	0/7/25/26	0/2/2/2
1	UFT	A	182	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CFZ	A	131	1	-	0/7/25/26	0/2/2/2

The worst 5 of 1063 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	163	UFT	C2-N1	5.15	1.46	1.38
1	A	46	UFT	C2-N1	5.13	1.46	1.38
1	A	86	UFT	C2-N1	5.10	1.46	1.38
1	A	91	UFT	C2-N1	5.09	1.46	1.38
1	A	10	UFT	C2-N1	5.06	1.46	1.38

The worst 5 of 621 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	UFT	C4-N3-C2	-6.31	118.77	126.61
1	A	147	UFT	C4-N3-C2	-6.19	118.93	126.61
1	A	184	UFT	C4-N3-C2	-6.12	119.02	126.61
1	A	228	UFT	C4-N3-C2	-6.09	119.05	126.61
1	A	163	UFT	C4-N3-C2	-6.07	119.07	126.61

There are no chirality outliers.

5 of 68 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	19	UFT	O4'-C4'-C5'-O5'
1	A	21	CFZ	C2'-C1'-N1-C6
1	A	21	CFZ	O4'-C4'-C5'-O5'
1	A	57	CFZ	C4'-C5'-O5'-P
1	A	91	UFT	O4'-C4'-C5'-O5'

There are no ring outliers.

93 monomers are involved in 163 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	123	CFZ	2	0
1	A	238	CFZ	2	0
1	A	124	UFT	3	0
1	A	194	UFT	1	0
1	A	73	UFT	3	0
1	A	229	UFT	3	0
1	A	84	UFT	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	199	CFZ	3	0
1	A	153	UFT	2	0
1	A	114	CFZ	2	0
1	A	213	CFZ	2	0
1	A	104	CFZ	1	0
1	A	169	CFZ	1	0
1	A	137	CFZ	4	0
1	A	228	UFT	3	0
1	A	23	UFT	5	0
1	A	140	CFZ	1	0
1	A	61	CFZ	1	0
1	A	222	UFT	3	0
1	A	227	CFZ	2	0
1	A	51	CFZ	2	0
1	A	166	UFT	4	0
1	A	163	UFT	2	0
1	A	72	UFT	2	0
1	A	27	CFZ	2	0
1	A	91	UFT	1	0
1	A	234	UFT	2	0
1	A	86	UFT	2	0
1	A	149	CFZ	1	0
1	A	144	UFT	3	0
1	A	7	UFT	2	0
1	A	154	CFZ	2	0
1	A	46	UFT	1	0
1	A	88	UFT	3	0
1	A	152	CFZ	2	0
1	A	76	CFZ	2	0
1	A	80	CFZ	2	0
1	A	70	CFZ	2	0
1	A	44	UFT	3	0
1	A	24	CFZ	3	0
1	A	141	UFT	3	0
1	A	236	CFZ	1	0
1	A	90	CFZ	2	0
1	A	175	CFZ	2	0
1	A	48	UFT	1	0
1	A	40	CFZ	2	0
1	A	94	CFZ	1	0
1	A	109	UFT	3	0
1	A	226	UFT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	112	UFT	3	0
1	A	42	CFZ	3	0
1	A	235	CFZ	1	0
1	A	85	UFT	2	0
1	A	113	CFZ	3	0
1	A	29	UFT	2	0
1	A	13	UFT	1	0
1	A	161	CFZ	3	0
1	A	120	UFT	2	0
1	A	41	UFT	3	0
1	A	208	CFZ	3	0
1	A	8	CFZ	1	0
1	A	35	UFT	3	0
1	A	142	CFZ	3	0
1	A	26	CFZ	1	0
1	A	198	CFZ	2	0
1	A	75	UFT	3	0
1	A	116	CFZ	4	0
1	A	212	CFZ	2	0
1	A	81	CFZ	3	0
1	A	47	CFZ	2	0
1	A	164	CFZ	1	0
1	A	10	UFT	2	0
1	A	21	CFZ	1	0
1	A	219	CFZ	2	0
1	A	126	UFT	2	0
1	A	203	UFT	2	0
1	A	63	CFZ	1	0
1	A	187	UFT	3	0
1	A	34	CFZ	2	0
1	A	64	UFT	2	0
1	A	98	UFT	3	0
1	A	121	CFZ	1	0
1	A	210	UFT	1	0
1	A	71	CFZ	2	0
1	A	147	UFT	1	0
1	A	77	UFT	2	0
1	A	57	CFZ	1	0
1	A	177	CFZ	2	0
1	A	11	CFZ	1	0
1	A	69	UFT	2	0
1	A	100	UFT	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	5	UFT	3	0
1	A	182	UFT	3	0

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.

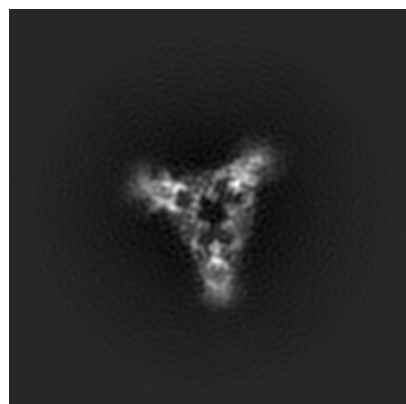
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53787. These allow visual inspection of the internal detail of the map and identification of artifacts.

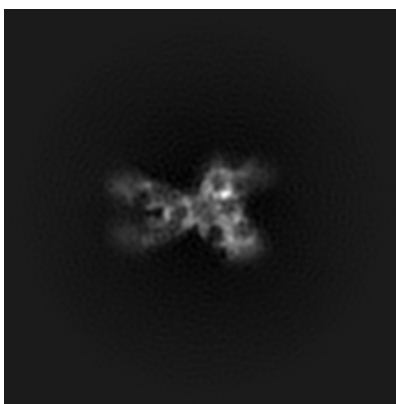
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

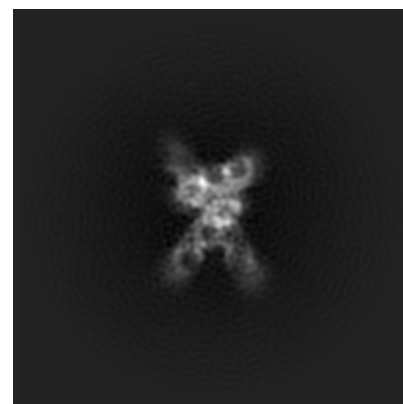
6.1.1 Primary map



X

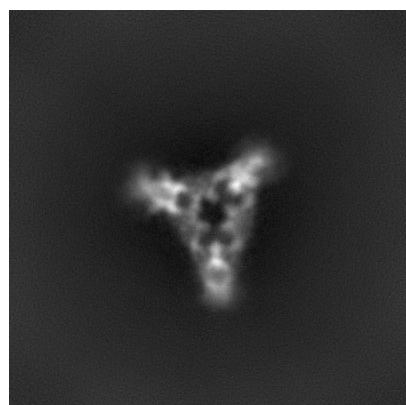


Y

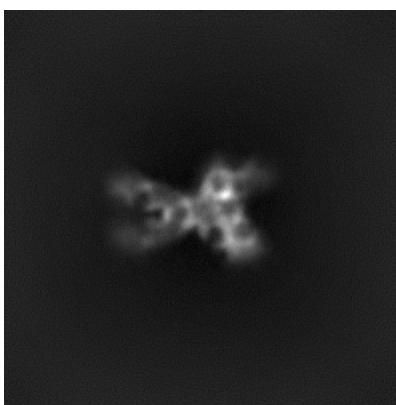


Z

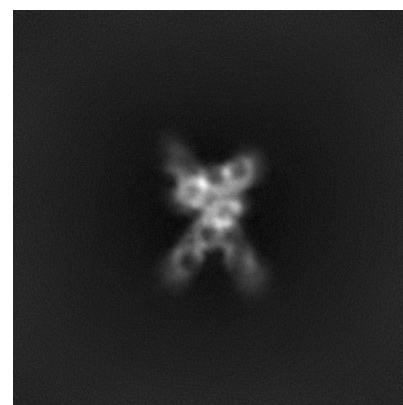
6.1.2 Raw map



X



Y

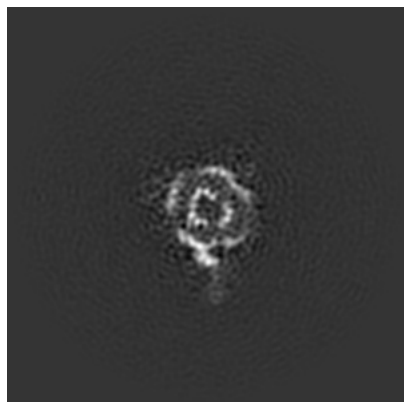


Z

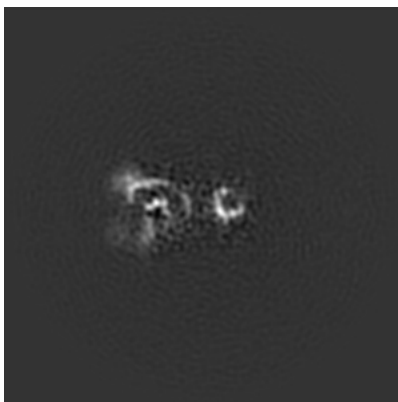
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

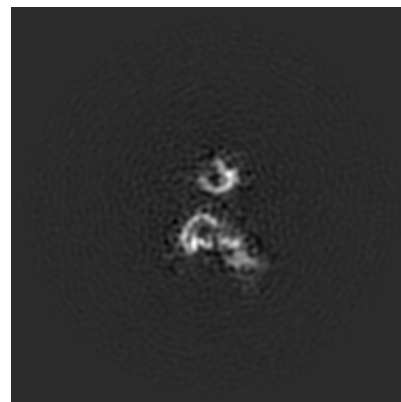
6.2.1 Primary map



X Index: 200

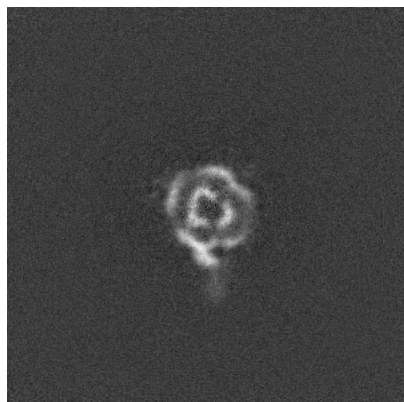


Y Index: 200

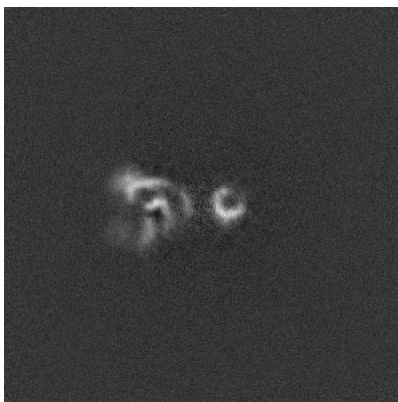


Z Index: 200

6.2.2 Raw map



X Index: 200



Y Index: 200

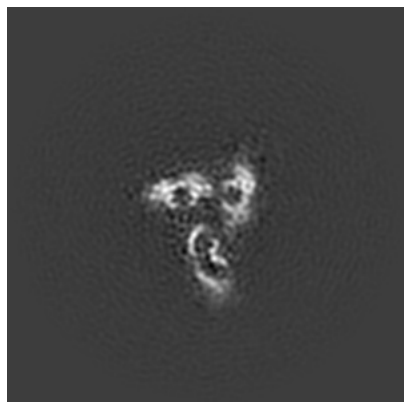


Z Index: 200

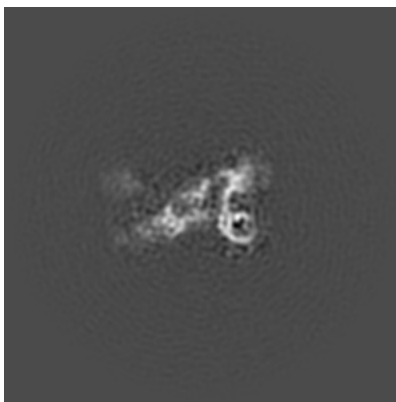
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

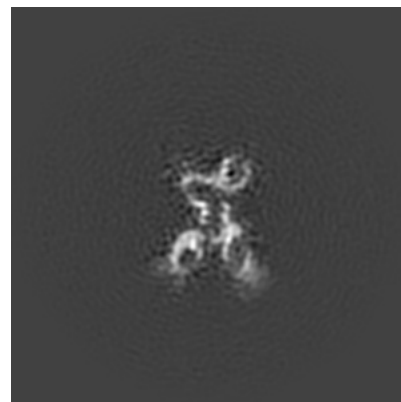
6.3.1 Primary map



X Index: 214

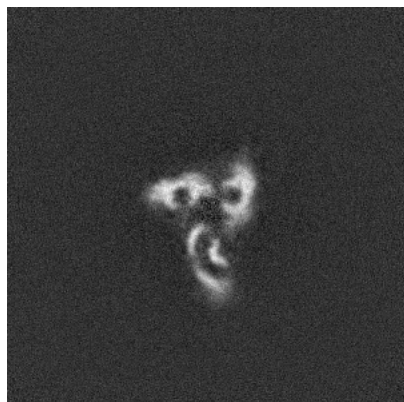


Y Index: 227

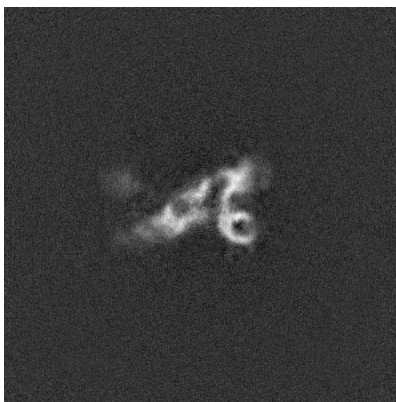


Z Index: 221

6.3.2 Raw map



X Index: 214



Y Index: 227

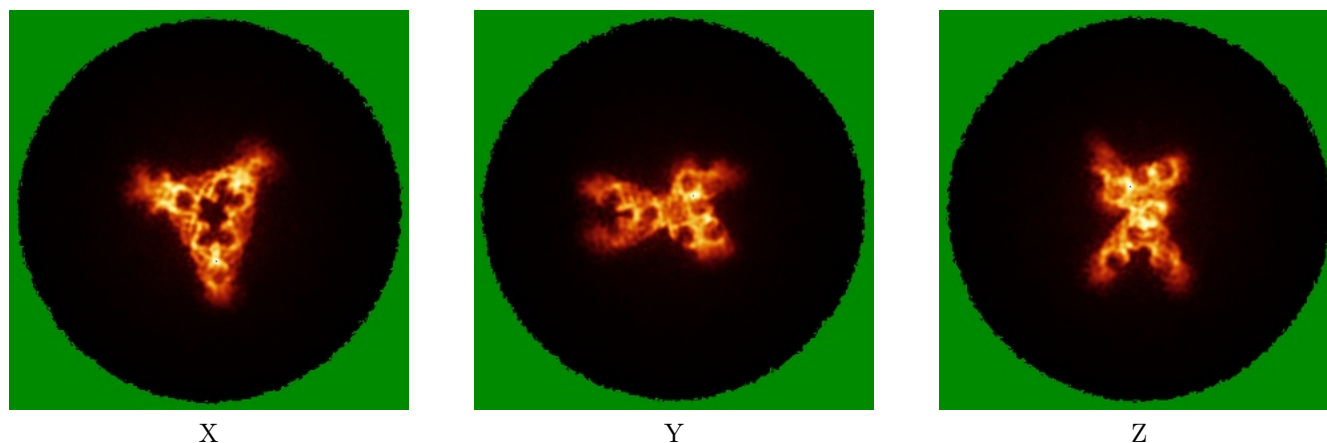


Z Index: 223

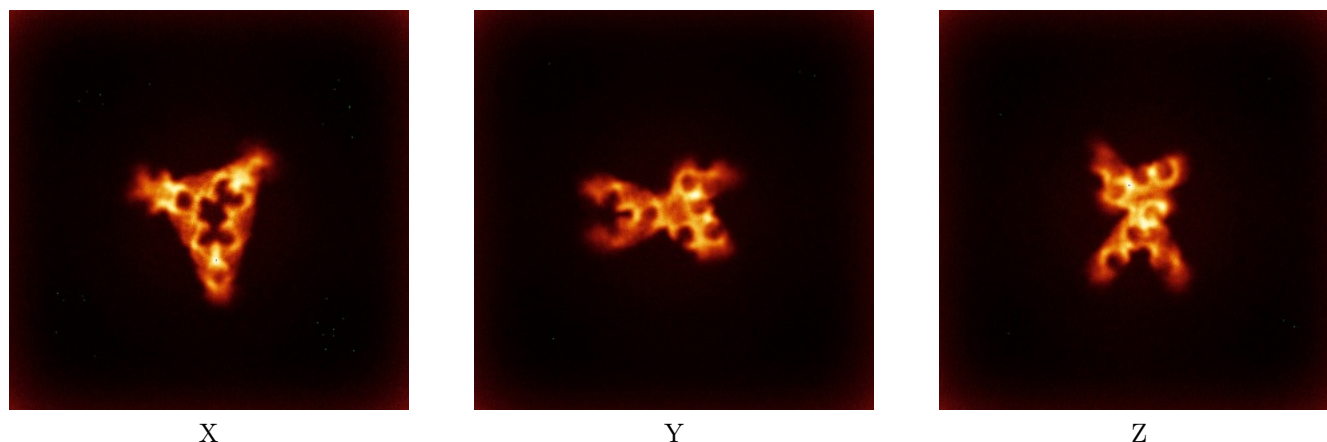
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

This section was not generated.

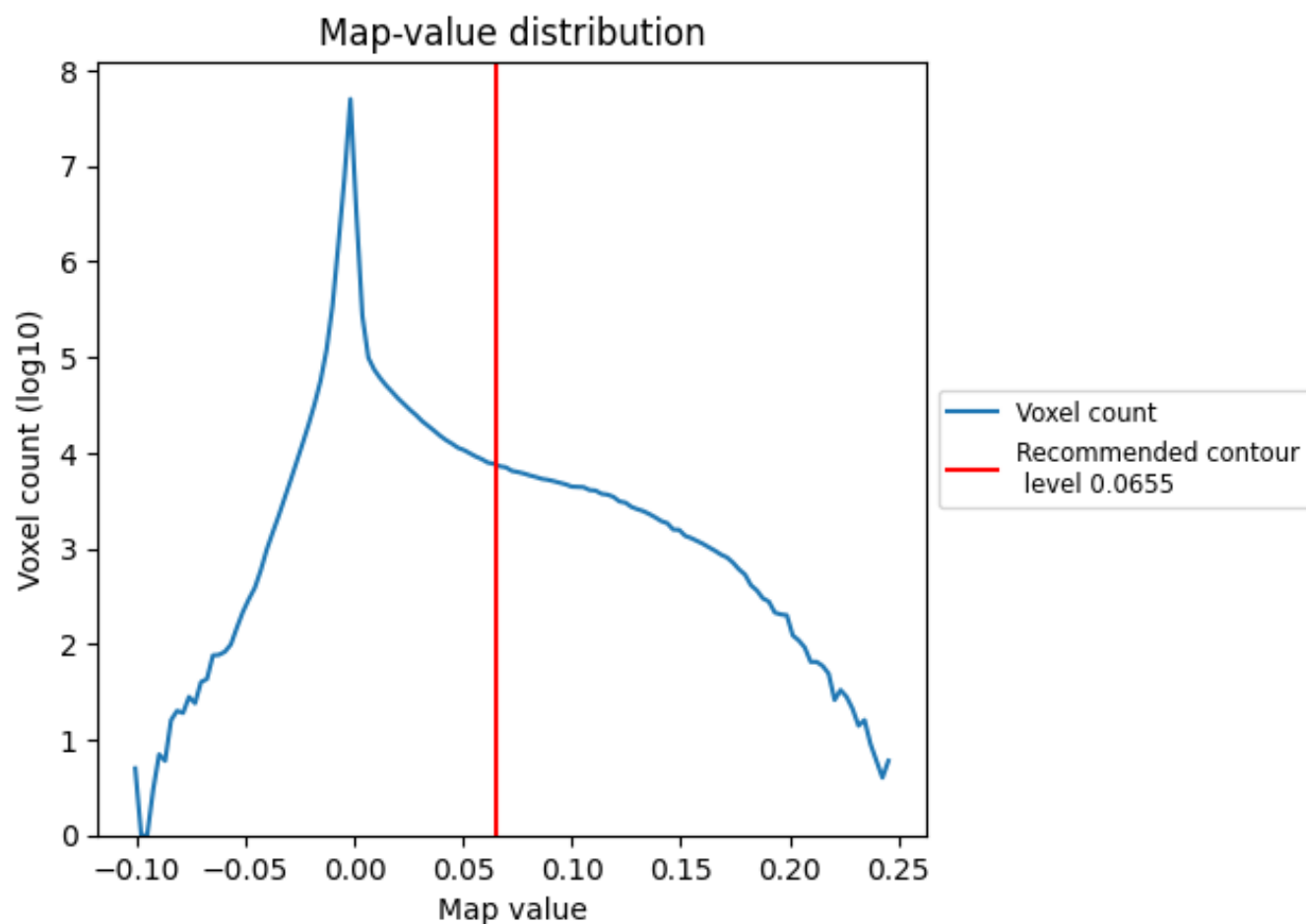
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

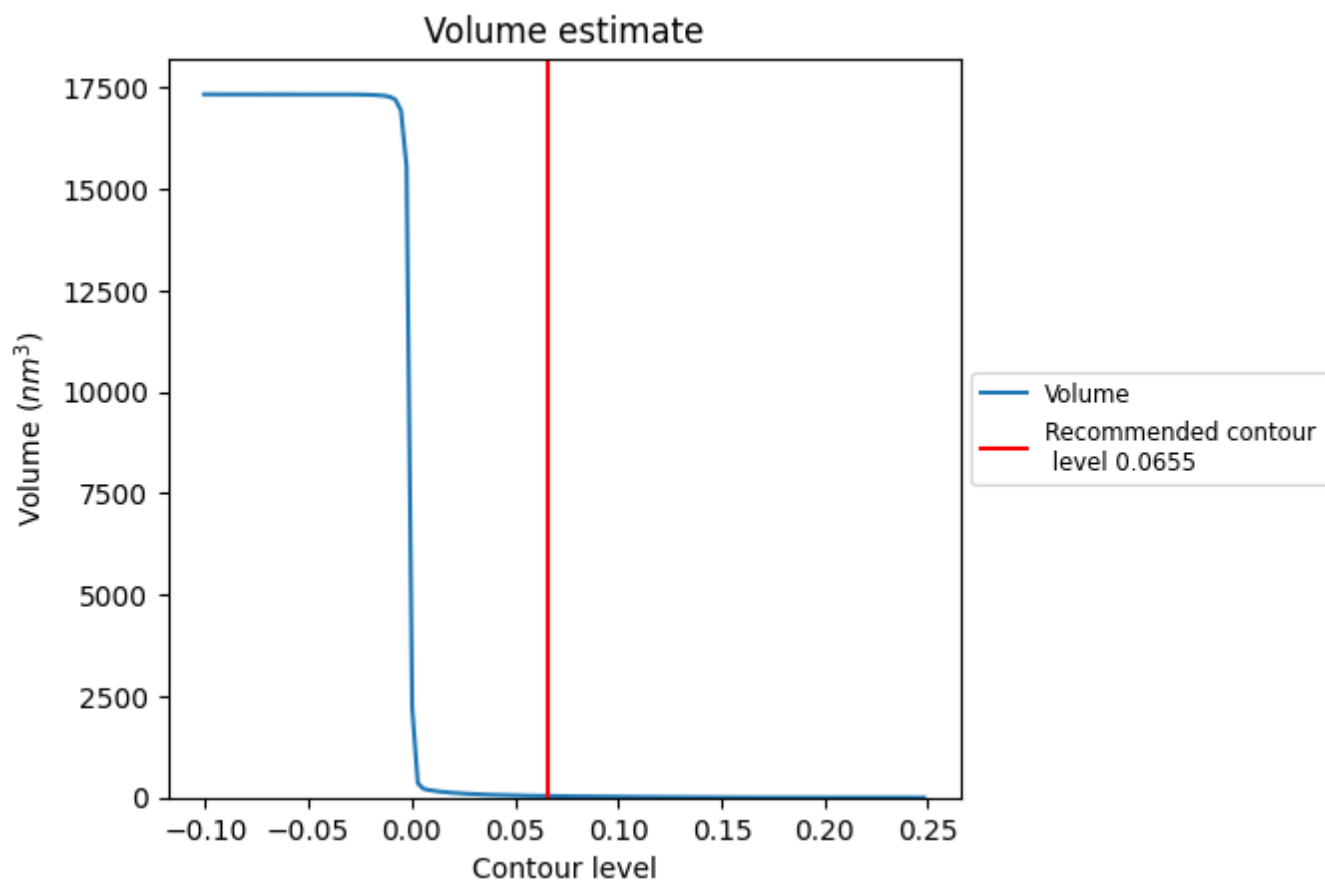
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

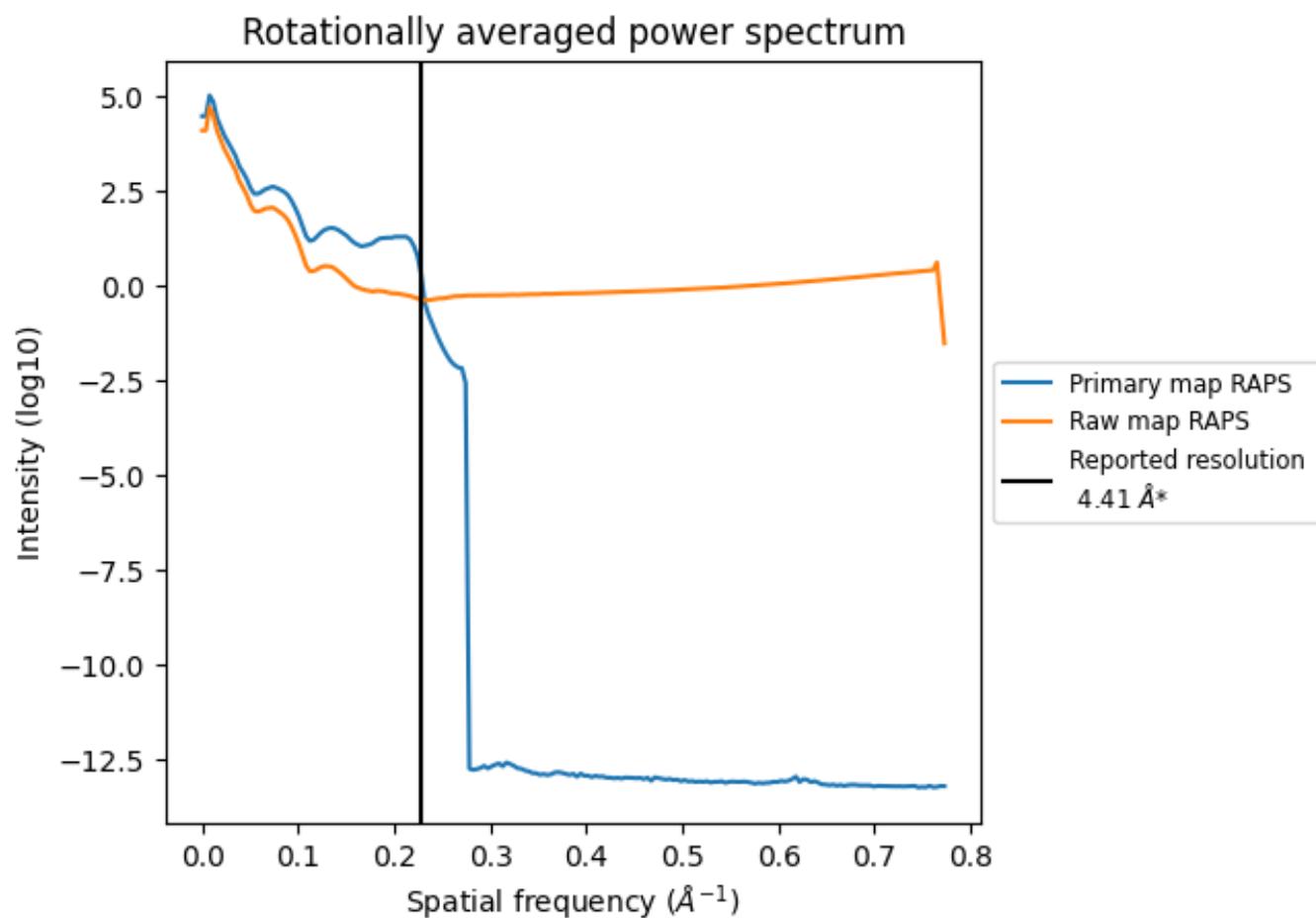
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 39 nm^3 ; this corresponds to an approximate mass of 35 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 ⓘ

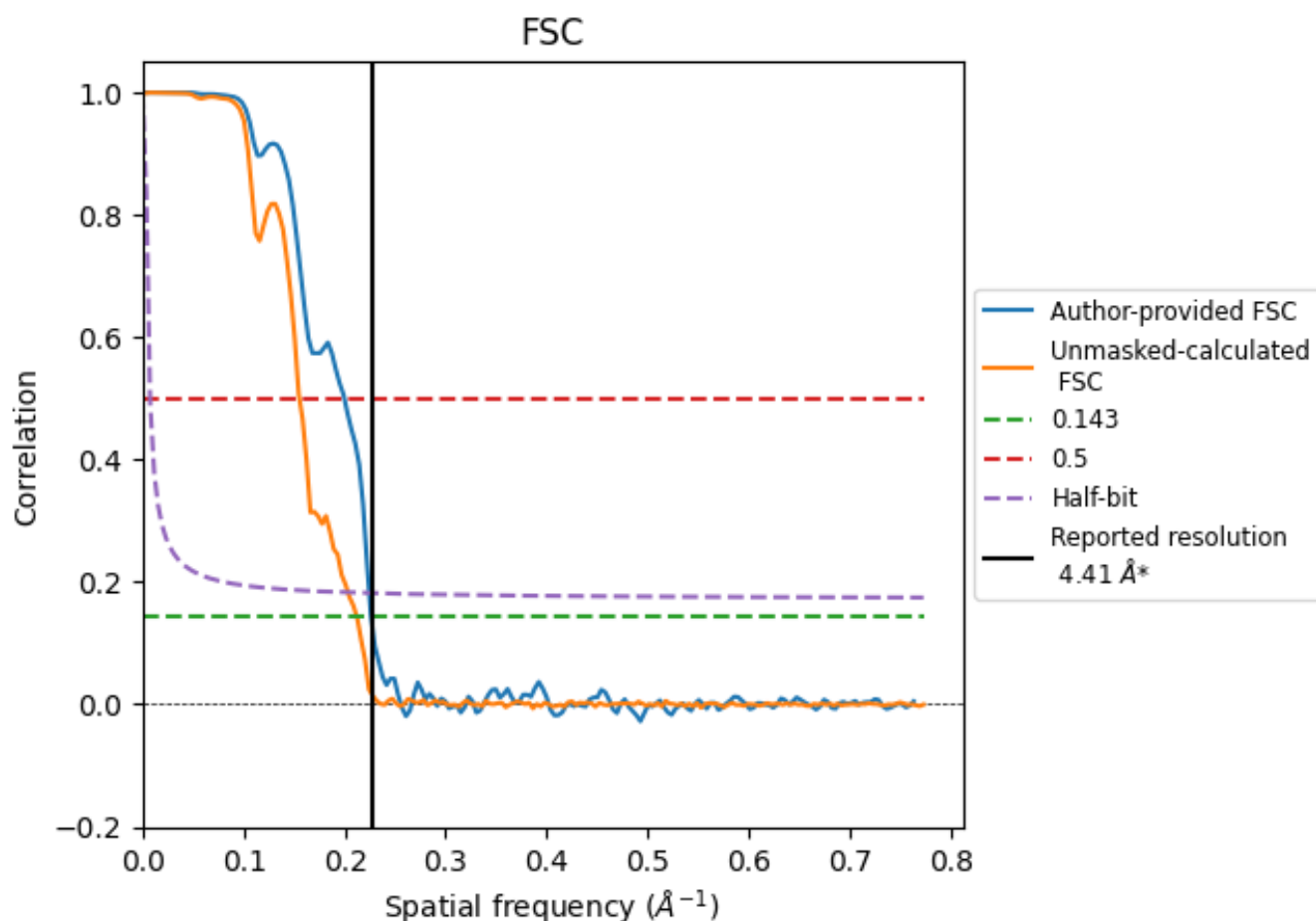


*Reported resolution corresponds to spatial frequency of 0.227 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.227 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.41	-	-
Author-provided FSC curve	4.42	5.01	4.46
Unmasked-calculated*	4.71	6.44	4.92

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

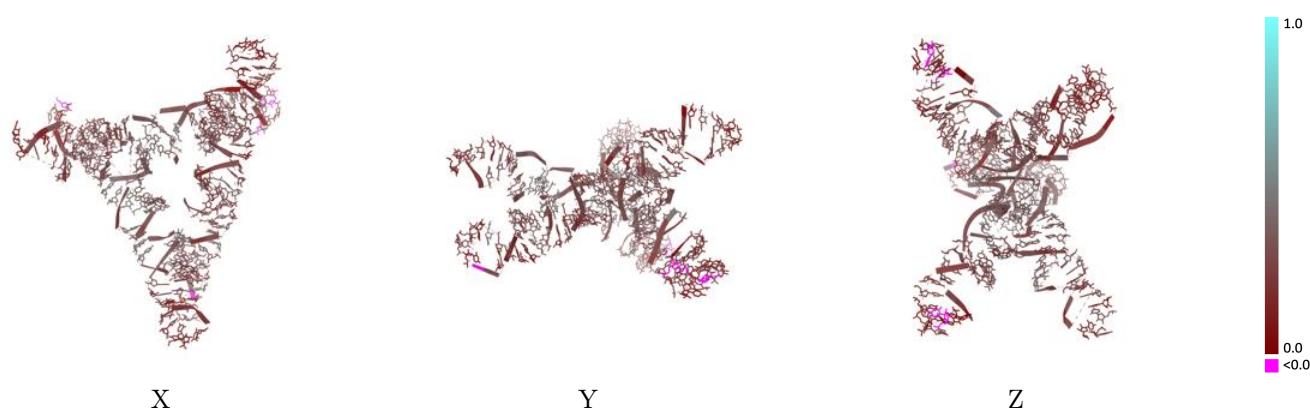
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53787 and PDB model 9R7Q. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)

This section was not generated.

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

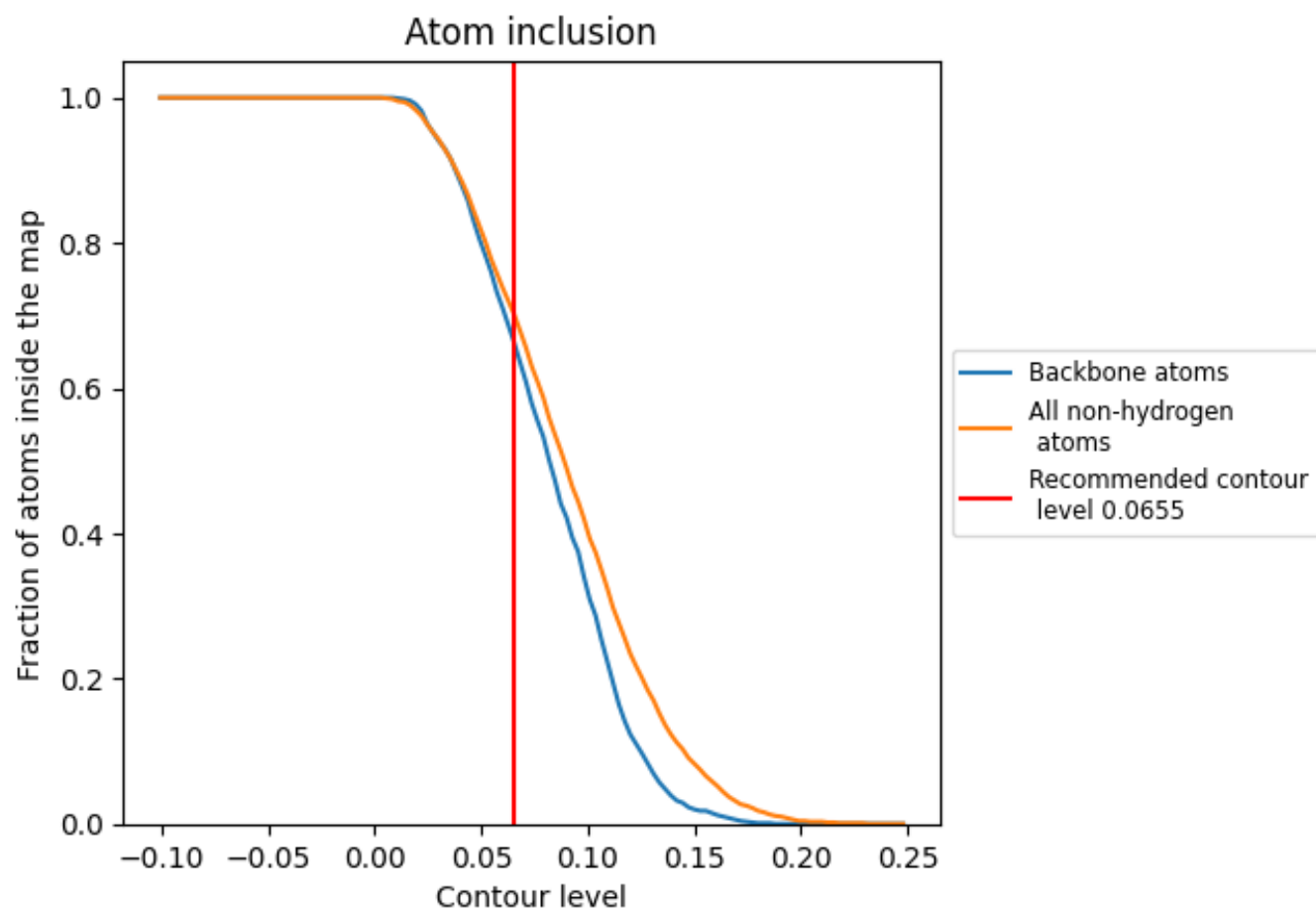


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 70% 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 (0.0655) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7020	<div></div> 0.2610
A	<div></div> 0.7020	<div></div> 0.2610

