



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 10:46 AM UTC

PDB ID : 9R7W / pdb_00009r7w
EMDB ID : EMD-53795
Title : 5-Helix Tile - Twist Corrected (5HT-TC) with 2'-Fluoro-modified pyrimidines (FY RNA)
Authors : Kristoffersen, E.L.; Andersen, E.S.; Zwergius, N.H.
Deposited on : 2025-05-15
Resolution : 6.06 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

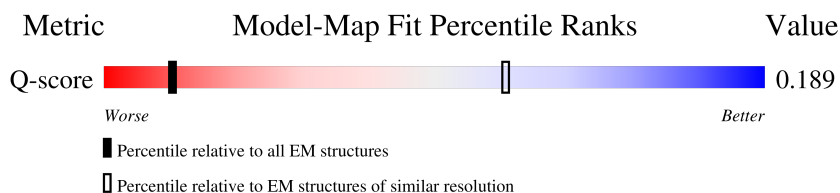
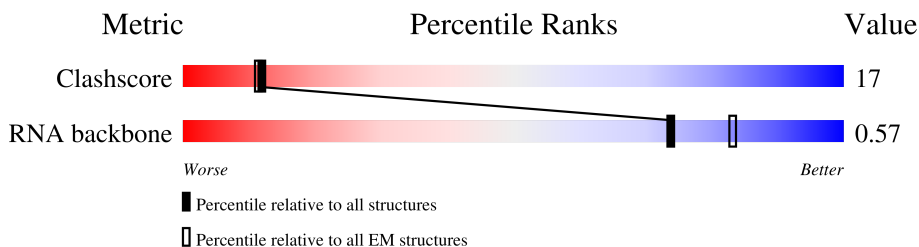
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

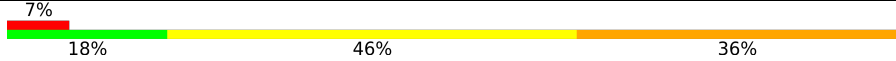
The reported resolution of this entry is 6.06 Å.

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	490 (5.57 - 6.56)

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	552	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 11752 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.

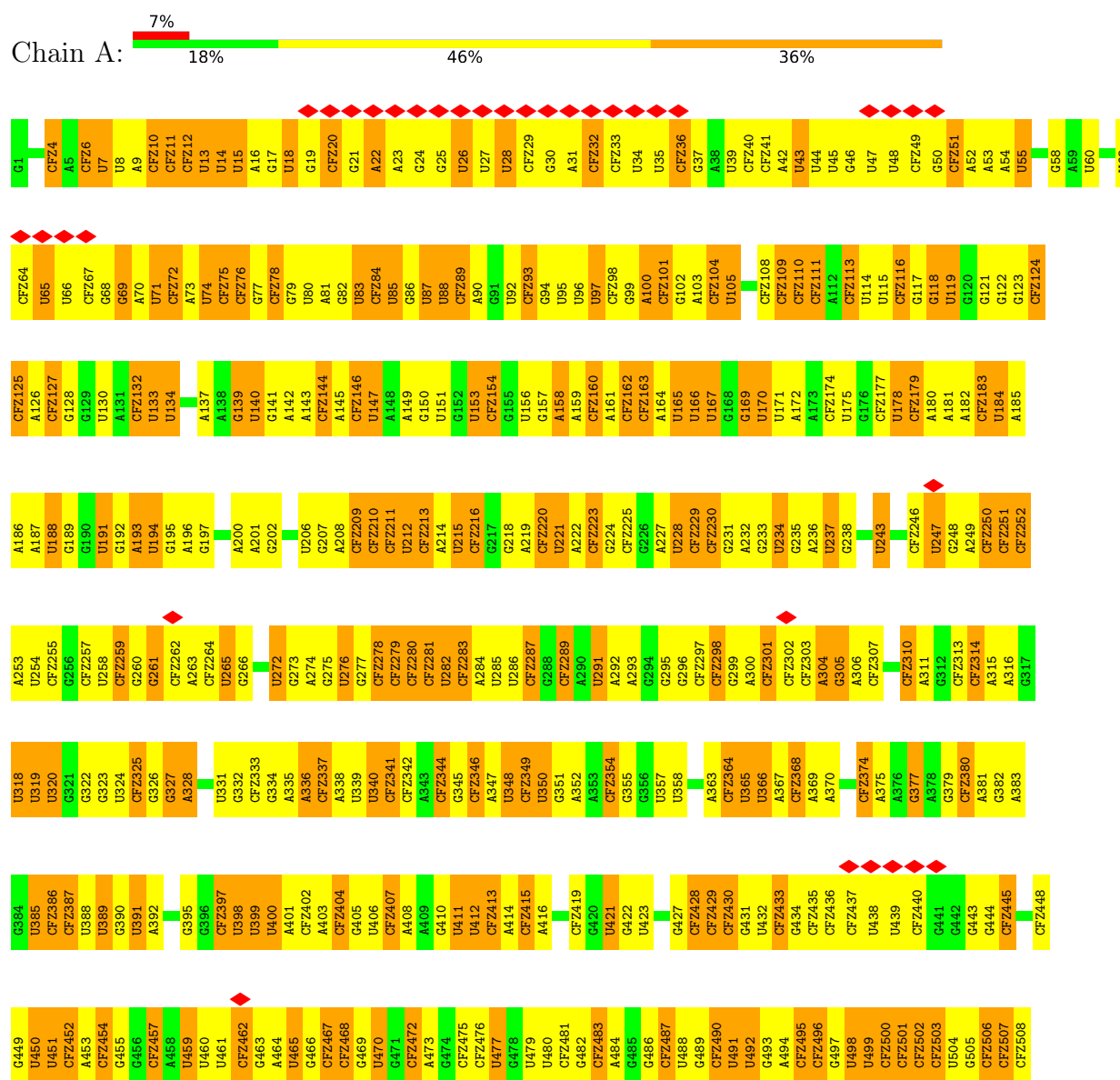
- Molecule 1 is a RNA chain called DNA/RNA (552-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	F	N	O	P		
1	A	552	11752	5246	274	2080	3600	552	0	0

3 Residue-property plots [i](#)

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 (552-MER)



U509	U510	U511	CFZ512	G513	A514	CFZ518	CFZ522	U523	A524	CFZ525	U526	CFZ527	U528	U529	CFZ530	G531	G532	A533	G534	U535	A536	G537	U538	CFZ539	U540	U541	A542	U543	G544	U545	G546	A547	A548	U549	G550	A551	G552

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	314600	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	0.497	Depositor
Minimum map value	-0.131	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.14	Depositor
Map size (Å)	331.264, 331.264, 331.264	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.294, 1.294, 1.294	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	0.49	43/7031 (0.6%)	0.24	0/10854

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	276	UFT	O3'-P	6.26	1.62	1.56
1	A	543	UFT	O3'-P	6.19	1.62	1.56
1	A	206	UFT	O3'-P	6.07	1.62	1.56
1	A	85	UFT	O3'-P	6.07	1.62	1.56
1	A	320	UFT	O3'-P	6.06	1.62	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	11752	0	5667	302	0
All	All	11752	0	5667	302	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 17.

The worst 5 of 302 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:25:G:H1	1:A:32:CFZ:HN4	1.02	1.02
1:A:430:CFZ:HN4	1:A:449:G:H1	1.00	0.98
1:A:459:UFT:HN3	1:A:464:A:N6	1.61	0.97
1:A:328:A:H61	1:A:350:UFT:HN3	0.92	0.92
1:A:328:A:N6	1:A:350:UFT:HN3	1.68	0.91

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	149/552 (26%)	27 (18%)	1 (0%)

5 of 27 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	22	A
1	A	23	A
1	A	24	G
1	A	58	G
1	A	69	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	304	A

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

274 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	CFZ	A	374	1	18,21,22	2.52	7 (38%)	25,30,33	1.23	2 (8%)
1	UFT	A	543	1	18,21,22	2.71	9 (50%)	25,30,33	2.00	6 (24%)
1	CFZ	A	487	1	18,21,22	2.55	7 (38%)	25,30,33	1.35	3 (12%)
1	CFZ	A	476	1	18,21,22	2.55	7 (38%)	25,30,33	1.25	2 (8%)
1	UFT	A	65	1	18,21,22	2.58	10 (55%)	25,30,33	2.28	8 (32%)
1	CFZ	A	104	1	18,21,22	2.56	7 (38%)	25,30,33	1.31	2 (8%)
1	CFZ	A	252	1	18,21,22	2.51	7 (38%)	25,30,33	1.41	3 (12%)
1	CFZ	A	281	1	18,21,22	2.54	7 (38%)	25,30,33	1.33	2 (8%)
1	UFT	A	391	1	18,21,22	2.66	10 (55%)	25,30,33	2.18	8 (32%)
1	CFZ	A	429	1	18,21,22	2.52	7 (38%)	25,30,33	1.54	3 (12%)
1	UFT	A	438	1	18,21,22	2.66	10 (55%)	25,30,33	2.03	7 (28%)
1	UFT	A	480	1	18,21,22	2.59	10 (55%)	25,30,33	2.21	8 (32%)
1	CFZ	A	530	1	18,21,22	2.47	7 (38%)	25,30,33	1.44	4 (16%)
1	CFZ	A	250	1	18,21,22	2.55	7 (38%)	25,30,33	1.23	2 (8%)
1	UFT	A	119	1	18,21,22	2.67	9 (50%)	25,30,33	1.90	6 (24%)
1	CFZ	A	4	1	18,21,22	2.54	7 (38%)	25,30,33	1.27	1 (4%)
1	CFZ	A	397	1	18,21,22	2.54	7 (38%)	25,30,33	1.26	2 (8%)
1	CFZ	A	162	1	18,21,22	2.55	7 (38%)	25,30,33	1.37	2 (8%)
1	CFZ	A	160	1	18,21,22	2.54	7 (38%)	25,30,33	1.35	3 (12%)
1	UFT	A	265	1	18,21,22	2.63	9 (50%)	25,30,33	1.95	7 (28%)
1	CFZ	A	32	1	18,21,22	2.51	6 (33%)	25,30,33	1.60	2 (8%)
1	UFT	A	88	1	18,21,22	2.60	9 (50%)	25,30,33	2.00	7 (28%)
1	UFT	A	167	1	18,21,22	2.66	9 (50%)	25,30,33	2.02	5 (20%)
1	UFT	A	451	1	18,21,22	2.62	9 (50%)	25,30,33	1.80	6 (24%)
1	CFZ	A	527	1	18,21,22	2.53	7 (38%)	25,30,33	1.23	2 (8%)
1	CFZ	A	539	1	18,21,22	2.53	6 (33%)	25,30,33	1.38	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CFZ	A	502	1	18,21,22	2.53	7 (38%)	25,30,33	1.28	3 (12%)
1	UFT	A	488	1	18,21,22	2.65	10 (55%)	25,30,33	2.03	7 (28%)
1	CFZ	A	211	1	18,21,22	2.55	7 (38%)	25,30,33	1.26	1 (4%)
1	CFZ	A	448	1	18,21,22	2.52	7 (38%)	25,30,33	1.26	3 (12%)
1	CFZ	A	472	1	18,21,22	2.53	7 (38%)	25,30,33	1.29	2 (8%)
1	CFZ	A	481	1	18,21,22	2.48	7 (38%)	25,30,33	1.24	2 (8%)
1	CFZ	A	11	1	18,21,22	2.54	7 (38%)	25,30,33	1.31	2 (8%)
1	CFZ	A	110	1	18,21,22	2.53	7 (38%)	25,30,33	1.27	3 (12%)
1	CFZ	A	255	1	18,21,22	2.52	7 (38%)	25,30,33	1.32	3 (12%)
1	UFT	A	95	1	18,21,22	2.61	10 (55%)	25,30,33	2.25	7 (28%)
1	UFT	A	178	1	18,21,22	2.67	10 (55%)	25,30,33	2.09	5 (20%)
1	UFT	A	331	1	18,21,22	2.64	9 (50%)	25,30,33	1.88	6 (24%)
1	UFT	A	234	1	18,21,22	2.64	10 (55%)	25,30,33	1.97	5 (20%)
1	CFZ	A	501	1	18,21,22	2.54	7 (38%)	25,30,33	1.23	2 (8%)
1	CFZ	A	506	1	18,21,22	2.57	7 (38%)	25,30,33	1.21	3 (12%)
1	CFZ	A	310	1	18,21,22	2.53	7 (38%)	25,30,33	1.28	3 (12%)
1	UFT	A	276	1	18,21,22	2.67	9 (50%)	25,30,33	1.94	6 (24%)
1	CFZ	A	462	1	18,21,22	2.46	7 (38%)	25,30,33	1.43	2 (8%)
1	CFZ	A	64	1	18,21,22	2.52	7 (38%)	25,30,33	1.23	2 (8%)
1	UFT	A	39	1	18,21,22	2.64	9 (50%)	25,30,33	2.09	7 (28%)
1	UFT	A	286	1	18,21,22	2.68	10 (55%)	25,30,33	2.18	6 (24%)
1	CFZ	A	525	1	18,21,22	2.53	7 (38%)	25,30,33	1.28	3 (12%)
1	CFZ	A	428	1	18,21,22	2.56	7 (38%)	25,30,33	1.26	2 (8%)
1	CFZ	A	402	1	18,21,22	2.55	7 (38%)	25,30,33	1.31	1 (4%)
1	CFZ	A	109	1	18,21,22	2.53	7 (38%)	25,30,33	1.28	2 (8%)
1	CFZ	A	33	1	18,21,22	2.49	7 (38%)	25,30,33	1.59	2 (8%)
1	UFT	A	357	1	18,21,22	2.67	9 (50%)	25,30,33	1.88	5 (20%)
1	CFZ	A	435	1	18,21,22	2.53	7 (38%)	25,30,33	1.29	2 (8%)
1	CFZ	A	483	1	18,21,22	2.54	7 (38%)	25,30,33	1.23	2 (8%)
1	CFZ	A	78	1	18,21,22	2.54	7 (38%)	25,30,33	1.47	4 (16%)
1	CFZ	A	146	1	18,21,22	2.55	7 (38%)	25,30,33	1.25	2 (8%)
1	CFZ	A	174	1	18,21,22	2.54	7 (38%)	25,30,33	1.31	3 (12%)
1	UFT	A	147	1	18,21,22	2.63	9 (50%)	25,30,33	2.18	8 (32%)
1	UFT	A	459	1	18,21,22	2.69	10 (55%)	25,30,33	1.99	6 (24%)
1	UFT	A	479	1	18,21,22	2.62	10 (55%)	25,30,33	2.14	8 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CFZ	A	251	1	18,21,22	2.54	7 (38%)	25,30,33	1.27	2 (8%)
1	CFZ	A	452	1	18,21,22	2.50	7 (38%)	25,30,33	1.42	2 (8%)
1	CFZ	A	179	1	18,21,22	2.55	7 (38%)	25,30,33	1.31	1 (4%)
1	CFZ	A	223	1	18,21,22	2.55	7 (38%)	25,30,33	1.28	2 (8%)
1	UFT	A	365	1	18,21,22	2.64	9 (50%)	25,30,33	1.98	7 (28%)
1	UFT	A	14	1	18,21,22	2.67	10 (55%)	25,30,33	2.03	7 (28%)
1	CFZ	A	116	1	18,21,22	2.50	7 (38%)	25,30,33	1.43	2 (8%)
1	CFZ	A	229	1	18,21,22	2.52	7 (38%)	25,30,33	1.51	3 (12%)
1	CFZ	A	430	1	18,21,22	2.53	6 (33%)	25,30,33	1.27	1 (4%)
1	UFT	A	153	1	18,21,22	2.66	10 (55%)	25,30,33	2.09	7 (28%)
1	CFZ	A	380	1	18,21,22	2.54	7 (38%)	25,30,33	1.19	2 (8%)
1	UFT	A	60	1	18,21,22	2.65	9 (50%)	25,30,33	1.93	5 (20%)
1	UFT	A	34	1	18,21,22	2.62	10 (55%)	25,30,33	2.09	7 (28%)
1	CFZ	A	344	1	18,21,22	2.52	7 (38%)	25,30,33	1.26	3 (12%)
1	CFZ	A	457	1	18,21,22	2.54	7 (38%)	25,30,33	1.24	1 (4%)
1	CFZ	A	468	1	18,21,22	2.53	7 (38%)	25,30,33	1.25	3 (12%)
1	CFZ	A	490	1	18,21,22	2.53	7 (38%)	25,30,33	1.42	2 (8%)
1	UFT	A	66	1	18,21,22	2.57	10 (55%)	25,30,33	2.19	8 (32%)
1	CFZ	A	349	1	18,21,22	2.54	7 (38%)	25,30,33	1.21	3 (12%)
1	CFZ	A	445	1	18,21,22	2.48	7 (38%)	25,30,33	1.55	3 (12%)
1	CFZ	A	454	1	18,21,22	2.55	7 (38%)	25,30,33	1.23	2 (8%)
1	CFZ	A	495	1	18,21,22	2.56	7 (38%)	25,30,33	1.24	2 (8%)
1	UFT	A	504	1	18,21,22	2.62	10 (55%)	25,30,33	2.18	7 (28%)
1	CFZ	A	40	1	18,21,22	2.50	7 (38%)	25,30,33	1.42	2 (8%)
1	CFZ	A	386	1	18,21,22	2.55	7 (38%)	25,30,33	1.32	3 (12%)
1	UFT	A	423	1	18,21,22	2.68	9 (50%)	25,30,33	1.90	6 (24%)
1	CFZ	A	113	1	18,21,22	2.53	7 (38%)	25,30,33	1.40	2 (8%)
1	UFT	A	538	1	18,21,22	2.62	9 (50%)	25,30,33	1.93	7 (28%)
1	UFT	A	87	1	18,21,22	2.63	10 (55%)	25,30,33	2.11	6 (24%)
1	UFT	A	92	1	18,21,22	2.66	9 (50%)	25,30,33	1.96	5 (20%)
1	CFZ	A	177	1	18,21,22	2.53	7 (38%)	25,30,33	1.39	3 (12%)
1	UFT	A	97	1	18,21,22	2.61	10 (55%)	25,30,33	2.11	6 (24%)
1	CFZ	A	124	1	18,21,22	2.54	7 (38%)	25,30,33	1.31	3 (12%)
1	UFT	A	282	1	18,21,22	2.64	9 (50%)	25,30,33	1.89	6 (24%)
1	UFT	A	35	1	18,21,22	2.63	10 (55%)	25,30,33	2.00	8 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	UFT	A	151	1	18,21,22	2.65	10 (55%)	25,30,33	1.95	7 (28%)
1	UFT	A	206	1	18,21,22	2.67	10 (55%)	25,30,33	2.07	5 (20%)
1	CFZ	A	101	1	18,21,22	2.52	6 (33%)	25,30,33	1.18	3 (12%)
1	UFT	A	170	1	18,21,22	2.66	10 (55%)	25,30,33	2.20	6 (24%)
1	UFT	A	320	1	18,21,22	2.62	10 (55%)	25,30,33	2.03	6 (24%)
1	UFT	A	509	1	18,21,22	2.66	10 (55%)	25,30,33	2.08	6 (24%)
1	UFT	A	254	1	18,21,22	2.61	9 (50%)	25,30,33	1.96	7 (28%)
1	UFT	A	411	1	18,21,22	2.65	10 (55%)	25,30,33	2.06	7 (28%)
1	UFT	A	388	1	18,21,22	2.65	10 (55%)	25,30,33	2.07	8 (32%)
1	CFZ	A	440	1	18,21,22	2.48	7 (38%)	25,30,33	1.34	2 (8%)
1	UFT	A	44	1	18,21,22	2.67	10 (55%)	25,30,33	2.01	6 (24%)
1	UFT	A	80	1	18,21,22	2.66	9 (50%)	25,30,33	1.87	5 (20%)
1	CFZ	A	354	1	18,21,22	2.55	7 (38%)	25,30,33	1.22	1 (4%)
1	UFT	A	366	1	18,21,22	2.63	9 (50%)	25,30,33	1.97	6 (24%)
1	CFZ	A	500	1	18,21,22	2.46	7 (38%)	25,30,33	1.44	2 (8%)
1	CFZ	A	111	1	18,21,22	2.53	7 (38%)	25,30,33	1.27	3 (12%)
1	UFT	A	358	1	18,21,22	2.67	10 (55%)	25,30,33	2.13	6 (24%)
1	CFZ	A	29	1	18,21,22	2.48	7 (38%)	25,30,33	1.54	3 (12%)
1	CFZ	A	127	1	18,21,22	2.56	7 (38%)	25,30,33	1.21	1 (4%)
1	UFT	A	212	1	18,21,22	2.66	10 (55%)	25,30,33	2.11	7 (28%)
1	CFZ	A	76	1	18,21,22	2.54	7 (38%)	25,30,33	1.20	2 (8%)
1	UFT	A	156	1	18,21,22	2.66	10 (55%)	25,30,33	2.09	7 (28%)
1	CFZ	A	98	1	18,21,22	2.48	7 (38%)	25,30,33	1.51	3 (12%)
1	UFT	A	450	1	18,21,22	2.65	10 (55%)	25,30,33	2.03	7 (28%)
1	UFT	A	83	1	18,21,22	2.67	10 (55%)	25,30,33	2.00	6 (24%)
1	CFZ	A	283	1	18,21,22	2.54	7 (38%)	25,30,33	1.28	3 (12%)
1	UFT	A	188	1	18,21,22	2.64	10 (55%)	25,30,33	2.03	7 (28%)
1	UFT	A	291	1	18,21,22	2.66	9 (50%)	25,30,33	1.92	6 (24%)
1	CFZ	A	93	1	18,21,22	2.53	7 (38%)	25,30,33	1.36	3 (12%)
1	UFT	A	319	1	18,21,22	2.62	10 (55%)	25,30,33	1.99	7 (28%)
1	UFT	A	385	1	18,21,22	2.65	9 (50%)	25,30,33	2.06	7 (28%)
1	UFT	A	47	1	18,21,22	2.65	9 (50%)	25,30,33	2.20	7 (28%)
1	CFZ	A	287	1	18,21,22	2.53	7 (38%)	25,30,33	1.40	2 (8%)
1	CFZ	A	298	1	18,21,22	2.55	7 (38%)	25,30,33	1.29	2 (8%)
1	CFZ	A	433	1	18,21,22	2.52	7 (38%)	25,30,33	1.34	3 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	UFT	A	339	1	18,21,22	2.61	9 (50%)	25,30,33	1.99	7 (28%)
1	UFT	A	477	1	18,21,22	2.67	10 (55%)	25,30,33	2.11	5 (20%)
1	CFZ	A	496	1	18,21,22	2.53	7 (38%)	25,30,33	1.43	4 (16%)
1	CFZ	A	132	1	18,21,22	2.53	7 (38%)	25,30,33	1.31	3 (12%)
1	UFT	A	398	1	18,21,22	2.61	10 (55%)	25,30,33	2.12	7 (28%)
1	CFZ	A	415	1	18,21,22	2.53	7 (38%)	25,30,33	1.21	2 (8%)
1	UFT	A	48	1	18,21,22	2.60	10 (55%)	25,30,33	2.13	8 (32%)
1	CFZ	A	512	1	18,21,22	2.48	7 (38%)	25,30,33	1.54	3 (12%)
1	UFT	A	194	1	18,21,22	2.64	10 (55%)	25,30,33	2.16	7 (28%)
1	CFZ	A	289	1	18,21,22	2.55	7 (38%)	25,30,33	1.37	2 (8%)
1	CFZ	A	216	1	18,21,22	2.54	7 (38%)	25,30,33	1.16	2 (8%)
1	CFZ	A	404	1	18,21,22	2.49	7 (38%)	25,30,33	1.50	2 (8%)
1	CFZ	A	230	1	18,21,22	2.55	7 (38%)	25,30,33	1.37	1 (4%)
1	CFZ	A	41	1	18,21,22	2.51	7 (38%)	25,30,33	1.33	3 (12%)
1	CFZ	A	246	1	18,21,22	2.56	7 (38%)	25,30,33	1.43	3 (12%)
1	UFT	A	389	1	18,21,22	2.66	10 (55%)	25,30,33	2.04	7 (28%)
1	CFZ	A	280	1	18,21,22	2.55	7 (38%)	25,30,33	1.36	3 (12%)
1	UFT	A	171	1	18,21,22	2.61	10 (55%)	25,30,33	2.20	8 (32%)
1	CFZ	A	503	1	18,21,22	2.49	7 (38%)	25,30,33	1.44	3 (12%)
1	UFT	A	184	1	18,21,22	2.65	10 (55%)	25,30,33	1.98	6 (24%)
1	CFZ	A	437	1	18,21,22	2.55	7 (38%)	25,30,33	1.32	2 (8%)
1	CFZ	A	75	1	18,21,22	2.54	6 (33%)	25,30,33	1.27	3 (12%)
1	CFZ	A	12	1	18,21,22	2.53	7 (38%)	25,30,33	1.33	2 (8%)
1	CFZ	A	407	1	18,21,22	2.50	7 (38%)	25,30,33	1.36	2 (8%)
1	CFZ	A	84	1	18,21,22	2.56	7 (38%)	25,30,33	1.26	2 (8%)
1	UFT	A	529	1	18,21,22	2.61	10 (55%)	25,30,33	2.18	8 (32%)
1	CFZ	A	436	1	18,21,22	2.54	7 (38%)	25,30,33	1.27	2 (8%)
1	UFT	A	130	1	18,21,22	2.66	10 (55%)	25,30,33	2.02	6 (24%)
1	UFT	A	470	1	18,21,22	2.66	10 (55%)	25,30,33	2.01	7 (28%)
1	UFT	A	535	1	18,21,22	2.67	9 (50%)	25,30,33	1.90	6 (24%)
1	UFT	A	28	1	18,21,22	2.65	10 (55%)	25,30,33	1.99	7 (28%)
1	CFZ	A	522	1	18,21,22	2.53	7 (38%)	25,30,33	1.27	2 (8%)
1	UFT	A	465	1	18,21,22	2.65	9 (50%)	25,30,33	2.06	7 (28%)
1	CFZ	A	20	1	18,21,22	2.50	7 (38%)	25,30,33	1.49	3 (12%)
1	UFT	A	18	1	18,21,22	2.68	10 (55%)	25,30,33	2.05	6 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	UFT	A	340	1	18,21,22	2.63	9 (50%)	25,30,33	2.13	8 (32%)
1	UFT	A	134	1	18,21,22	2.66	10 (55%)	25,30,33	2.14	7 (28%)
1	UFT	A	8	1	18,21,22	2.67	10 (55%)	25,30,33	2.09	7 (28%)
1	CFZ	A	163	1	18,21,22	2.54	7 (38%)	25,30,33	1.24	3 (12%)
1	CFZ	A	209	1	18,21,22	2.54	7 (38%)	25,30,33	1.32	3 (12%)
1	CFZ	A	210	1	18,21,22	2.50	7 (38%)	25,30,33	1.46	3 (12%)
1	UFT	A	324	1	18,21,22	2.62	10 (55%)	25,30,33	2.18	7 (28%)
1	CFZ	A	518	1	18,21,22	2.54	7 (38%)	25,30,33	1.29	3 (12%)
1	UFT	A	27	1	18,21,22	2.59	10 (55%)	25,30,33	2.18	8 (32%)
1	UFT	A	85	1	18,21,22	2.66	10 (55%)	25,30,33	2.11	6 (24%)
1	UFT	A	74	1	18,21,22	2.67	9 (50%)	25,30,33	1.91	6 (24%)
1	CFZ	A	257	1	18,21,22	2.51	7 (38%)	25,30,33	1.46	2 (8%)
1	UFT	A	526	1	18,21,22	2.68	10 (55%)	25,30,33	2.10	6 (24%)
1	CFZ	A	220	1	18,21,22	2.55	7 (38%)	25,30,33	1.37	2 (8%)
1	CFZ	A	413	1	18,21,22	2.54	7 (38%)	25,30,33	1.23	3 (12%)
1	UFT	A	460	1	18,21,22	2.61	10 (55%)	25,30,33	2.12	6 (24%)
1	UFT	A	492	1	18,21,22	2.63	10 (55%)	25,30,33	2.10	7 (28%)
1	CFZ	A	279	1	18,21,22	2.55	7 (38%)	25,30,33	1.31	2 (8%)
1	CFZ	A	419	1	18,21,22	2.52	7 (38%)	25,30,33	1.34	3 (12%)
1	UFT	A	540	1	18,21,22	2.67	10 (55%)	25,30,33	2.14	6 (24%)
1	UFT	A	26	1	18,21,22	2.68	10 (55%)	25,30,33	2.18	6 (24%)
1	UFT	A	191	1	18,21,22	2.63	10 (55%)	25,30,33	2.13	7 (28%)
1	UFT	A	96	1	18,21,22	2.63	10 (55%)	25,30,33	2.04	7 (28%)
1	UFT	A	541	1	18,21,22	2.67	10 (55%)	25,30,33	2.05	7 (28%)
1	UFT	A	71	1	18,21,22	2.65	9 (50%)	25,30,33	1.90	6 (24%)
1	CFZ	A	89	1	18,21,22	2.56	7 (38%)	25,30,33	1.18	2 (8%)
1	CFZ	A	225	1	18,21,22	2.50	7 (38%)	25,30,33	1.47	3 (12%)
1	CFZ	A	302	1	18,21,22	2.52	7 (38%)	25,30,33	1.44	2 (8%)
1	CFZ	A	313	1	18,21,22	2.53	7 (38%)	25,30,33	1.59	2 (8%)
1	CFZ	A	341	1	18,21,22	2.50	7 (38%)	25,30,33	1.33	3 (12%)
1	CFZ	A	342	1	18,21,22	2.51	7 (38%)	25,30,33	1.24	3 (12%)
1	UFT	A	461	1	18,21,22	2.60	10 (55%)	25,30,33	2.20	8 (32%)
1	UFT	A	511	1	18,21,22	2.61	10 (55%)	25,30,33	2.10	6 (24%)
1	CFZ	A	368	1	18,21,22	2.54	7 (38%)	25,30,33	1.33	2 (8%)
1	CFZ	A	467	1	18,21,22	2.54	7 (38%)	25,30,33	1.31	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	UFT	A	272	1	18,21,22	2.66	10 (55%)	25,30,33	2.02	7 (28%)
1	UFT	A	285	1	18,21,22	2.64	10 (55%)	25,30,33	2.02	7 (28%)
1	CFZ	A	51	1	18,21,22	2.53	7 (38%)	25,30,33	1.35	4 (16%)
1	UFT	A	399	1	18,21,22	2.70	10 (55%)	25,30,33	2.03	7 (28%)
1	UFT	A	7	1	18,21,22	2.65	9 (50%)	25,30,33	1.90	5 (20%)
1	CFZ	A	307	1	18,21,22	2.51	7 (38%)	25,30,33	1.33	3 (12%)
1	CFZ	A	325	1	18,21,22	2.52	7 (38%)	25,30,33	1.34	3 (12%)
1	CFZ	A	301	1	18,21,22	2.53	7 (38%)	25,30,33	1.35	3 (12%)
1	UFT	A	406	1	18,21,22	2.65	10 (55%)	25,30,33	2.17	7 (28%)
1	UFT	A	166	1	18,21,22	2.68	10 (55%)	25,30,33	2.11	7 (28%)
1	CFZ	A	475	1	18,21,22	2.52	7 (38%)	25,30,33	1.26	3 (12%)
1	CFZ	A	333	1	18,21,22	2.48	7 (38%)	25,30,33	1.56	3 (12%)
1	UFT	A	412	1	18,21,22	2.65	10 (55%)	25,30,33	2.01	7 (28%)
1	UFT	A	510	1	18,21,22	2.60	10 (55%)	25,30,33	2.06	6 (24%)
1	UFT	A	545	1	18,21,22	2.63	9 (50%)	25,30,33	2.24	7 (28%)
1	CFZ	A	262	1	18,21,22	2.53	7 (38%)	25,30,33	1.33	3 (12%)
1	UFT	A	140	1	18,21,22	2.63	9 (50%)	25,30,33	1.96	6 (24%)
1	UFT	A	175	1	18,21,22	2.64	9 (50%)	25,30,33	1.96	6 (24%)
1	CFZ	A	10	1	18,21,22	2.53	7 (38%)	25,30,33	1.25	2 (8%)
1	UFT	A	165	1	18,21,22	2.67	10 (55%)	25,30,33	2.09	7 (28%)
1	UFT	A	63	1	18,21,22	2.63	9 (50%)	25,30,33	2.04	7 (28%)
1	UFT	A	15	1	18,21,22	2.68	10 (55%)	25,30,33	2.11	6 (24%)
1	CFZ	A	213	1	18,21,22	2.53	7 (38%)	25,30,33	1.29	3 (12%)
1	UFT	A	221	1	18,21,22	2.66	10 (55%)	25,30,33	1.97	6 (24%)
1	UFT	A	350	1	18,21,22	2.67	10 (55%)	25,30,33	2.14	7 (28%)
1	CFZ	A	507	1	18,21,22	2.54	7 (38%)	25,30,33	1.25	3 (12%)
1	CFZ	A	314	1	18,21,22	2.56	6 (33%)	25,30,33	1.24	2 (8%)
1	UFT	A	215	1	18,21,22	2.67	10 (55%)	25,30,33	2.18	7 (28%)
1	CFZ	A	36	1	18,21,22	2.47	7 (38%)	25,30,33	1.22	2 (8%)
1	CFZ	A	125	1	18,21,22	2.54	7 (38%)	25,30,33	1.28	2 (8%)
1	UFT	A	439	1	18,21,22	2.62	10 (55%)	25,30,33	2.15	8 (32%)
1	CFZ	A	259	1	18,21,22	2.50	7 (38%)	25,30,33	1.38	4 (16%)
1	UFT	A	491	1	18,21,22	2.67	10 (55%)	25,30,33	2.07	7 (28%)
1	UFT	A	523	1	18,21,22	2.65	10 (55%)	25,30,33	2.05	7 (28%)
1	UFT	A	247	1	18,21,22	2.71	10 (55%)	25,30,33	2.07	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	UFT	A	400	1	18,21,22	2.66	9 (50%)	25,30,33	1.96	5 (20%)
1	CFZ	A	346	1	18,21,22	2.54	7 (38%)	25,30,33	1.29	3 (12%)
1	CFZ	A	297	1	18,21,22	2.49	6 (33%)	25,30,33	1.55	3 (12%)
1	UFT	A	528	1	18,21,22	2.67	9 (50%)	25,30,33	1.97	5 (20%)
1	CFZ	A	72	1	18,21,22	2.55	7 (38%)	25,30,33	1.27	2 (8%)
1	CFZ	A	154	1	18,21,22	2.50	7 (38%)	25,30,33	1.40	4 (16%)
1	CFZ	A	303	1	18,21,22	2.54	7 (38%)	25,30,33	1.28	3 (12%)
1	UFT	A	13	1	18,21,22	2.67	10 (55%)	25,30,33	2.02	6 (24%)
1	UFT	A	228	1	18,21,22	2.64	9 (50%)	25,30,33	1.85	6 (24%)
1	UFT	A	549	1	18,21,22	2.65	10 (55%)	25,30,33	1.99	7 (28%)
1	UFT	A	133	1	18,21,22	2.66	10 (55%)	25,30,33	2.03	7 (28%)
1	CFZ	A	183	1	18,21,22	2.53	7 (38%)	25,30,33	1.24	2 (8%)
1	CFZ	A	337	1	18,21,22	2.52	7 (38%)	25,30,33	1.27	3 (12%)
1	UFT	A	258	1	18,21,22	2.60	9 (50%)	25,30,33	1.97	8 (32%)
1	UFT	A	105	1	18,21,22	2.61	9 (50%)	25,30,33	2.09	7 (28%)
1	CFZ	A	108	1	18,21,22	2.55	7 (38%)	25,30,33	1.24	2 (8%)
1	UFT	A	55	1	18,21,22	2.64	10 (55%)	25,30,33	2.10	8 (32%)
1	UFT	A	115	1	18,21,22	2.59	10 (55%)	25,30,33	2.07	6 (24%)
1	UFT	A	243	1	18,21,22	2.65	10 (55%)	25,30,33	2.14	8 (32%)
1	UFT	A	498	1	18,21,22	2.62	10 (55%)	25,30,33	2.27	7 (28%)
1	CFZ	A	264	1	18,21,22	2.54	7 (38%)	25,30,33	1.41	3 (12%)
1	CFZ	A	508	1	18,21,22	2.54	7 (38%)	25,30,33	1.34	3 (12%)
1	CFZ	A	144	1	18,21,22	2.54	7 (38%)	25,30,33	1.22	2 (8%)
1	UFT	A	348	1	18,21,22	2.68	10 (55%)	25,30,33	1.98	7 (28%)
1	UFT	A	499	1	18,21,22	2.63	10 (55%)	25,30,33	2.32	10 (40%)
1	CFZ	A	67	1	18,21,22	2.50	7 (38%)	25,30,33	1.49	3 (12%)
1	CFZ	A	278	1	18,21,22	2.56	7 (38%)	25,30,33	1.25	2 (8%)
1	UFT	A	318	1	18,21,22	2.66	10 (55%)	25,30,33	2.16	7 (28%)
1	CFZ	A	49	1	18,21,22	2.48	7 (38%)	25,30,33	1.56	3 (12%)
1	UFT	A	237	1	18,21,22	2.67	9 (50%)	25,30,33	1.99	6 (24%)
1	CFZ	A	6	1	18,21,22	2.54	7 (38%)	25,30,33	1.30	3 (12%)
1	UFT	A	45	1	18,21,22	2.69	10 (55%)	25,30,33	2.00	5 (20%)
1	CFZ	A	387	1	18,21,22	2.51	7 (38%)	25,30,33	1.47	2 (8%)
1	CFZ	A	364	1	18,21,22	2.53	7 (38%)	25,30,33	1.32	3 (12%)
1	UFT	A	43	1	18,21,22	2.65	10 (55%)	25,30,33	1.95	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	UFT	A	421	1	18,21,22	2.65	10 (55%)	25,30,33	2.00	7 (28%)
1	UFT	A	114	1	18,21,22	2.62	9 (50%)	25,30,33	2.07	7 (28%)
1	UFT	A	432	1	18,21,22	2.64	10 (55%)	25,30,33	2.01	7 (28%)

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	CFZ	A	374	1	-	0/7/25/26	0/2/2/2
1	UFT	A	543	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	487	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	476	1	-	0/7/25/26	0/2/2/2
1	UFT	A	65	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	104	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	252	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	281	1	-	0/7/25/26	0/2/2/2
1	UFT	A	391	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	429	1	-	1/7/25/26	0/2/2/2
1	UFT	A	438	1	-	2/7/25/26	0/2/2/2
1	UFT	A	480	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	530	1	-	5/7/25/26	0/2/2/2
1	CFZ	A	250	1	-	0/7/25/26	0/2/2/2
1	UFT	A	119	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	4	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	397	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	162	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	160	1	-	0/7/25/26	0/2/2/2
1	UFT	A	265	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	32	1	-	0/7/25/26	0/2/2/2
1	UFT	A	88	1	-	2/7/25/26	0/2/2/2
1	UFT	A	167	1	-	0/7/25/26	0/2/2/2
1	UFT	A	451	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	527	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	539	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	502	1	-	0/7/25/26	0/2/2/2
1	UFT	A	488	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	211	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	448	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	472	1	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CFZ	A	481	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	11	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	110	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	255	1	-	0/7/25/26	0/2/2/2
1	UFT	A	95	1	-	2/7/25/26	0/2/2/2
1	UFT	A	178	1	-	1/7/25/26	0/2/2/2
1	UFT	A	331	1	-	2/7/25/26	0/2/2/2
1	UFT	A	234	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	501	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	506	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	310	1	-	1/7/25/26	0/2/2/2
1	UFT	A	276	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	462	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	64	1	-	0/7/25/26	0/2/2/2
1	UFT	A	39	1	-	2/7/25/26	0/2/2/2
1	UFT	A	286	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	525	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	428	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	402	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	109	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	33	1	-	0/7/25/26	0/2/2/2
1	UFT	A	357	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	435	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	483	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	78	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	146	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	174	1	-	0/7/25/26	0/2/2/2
1	UFT	A	147	1	-	0/7/25/26	0/2/2/2
1	UFT	A	459	1	-	1/7/25/26	0/2/2/2
1	UFT	A	479	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	251	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	452	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	179	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	223	1	-	0/7/25/26	0/2/2/2
1	UFT	A	365	1	-	0/7/25/26	0/2/2/2
1	UFT	A	14	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	116	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	229	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	430	1	-	0/7/25/26	0/2/2/2
1	UFT	A	153	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	380	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UFT	A	60	1	-	0/7/25/26	0/2/2/2
1	UFT	A	34	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	344	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	457	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	468	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	490	1	-	0/7/25/26	0/2/2/2
1	UFT	A	66	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	349	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	445	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	454	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	495	1	-	0/7/25/26	0/2/2/2
1	UFT	A	504	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	40	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	386	1	-	0/7/25/26	0/2/2/2
1	UFT	A	423	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	113	1	-	0/7/25/26	0/2/2/2
1	UFT	A	538	1	-	0/7/25/26	0/2/2/2
1	UFT	A	87	1	-	3/7/25/26	0/2/2/2
1	UFT	A	92	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	177	1	-	2/7/25/26	0/2/2/2
1	UFT	A	97	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	124	1	-	0/7/25/26	0/2/2/2
1	UFT	A	282	1	-	0/7/25/26	0/2/2/2
1	UFT	A	35	1	-	1/7/25/26	0/2/2/2
1	UFT	A	151	1	-	0/7/25/26	0/2/2/2
1	UFT	A	206	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	101	1	-	0/7/25/26	0/2/2/2
1	UFT	A	170	1	-	2/7/25/26	0/2/2/2
1	UFT	A	320	1	-	0/7/25/26	0/2/2/2
1	UFT	A	509	1	-	2/7/25/26	0/2/2/2
1	UFT	A	254	1	-	0/7/25/26	0/2/2/2
1	UFT	A	411	1	-	1/7/25/26	0/2/2/2
1	UFT	A	388	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	440	1	-	2/7/25/26	0/2/2/2
1	UFT	A	44	1	-	0/7/25/26	0/2/2/2
1	UFT	A	80	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	354	1	-	0/7/25/26	0/2/2/2
1	UFT	A	366	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	500	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	111	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UFT	A	358	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	29	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	127	1	-	0/7/25/26	0/2/2/2
1	UFT	A	212	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	76	1	-	0/7/25/26	0/2/2/2
1	UFT	A	156	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	98	1	-	2/7/25/26	0/2/2/2
1	UFT	A	450	1	-	0/7/25/26	0/2/2/2
1	UFT	A	83	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	283	1	-	0/7/25/26	0/2/2/2
1	UFT	A	188	1	-	0/7/25/26	0/2/2/2
1	UFT	A	291	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	93	1	-	1/7/25/26	0/2/2/2
1	UFT	A	319	1	-	2/7/25/26	0/2/2/2
1	UFT	A	385	1	-	2/7/25/26	0/2/2/2
1	UFT	A	47	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	287	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	298	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	433	1	-	0/7/25/26	0/2/2/2
1	UFT	A	339	1	-	0/7/25/26	0/2/2/2
1	UFT	A	477	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	496	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	132	1	-	0/7/25/26	0/2/2/2
1	UFT	A	398	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	415	1	-	0/7/25/26	0/2/2/2
1	UFT	A	48	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	512	1	-	2/7/25/26	0/2/2/2
1	UFT	A	194	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	289	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	216	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	404	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	230	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	41	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	246	1	-	0/7/25/26	0/2/2/2
1	UFT	A	389	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	280	1	-	0/7/25/26	0/2/2/2
1	UFT	A	171	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	503	1	-	0/7/25/26	0/2/2/2
1	UFT	A	184	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CFZ	A	437	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	75	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	12	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	407	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	84	1	-	0/7/25/26	0/2/2/2
1	UFT	A	529	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	436	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	470	1	-	0/7/25/26	0/2/2/2
1	UFT	A	535	1	-	0/7/25/26	0/2/2/2
1	UFT	A	28	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	522	1	-	0/7/25/26	0/2/2/2
1	UFT	A	465	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	20	1	-	0/7/25/26	0/2/2/2
1	UFT	A	18	1	-	0/7/25/26	0/2/2/2
1	UFT	A	340	1	-	1/7/25/26	0/2/2/2
1	UFT	A	134	1	-	0/7/25/26	0/2/2/2
1	UFT	A	8	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	163	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	209	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	210	1	-	0/7/25/26	0/2/2/2
1	UFT	A	324	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	518	1	-	0/7/25/26	0/2/2/2
1	UFT	A	27	1	-	2/7/25/26	0/2/2/2
1	UFT	A	85	1	-	0/7/25/26	0/2/2/2
1	UFT	A	74	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	257	1	-	0/7/25/26	0/2/2/2
1	UFT	A	526	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	220	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	413	1	-	0/7/25/26	0/2/2/2
1	UFT	A	460	1	-	2/7/25/26	0/2/2/2
1	UFT	A	492	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	279	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	419	1	-	2/7/25/26	0/2/2/2
1	UFT	A	540	1	-	0/7/25/26	0/2/2/2
1	UFT	A	26	1	-	1/7/25/26	0/2/2/2
1	UFT	A	191	1	-	3/7/25/26	0/2/2/2
1	UFT	A	96	1	-	0/7/25/26	0/2/2/2
1	UFT	A	541	1	-	0/7/25/26	0/2/2/2
1	UFT	A	71	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	89	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CFZ	A	225	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	302	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	313	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	341	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	342	1	-	0/7/25/26	0/2/2/2
1	UFT	A	461	1	-	0/7/25/26	0/2/2/2
1	UFT	A	511	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	368	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	467	1	-	0/7/25/26	0/2/2/2
1	UFT	A	272	1	-	0/7/25/26	0/2/2/2
1	UFT	A	285	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	51	1	-	0/7/25/26	0/2/2/2
1	UFT	A	399	1	-	3/7/25/26	0/2/2/2
1	UFT	A	7	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	307	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	325	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	301	1	-	0/7/25/26	0/2/2/2
1	UFT	A	406	1	-	1/7/25/26	0/2/2/2
1	UFT	A	166	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	475	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	333	1	-	0/7/25/26	0/2/2/2
1	UFT	A	412	1	-	0/7/25/26	0/2/2/2
1	UFT	A	510	1	-	2/7/25/26	0/2/2/2
1	UFT	A	545	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	262	1	-	0/7/25/26	0/2/2/2
1	UFT	A	140	1	-	0/7/25/26	0/2/2/2
1	UFT	A	175	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	10	1	-	0/7/25/26	0/2/2/2
1	UFT	A	165	1	-	0/7/25/26	0/2/2/2
1	UFT	A	63	1	-	0/7/25/26	0/2/2/2
1	UFT	A	15	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	213	1	-	0/7/25/26	0/2/2/2
1	UFT	A	221	1	-	0/7/25/26	0/2/2/2
1	UFT	A	350	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	507	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	314	1	-	1/7/25/26	0/2/2/2
1	UFT	A	215	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	36	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	125	1	-	0/7/25/26	0/2/2/2
1	UFT	A	439	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	259	1	-	0/7/25/26	0/2/2/2
1	UFT	A	491	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UFT	A	523	1	-	0/7/25/26	0/2/2/2
1	UFT	A	247	1	-	2/7/25/26	0/2/2/2
1	UFT	A	400	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	346	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	297	1	-	0/7/25/26	0/2/2/2
1	UFT	A	528	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	72	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	154	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	303	1	-	2/7/25/26	0/2/2/2
1	UFT	A	13	1	-	2/7/25/26	0/2/2/2
1	UFT	A	228	1	-	0/7/25/26	0/2/2/2
1	UFT	A	549	1	-	0/7/25/26	0/2/2/2
1	UFT	A	133	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	183	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	337	1	-	0/7/25/26	0/2/2/2
1	UFT	A	258	1	-	2/7/25/26	0/2/2/2
1	UFT	A	105	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	108	1	-	0/7/25/26	0/2/2/2
1	UFT	A	55	1	-	0/7/25/26	0/2/2/2
1	UFT	A	115	1	-	2/7/25/26	0/2/2/2
1	UFT	A	243	1	-	0/7/25/26	0/2/2/2
1	UFT	A	498	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	264	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	508	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	144	1	-	0/7/25/26	0/2/2/2
1	UFT	A	348	1	-	0/7/25/26	0/2/2/2
1	UFT	A	499	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	67	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	278	1	-	0/7/25/26	0/2/2/2
1	UFT	A	318	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	49	1	-	0/7/25/26	0/2/2/2
1	UFT	A	237	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	6	1	-	0/7/25/26	0/2/2/2
1	UFT	A	45	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	387	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	364	1	-	0/7/25/26	0/2/2/2
1	UFT	A	43	1	-	1/7/25/26	0/2/2/2
1	UFT	A	421	1	-	0/7/25/26	0/2/2/2
1	UFT	A	114	1	-	2/7/25/26	0/2/2/2
1	UFT	A	432	1	-	2/7/25/26	0/2/2/2

The worst 5 of 2266 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	47	UFT	C2-N1	5.29	1.46	1.38
1	A	399	UFT	C2-N1	5.23	1.46	1.38
1	A	543	UFT	C2-N1	5.18	1.46	1.38
1	A	385	UFT	C2-N1	5.09	1.46	1.38
1	A	247	UFT	C2-N1	5.08	1.46	1.38

The worst 5 of 1224 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	UFT	C4-N3-C2	-5.93	119.25	126.61
1	A	215	UFT	C4-N3-C2	-5.89	119.30	126.61
1	A	391	UFT	C4-N3-C2	-5.89	119.31	126.61
1	A	545	UFT	C4-N3-C2	-5.86	119.34	126.61
1	A	350	UFT	C4-N3-C2	-5.85	119.35	126.61

There are no chirality outliers.

5 of 142 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	8	UFT	O4'-C4'-C5'-O5'
1	A	27	UFT	O4'-C4'-C5'-O5'
1	A	45	UFT	O4'-C4'-C5'-O5'
1	A	48	UFT	O4'-C4'-C5'-O5'
1	A	87	UFT	C4'-C5'-O5'-P

There are no ring outliers.

182 monomers are involved in 230 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	374	CFZ	1	0
1	A	487	CFZ	1	0
1	A	65	UFT	1	0
1	A	104	CFZ	2	0
1	A	252	CFZ	1	0
1	A	281	CFZ	2	0
1	A	391	UFT	3	0
1	A	429	CFZ	1	0
1	A	530	CFZ	1	0
1	A	250	CFZ	3	0
1	A	119	UFT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	4	CFZ	1	0
1	A	397	CFZ	1	0
1	A	162	CFZ	3	0
1	A	160	CFZ	1	0
1	A	265	UFT	1	0
1	A	32	CFZ	3	0
1	A	88	UFT	3	0
1	A	167	UFT	2	0
1	A	451	UFT	2	0
1	A	539	CFZ	2	0
1	A	502	CFZ	3	0
1	A	211	CFZ	3	0
1	A	472	CFZ	1	0
1	A	11	CFZ	2	0
1	A	110	CFZ	2	0
1	A	178	UFT	1	0
1	A	234	UFT	1	0
1	A	501	CFZ	2	0
1	A	506	CFZ	2	0
1	A	310	CFZ	1	0
1	A	276	UFT	1	0
1	A	462	CFZ	2	0
1	A	428	CFZ	2	0
1	A	109	CFZ	1	0
1	A	483	CFZ	2	0
1	A	78	CFZ	2	0
1	A	146	CFZ	1	0
1	A	147	UFT	1	0
1	A	459	UFT	3	0
1	A	251	CFZ	3	0
1	A	452	CFZ	1	0
1	A	179	CFZ	1	0
1	A	223	CFZ	2	0
1	A	365	UFT	1	0
1	A	14	UFT	2	0
1	A	116	CFZ	1	0
1	A	229	CFZ	1	0
1	A	430	CFZ	4	0
1	A	153	UFT	1	0
1	A	380	CFZ	3	0
1	A	344	CFZ	4	0
1	A	457	CFZ	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	468	CFZ	3	0
1	A	490	CFZ	1	0
1	A	349	CFZ	2	0
1	A	445	CFZ	1	0
1	A	454	CFZ	3	0
1	A	495	CFZ	2	0
1	A	386	CFZ	2	0
1	A	113	CFZ	1	0
1	A	538	UFT	1	0
1	A	87	UFT	2	0
1	A	97	UFT	1	0
1	A	124	CFZ	2	0
1	A	282	UFT	2	0
1	A	101	CFZ	2	0
1	A	170	UFT	1	0
1	A	320	UFT	3	0
1	A	411	UFT	1	0
1	A	354	CFZ	1	0
1	A	366	UFT	2	0
1	A	500	CFZ	1	0
1	A	111	CFZ	1	0
1	A	127	CFZ	3	0
1	A	212	UFT	3	0
1	A	76	CFZ	3	0
1	A	450	UFT	1	0
1	A	83	UFT	1	0
1	A	283	CFZ	3	0
1	A	188	UFT	1	0
1	A	291	UFT	1	0
1	A	93	CFZ	1	0
1	A	319	UFT	2	0
1	A	385	UFT	1	0
1	A	287	CFZ	3	0
1	A	298	CFZ	1	0
1	A	433	CFZ	1	0
1	A	477	UFT	2	0
1	A	496	CFZ	1	0
1	A	132	CFZ	1	0
1	A	398	UFT	1	0
1	A	415	CFZ	3	0
1	A	194	UFT	1	0
1	A	289	CFZ	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	216	CFZ	1	0
1	A	404	CFZ	1	0
1	A	230	CFZ	2	0
1	A	389	UFT	2	0
1	A	280	CFZ	2	0
1	A	503	CFZ	1	0
1	A	184	UFT	2	0
1	A	75	CFZ	2	0
1	A	12	CFZ	2	0
1	A	407	CFZ	3	0
1	A	84	CFZ	2	0
1	A	470	UFT	1	0
1	A	535	UFT	1	0
1	A	28	UFT	1	0
1	A	465	UFT	1	0
1	A	20	CFZ	1	0
1	A	18	UFT	1	0
1	A	340	UFT	1	0
1	A	134	UFT	1	0
1	A	163	CFZ	4	0
1	A	209	CFZ	1	0
1	A	210	CFZ	1	0
1	A	85	UFT	1	0
1	A	74	UFT	2	0
1	A	220	CFZ	1	0
1	A	413	CFZ	3	0
1	A	492	UFT	1	0
1	A	279	CFZ	2	0
1	A	540	UFT	2	0
1	A	26	UFT	2	0
1	A	191	UFT	1	0
1	A	541	UFT	1	0
1	A	71	UFT	2	0
1	A	89	CFZ	1	0
1	A	341	CFZ	1	0
1	A	368	CFZ	3	0
1	A	467	CFZ	1	0
1	A	272	UFT	2	0
1	A	51	CFZ	1	0
1	A	399	UFT	1	0
1	A	7	UFT	1	0
1	A	325	CFZ	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	301	CFZ	1	0
1	A	166	UFT	1	0
1	A	412	UFT	2	0
1	A	545	UFT	1	0
1	A	140	UFT	1	0
1	A	10	CFZ	1	0
1	A	165	UFT	2	0
1	A	15	UFT	1	0
1	A	213	CFZ	2	0
1	A	221	UFT	1	0
1	A	350	UFT	3	0
1	A	507	CFZ	1	0
1	A	314	CFZ	1	0
1	A	215	UFT	1	0
1	A	36	CFZ	1	0
1	A	125	CFZ	3	0
1	A	259	CFZ	1	0
1	A	491	UFT	2	0
1	A	247	UFT	2	0
1	A	400	UFT	3	0
1	A	346	CFZ	2	0
1	A	528	UFT	1	0
1	A	72	CFZ	2	0
1	A	154	CFZ	1	0
1	A	13	UFT	2	0
1	A	228	UFT	1	0
1	A	549	UFT	1	0
1	A	133	UFT	2	0
1	A	183	CFZ	1	0
1	A	337	CFZ	2	0
1	A	105	UFT	1	0
1	A	55	UFT	2	0
1	A	243	UFT	1	0
1	A	498	UFT	1	0
1	A	144	CFZ	2	0
1	A	348	UFT	2	0
1	A	499	UFT	1	0
1	A	278	CFZ	2	0
1	A	318	UFT	1	0
1	A	237	UFT	3	0
1	A	6	CFZ	1	0
1	A	387	CFZ	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	364	CFZ	1	0
1	A	43	UFT	1	0
1	A	421	UFT	1	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.

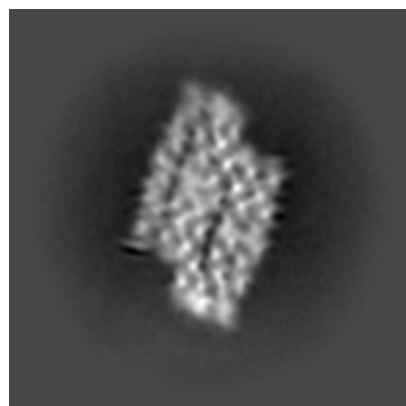
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53795. These allow visual inspection of the internal detail of the map and identification of artifacts.

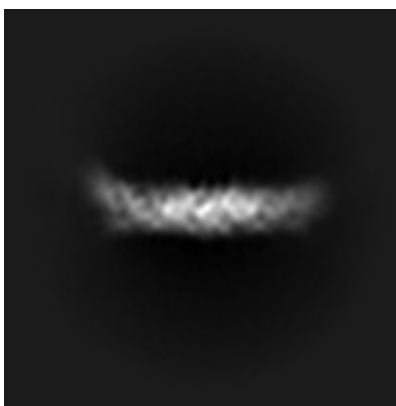
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

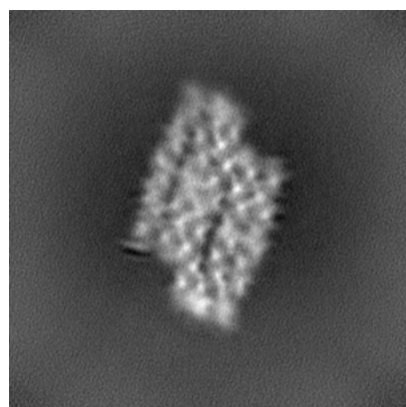


Y

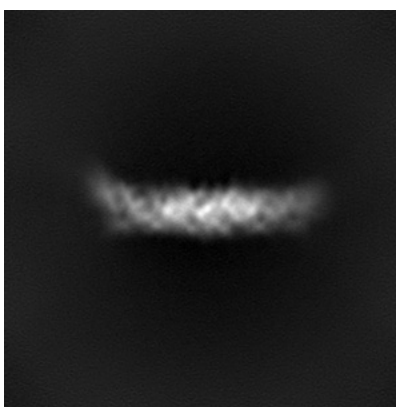


Z

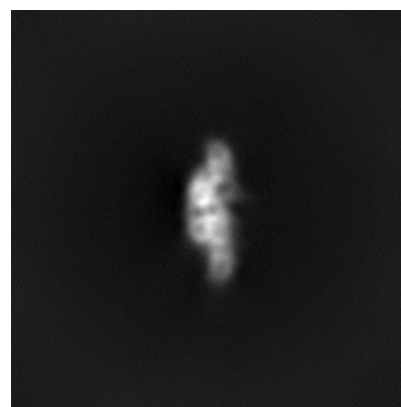
6.1.2 Raw map



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

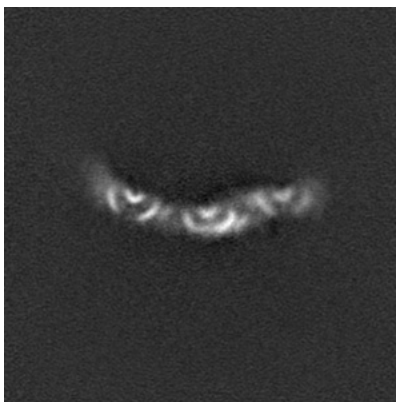


Z Index: 128

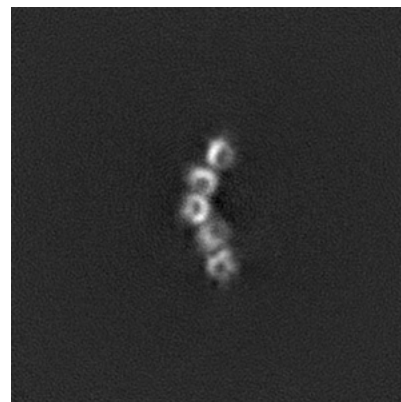
6.2.2 Raw map



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: 130

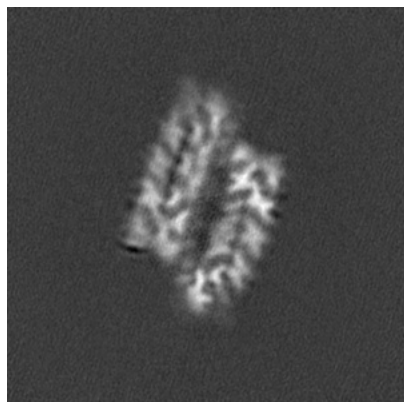


Y Index: 133

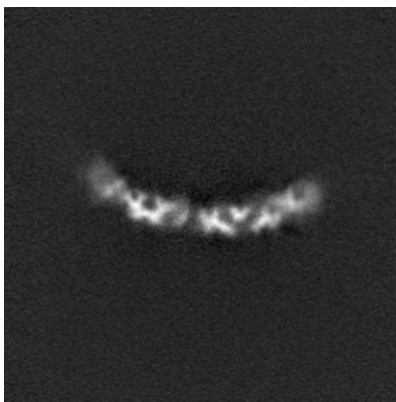


Z Index: 143

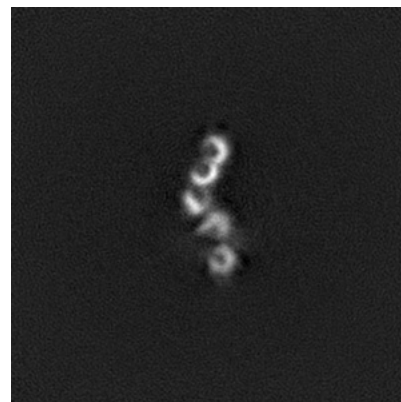
6.3.2 Raw map



X Index: 130



Y Index: 133

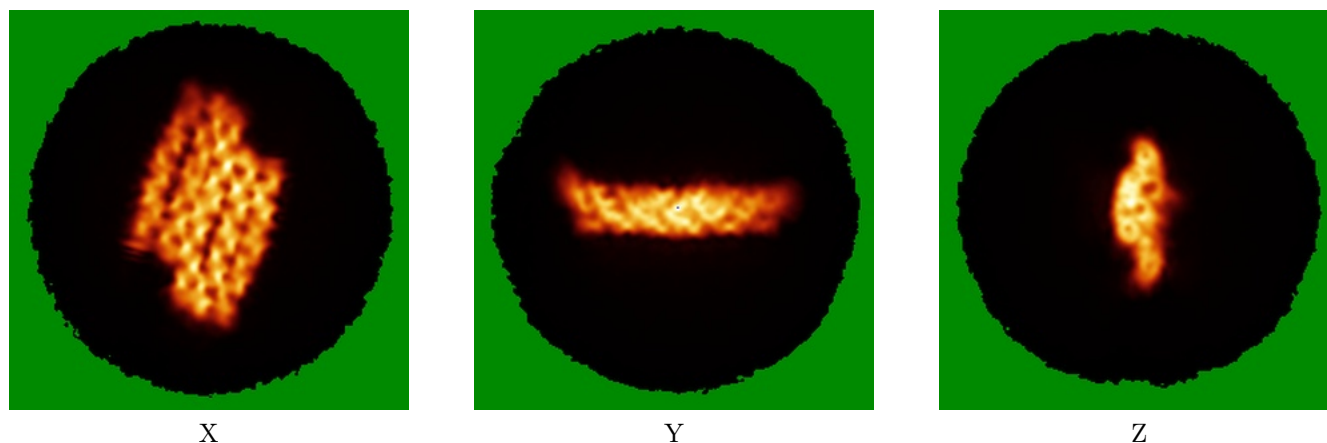


Z Index: 143

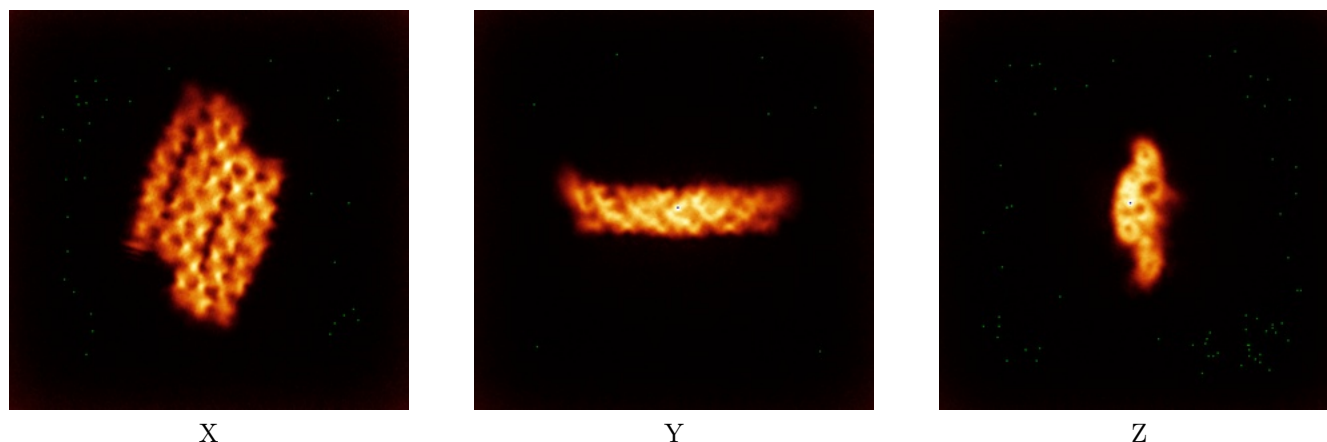
The images above show the largest variance slices of the map in three orthogonal directions.

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.

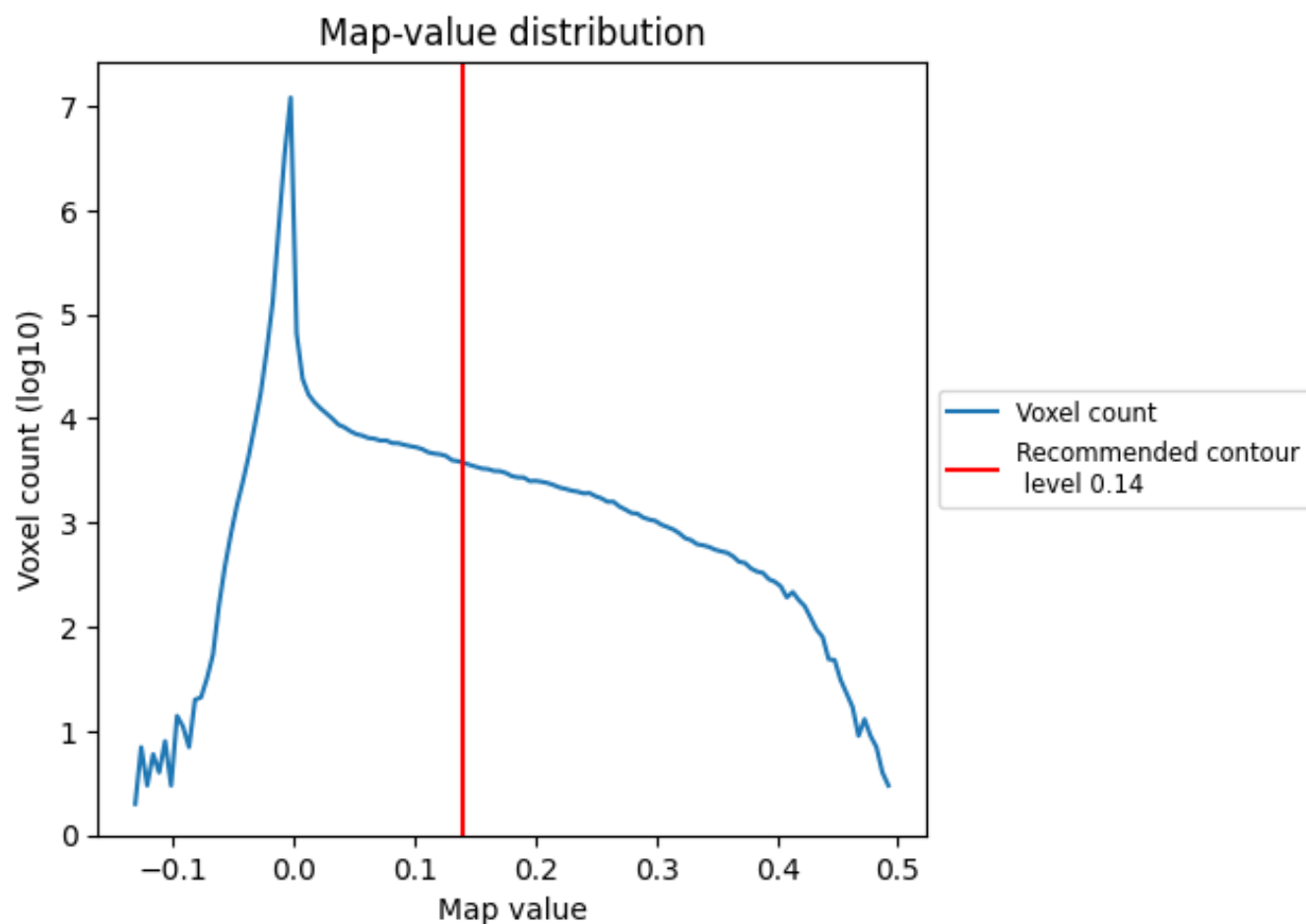
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

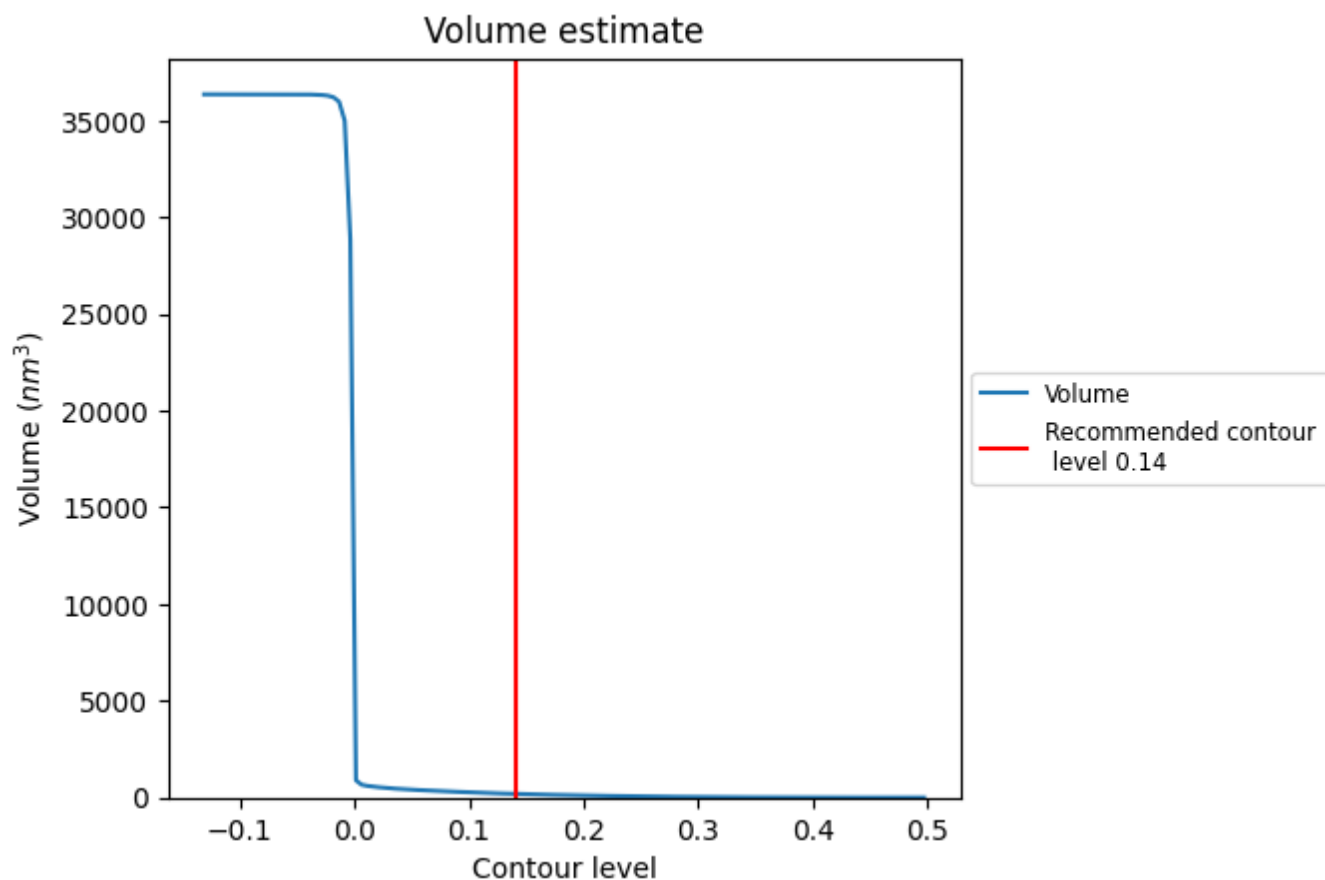
This section contains the results of statistical analysis of the map.

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.

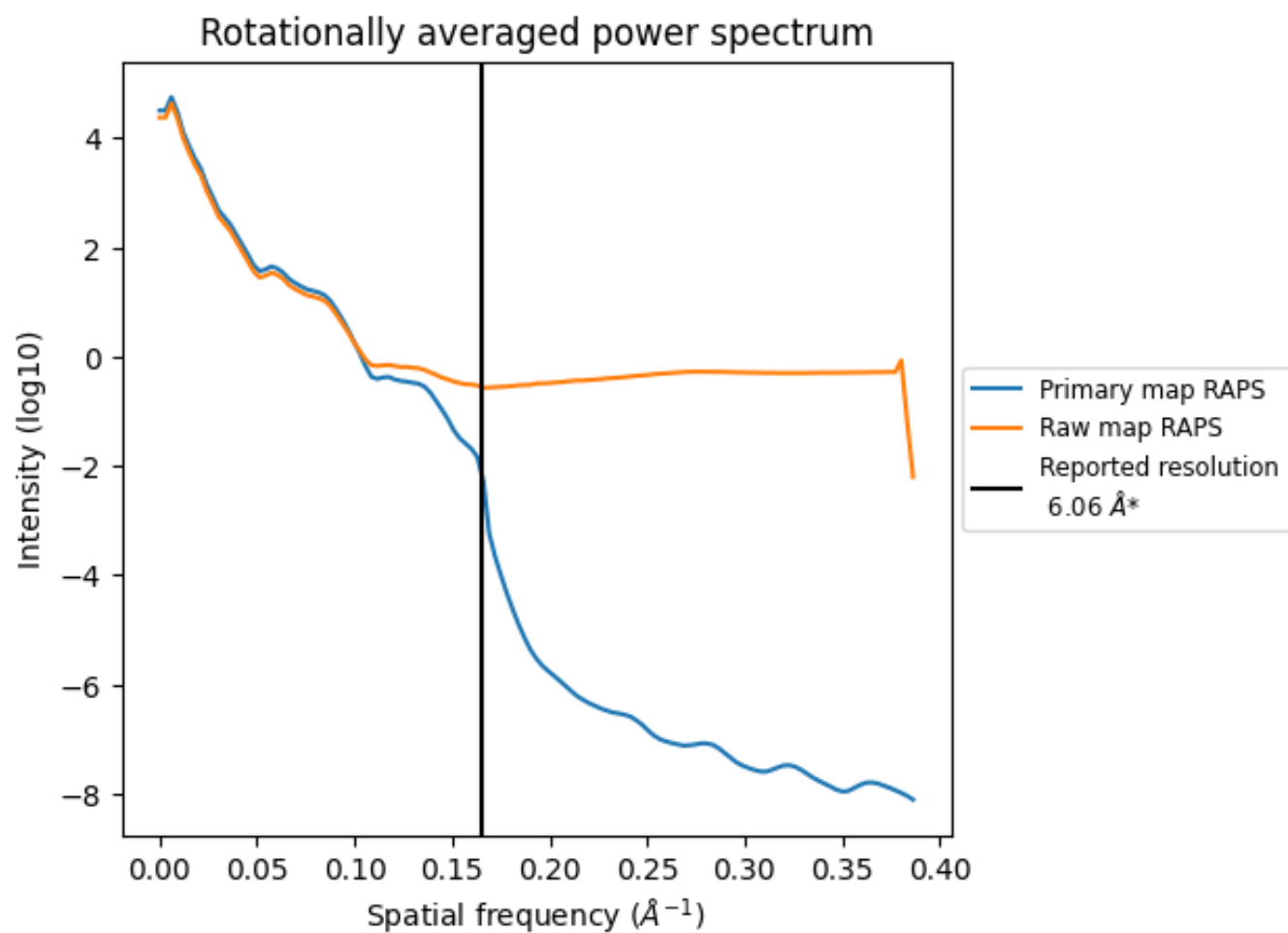
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 190 nm³; this corresponds to an approximate mass of 172 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 [i](#)

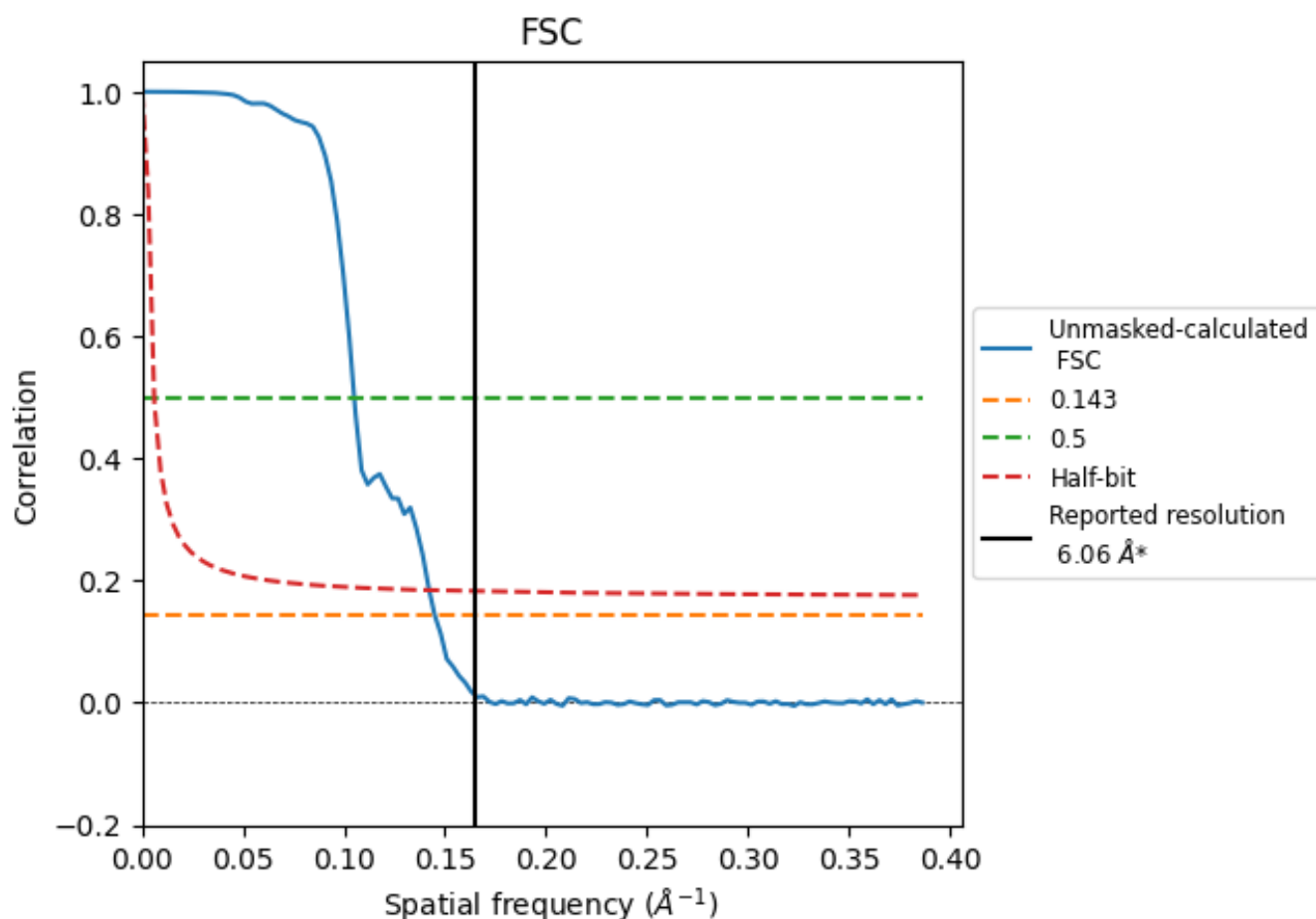


*Reported resolution corresponds to spatial frequency of 0.165 \AA^{-1}

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 0.165 Å⁻¹

8.2 Resolution estimates [i](#)

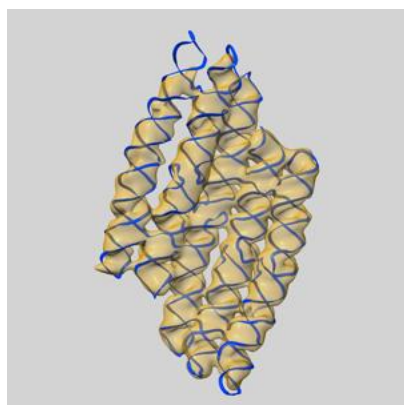
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.06	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.90	9.52	7.03

*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 6.90 differs from the reported value 6.06 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53795 and PDB model 9R7W. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

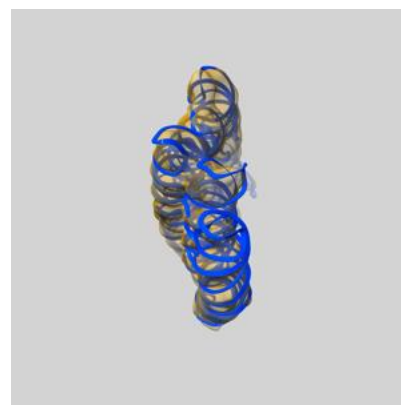
9.1 Map-model overlay [i](#)



X



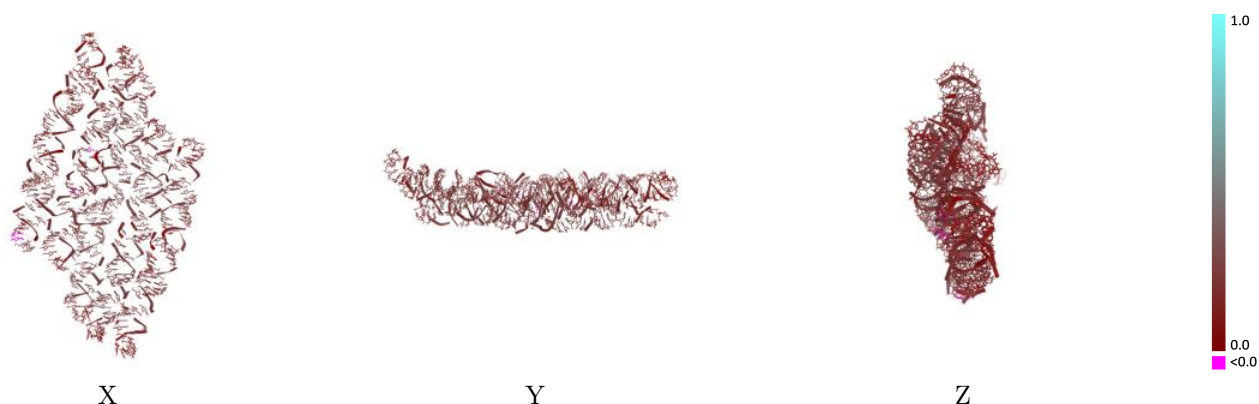
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.14 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](#)

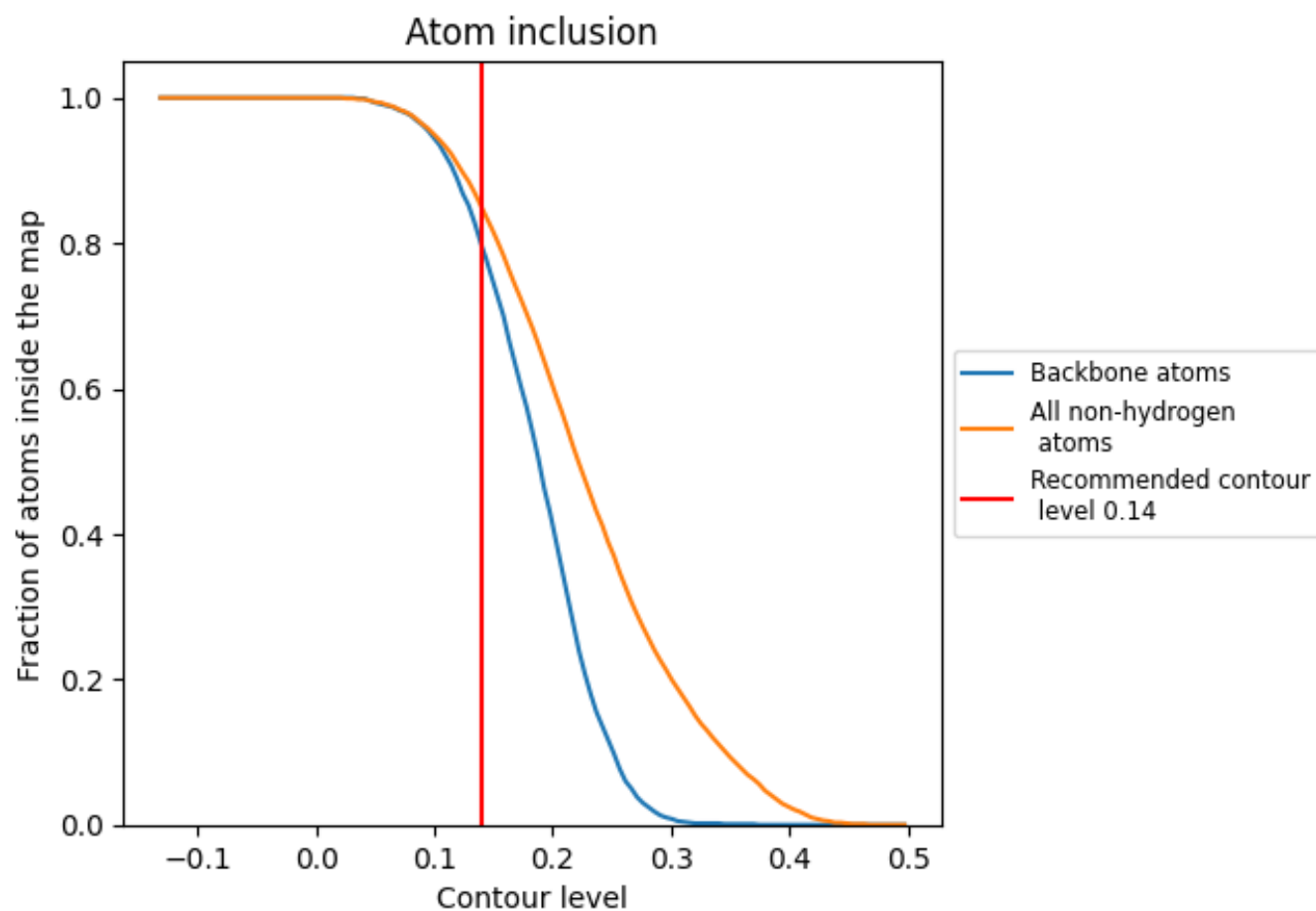


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 85% 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 (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8490	<div></div> 0.1890
A	<div></div> 0.8490	<div></div> 0.1890

