



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 06:23 AM UTC

PDB ID : 9R82 / pdb_00009r82
EMDB ID : EMD-53803
Title : 6-Helix Bundle - with a Clasp (6HB-C)-monomer with 2'-Fluoro-modified pyrimidines (FY RNA)
Authors : Kristoffersen, E.L.; Andersen, E.S.; Zwergius, N.H.
Deposited on : 2025-05-15
Resolution : 9.33 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

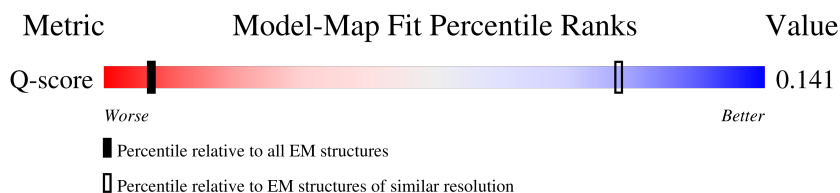
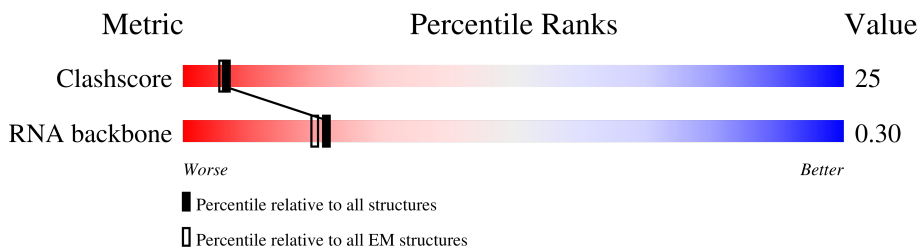
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY


The reported resolution of this entry is 9.33 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	215 (8.90 - 9.83)

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	728	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15523 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.

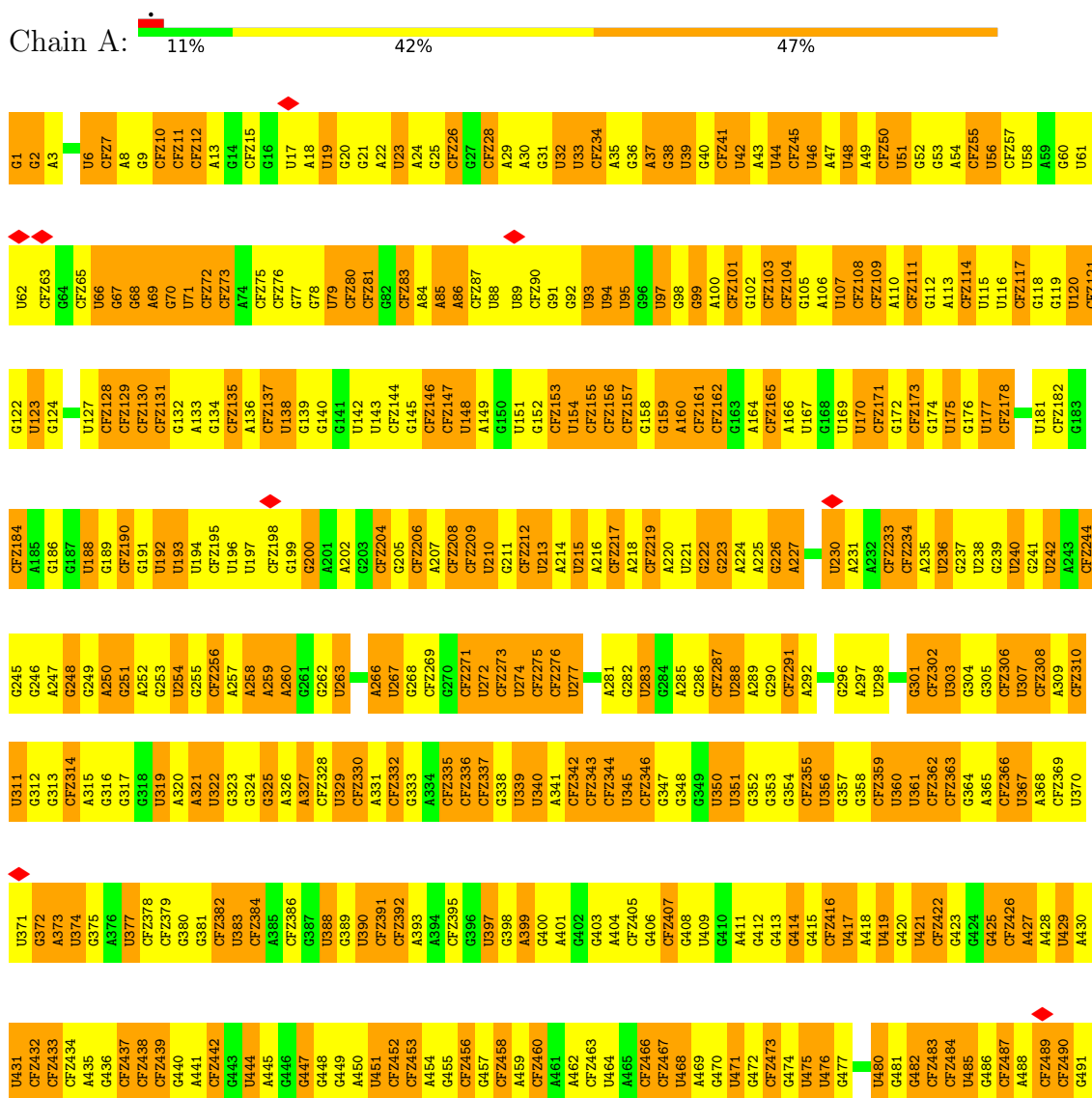
- Molecule 1 is a RNA chain called DNA/RNA (728-MER).

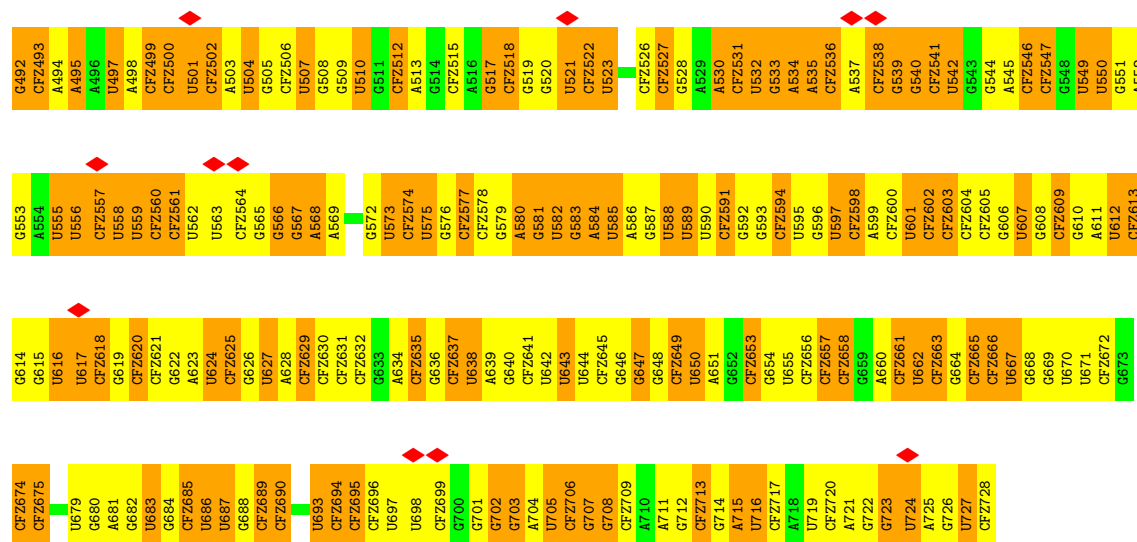
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	F	N	O	P		
1	A	728	15523	6919	361	2758	4757	728	0	0

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 (728-MER)





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	11445	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	0.416	Depositor
Minimum map value	-0.106	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.1	Depositor
Map size (\AA)	331.264, 331.264, 331.264	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.294, 1.294, 1.294	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.51	44/9303 (0.5%)	0.39	0/14367

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	175	UFT	O3'-P	6.75	1.63	1.56
1	A	497	UFT	O3'-P	6.62	1.62	1.56
1	A	322	UFT	O3'-P	6.38	1.62	1.56
1	A	66	UFT	O3'-P	6.36	1.62	1.56
1	A	17	UFT	O3'-P	6.30	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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	15523	0	7488	574	0
All	All	15523	0	7488	574	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 25.

The worst 5 of 574 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:377:UFT:HN3	1:A:715:A:N6	1.43	1.16
1:A:377:UFT:O4	1:A:715:A:N1	1.97	0.97
1:A:260:A:N6	1:A:468:UFT:HN3	1.64	0.95
1:A:377:UFT:HN3	1:A:715:A:H61	0.95	0.93
1:A:29:A:H61	1:A:37:A:N6	1.69	0.89

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	196/728 (26%)	76 (38%)	15 (7%)

5 of 76 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	G
1	A	30	A
1	A	31	G
1	A	37	A
1	A	38	G

5 of 15 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	250	A
1	A	583	G

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Mol	Chain	Res	Type
1	A	372	G
1	A	707	G
1	A	539	G

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

361 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	161	1	18,21,22	2.51	7 (38%)	25,30,33	1.29	2 (8%)
1	CFZ	A	11	1	18,21,22	2.52	7 (38%)	25,30,33	1.58	2 (8%)
1	CFZ	A	378	1	18,21,22	2.45	7 (38%)	25,30,33	1.56	3 (12%)
1	UFT	A	485	1	18,21,22	2.67	10 (55%)	25,30,33	2.01	6 (24%)
1	UFT	A	409	1	18,21,22	2.67	10 (55%)	25,30,33	2.20	7 (28%)
1	CFZ	A	717	1	18,21,22	2.45	6 (33%)	25,30,33	1.61	2 (8%)
1	CFZ	A	426	1	18,21,22	2.45	7 (38%)	25,30,33	1.34	3 (12%)
1	UFT	A	542	1	18,21,22	2.62	10 (55%)	25,30,33	2.14	8 (32%)
1	CFZ	A	632	1	18,21,22	2.54	6 (33%)	25,30,33	1.36	3 (12%)
1	CFZ	A	661	1	18,21,22	2.50	7 (38%)	25,30,33	1.35	3 (12%)
1	UFT	A	595	1	18,21,22	2.60	10 (55%)	25,30,33	2.16	6 (24%)
1	UFT	A	627	1	18,21,22	2.65	10 (55%)	25,30,33	1.88	5 (20%)
1	CFZ	A	405	1	18,21,22	2.50	7 (38%)	25,30,33	1.23	3 (12%)
1	CFZ	A	346	1	18,21,22	2.44	7 (38%)	25,30,33	1.52	3 (12%)
1	UFT	A	670	1	18,21,22	2.61	10 (55%)	25,30,33	2.05	8 (32%)
1	CFZ	A	128	1	18,21,22	2.45	7 (38%)	25,30,33	1.44	3 (12%)
1	UFT	A	236	1	18,21,22	2.66	10 (55%)	25,30,33	2.17	7 (28%)
1	CFZ	A	658	1	18,21,22	2.47	7 (38%)	25,30,33	1.56	3 (12%)
1	CFZ	A	206	1	18,21,22	2.47	7 (38%)	25,30,33	1.37	2 (8%)
1	CFZ	A	275	1	18,21,22	2.54	7 (38%)	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	UFT	A	61	1	18,21,22	2.63	10 (55%)	25,30,33	2.09	8 (32%)
1	UFT	A	51	1	18,21,22	2.69	10 (55%)	25,30,33	2.33	7 (28%)
1	CFZ	A	577	1	18,21,22	2.50	6 (33%)	25,30,33	1.34	3 (12%)
1	UFT	A	95	1	18,21,22	2.59	10 (55%)	25,30,33	2.13	7 (28%)
1	UFT	A	283	1	18,21,22	2.67	10 (55%)	25,30,33	2.26	7 (28%)
1	CFZ	A	518	1	18,21,22	2.55	6 (33%)	25,30,33	1.24	2 (8%)
1	UFT	A	471	1	18,21,22	2.72	10 (55%)	25,30,33	2.38	7 (28%)
1	UFT	A	329	1	18,21,22	2.64	9 (50%)	25,30,33	2.12	7 (28%)
1	CFZ	A	45	1	18,21,22	2.54	7 (38%)	25,30,33	1.29	2 (8%)
1	UFT	A	687	1	18,21,22	2.68	10 (55%)	25,30,33	2.09	7 (28%)
1	CFZ	A	72	1	18,21,22	2.51	7 (38%)	25,30,33	1.28	2 (8%)
1	UFT	A	196	1	18,21,22	2.57	10 (55%)	25,30,33	2.07	7 (28%)
1	CFZ	A	675	1	18,21,22	2.49	7 (38%)	25,30,33	1.47	2 (8%)
1	UFT	A	175	1	18,21,22	2.61	10 (55%)	25,30,33	1.98	7 (28%)
1	CFZ	A	63	1	18,21,22	2.48	7 (38%)	25,30,33	1.54	3 (12%)
1	UFT	A	475	1	18,21,22	2.62	8 (44%)	25,30,33	2.12	7 (28%)
1	UFT	A	667	1	18,21,22	2.57	9 (50%)	25,30,33	2.06	7 (28%)
1	CFZ	A	50	1	18,21,22	2.51	6 (33%)	25,30,33	1.63	3 (12%)
1	UFT	A	585	1	18,21,22	2.62	10 (55%)	25,30,33	2.17	7 (28%)
1	CFZ	A	165	1	18,21,22	2.52	6 (33%)	25,30,33	1.46	2 (8%)
1	UFT	A	56	1	18,21,22	2.68	10 (55%)	25,30,33	2.27	8 (32%)
1	CFZ	A	433	1	18,21,22	2.50	7 (38%)	25,30,33	1.37	3 (12%)
1	UFT	A	575	1	18,21,22	2.68	10 (55%)	25,30,33	2.17	8 (32%)
1	UFT	A	444	1	18,21,22	2.60	9 (50%)	25,30,33	1.91	7 (28%)
1	UFT	A	650	1	18,21,22	2.65	10 (55%)	25,30,33	2.36	8 (32%)
1	UFT	A	115	1	18,21,22	2.63	10 (55%)	25,30,33	2.06	7 (28%)
1	CFZ	A	195	1	18,21,22	2.48	7 (38%)	25,30,33	1.29	2 (8%)
1	CFZ	A	75	1	18,21,22	2.52	7 (38%)	25,30,33	1.47	3 (12%)
1	CFZ	A	602	1	18,21,22	2.50	7 (38%)	25,30,33	1.47	5 (20%)
1	UFT	A	683	1	18,21,22	2.59	10 (55%)	25,30,33	2.24	7 (28%)
1	CFZ	A	137	1	18,21,22	2.55	7 (38%)	25,30,33	1.36	2 (8%)
1	CFZ	A	500	1	18,21,22	2.44	7 (38%)	25,30,33	1.47	3 (12%)
1	CFZ	A	416	1	18,21,22	2.54	6 (33%)	25,30,33	1.42	3 (12%)
1	UFT	A	607	1	18,21,22	2.67	10 (55%)	25,30,33	2.37	6 (24%)
1	CFZ	A	101	1	18,21,22	2.50	6 (33%)	25,30,33	1.41	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CFZ	A	184	1	18,21,22	2.50	6 (33%)	25,30,33	1.39	3 (12%)
1	UFT	A	298	1	18,21,22	2.64	9 (50%)	25,30,33	1.89	5 (20%)
1	CFZ	A	460	1	18,21,22	2.46	7 (38%)	25,30,33	1.39	2 (8%)
1	CFZ	A	578	1	18,21,22	2.51	7 (38%)	25,30,33	1.63	3 (12%)
1	CFZ	A	233	1	18,21,22	2.53	7 (38%)	25,30,33	1.37	3 (12%)
1	CFZ	A	355	1	18,21,22	2.53	7 (38%)	25,30,33	1.27	2 (8%)
1	CFZ	A	442	1	18,21,22	2.48	7 (38%)	25,30,33	1.49	3 (12%)
1	UFT	A	193	1	18,21,22	2.62	10 (55%)	25,30,33	2.07	7 (28%)
1	CFZ	A	308	1	18,21,22	2.55	6 (33%)	25,30,33	1.23	2 (8%)
1	CFZ	A	609	1	18,21,22	2.51	7 (38%)	25,30,33	1.43	2 (8%)
1	UFT	A	62	1	18,21,22	2.59	10 (55%)	25,30,33	2.16	8 (32%)
1	UFT	A	311	1	18,21,22	2.69	10 (55%)	25,30,33	2.19	9 (36%)
1	CFZ	A	649	1	18,21,22	2.54	6 (33%)	25,30,33	1.32	2 (8%)
1	UFT	A	464	1	18,21,22	2.63	10 (55%)	25,30,33	2.18	8 (32%)
1	CFZ	A	337	1	18,21,22	2.56	7 (38%)	25,30,33	1.14	2 (8%)
1	CFZ	A	618	1	18,21,22	2.46	7 (38%)	25,30,33	1.49	2 (8%)
1	UFT	A	221	1	18,21,22	2.69	9 (50%)	25,30,33	1.92	6 (24%)
1	UFT	A	727	1	18,21,22	2.66	9 (50%)	25,30,33	2.03	8 (32%)
1	CFZ	A	57	1	18,21,22	2.56	7 (38%)	25,30,33	1.43	3 (12%)
1	CFZ	A	621	1	18,21,22	2.47	7 (38%)	25,30,33	1.49	3 (12%)
1	CFZ	A	392	1	18,21,22	2.47	7 (38%)	25,30,33	1.36	3 (12%)
1	UFT	A	274	1	18,21,22	2.65	10 (55%)	25,30,33	2.04	7 (28%)
1	UFT	A	679	1	18,21,22	2.63	10 (55%)	25,30,33	2.21	6 (24%)
1	CFZ	A	637	1	18,21,22	2.49	7 (38%)	25,30,33	1.28	2 (8%)
1	UFT	A	93	1	18,21,22	2.65	10 (55%)	25,30,33	2.19	7 (28%)
1	UFT	A	194	1	18,21,22	2.71	10 (55%)	25,30,33	2.33	7 (28%)
1	UFT	A	154	1	18,21,22	2.62	9 (50%)	25,30,33	2.11	10 (40%)
1	UFT	A	215	1	18,21,22	2.66	9 (50%)	25,30,33	2.01	6 (24%)
1	CFZ	A	144	1	18,21,22	2.49	7 (38%)	25,30,33	1.13	1 (4%)
1	CFZ	A	382	1	18,21,22	2.54	6 (33%)	25,30,33	1.35	2 (8%)
1	CFZ	A	162	1	18,21,22	2.53	7 (38%)	25,30,33	1.28	2 (8%)
1	CFZ	A	90	1	18,21,22	2.45	7 (38%)	25,30,33	1.34	2 (8%)
1	CFZ	A	129	1	18,21,22	2.53	7 (38%)	25,30,33	1.39	2 (8%)
1	CFZ	A	111	1	18,21,22	2.52	7 (38%)	25,30,33	1.35	3 (12%)
1	UFT	A	556	1	18,21,22	2.64	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	CFZ	A	506	1	18,21,22	2.51	7 (38%)	25,30,33	1.30	2 (8%)
1	UFT	A	138	1	18,21,22	2.61	10 (55%)	25,30,33	2.12	8 (32%)
1	UFT	A	127	1	18,21,22	2.61	10 (55%)	25,30,33	2.18	8 (32%)
1	CFZ	A	332	1	18,21,22	2.55	6 (33%)	25,30,33	1.28	2 (8%)
1	CFZ	A	391	1	18,21,22	2.49	6 (33%)	25,30,33	1.53	2 (8%)
1	CFZ	A	15	1	18,21,22	2.48	7 (38%)	25,30,33	1.54	3 (12%)
1	UFT	A	724	1	18,21,22	2.57	9 (50%)	25,30,33	1.98	6 (24%)
1	CFZ	A	656	1	18,21,22	2.47	7 (38%)	25,30,33	1.50	3 (12%)
1	CFZ	A	153	1	18,21,22	2.52	7 (38%)	25,30,33	1.42	2 (8%)
1	UFT	A	48	1	18,21,22	2.69	9 (50%)	25,30,33	1.93	7 (28%)
1	CFZ	A	483	1	18,21,22	2.51	7 (38%)	25,30,33	1.25	2 (8%)
1	CFZ	A	438	1	18,21,22	2.48	7 (38%)	25,30,33	1.32	2 (8%)
1	CFZ	A	515	1	18,21,22	2.50	6 (33%)	25,30,33	1.80	6 (24%)
1	UFT	A	388	1	18,21,22	2.64	10 (55%)	25,30,33	2.08	6 (24%)
1	UFT	A	698	1	18,21,22	2.61	10 (55%)	25,30,33	2.07	7 (28%)
1	UFT	A	116	1	18,21,22	2.63	10 (55%)	25,30,33	1.94	5 (20%)
1	UFT	A	169	1	18,21,22	2.61	9 (50%)	25,30,33	2.19	7 (28%)
1	UFT	A	360	1	18,21,22	2.67	9 (50%)	25,30,33	2.08	7 (28%)
1	UFT	A	123	1	18,21,22	2.63	10 (55%)	25,30,33	2.15	7 (28%)
1	CFZ	A	526	1	18,21,22	2.51	7 (38%)	25,30,33	1.61	4 (16%)
1	CFZ	A	208	1	18,21,22	2.54	7 (38%)	25,30,33	1.41	3 (12%)
1	CFZ	A	641	1	18,21,22	2.49	7 (38%)	25,30,33	1.24	2 (8%)
1	UFT	A	451	1	18,21,22	2.65	9 (50%)	25,30,33	1.95	6 (24%)
1	CFZ	A	439	1	18,21,22	2.55	7 (38%)	25,30,33	1.26	3 (12%)
1	CFZ	A	690	1	18,21,22	2.48	7 (38%)	25,30,33	1.43	2 (8%)
1	CFZ	A	121	1	18,21,22	2.50	7 (38%)	25,30,33	1.24	3 (12%)
1	UFT	A	345	1	18,21,22	2.60	10 (55%)	25,30,33	2.06	7 (28%)
1	CFZ	A	108	1	18,21,22	2.55	7 (38%)	25,30,33	1.35	2 (8%)
1	CFZ	A	456	1	18,21,22	2.52	7 (38%)	25,30,33	1.32	3 (12%)
1	UFT	A	417	1	18,21,22	2.61	9 (50%)	25,30,33	1.93	7 (28%)
1	CFZ	A	330	1	18,21,22	2.52	7 (38%)	25,30,33	1.44	4 (16%)
1	UFT	A	361	1	18,21,22	2.58	9 (50%)	25,30,33	2.15	7 (28%)
1	UFT	A	350	1	18,21,22	2.66	10 (55%)	25,30,33	2.01	6 (24%)
1	UFT	A	319	1	18,21,22	2.62	9 (50%)	25,30,33	2.05	6 (24%)
1	CFZ	A	502	1	18,21,22	2.46	7 (38%)	25,30,33	1.48	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	UFT	A	573	1	18,21,22	2.69	9 (50%)	25,30,33	2.13	7 (28%)
1	CFZ	A	625	1	18,21,22	2.51	7 (38%)	25,30,33	1.19	2 (8%)
1	UFT	A	240	1	18,21,22	2.61	10 (55%)	25,30,33	2.08	8 (32%)
1	CFZ	A	466	1	18,21,22	2.55	7 (38%)	25,30,33	1.27	3 (12%)
1	CFZ	A	603	1	18,21,22	2.47	7 (38%)	25,30,33	1.56	3 (12%)
1	UFT	A	555	1	18,21,22	2.66	10 (55%)	25,30,33	1.93	6 (24%)
1	CFZ	A	190	1	18,21,22	2.54	7 (38%)	25,30,33	1.29	2 (8%)
1	CFZ	A	384	1	18,21,22	2.55	7 (38%)	25,30,33	1.33	2 (8%)
1	CFZ	A	452	1	18,21,22	2.54	7 (38%)	25,30,33	1.26	2 (8%)
1	CFZ	A	657	1	18,21,22	2.49	7 (38%)	25,30,33	1.47	4 (16%)
1	CFZ	A	473	1	18,21,22	2.46	7 (38%)	25,30,33	1.21	2 (8%)
1	UFT	A	612	1	18,21,22	2.69	10 (55%)	25,30,33	2.05	5 (20%)
1	CFZ	A	674	1	18,21,22	2.49	7 (38%)	25,30,33	1.49	2 (8%)
1	CFZ	A	103	1	18,21,22	2.51	6 (33%)	25,30,33	1.25	2 (8%)
1	CFZ	A	557	1	18,21,22	2.54	6 (33%)	25,30,33	1.54	3 (12%)
1	UFT	A	307	1	18,21,22	2.64	9 (50%)	25,30,33	1.87	6 (24%)
1	CFZ	A	709	1	18,21,22	2.51	6 (33%)	25,30,33	1.55	5 (20%)
1	CFZ	A	273	1	18,21,22	2.50	6 (33%)	25,30,33	1.45	2 (8%)
1	UFT	A	532	1	18,21,22	2.55	9 (50%)	25,30,33	1.90	8 (32%)
1	UFT	A	497	1	18,21,22	2.71	9 (50%)	25,30,33	2.16	8 (32%)
1	CFZ	A	538	1	18,21,22	2.56	7 (38%)	25,30,33	1.26	3 (12%)
1	UFT	A	601	1	18,21,22	2.64	10 (55%)	25,30,33	2.41	9 (36%)
1	CFZ	A	28	1	18,21,22	2.47	7 (38%)	25,30,33	1.52	6 (24%)
1	CFZ	A	629	1	18,21,22	2.43	7 (38%)	25,30,33	1.74	5 (20%)
1	UFT	A	167	1	18,21,22	2.62	10 (55%)	25,30,33	2.07	8 (32%)
1	CFZ	A	695	1	18,21,22	2.52	6 (33%)	25,30,33	1.36	3 (12%)
1	UFT	A	177	1	18,21,22	2.64	10 (55%)	25,30,33	2.12	7 (28%)
1	UFT	A	23	1	18,21,22	2.75	10 (55%)	25,30,33	2.10	6 (24%)
1	CFZ	A	209	1	18,21,22	2.54	6 (33%)	25,30,33	1.30	3 (12%)
1	CFZ	A	156	1	18,21,22	2.54	7 (38%)	25,30,33	1.27	2 (8%)
1	UFT	A	642	1	18,21,22	2.62	9 (50%)	25,30,33	1.89	6 (24%)
1	UFT	A	170	1	18,21,22	2.65	10 (55%)	25,30,33	2.00	7 (28%)
1	UFT	A	671	1	18,21,22	2.61	10 (55%)	25,30,33	2.15	7 (28%)
1	CFZ	A	104	1	18,21,22	2.54	7 (38%)	25,30,33	1.20	2 (8%)
1	UFT	A	397	1	18,21,22	2.63	10 (55%)	25,30,33	2.09	8 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	UFT	A	510	1	18,21,22	2.59	9 (50%)	25,30,33	2.13	7 (28%)
1	UFT	A	89	1	18,21,22	2.59	10 (55%)	25,30,33	2.17	8 (32%)
1	CFZ	A	594	1	18,21,22	2.51	7 (38%)	25,30,33	1.43	2 (8%)
1	UFT	A	419	1	18,21,22	2.68	9 (50%)	25,30,33	1.95	7 (28%)
1	CFZ	A	335	1	18,21,22	2.53	6 (33%)	25,30,33	1.61	4 (16%)
1	UFT	A	197	1	18,21,22	2.63	10 (55%)	25,30,33	2.06	8 (32%)
1	CFZ	A	379	1	18,21,22	2.56	8 (44%)	25,30,33	1.33	4 (16%)
1	CFZ	A	685	1	18,21,22	2.50	7 (38%)	25,30,33	1.58	2 (8%)
1	CFZ	A	12	1	18,21,22	2.56	7 (38%)	25,30,33	1.38	2 (8%)
1	CFZ	A	306	1	18,21,22	2.54	6 (33%)	25,30,33	1.20	1 (4%)
1	UFT	A	39	1	18,21,22	2.65	9 (50%)	25,30,33	1.76	6 (24%)
1	CFZ	A	363	1	18,21,22	2.55	7 (38%)	25,30,33	1.29	2 (8%)
1	CFZ	A	467	1	18,21,22	2.53	7 (38%)	25,30,33	1.31	2 (8%)
1	CFZ	A	366	1	18,21,22	2.54	7 (38%)	25,30,33	1.36	4 (16%)
1	CFZ	A	604	1	18,21,22	2.51	7 (38%)	25,30,33	1.15	1 (4%)
1	CFZ	A	696	1	18,21,22	2.53	6 (33%)	25,30,33	1.23	2 (8%)
1	UFT	A	263	1	18,21,22	2.64	10 (55%)	25,30,33	2.18	8 (32%)
1	CFZ	A	310	1	18,21,22	2.58	7 (38%)	25,30,33	1.41	3 (12%)
1	UFT	A	476	1	18,21,22	2.63	10 (55%)	25,30,33	2.05	6 (24%)
1	UFT	A	590	1	18,21,22	2.60	9 (50%)	25,30,33	2.12	8 (32%)
1	UFT	A	272	1	18,21,22	2.62	9 (50%)	25,30,33	1.98	6 (24%)
1	CFZ	A	157	1	18,21,22	2.47	7 (38%)	25,30,33	1.39	3 (12%)
1	CFZ	A	395	1	18,21,22	2.50	7 (38%)	25,30,33	1.35	3 (12%)
1	CFZ	A	7	1	18,21,22	2.56	7 (38%)	25,30,33	1.25	2 (8%)
1	UFT	A	597	1	18,21,22	2.63	10 (55%)	25,30,33	2.11	7 (28%)
1	UFT	A	521	1	18,21,22	2.64	10 (55%)	25,30,33	2.12	9 (36%)
1	UFT	A	351	1	18,21,22	2.56	10 (55%)	25,30,33	2.00	8 (32%)
1	CFZ	A	487	1	18,21,22	2.53	7 (38%)	25,30,33	1.39	4 (16%)
1	CFZ	A	598	1	18,21,22	2.53	7 (38%)	25,30,33	1.51	3 (12%)
1	CFZ	A	631	1	18,21,22	2.57	7 (38%)	25,30,33	1.27	2 (8%)
1	CFZ	A	434	1	18,21,22	2.57	6 (33%)	25,30,33	1.26	3 (12%)
1	CFZ	A	212	1	18,21,22	2.54	6 (33%)	25,30,33	1.42	3 (12%)
1	CFZ	A	155	1	18,21,22	2.46	7 (38%)	25,30,33	1.47	4 (16%)
1	UFT	A	480	1	18,21,22	2.59	9 (50%)	25,30,33	2.08	7 (28%)
1	UFT	A	242	1	18,21,22	2.61	10 (55%)	25,30,33	2.15	7 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CFZ	A	531	1	18,21,22	2.47	6 (33%)	25,30,33	1.57	2 (8%)
1	UFT	A	662	1	18,21,22	2.65	10 (55%)	25,30,33	2.10	9 (36%)
1	CFZ	A	302	1	18,21,22	2.54	7 (38%)	25,30,33	1.36	2 (8%)
1	CFZ	A	369	1	18,21,22	2.52	7 (38%)	25,30,33	1.31	2 (8%)
1	CFZ	A	26	1	18,21,22	2.48	7 (38%)	25,30,33	1.33	3 (12%)
1	UFT	A	377	1	18,21,22	2.75	9 (50%)	25,30,33	2.69	10 (40%)
1	CFZ	A	234	1	18,21,22	2.56	7 (38%)	25,30,33	1.38	2 (8%)
1	CFZ	A	343	1	18,21,22	2.53	7 (38%)	25,30,33	1.25	2 (8%)
1	UFT	A	356	1	18,21,22	2.61	10 (55%)	25,30,33	2.14	6 (24%)
1	CFZ	A	564	1	18,21,22	2.47	7 (38%)	25,30,33	1.23	2 (8%)
1	CFZ	A	76	1	18,21,22	2.53	7 (38%)	25,30,33	1.28	1 (4%)
1	CFZ	A	574	1	18,21,22	2.50	7 (38%)	25,30,33	1.33	3 (12%)
1	CFZ	A	699	1	18,21,22	2.49	7 (38%)	25,30,33	1.29	2 (8%)
1	UFT	A	563	1	18,21,22	2.62	10 (55%)	25,30,33	2.08	8 (32%)
1	CFZ	A	130	1	18,21,22	2.52	7 (38%)	25,30,33	1.27	3 (12%)
1	CFZ	A	432	1	18,21,22	2.51	7 (38%)	25,30,33	1.45	3 (12%)
1	UFT	A	421	1	18,21,22	2.64	10 (55%)	25,30,33	2.01	7 (28%)
1	CFZ	A	666	1	18,21,22	2.53	6 (33%)	25,30,33	1.45	2 (8%)
1	CFZ	A	117	1	18,21,22	2.47	7 (38%)	25,30,33	1.46	3 (12%)
1	UFT	A	367	1	18,21,22	2.71	10 (55%)	25,30,33	2.27	6 (24%)
1	CFZ	A	437	1	18,21,22	2.57	7 (38%)	25,30,33	1.34	2 (8%)
1	UFT	A	66	1	18,21,22	2.69	10 (55%)	25,30,33	2.25	8 (32%)
1	CFZ	A	109	1	18,21,22	2.54	6 (33%)	25,30,33	1.53	4 (16%)
1	UFT	A	210	1	18,21,22	2.70	10 (55%)	25,30,33	2.17	8 (32%)
1	UFT	A	288	1	18,21,22	2.65	10 (55%)	25,30,33	2.12	6 (24%)
1	CFZ	A	489	1	18,21,22	2.51	7 (38%)	25,30,33	1.25	3 (12%)
1	UFT	A	142	1	18,21,22	2.59	10 (55%)	25,30,33	2.07	7 (28%)
1	UFT	A	719	1	18,21,22	2.60	9 (50%)	25,30,33	2.01	7 (28%)
1	CFZ	A	512	1	18,21,22	2.53	7 (38%)	25,30,33	1.35	2 (8%)
1	CFZ	A	453	1	18,21,22	2.52	7 (38%)	25,30,33	1.31	2 (8%)
1	CFZ	A	386	1	18,21,22	2.50	7 (38%)	25,30,33	1.40	3 (12%)
1	CFZ	A	600	1	18,21,22	2.56	6 (33%)	25,30,33	1.36	2 (8%)
1	CFZ	A	728	1	18,21,22	2.46	7 (38%)	25,30,33	1.36	3 (12%)
1	CFZ	A	605	1	18,21,22	2.51	7 (38%)	25,30,33	1.20	2 (8%)
1	CFZ	A	219	1	18,21,22	2.51	7 (38%)	25,30,33	1.50	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CFZ	A	328	1	18,21,22	2.55	7 (38%)	25,30,33	1.35	3 (12%)
1	UFT	A	107	1	18,21,22	2.69	10 (55%)	25,30,33	2.08	6 (24%)
1	CFZ	A	271	1	18,21,22	2.51	7 (38%)	25,30,33	1.50	3 (12%)
1	CFZ	A	407	1	18,21,22	2.49	7 (38%)	25,30,33	1.36	3 (12%)
1	CFZ	A	665	1	18,21,22	2.53	7 (38%)	25,30,33	1.49	2 (8%)
1	UFT	A	44	1	18,21,22	2.66	10 (55%)	25,30,33	2.16	7 (28%)
1	UFT	A	643	1	18,21,22	2.62	9 (50%)	25,30,33	1.97	6 (24%)
1	CFZ	A	484	1	18,21,22	2.59	7 (38%)	25,30,33	1.28	1 (4%)
1	CFZ	A	314	1	18,21,22	2.48	7 (38%)	25,30,33	1.38	2 (8%)
1	UFT	A	559	1	18,21,22	2.70	10 (55%)	25,30,33	2.24	7 (28%)
1	CFZ	A	147	1	18,21,22	2.50	7 (38%)	25,30,33	1.43	2 (8%)
1	CFZ	A	80	1	18,21,22	2.52	7 (38%)	25,30,33	1.32	4 (16%)
1	CFZ	A	55	1	18,21,22	2.56	7 (38%)	25,30,33	1.26	2 (8%)
1	UFT	A	88	1	18,21,22	2.60	10 (55%)	25,30,33	2.08	8 (32%)
1	UFT	A	617	1	18,21,22	2.62	10 (55%)	25,30,33	2.10	6 (24%)
1	UFT	A	46	1	18,21,22	2.69	10 (55%)	25,30,33	1.85	6 (24%)
1	CFZ	A	41	1	18,21,22	2.53	7 (38%)	25,30,33	1.23	2 (8%)
1	UFT	A	504	1	18,21,22	2.68	10 (55%)	25,30,33	2.24	6 (24%)
1	UFT	A	254	1	18,21,22	2.65	10 (55%)	25,30,33	2.00	7 (28%)
1	CFZ	A	645	1	18,21,22	2.48	7 (38%)	25,30,33	1.50	3 (12%)
1	UFT	A	374	1	18,21,22	2.67	10 (55%)	25,30,33	2.16	7 (28%)
1	CFZ	A	522	1	18,21,22	2.53	6 (33%)	25,30,33	1.33	2 (8%)
1	CFZ	A	620	1	18,21,22	2.49	7 (38%)	25,30,33	1.21	2 (8%)
1	UFT	A	79	1	18,21,22	2.61	9 (50%)	25,30,33	2.04	6 (24%)
1	CFZ	A	541	1	18,21,22	2.55	7 (38%)	25,30,33	1.21	1 (4%)
1	CFZ	A	527	1	18,21,22	2.51	7 (38%)	25,30,33	1.54	2 (8%)
1	UFT	A	238	1	18,21,22	2.64	10 (55%)	25,30,33	2.02	8 (32%)
1	UFT	A	71	1	18,21,22	2.67	10 (55%)	25,30,33	2.00	6 (24%)
1	CFZ	A	276	1	18,21,22	2.52	7 (38%)	25,30,33	1.39	2 (8%)
1	UFT	A	507	1	18,21,22	2.68	10 (55%)	25,30,33	1.92	6 (24%)
1	CFZ	A	630	1	18,21,22	2.48	7 (38%)	25,30,33	1.55	2 (8%)
1	UFT	A	644	1	18,21,22	2.63	10 (55%)	25,30,33	2.00	7 (28%)
1	CFZ	A	244	1	18,21,22	2.53	7 (38%)	25,30,33	1.26	3 (12%)
1	UFT	A	582	1	18,21,22	2.65	9 (50%)	25,30,33	1.95	6 (24%)
1	UFT	A	151	1	18,21,22	2.63	9 (50%)	25,30,33	2.02	8 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CFZ	A	217	1	18,21,22	2.56	7 (38%)	25,30,33	1.44	2 (8%)
1	CFZ	A	342	1	18,21,22	2.56	7 (38%)	25,30,33	1.26	2 (8%)
1	UFT	A	33	1	18,21,22	2.66	10 (55%)	25,30,33	2.08	7 (28%)
1	UFT	A	624	1	18,21,22	2.63	10 (55%)	25,30,33	2.04	7 (28%)
1	UFT	A	94	1	18,21,22	2.68	10 (55%)	25,30,33	2.17	7 (28%)
1	UFT	A	468	1	18,21,22	2.58	9 (50%)	25,30,33	1.99	7 (28%)
1	CFZ	A	178	1	18,21,22	2.49	7 (38%)	25,30,33	1.47	3 (12%)
1	CFZ	A	34	1	18,21,22	2.46	6 (33%)	25,30,33	1.27	2 (8%)
1	CFZ	A	204	1	18,21,22	2.51	7 (38%)	25,30,33	1.33	2 (8%)
1	CFZ	A	182	1	18,21,22	2.50	7 (38%)	25,30,33	1.48	3 (12%)
1	CFZ	A	672	1	18,21,22	2.47	7 (38%)	25,30,33	1.16	3 (12%)
1	CFZ	A	287	1	18,21,22	2.53	7 (38%)	25,30,33	1.24	2 (8%)
1	CFZ	A	359	1	18,21,22	2.53	7 (38%)	25,30,33	1.81	6 (24%)
1	CFZ	A	613	1	18,21,22	2.49	6 (33%)	25,30,33	1.37	2 (8%)
1	UFT	A	213	1	18,21,22	2.72	9 (50%)	25,30,33	2.40	8 (32%)
1	CFZ	A	713	1	18,21,22	2.54	6 (33%)	25,30,33	1.77	6 (24%)
1	UFT	A	390	1	18,21,22	2.68	10 (55%)	25,30,33	2.13	6 (24%)
1	UFT	A	705	1	18,21,22	2.62	9 (50%)	25,30,33	1.95	7 (28%)
1	UFT	A	340	1	18,21,22	2.67	10 (55%)	25,30,33	2.01	7 (28%)
1	UFT	A	192	1	18,21,22	2.62	9 (50%)	25,30,33	1.92	6 (24%)
1	CFZ	A	87	1	18,21,22	2.53	7 (38%)	25,30,33	1.30	2 (8%)
1	UFT	A	370	1	18,21,22	2.69	9 (50%)	25,30,33	2.08	6 (24%)
1	CFZ	A	536	1	18,21,22	2.50	7 (38%)	25,30,33	1.27	2 (8%)
1	CFZ	A	561	1	18,21,22	2.51	7 (38%)	25,30,33	1.33	2 (8%)
1	UFT	A	693	1	18,21,22	2.68	10 (55%)	25,30,33	2.09	6 (24%)
1	UFT	A	371	1	18,21,22	2.66	10 (55%)	25,30,33	2.25	8 (32%)
1	UFT	A	383	1	18,21,22	2.64	9 (50%)	25,30,33	1.95	6 (24%)
1	UFT	A	97	1	18,21,22	2.71	9 (50%)	25,30,33	1.94	5 (20%)
1	CFZ	A	591	1	18,21,22	2.45	7 (38%)	25,30,33	1.39	2 (8%)
1	UFT	A	143	1	18,21,22	2.61	10 (55%)	25,30,33	2.05	8 (32%)
1	CFZ	A	344	1	18,21,22	2.53	7 (38%)	25,30,33	1.36	3 (12%)
1	UFT	A	188	1	18,21,22	2.64	9 (50%)	25,30,33	1.92	7 (28%)
1	UFT	A	589	1	18,21,22	2.57	10 (55%)	25,30,33	2.02	7 (28%)
1	CFZ	A	114	1	18,21,22	2.51	7 (38%)	25,30,33	1.41	2 (8%)
1	UFT	A	17	1	18,21,22	2.64	9 (50%)	25,30,33	1.98	7 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	UFT	A	562	1	18,21,22	2.60	9 (50%)	25,30,33	2.11	8 (32%)
1	UFT	A	501	1	18,21,22	2.61	9 (50%)	25,30,33	1.93	7 (28%)
1	CFZ	A	422	1	18,21,22	2.54	7 (38%)	25,30,33	1.25	2 (8%)
1	UFT	A	32	1	18,21,22	2.62	10 (55%)	25,30,33	2.06	8 (32%)
1	UFT	A	181	1	18,21,22	2.57	9 (50%)	25,30,33	1.87	7 (28%)
1	CFZ	A	291	1	18,21,22	2.52	7 (38%)	25,30,33	1.27	3 (12%)
1	CFZ	A	547	1	18,21,22	2.47	7 (38%)	25,30,33	1.43	2 (8%)
1	CFZ	A	490	1	18,21,22	2.55	7 (38%)	25,30,33	1.22	3 (12%)
1	CFZ	A	653	1	18,21,22	2.49	7 (38%)	25,30,33	1.21	2 (8%)
1	CFZ	A	499	1	18,21,22	2.52	7 (38%)	25,30,33	1.58	2 (8%)
1	UFT	A	523	1	18,21,22	2.61	9 (50%)	25,30,33	1.94	6 (24%)
1	CFZ	A	171	1	18,21,22	2.46	7 (38%)	25,30,33	1.51	2 (8%)
1	UFT	A	267	1	18,21,22	2.66	10 (55%)	25,30,33	2.15	7 (28%)
1	CFZ	A	463	1	18,21,22	2.54	8 (44%)	25,30,33	1.58	4 (16%)
1	CFZ	A	256	1	18,21,22	2.51	7 (38%)	25,30,33	1.59	3 (12%)
1	CFZ	A	493	1	18,21,22	2.52	7 (38%)	25,30,33	1.33	2 (8%)
1	CFZ	A	173	1	18,21,22	2.50	6 (33%)	25,30,33	1.13	2 (8%)
1	UFT	A	616	1	18,21,22	2.62	10 (55%)	25,30,33	2.06	8 (32%)
1	CFZ	A	663	1	18,21,22	2.50	7 (38%)	25,30,33	1.38	4 (16%)
1	UFT	A	638	1	18,21,22	2.66	10 (55%)	25,30,33	2.24	8 (32%)
1	UFT	A	549	1	18,21,22	2.65	10 (55%)	25,30,33	1.90	7 (28%)
1	UFT	A	58	1	18,21,22	2.60	10 (55%)	25,30,33	2.31	7 (28%)
1	CFZ	A	135	1	18,21,22	2.55	7 (38%)	25,30,33	1.28	2 (8%)
1	CFZ	A	689	1	18,21,22	2.52	7 (38%)	25,30,33	1.25	2 (8%)
1	CFZ	A	81	1	18,21,22	2.50	7 (38%)	25,30,33	1.32	2 (8%)
1	UFT	A	339	1	18,21,22	2.69	9 (50%)	25,30,33	2.06	7 (28%)
1	CFZ	A	635	1	18,21,22	2.54	7 (38%)	25,30,33	1.32	3 (12%)
1	UFT	A	120	1	18,21,22	2.63	10 (55%)	25,30,33	2.20	7 (28%)
1	UFT	A	697	1	18,21,22	2.60	9 (50%)	25,30,33	2.06	8 (32%)
1	UFT	A	322	1	18,21,22	2.59	10 (55%)	25,30,33	2.14	9 (36%)
1	UFT	A	429	1	18,21,22	2.72	9 (50%)	25,30,33	1.89	7 (28%)
1	CFZ	A	269	1	18,21,22	2.46	7 (38%)	25,30,33	1.38	3 (12%)
1	UFT	A	431	1	18,21,22	2.64	9 (50%)	25,30,33	2.13	7 (28%)
1	CFZ	A	694	1	18,21,22	2.51	7 (38%)	25,30,33	1.28	2 (8%)
1	CFZ	A	362	1	18,21,22	2.50	7 (38%)	25,30,33	1.50	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	UFT	A	558	1	18,21,22	2.66	10 (55%)	25,30,33	2.08	7 (28%)
1	UFT	A	716	1	18,21,22	2.66	10 (55%)	25,30,33	2.06	6 (24%)
1	UFT	A	686	1	18,21,22	2.65	9 (50%)	25,30,33	2.06	9 (36%)
1	CFZ	A	458	1	18,21,22	2.52	7 (38%)	25,30,33	1.28	3 (12%)
1	CFZ	A	706	1	18,21,22	2.47	6 (33%)	25,30,33	1.31	2 (8%)
1	UFT	A	42	1	18,21,22	2.66	10 (55%)	25,30,33	1.97	6 (24%)
1	UFT	A	19	1	18,21,22	2.66	10 (55%)	25,30,33	2.00	6 (24%)
1	CFZ	A	336	1	18,21,22	2.55	7 (38%)	25,30,33	1.40	2 (8%)
1	UFT	A	588	1	18,21,22	2.57	10 (55%)	25,30,33	2.17	8 (32%)
1	CFZ	A	146	1	18,21,22	2.43	7 (38%)	25,30,33	1.33	3 (12%)
1	UFT	A	277	1	18,21,22	2.61	10 (55%)	25,30,33	2.25	7 (28%)
1	CFZ	A	720	1	18,21,22	2.47	7 (38%)	25,30,33	1.42	3 (12%)
1	CFZ	A	198	1	18,21,22	2.56	7 (38%)	25,30,33	1.24	2 (8%)
1	UFT	A	303	1	18,21,22	2.64	10 (55%)	25,30,33	2.20	7 (28%)
1	UFT	A	655	1	18,21,22	2.61	9 (50%)	25,30,33	2.03	7 (28%)
1	UFT	A	148	1	18,21,22	2.69	10 (55%)	25,30,33	1.89	6 (24%)
1	CFZ	A	65	1	18,21,22	2.48	7 (38%)	25,30,33	1.42	3 (12%)
1	UFT	A	230	1	18,21,22	2.66	10 (55%)	25,30,33	2.06	5 (20%)
1	CFZ	A	560	1	18,21,22	2.51	7 (38%)	25,30,33	1.24	2 (8%)
1	CFZ	A	73	1	18,21,22	2.44	7 (38%)	25,30,33	1.55	2 (8%)
1	CFZ	A	83	1	18,21,22	2.60	7 (38%)	25,30,33	1.25	2 (8%)
1	CFZ	A	546	1	18,21,22	2.53	7 (38%)	25,30,33	1.22	1 (4%)
1	UFT	A	550	1	18,21,22	2.67	10 (55%)	25,30,33	2.19	8 (32%)
1	CFZ	A	10	1	18,21,22	2.54	7 (38%)	25,30,33	1.33	2 (8%)
1	UFT	A	6	1	18,21,22	2.65	10 (55%)	25,30,33	1.97	6 (24%)
1	CFZ	A	131	1	18,21,22	2.48	7 (38%)	25,30,33	1.55	3 (12%)

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	161	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	11	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	378	1	-	0/7/25/26	0/2/2/2
1	UFT	A	485	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UFT	A	409	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	717	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	426	1	-	0/7/25/26	0/2/2/2
1	UFT	A	542	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	632	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	661	1	-	2/7/25/26	0/2/2/2
1	UFT	A	595	1	-	1/7/25/26	0/2/2/2
1	UFT	A	627	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	405	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	346	1	-	1/7/25/26	0/2/2/2
1	UFT	A	670	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	128	1	-	7/7/25/26	0/2/2/2
1	UFT	A	236	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	658	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	206	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	275	1	-	0/7/25/26	0/2/2/2
1	UFT	A	61	1	-	2/7/25/26	0/2/2/2
1	UFT	A	51	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	577	1	-	0/7/25/26	0/2/2/2
1	UFT	A	95	1	-	0/7/25/26	0/2/2/2
1	UFT	A	283	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	471	1	-	0/7/25/26	0/2/2/2
1	UFT	A	329	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	45	1	-	0/7/25/26	0/2/2/2
1	UFT	A	687	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	72	1	-	4/7/25/26	0/2/2/2
1	UFT	A	196	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	675	1	-	3/7/25/26	0/2/2/2
1	UFT	A	175	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	475	1	-	3/7/25/26	0/2/2/2
1	UFT	A	667	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	50	1	-	0/7/25/26	0/2/2/2
1	UFT	A	585	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	165	1	-	0/7/25/26	0/2/2/2
1	UFT	A	56	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	433	1	-	0/7/25/26	0/2/2/2
1	UFT	A	575	1	-	4/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UFT	A	444	1	-	0/7/25/26	0/2/2/2
1	UFT	A	650	1	-	2/7/25/26	0/2/2/2
1	UFT	A	115	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	195	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	75	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	602	1	-	2/7/25/26	0/2/2/2
1	UFT	A	683	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	137	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	500	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	416	1	-	0/7/25/26	0/2/2/2
1	UFT	A	607	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	101	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	184	1	-	0/7/25/26	0/2/2/2
1	UFT	A	298	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	460	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	578	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	233	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	355	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	442	1	-	0/7/25/26	0/2/2/2
1	UFT	A	193	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	308	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	609	1	-	0/7/25/26	0/2/2/2
1	UFT	A	62	1	-	3/7/25/26	0/2/2/2
1	UFT	A	311	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	649	1	-	2/7/25/26	0/2/2/2
1	UFT	A	464	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	337	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	618	1	-	2/7/25/26	0/2/2/2
1	UFT	A	221	1	-	3/7/25/26	0/2/2/2
1	UFT	A	727	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	57	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	621	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	392	1	-	0/7/25/26	0/2/2/2
1	UFT	A	274	1	-	3/7/25/26	0/2/2/2
1	UFT	A	679	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	637	1	-	0/7/25/26	0/2/2/2
1	UFT	A	93	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	154	1	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UFT	A	215	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	144	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	382	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	162	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	90	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	129	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	111	1	-	0/7/25/26	0/2/2/2
1	UFT	A	556	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	506	1	-	0/7/25/26	0/2/2/2
1	UFT	A	138	1	-	0/7/25/26	0/2/2/2
1	UFT	A	127	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	332	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	391	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	15	1	-	0/7/25/26	0/2/2/2
1	UFT	A	724	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	656	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	153	1	-	0/7/25/26	0/2/2/2
1	UFT	A	48	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	483	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	438	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	515	1	-	2/7/25/26	0/2/2/2
1	UFT	A	388	1	-	0/7/25/26	0/2/2/2
1	UFT	A	698	1	-	0/7/25/26	0/2/2/2
1	UFT	A	116	1	-	2/7/25/26	0/2/2/2
1	UFT	A	169	1	-	0/7/25/26	0/2/2/2
1	UFT	A	360	1	-	3/7/25/26	0/2/2/2
1	UFT	A	123	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	526	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	208	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	641	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	439	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	690	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	345	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	108	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	456	1	-	0/7/25/26	0/2/2/2
1	UFT	A	417	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	330	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UFT	A	361	1	-	0/7/25/26	0/2/2/2
1	UFT	A	350	1	-	0/7/25/26	0/2/2/2
1	UFT	A	319	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	502	1	-	3/7/25/26	0/2/2/2
1	UFT	A	573	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	625	1	-	0/7/25/26	0/2/2/2
1	UFT	A	240	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	466	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	603	1	-	2/7/25/26	0/2/2/2
1	UFT	A	555	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	190	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	384	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	657	1	-	6/7/25/26	0/2/2/2
1	CFZ	A	473	1	-	0/7/25/26	0/2/2/2
1	UFT	A	612	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	674	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	103	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	557	1	-	1/7/25/26	0/2/2/2
1	UFT	A	307	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	709	1	-	4/7/25/26	0/2/2/2
1	CFZ	A	273	1	-	1/7/25/26	0/2/2/2
1	UFT	A	532	1	-	0/7/25/26	0/2/2/2
1	UFT	A	497	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	538	1	-	0/7/25/26	0/2/2/2
1	UFT	A	601	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	28	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	629	1	-	0/7/25/26	0/2/2/2
1	UFT	A	167	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	695	1	-	0/7/25/26	0/2/2/2
1	UFT	A	177	1	-	1/7/25/26	0/2/2/2
1	UFT	A	23	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	209	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	156	1	-	0/7/25/26	0/2/2/2
1	UFT	A	642	1	-	1/7/25/26	0/2/2/2
1	UFT	A	170	1	-	0/7/25/26	0/2/2/2
1	UFT	A	671	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	104	1	-	0/7/25/26	0/2/2/2
1	UFT	A	397	1	-	1/7/25/26	0/2/2/2
1	UFT	A	510	1	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UFT	A	89	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	594	1	-	0/7/25/26	0/2/2/2
1	UFT	A	419	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	335	1	-	1/7/25/26	0/2/2/2
1	UFT	A	197	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	379	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	685	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	12	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	306	1	-	0/7/25/26	0/2/2/2
1	UFT	A	39	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	363	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	467	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	366	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	604	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	696	1	-	2/7/25/26	0/2/2/2
1	UFT	A	263	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	310	1	-	0/7/25/26	0/2/2/2
1	UFT	A	476	1	-	3/7/25/26	0/2/2/2
1	UFT	A	590	1	-	2/7/25/26	0/2/2/2
1	UFT	A	272	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	157	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	395	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	7	1	-	0/7/25/26	0/2/2/2
1	UFT	A	597	1	-	0/7/25/26	0/2/2/2
1	UFT	A	521	1	-	2/7/25/26	0/2/2/2
1	UFT	A	351	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	487	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	598	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	631	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	434	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	212	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	155	1	-	0/7/25/26	0/2/2/2
1	UFT	A	480	1	-	0/7/25/26	0/2/2/2
1	UFT	A	242	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	531	1	-	2/7/25/26	0/2/2/2
1	UFT	A	662	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	302	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	369	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	26	1	-	0/7/25/26	0/2/2/2
1	UFT	A	377	1	-	6/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CFZ	A	234	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	343	1	-	0/7/25/26	0/2/2/2
1	UFT	A	356	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	564	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	76	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	574	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	699	1	-	0/7/25/26	0/2/2/2
1	UFT	A	563	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	130	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	432	1	-	0/7/25/26	0/2/2/2
1	UFT	A	421	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	666	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	117	1	-	0/7/25/26	0/2/2/2
1	UFT	A	367	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	437	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	109	1	-	0/7/25/26	0/2/2/2
1	UFT	A	210	1	-	0/7/25/26	0/2/2/2
1	UFT	A	288	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	489	1	-	0/7/25/26	0/2/2/2
1	UFT	A	142	1	-	3/7/25/26	0/2/2/2
1	UFT	A	719	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	512	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	453	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	386	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	600	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	728	1	-	5/7/25/26	0/2/2/2
1	CFZ	A	605	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	219	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	328	1	-	0/7/25/26	0/2/2/2
1	UFT	A	107	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	271	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	407	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	665	1	-	0/7/25/26	0/2/2/2
1	UFT	A	44	1	-	1/7/25/26	0/2/2/2
1	UFT	A	643	1	-	4/7/25/26	0/2/2/2
1	CFZ	A	484	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	314	1	-	0/7/25/26	0/2/2/2
1	UFT	A	559	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	147	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CFZ	A	80	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	55	1	-	2/7/25/26	0/2/2/2
1	UFT	A	88	1	-	3/7/25/26	0/2/2/2
1	UFT	A	617	1	-	3/7/25/26	0/2/2/2
1	UFT	A	46	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	41	1	-	0/7/25/26	0/2/2/2
1	UFT	A	504	1	-	3/7/25/26	0/2/2/2
1	UFT	A	254	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	645	1	-	2/7/25/26	0/2/2/2
1	UFT	A	374	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	522	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	620	1	-	0/7/25/26	0/2/2/2
1	UFT	A	79	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	541	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	527	1	-	2/7/25/26	0/2/2/2
1	UFT	A	238	1	-	0/7/25/26	0/2/2/2
1	UFT	A	71	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	276	1	-	0/7/25/26	0/2/2/2
1	UFT	A	507	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	630	1	-	0/7/25/26	0/2/2/2
1	UFT	A	644	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	244	1	-	2/7/25/26	0/2/2/2
1	UFT	A	582	1	-	0/7/25/26	0/2/2/2
1	UFT	A	151	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	217	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	342	1	-	0/7/25/26	0/2/2/2
1	UFT	A	33	1	-	2/7/25/26	0/2/2/2
1	UFT	A	624	1	-	0/7/25/26	0/2/2/2
1	UFT	A	94	1	-	3/7/25/26	0/2/2/2
1	UFT	A	468	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	178	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	34	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	204	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	182	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	672	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	287	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	359	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	613	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UFT	A	213	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	713	1	-	3/7/25/26	0/2/2/2
1	UFT	A	390	1	-	0/7/25/26	0/2/2/2
1	UFT	A	705	1	-	0/7/25/26	0/2/2/2
1	UFT	A	340	1	-	0/7/25/26	0/2/2/2
1	UFT	A	192	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	87	1	-	0/7/25/26	0/2/2/2
1	UFT	A	370	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	536	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	561	1	-	0/7/25/26	0/2/2/2
1	UFT	A	693	1	-	0/7/25/26	0/2/2/2
1	UFT	A	371	1	-	2/7/25/26	0/2/2/2
1	UFT	A	383	1	-	0/7/25/26	0/2/2/2
1	UFT	A	97	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	591	1	-	3/7/25/26	0/2/2/2
1	UFT	A	143	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	344	1	-	0/7/25/26	0/2/2/2
1	UFT	A	188	1	-	1/7/25/26	0/2/2/2
1	UFT	A	589	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	114	1	-	2/7/25/26	0/2/2/2
1	UFT	A	17	1	-	2/7/25/26	0/2/2/2
1	UFT	A	562	1	-	0/7/25/26	0/2/2/2
1	UFT	A	501	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	422	1	-	0/7/25/26	0/2/2/2
1	UFT	A	32	1	-	2/7/25/26	0/2/2/2
1	UFT	A	181	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	291	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	547	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	490	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	653	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	499	1	-	2/7/25/26	0/2/2/2
1	UFT	A	523	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	171	1	-	2/7/25/26	0/2/2/2
1	UFT	A	267	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	463	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	256	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	493	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	173	1	-	0/7/25/26	0/2/2/2
1	UFT	A	616	1	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CFZ	A	663	1	-	0/7/25/26	0/2/2/2
1	UFT	A	638	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	58	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	135	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	689	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	81	1	-	0/7/25/26	0/2/2/2
1	UFT	A	339	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	635	1	-	0/7/25/26	0/2/2/2
1	UFT	A	120	1	-	1/7/25/26	0/2/2/2
1	UFT	A	697	1	-	1/7/25/26	0/2/2/2
1	UFT	A	322	1	-	2/7/25/26	0/2/2/2
1	UFT	A	429	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	269	1	-	0/7/25/26	0/2/2/2
1	UFT	A	431	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	694	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	362	1	-	2/7/25/26	0/2/2/2
1	UFT	A	558	1	-	0/7/25/26	0/2/2/2
1	UFT	A	716	1	-	2/7/25/26	0/2/2/2
1	UFT	A	686	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	458	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	706	1	-	0/7/25/26	0/2/2/2
1	UFT	A	42	1	-	0/7/25/26	0/2/2/2
1	UFT	A	19	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	336	1	-	1/7/25/26	0/2/2/2
1	UFT	A	588	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	146	1	-	1/7/25/26	0/2/2/2
1	UFT	A	277	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	720	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	198	1	-	2/7/25/26	0/2/2/2
1	UFT	A	303	1	-	1/7/25/26	0/2/2/2
1	UFT	A	655	1	-	3/7/25/26	0/2/2/2
1	UFT	A	148	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	65	1	-	0/7/25/26	0/2/2/2
1	UFT	A	230	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	560	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	73	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	83	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	546	1	-	0/7/25/26	0/2/2/2
1	UFT	A	550	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	10	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UFT	A	6	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	131	1	-	1/7/25/26	0/2/2/2

The worst 5 of 2919 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	573	UFT	C2-N1	5.43	1.47	1.38
1	A	23	UFT	C2-N1	5.38	1.46	1.38
1	A	194	UFT	C2-N1	5.36	1.46	1.38
1	A	71	UFT	C2-N1	5.34	1.46	1.38
1	A	429	UFT	C2-N1	5.33	1.46	1.38

The worst 5 of 1638 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	607	UFT	C4-N3-C2	-6.80	118.17	126.61
1	A	213	UFT	C4-N3-C2	-6.53	118.51	126.61
1	A	650	UFT	C4-N3-C2	-6.41	118.65	126.61
1	A	56	UFT	C4-N3-C2	-6.32	118.76	126.61
1	A	471	UFT	C4-N3-C2	-6.22	118.89	126.61

There are no chirality outliers.

5 of 299 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	32	UFT	O4'-C4'-C5'-O5'
1	A	61	UFT	O4'-C4'-C5'-O5'
1	A	62	UFT	O4'-C4'-C5'-O5'
1	A	62	UFT	C3'-C4'-C5'-O5'
1	A	72	CFZ	O4'-C4'-C5'-O5'

There are no ring outliers.

279 monomers are involved in 430 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	161	CFZ	1	0
1	A	11	CFZ	2	0
1	A	485	UFT	2	0
1	A	426	CFZ	1	0
1	A	542	UFT	2	0
1	A	661	CFZ	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	627	UFT	1	0
1	A	346	CFZ	1	0
1	A	128	CFZ	1	0
1	A	236	UFT	2	0
1	A	658	CFZ	1	0
1	A	206	CFZ	2	0
1	A	275	CFZ	4	0
1	A	51	UFT	2	0
1	A	577	CFZ	1	0
1	A	95	UFT	2	0
1	A	283	UFT	3	0
1	A	518	CFZ	2	0
1	A	471	UFT	4	0
1	A	329	UFT	1	0
1	A	45	CFZ	3	0
1	A	687	UFT	3	0
1	A	72	CFZ	2	0
1	A	675	CFZ	1	0
1	A	175	UFT	3	0
1	A	475	UFT	1	0
1	A	667	UFT	2	0
1	A	50	CFZ	1	0
1	A	585	UFT	2	0
1	A	165	CFZ	3	0
1	A	56	UFT	1	0
1	A	433	CFZ	1	0
1	A	575	UFT	2	0
1	A	444	UFT	2	0
1	A	650	UFT	3	0
1	A	602	CFZ	1	0
1	A	683	UFT	1	0
1	A	137	CFZ	2	0
1	A	500	CFZ	2	0
1	A	416	CFZ	3	0
1	A	607	UFT	3	0
1	A	101	CFZ	1	0
1	A	184	CFZ	1	0
1	A	460	CFZ	2	0
1	A	233	CFZ	1	0
1	A	355	CFZ	2	0
1	A	442	CFZ	1	0
1	A	193	UFT	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	308	CFZ	1	0
1	A	609	CFZ	3	0
1	A	311	UFT	2	0
1	A	649	CFZ	3	0
1	A	337	CFZ	3	0
1	A	618	CFZ	1	0
1	A	727	UFT	1	0
1	A	392	CFZ	3	0
1	A	274	UFT	3	0
1	A	637	CFZ	2	0
1	A	93	UFT	2	0
1	A	154	UFT	2	0
1	A	215	UFT	4	0
1	A	382	CFZ	3	0
1	A	162	CFZ	1	0
1	A	129	CFZ	3	0
1	A	111	CFZ	3	0
1	A	556	UFT	1	0
1	A	138	UFT	1	0
1	A	332	CFZ	3	0
1	A	391	CFZ	2	0
1	A	724	UFT	3	0
1	A	153	CFZ	1	0
1	A	48	UFT	2	0
1	A	483	CFZ	1	0
1	A	438	CFZ	2	0
1	A	388	UFT	1	0
1	A	360	UFT	2	0
1	A	123	UFT	1	0
1	A	208	CFZ	2	0
1	A	451	UFT	2	0
1	A	439	CFZ	3	0
1	A	690	CFZ	1	0
1	A	121	CFZ	3	0
1	A	345	UFT	2	0
1	A	108	CFZ	1	0
1	A	456	CFZ	2	0
1	A	417	UFT	4	0
1	A	330	CFZ	4	0
1	A	361	UFT	2	0
1	A	350	UFT	2	0
1	A	319	UFT	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	502	CFZ	2	0
1	A	573	UFT	1	0
1	A	625	CFZ	4	0
1	A	240	UFT	1	0
1	A	466	CFZ	1	0
1	A	603	CFZ	1	0
1	A	555	UFT	1	0
1	A	190	CFZ	3	0
1	A	384	CFZ	1	0
1	A	452	CFZ	3	0
1	A	657	CFZ	2	0
1	A	473	CFZ	1	0
1	A	612	UFT	2	0
1	A	674	CFZ	1	0
1	A	103	CFZ	3	0
1	A	557	CFZ	1	0
1	A	307	UFT	2	0
1	A	273	CFZ	3	0
1	A	532	UFT	1	0
1	A	497	UFT	1	0
1	A	538	CFZ	2	0
1	A	601	UFT	1	0
1	A	28	CFZ	3	0
1	A	629	CFZ	1	0
1	A	695	CFZ	1	0
1	A	177	UFT	2	0
1	A	23	UFT	2	0
1	A	209	CFZ	3	0
1	A	156	CFZ	1	0
1	A	170	UFT	1	0
1	A	104	CFZ	2	0
1	A	397	UFT	1	0
1	A	510	UFT	1	0
1	A	594	CFZ	3	0
1	A	419	UFT	3	0
1	A	335	CFZ	2	0
1	A	685	CFZ	1	0
1	A	12	CFZ	3	0
1	A	306	CFZ	3	0
1	A	39	UFT	2	0
1	A	363	CFZ	2	0
1	A	467	CFZ	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	366	CFZ	3	0
1	A	263	UFT	1	0
1	A	310	CFZ	1	0
1	A	476	UFT	1	0
1	A	272	UFT	2	0
1	A	157	CFZ	2	0
1	A	7	CFZ	3	0
1	A	597	UFT	1	0
1	A	521	UFT	5	0
1	A	351	UFT	3	0
1	A	487	CFZ	3	0
1	A	598	CFZ	1	0
1	A	212	CFZ	2	0
1	A	155	CFZ	1	0
1	A	480	UFT	1	0
1	A	242	UFT	1	0
1	A	531	CFZ	2	0
1	A	662	UFT	3	0
1	A	302	CFZ	3	0
1	A	26	CFZ	1	0
1	A	377	UFT	5	0
1	A	234	CFZ	4	0
1	A	343	CFZ	4	0
1	A	356	UFT	2	0
1	A	574	CFZ	2	0
1	A	130	CFZ	2	0
1	A	432	CFZ	1	0
1	A	421	UFT	2	0
1	A	666	CFZ	4	0
1	A	117	CFZ	1	0
1	A	367	UFT	3	0
1	A	437	CFZ	2	0
1	A	66	UFT	2	0
1	A	109	CFZ	2	0
1	A	210	UFT	2	0
1	A	288	UFT	1	0
1	A	489	CFZ	1	0
1	A	512	CFZ	2	0
1	A	453	CFZ	4	0
1	A	219	CFZ	3	0
1	A	107	UFT	2	0
1	A	271	CFZ	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	407	CFZ	3	0
1	A	665	CFZ	2	0
1	A	44	UFT	3	0
1	A	643	UFT	1	0
1	A	484	CFZ	1	0
1	A	314	CFZ	1	0
1	A	559	UFT	2	0
1	A	147	CFZ	1	0
1	A	80	CFZ	1	0
1	A	55	CFZ	3	0
1	A	617	UFT	1	0
1	A	46	UFT	3	0
1	A	41	CFZ	2	0
1	A	504	UFT	2	0
1	A	254	UFT	1	0
1	A	374	UFT	1	0
1	A	522	CFZ	4	0
1	A	620	CFZ	2	0
1	A	79	UFT	1	0
1	A	541	CFZ	3	0
1	A	527	CFZ	1	0
1	A	71	UFT	1	0
1	A	276	CFZ	3	0
1	A	507	UFT	1	0
1	A	244	CFZ	2	0
1	A	582	UFT	4	0
1	A	217	CFZ	4	0
1	A	342	CFZ	3	0
1	A	33	UFT	1	0
1	A	624	UFT	2	0
1	A	94	UFT	3	0
1	A	468	UFT	3	0
1	A	178	CFZ	2	0
1	A	34	CFZ	2	0
1	A	204	CFZ	2	0
1	A	287	CFZ	2	0
1	A	359	CFZ	1	0
1	A	613	CFZ	3	0
1	A	213	UFT	3	0
1	A	713	CFZ	4	0
1	A	390	UFT	1	0
1	A	705	UFT	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	340	UFT	5	0
1	A	192	UFT	3	0
1	A	536	CFZ	2	0
1	A	561	CFZ	1	0
1	A	693	UFT	1	0
1	A	383	UFT	3	0
1	A	97	UFT	3	0
1	A	591	CFZ	1	0
1	A	344	CFZ	2	0
1	A	188	UFT	3	0
1	A	589	UFT	1	0
1	A	114	CFZ	1	0
1	A	501	UFT	1	0
1	A	422	CFZ	3	0
1	A	32	UFT	1	0
1	A	291	CFZ	1	0
1	A	547	CFZ	2	0
1	A	490	CFZ	2	0
1	A	653	CFZ	2	0
1	A	499	CFZ	1	0
1	A	523	UFT	2	0
1	A	171	CFZ	2	0
1	A	267	UFT	2	0
1	A	256	CFZ	3	0
1	A	493	CFZ	1	0
1	A	173	CFZ	3	0
1	A	616	UFT	1	0
1	A	663	CFZ	3	0
1	A	638	UFT	2	0
1	A	549	UFT	2	0
1	A	135	CFZ	2	0
1	A	689	CFZ	2	0
1	A	81	CFZ	1	0
1	A	339	UFT	3	0
1	A	635	CFZ	3	0
1	A	120	UFT	1	0
1	A	322	UFT	1	0
1	A	429	UFT	1	0
1	A	431	UFT	1	0
1	A	694	CFZ	2	0
1	A	362	CFZ	1	0
1	A	558	UFT	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	716	UFT	1	0
1	A	686	UFT	2	0
1	A	458	CFZ	2	0
1	A	706	CFZ	4	0
1	A	42	UFT	3	0
1	A	19	UFT	1	0
1	A	336	CFZ	3	0
1	A	588	UFT	2	0
1	A	146	CFZ	1	0
1	A	277	UFT	2	0
1	A	303	UFT	2	0
1	A	148	UFT	3	0
1	A	230	UFT	2	0
1	A	560	CFZ	2	0
1	A	73	CFZ	1	0
1	A	83	CFZ	3	0
1	A	546	CFZ	2	0
1	A	550	UFT	3	0
1	A	10	CFZ	2	0
1	A	6	UFT	1	0
1	A	131	CFZ	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.

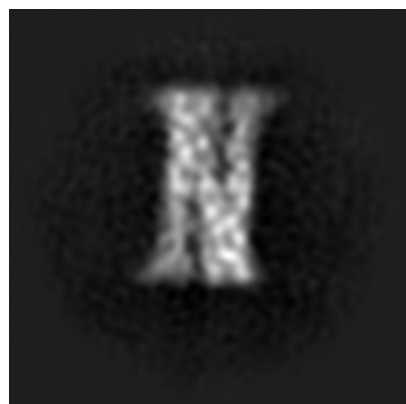
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53803. These allow visual inspection of the internal detail of the map and identification of artifacts.

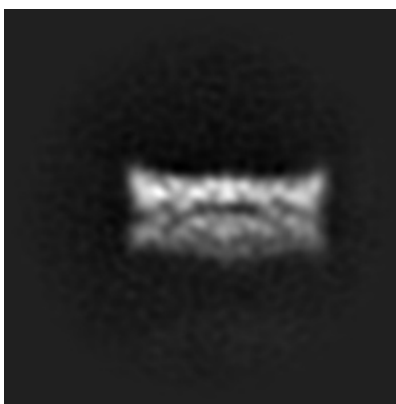
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

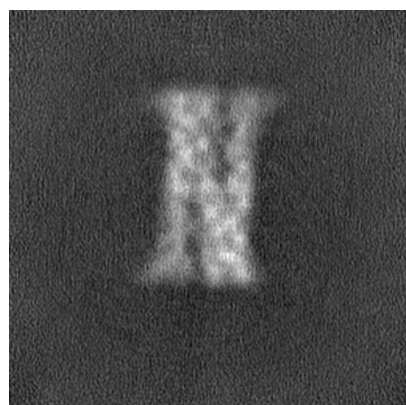


Y

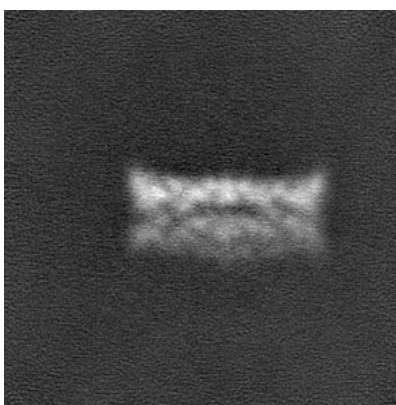


Z

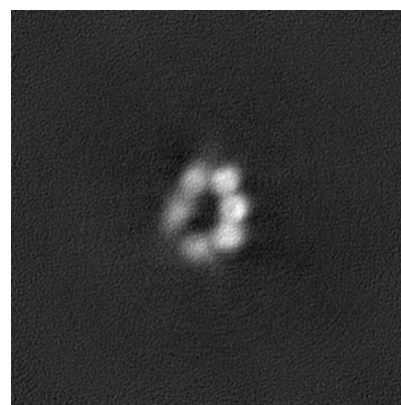
6.1.2 Raw map



X



Y

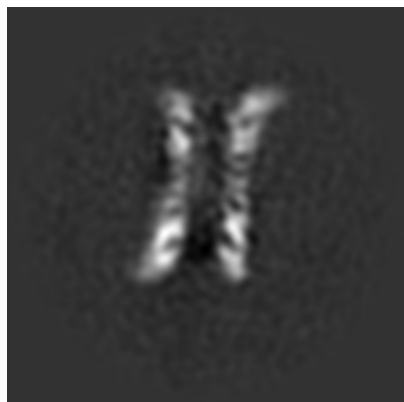


Z

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

6.2 Central slices [i](#)

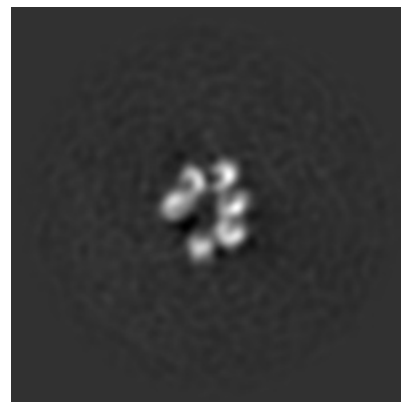
6.2.1 Primary map



X Index: 128

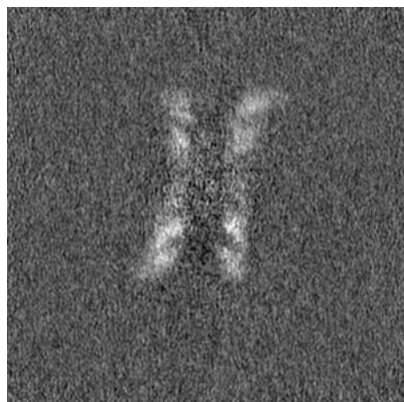


Y Index: 128

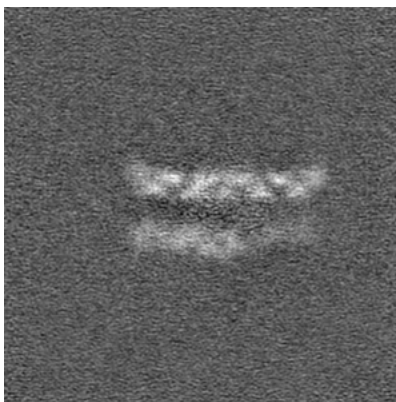


Z Index: 128

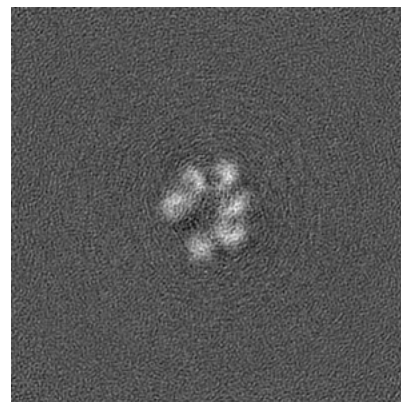
6.2.2 Raw map



X Index: 128



Y Index: 128



Z Index: 128

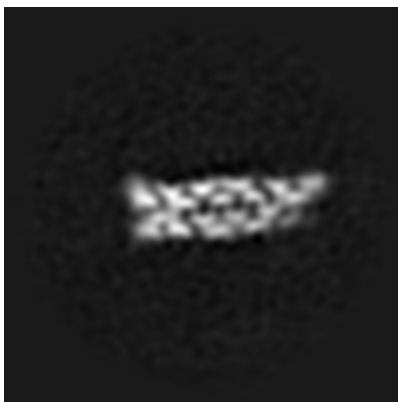
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

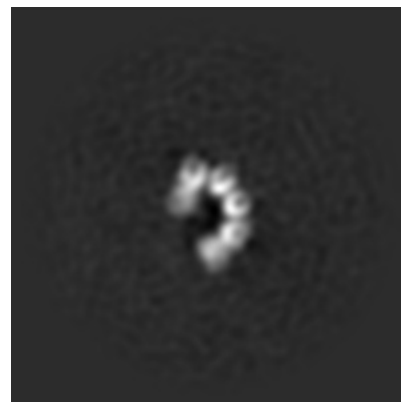
6.3.1 Primary map



X Index: 139

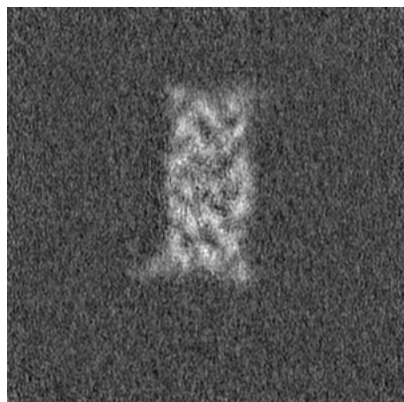


Y Index: 147

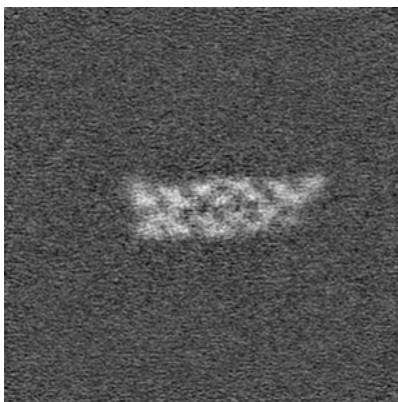


Z Index: 97

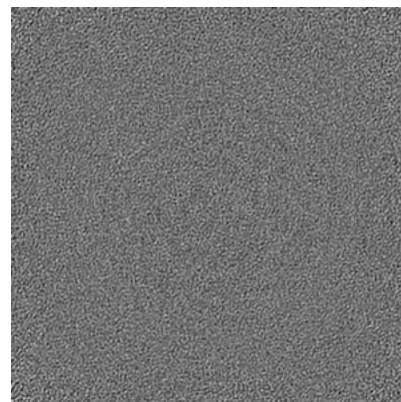
6.3.2 Raw map



X Index: 139



Y Index: 147

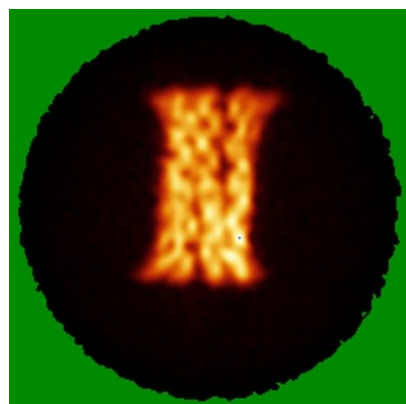


Z Index: 0

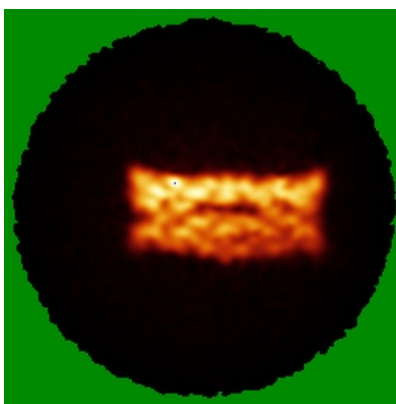
The images above show the largest variance slices of the map in three orthogonal directions.

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

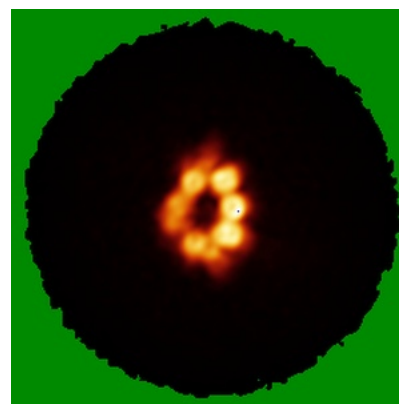
6.4.1 Primary map



X

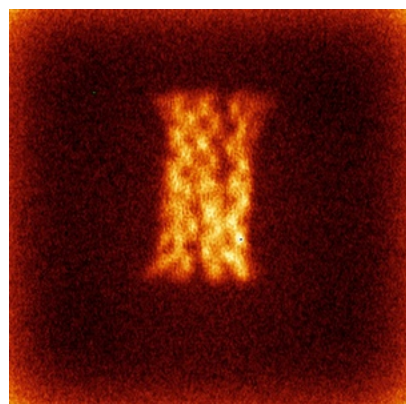


Y

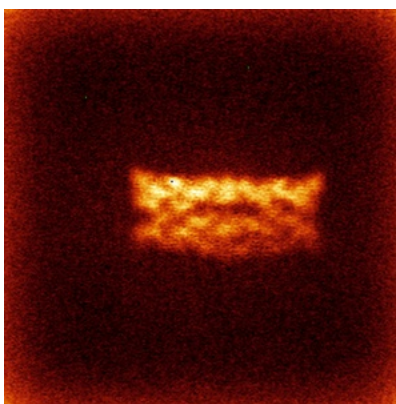


Z

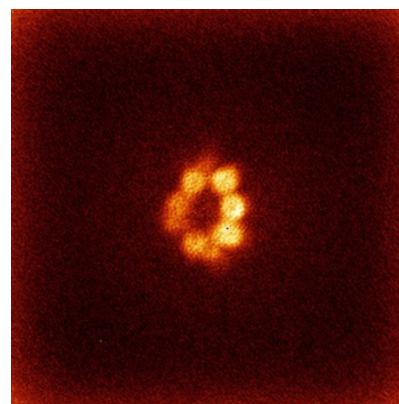
6.4.2 Raw map



X



Y

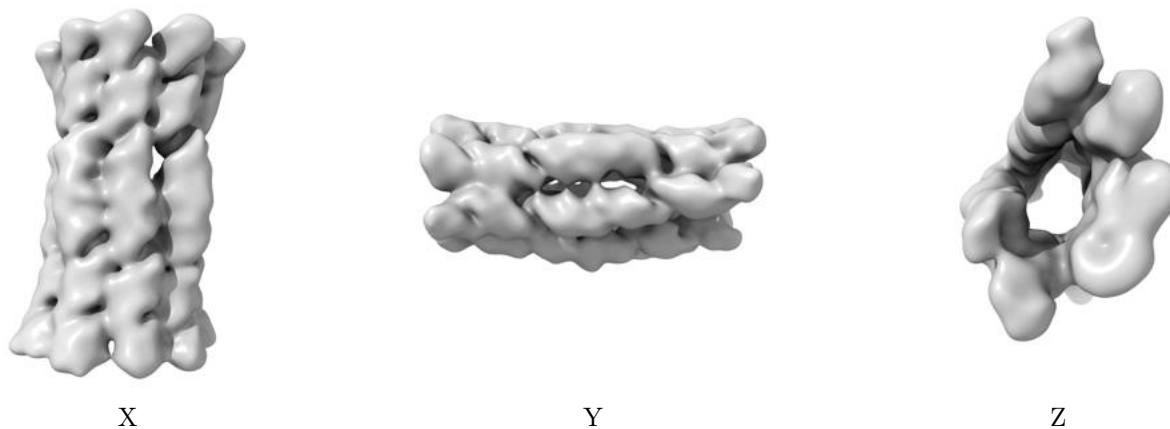


Z

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.

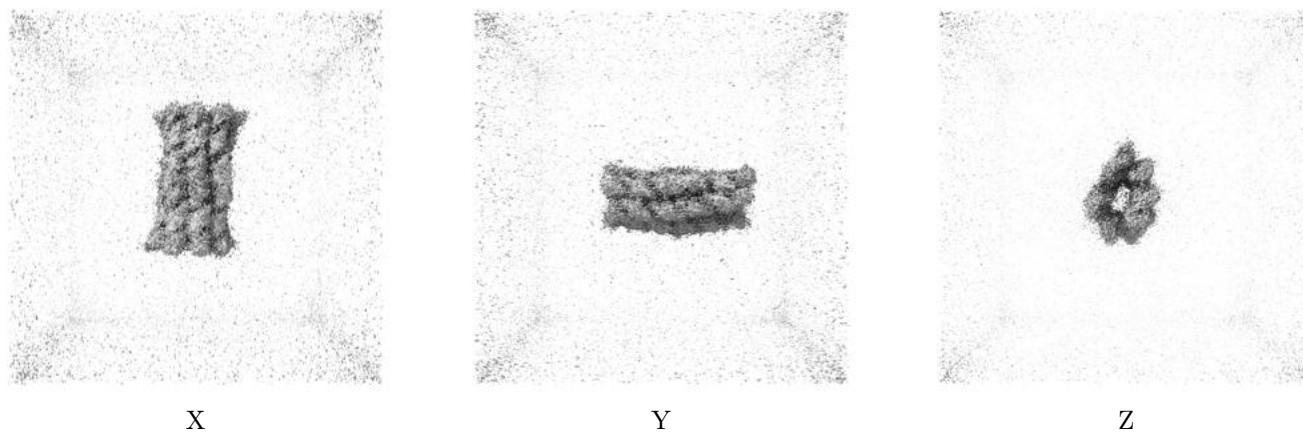
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

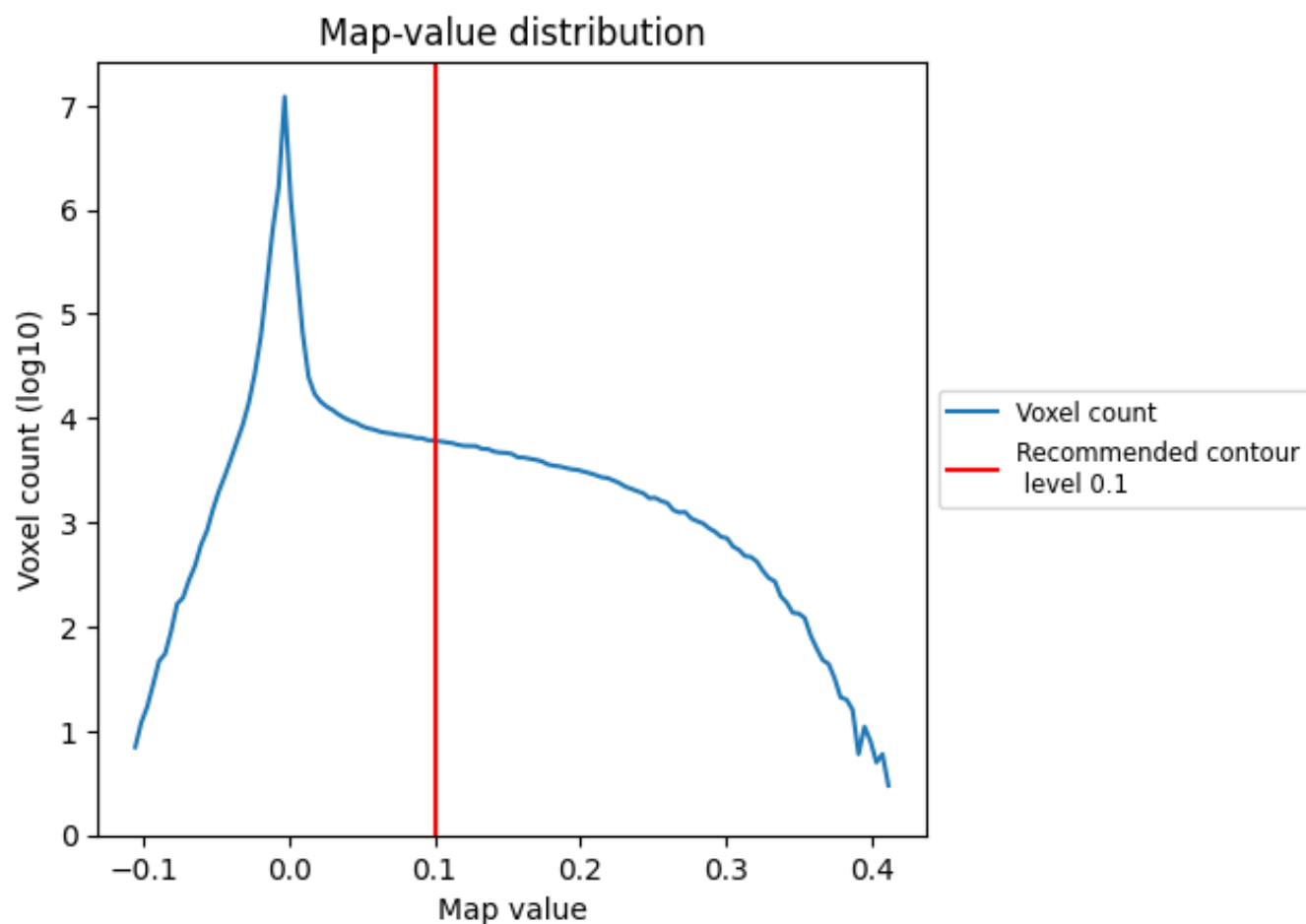
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

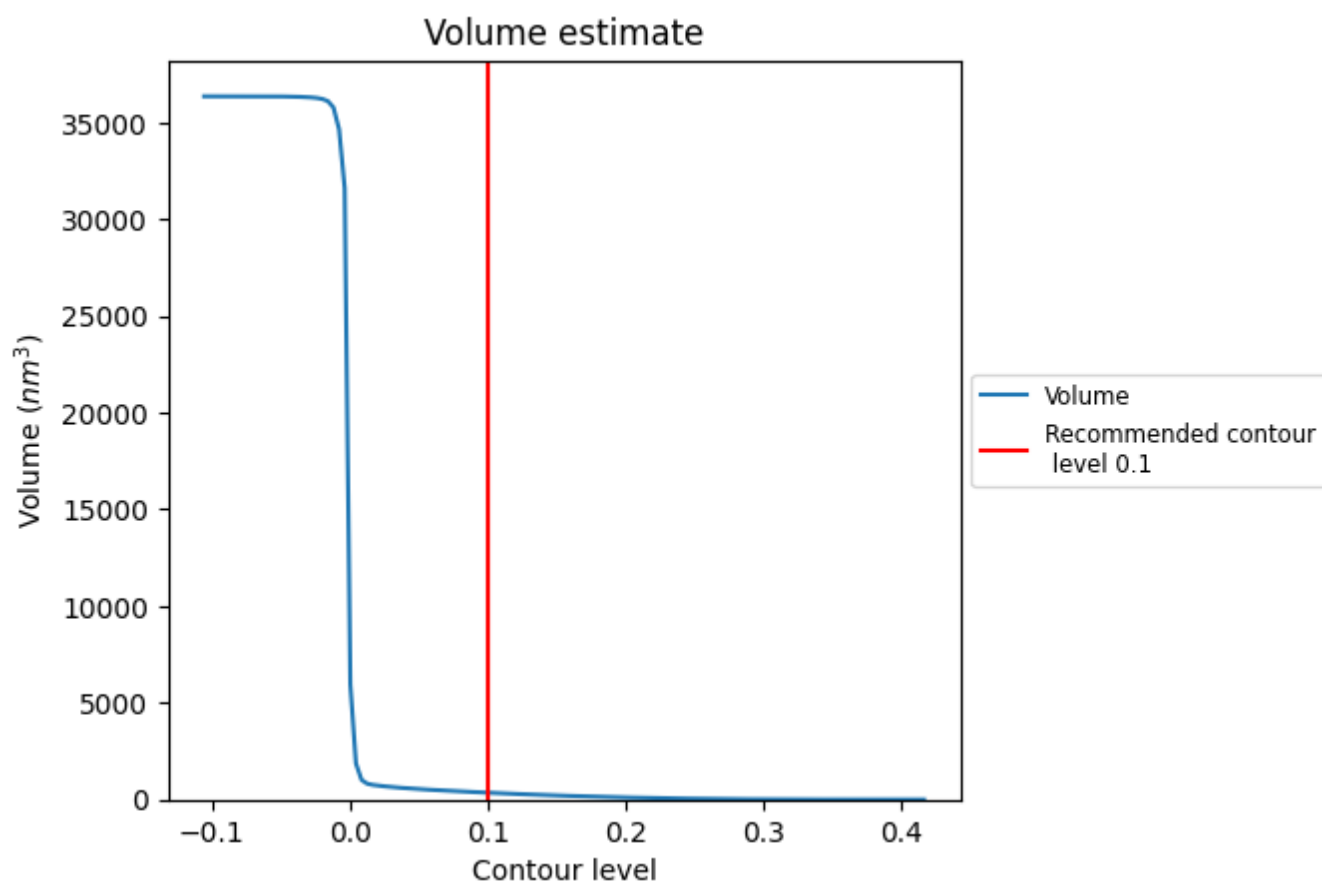
This section contains the results of statistical analysis of the map.

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.

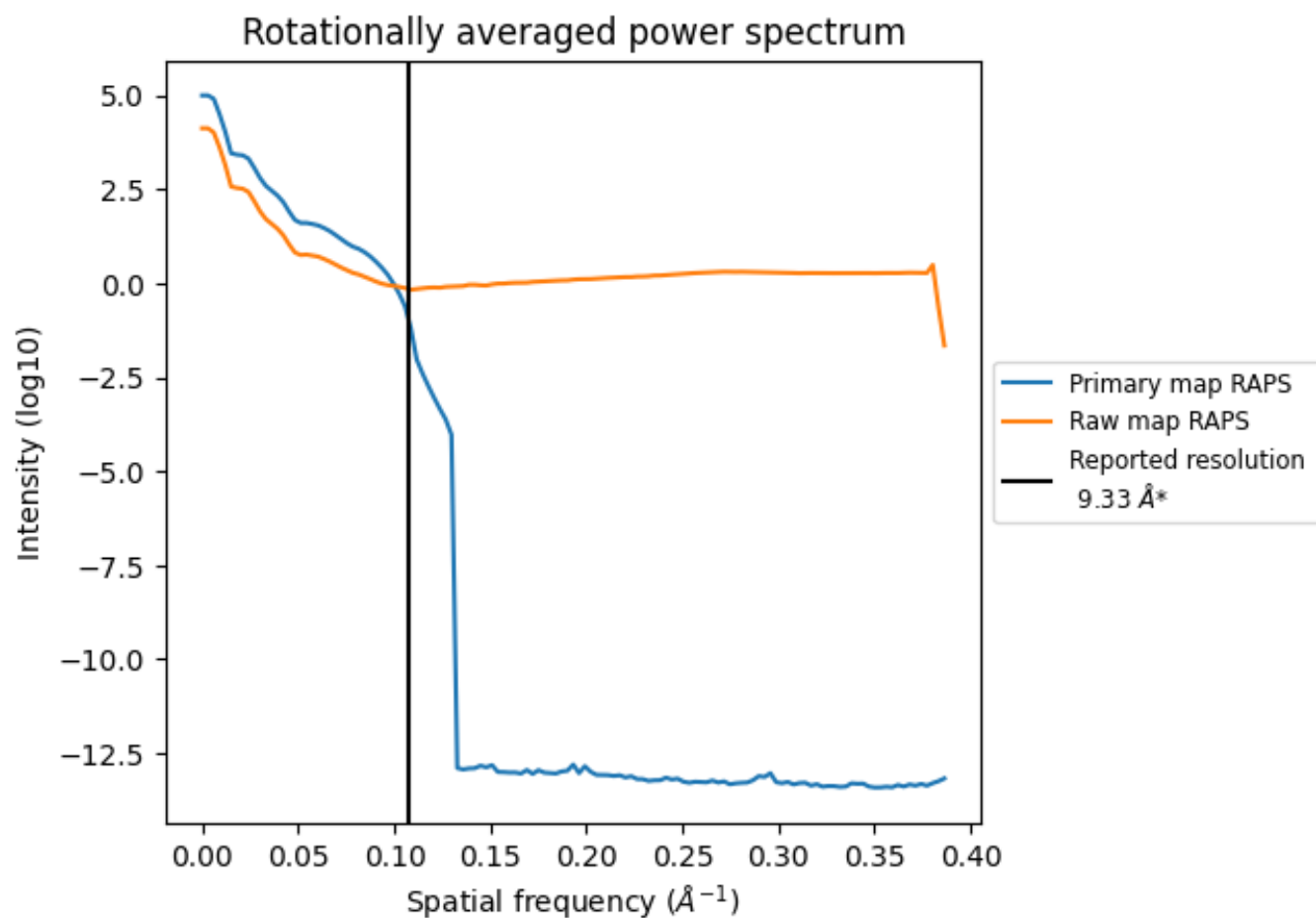
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 354 nm³; this corresponds to an approximate mass of 319 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 ⓘ

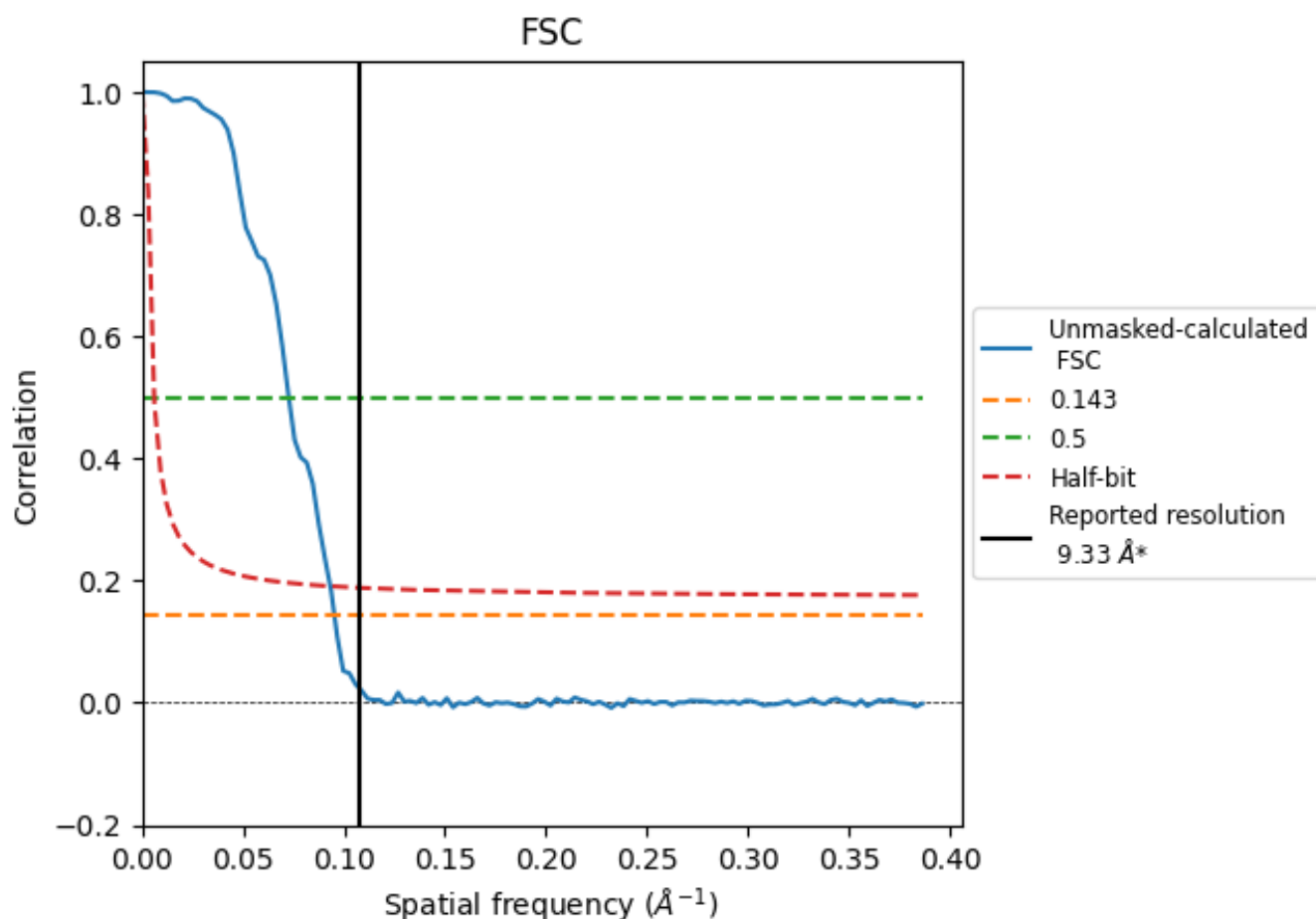


*Reported resolution corresponds to spatial frequency of 0.107 \AA^{-1}

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 0.107 Å⁻¹

8.2 Resolution estimates [i](#)

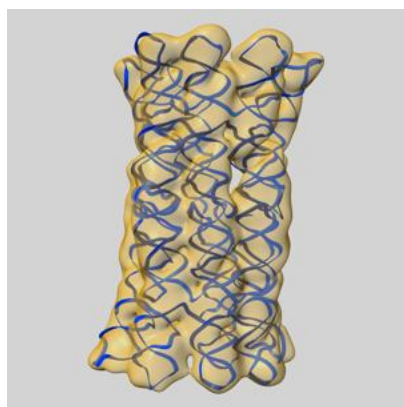
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.33	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	10.50	13.77	10.74

*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 10.50 differs from the reported value 9.33 by more than 10 %

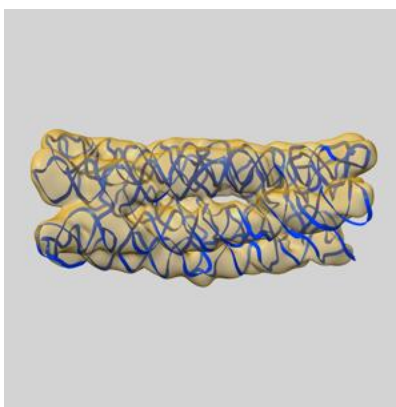
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53803 and PDB model 9R82. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

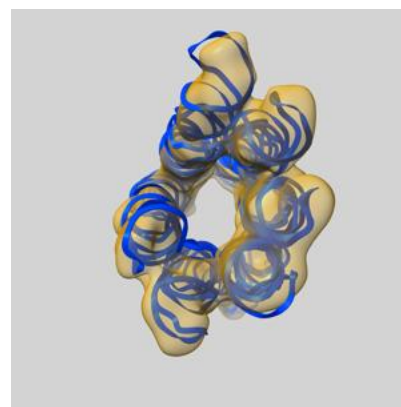
9.1 Map-model overlay [i](#)



X



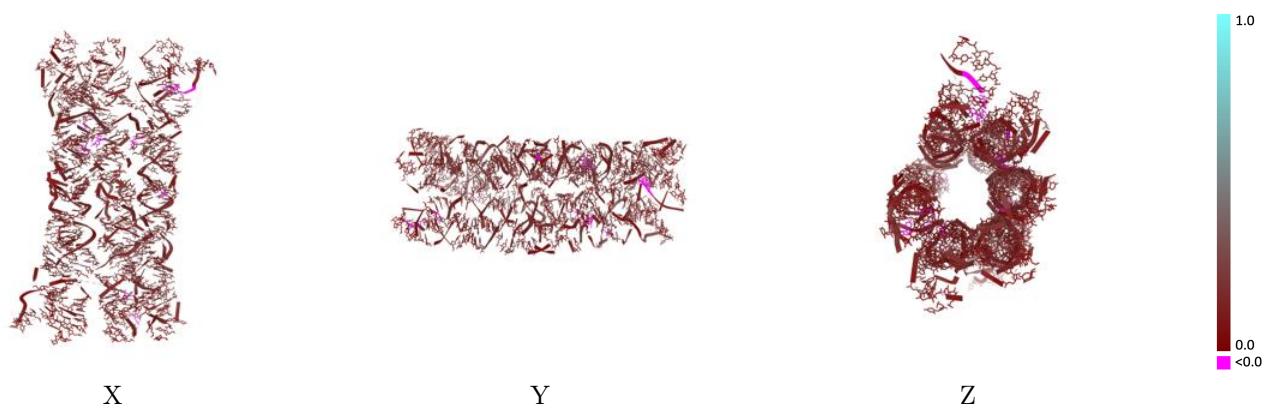
Y



Z

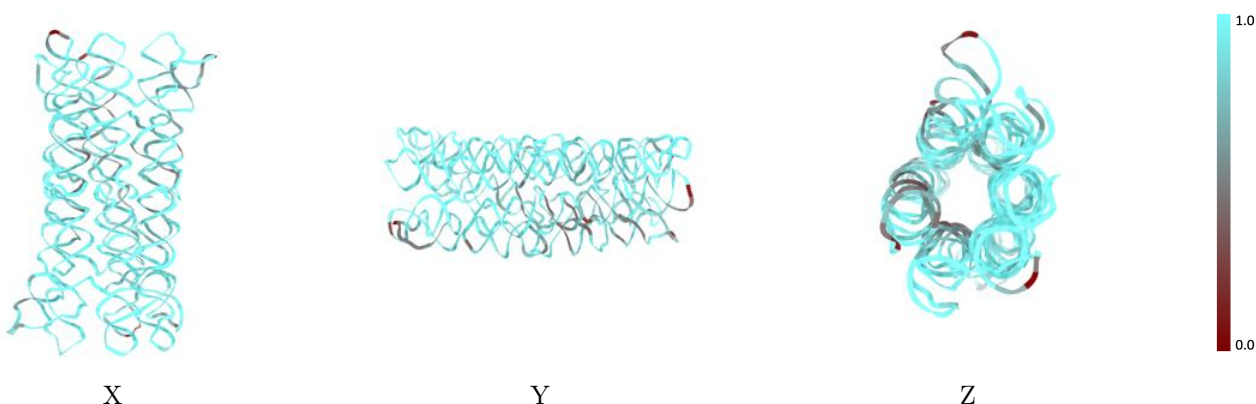
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



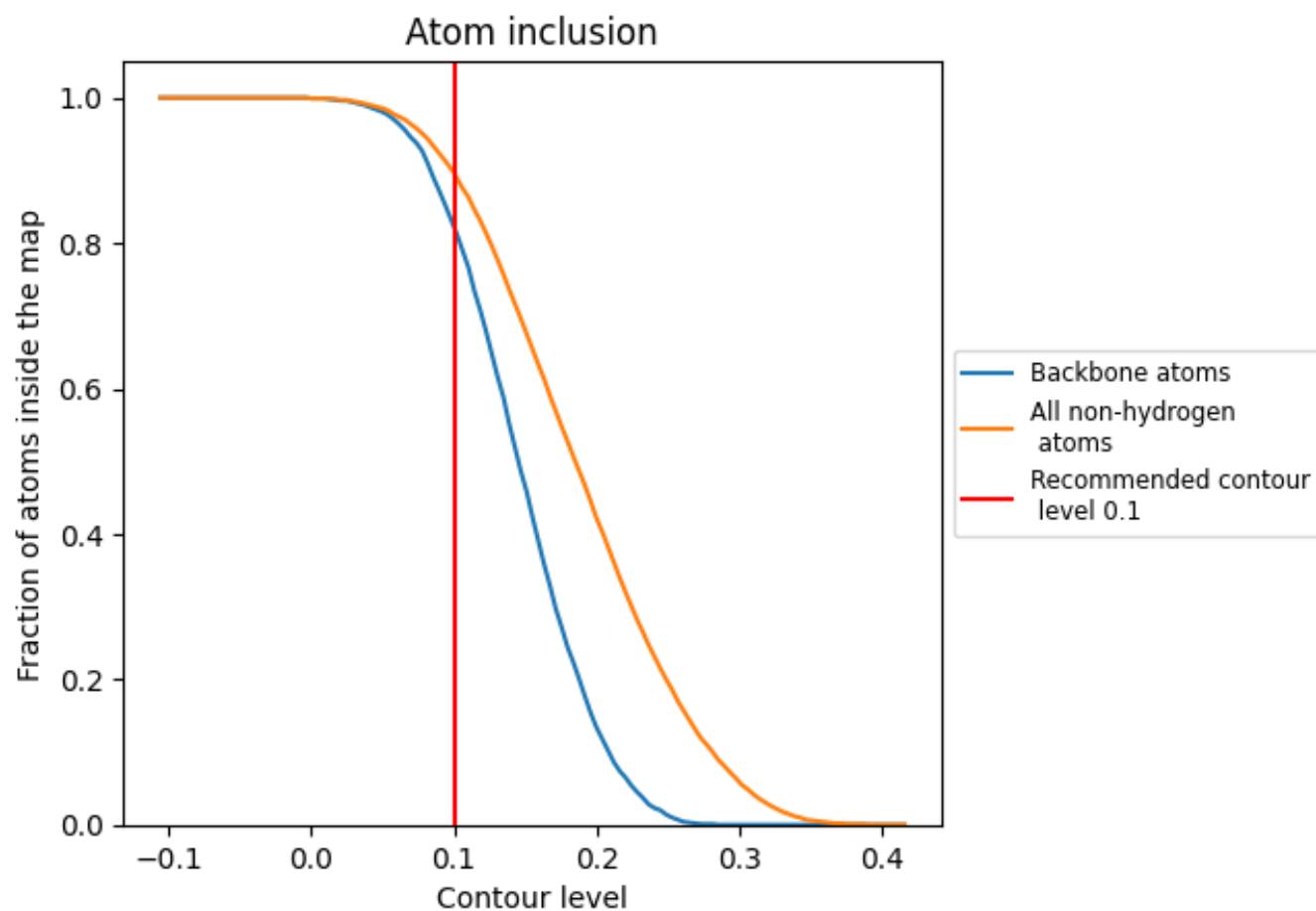
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 90% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8970	<div><div></div></div> 0.1410
A	<div><div></div></div> 0.8970	<div><div></div></div> 0.1410

