



wwPDB EM Validation Summary Report ⓘ

Jun 4, 2026 – 03:14 pm BST

PDB ID : 9SD9 / pdb_00009sd9
EMDB ID : EMD-54779
Title : 6-Helix Bundle - with a Clasp (6HB-C)-dimer with 2'-Fluoro-modified pyrimidines (FY RNA)
Authors : Kristoffersen, E.L.; Andersen, E.S.; Zwergius, N.H.
Deposited on : 2025-08-12
Resolution : 9.60 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 : 1.8.4, CSD as541be (2020)
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

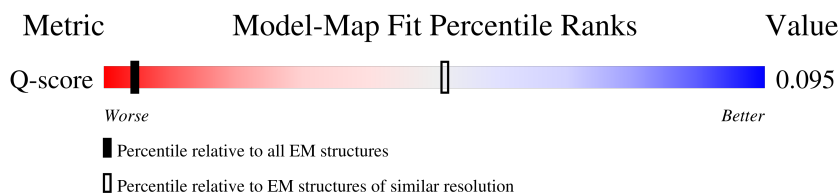
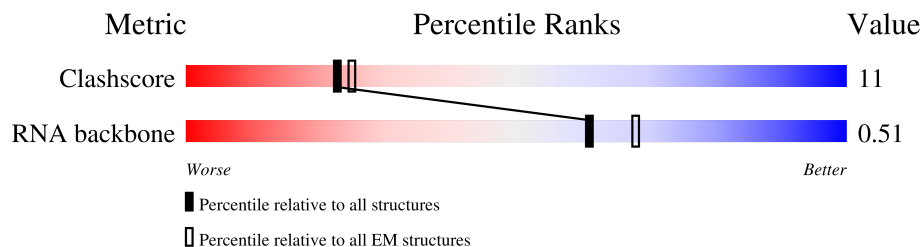
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

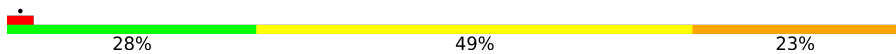
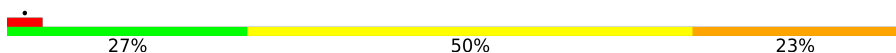
The reported resolution of this entry is 9.60 Å.

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	185 (9.10 - 10.10)

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	720	
1	B	720	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	UFT	B	720	X	-	-	-

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 30671 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.

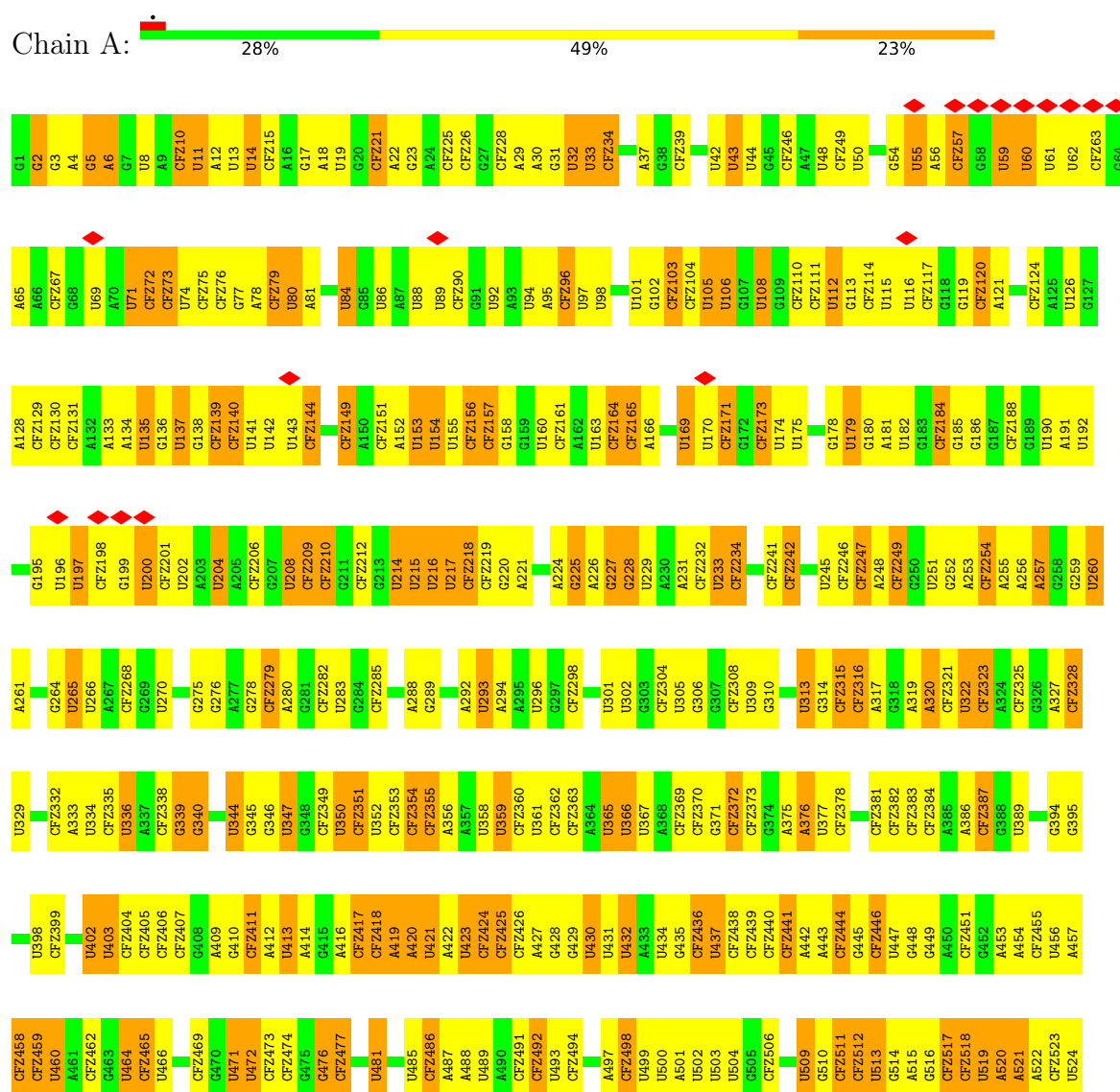
- Molecule 1 is a RNA chain called RNA (720-MER).

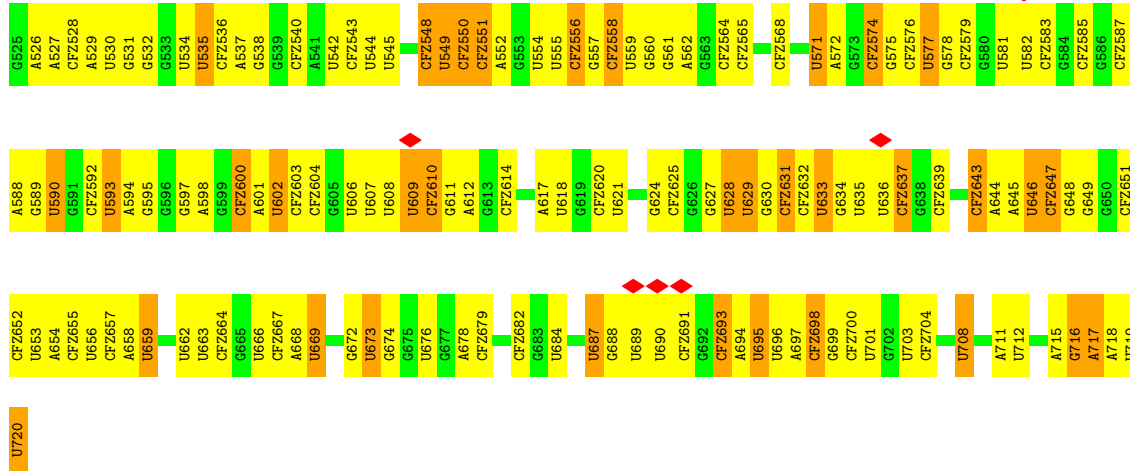
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	F	N	O	P		
1	A	720	15334	6843	357	2708	4707	719	0	0
1	B	720	15337	6843	357	2708	4709	720	0	0

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.

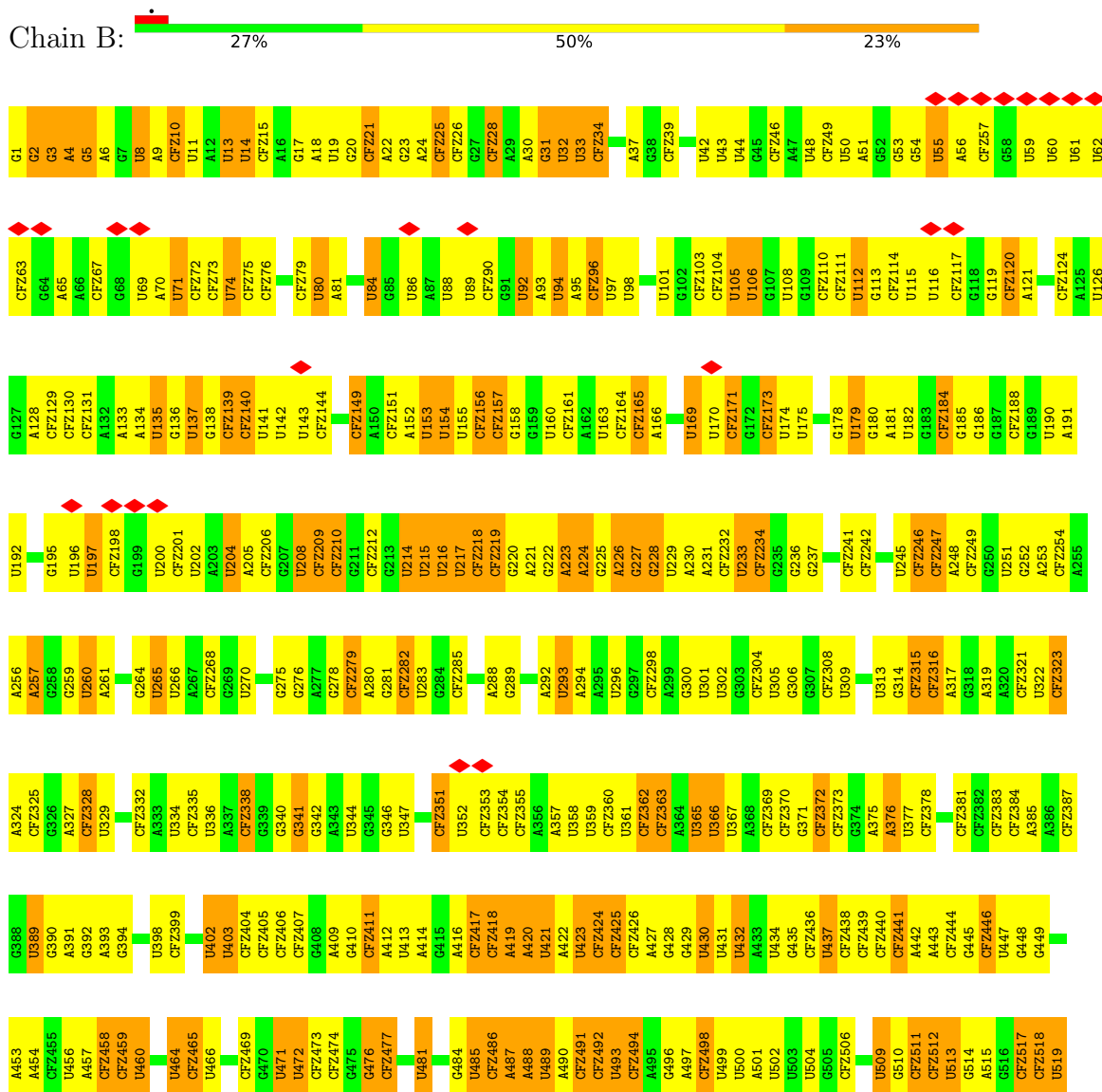
• Molecule 1: RNA (720-MER)





• Molecule 1: RNA (720-MER)

Chain B:





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	49938	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	0.650	Depositor
Minimum map value	-0.099	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.128	Depositor
Map size (Å)	465.8432, 465.8432, 465.8432	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.8197, 1.8197, 1.8197	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: 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	0.47	6/9186 (0.1%)	0.26	2/14187 (0.0%)
1	B	0.47	5/9189 (0.1%)	0.24	0/14191
All	All	0.47	11/18375 (0.1%)	0.25	2/28378 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	1	0

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	519	UFT	O3'-P	5.40	1.61	1.56
1	B	389	UFT	O3'-P	5.08	1.61	1.56
1	A	101	UFT	O3'-P	5.07	1.61	1.56
1	A	684	UFT	O3'-P	5.04	1.61	1.56
1	B	432	UFT	O3'-P	5.03	1.61	1.56

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	520	A	OP1-P-O3'	-8.91	81.27	108.00
1	A	520	A	OP2-P-O3'	-7.93	84.20	108.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	720	UFT	C2'

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	15334	0	7387	225	0
1	B	15337	0	7384	236	0
All	All	30671	0	14771	458	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 11.

The worst 5 of 458 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:225:G:H1	1:B:494:CFZ:HN4	1.19	0.87
1:A:481:UFT:HN3	1:A:501:A:H61	1.24	0.84
1:B:481:UFT:HN3	1:B:501:A:H61	1.25	0.83
1:B:135:UFT:HN3	1:B:152:A:H61	1.27	0.81
1:B:602:UFT:HN3	1:B:617:A:H61	1.30	0.78

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 ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	185/720 (25%)	43 (23%)	6 (3%)
1	B	186/720 (25%)	41 (22%)	5 (2%)
All	All	371/1440 (25%)	84 (22%)	11 (2%)

5 of 84 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	G
1	A	3	G
1	A	4	A
1	A	5	G
1	A	6	A

5 of 11 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B	227	G
1	B	230	A
1	B	487	A
1	B	419	A
1	A	419	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	UFT	B	155	1	18,21,22	2.58	9 (50%)	26,30,33	1.95	8 (30%)
1	UFT	A	530	1	18,21,22	2.64	9 (50%)	26,30,33	1.85	8 (30%)
1	UFT	A	143	1	18,21,22	2.58	9 (50%)	26,30,33	2.10	8 (30%)
1	UFT	A	200	1	18,21,22	2.54	9 (50%)	26,30,33	2.04	7 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CFZ	B	446	1	18,21,22	2.48	7 (38%)	26,30,33	1.43	3 (11%)
1	UFT	B	504	1	18,21,22	2.59	11 (61%)	26,30,33	1.95	8 (30%)
1	UFT	A	358	1	18,21,22	2.64	9 (50%)	26,30,33	1.84	7 (26%)
1	UFT	B	402	1	18,21,22	2.61	10 (55%)	26,30,33	1.90	7 (26%)
1	UFT	B	695	1	18,21,22	2.62	10 (55%)	26,30,33	1.90	8 (30%)
1	CFZ	B	328	1	18,21,22	2.46	7 (38%)	26,30,33	1.44	3 (11%)
1	UFT	B	42	1	18,21,22	2.68	9 (50%)	26,30,33	1.79	6 (23%)
1	UFT	A	662	1	18,21,22	2.58	9 (50%)	26,30,33	1.96	8 (30%)
1	UFT	A	542	1	18,21,22	2.59	10 (55%)	26,30,33	1.94	8 (30%)
1	CFZ	A	407	1	18,21,22	2.49	7 (38%)	26,30,33	1.24	3 (11%)
1	CFZ	B	458	1	18,21,22	2.53	7 (38%)	26,30,33	1.26	2 (7%)
1	UFT	A	115	1	18,21,22	2.57	10 (55%)	26,30,33	2.00	8 (30%)
1	CFZ	A	372	1	18,21,22	2.51	7 (38%)	26,30,33	1.29	3 (11%)
1	UFT	A	559	1	18,21,22	2.58	10 (55%)	26,30,33	1.98	7 (26%)
1	CFZ	B	540	1	18,21,22	2.52	7 (38%)	26,30,33	1.27	3 (11%)
1	CFZ	A	10	1	18,21,22	2.54	7 (38%)	26,30,33	1.15	3 (11%)
1	UFT	A	322	1	18,21,22	2.64	9 (50%)	26,30,33	1.85	7 (26%)
1	CFZ	A	111	1	18,21,22	2.49	7 (38%)	26,30,33	1.37	3 (11%)
1	CFZ	B	477	1	18,21,22	2.52	7 (38%)	26,30,33	1.14	3 (11%)
1	CFZ	A	198	1	18,21,22	2.49	7 (38%)	26,30,33	1.27	3 (11%)
1	UFT	B	116	1	18,21,22	2.58	9 (50%)	26,30,33	2.07	8 (30%)
1	CFZ	A	643	1	18,21,22	2.50	7 (38%)	26,30,33	1.24	3 (11%)
1	UFT	A	233	1	18,21,22	2.59	9 (50%)	26,30,33	1.86	6 (23%)
1	CFZ	B	372	1	18,21,22	2.50	7 (38%)	26,30,33	1.28	3 (11%)
1	CFZ	B	241	1	18,21,22	2.48	7 (38%)	26,30,33	1.57	4 (15%)
1	CFZ	A	438	1	18,21,22	2.48	7 (38%)	26,30,33	1.45	4 (15%)
1	UFT	A	367	1	18,21,22	2.63	9 (50%)	26,30,33	1.84	6 (23%)
1	CFZ	B	564	1	18,21,22	2.49	7 (38%)	26,30,33	1.38	2 (7%)
1	CFZ	A	462	1	18,21,22	2.50	7 (38%)	26,30,33	1.26	3 (11%)
1	UFT	A	251	1	18,21,22	2.62	10 (55%)	26,30,33	1.87	7 (26%)
1	UFT	A	636	1	18,21,22	2.57	9 (50%)	26,30,33	2.09	8 (30%)
1	UFT	B	509	1	18,21,22	2.61	10 (55%)	26,30,33	1.93	7 (26%)
1	CFZ	A	564	1	18,21,22	2.50	7 (38%)	26,30,33	1.39	2 (7%)
1	UFT	A	545	1	18,21,22	2.60	9 (50%)	26,30,33	1.92	7 (26%)
1	UFT	B	690	1	18,21,22	2.59	10 (55%)	26,30,33	1.90	8 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	UFT	B	59	1	18,21,22	2.59	9 (50%)	26,30,33	2.03	7 (26%)
1	CFZ	B	558	1	18,21,22	2.49	7 (38%)	26,30,33	1.16	3 (11%)
1	CFZ	B	90	1	18,21,22	2.47	7 (38%)	26,30,33	1.50	3 (11%)
1	UFT	A	142	1	18,21,22	2.58	9 (50%)	26,30,33	2.01	8 (30%)
1	CFZ	B	219	1	18,21,22	2.53	7 (38%)	26,30,33	1.17	3 (11%)
1	UFT	A	493	1	18,21,22	2.56	9 (50%)	26,30,33	1.98	7 (26%)
1	CFZ	A	548	1	18,21,22	2.50	7 (38%)	26,30,33	1.27	3 (11%)
1	UFT	A	513	1	18,21,22	2.64	9 (50%)	26,30,33	1.82	7 (26%)
1	UFT	B	293	1	18,21,22	2.62	9 (50%)	26,30,33	1.85	6 (23%)
1	UFT	A	42	1	18,21,22	2.64	9 (50%)	26,30,33	1.82	6 (23%)
1	UFT	B	549	1	18,21,22	2.60	9 (50%)	26,30,33	1.89	7 (26%)
1	UFT	B	719	1	18,21,22	2.59	10 (55%)	26,30,33	1.86	7 (26%)
1	UFT	B	684	1	18,21,22	2.64	9 (50%)	26,30,33	1.80	5 (19%)
1	CFZ	A	308	1	18,21,22	2.48	7 (38%)	26,30,33	1.50	4 (15%)
1	UFT	B	618	1	18,21,22	2.57	10 (55%)	26,30,33	2.04	8 (30%)
1	UFT	B	202	1	18,21,22	2.58	10 (55%)	26,30,33	2.00	8 (30%)
1	UFT	A	215	1	18,21,22	2.57	9 (50%)	26,30,33	1.97	7 (26%)
1	CFZ	B	210	1	18,21,22	2.48	7 (38%)	26,30,33	1.37	3 (11%)
1	CFZ	A	405	1	18,21,22	2.50	7 (38%)	26,30,33	1.29	3 (11%)
1	CFZ	B	67	1	18,21,22	2.48	7 (38%)	26,30,33	1.39	3 (11%)
1	CFZ	A	455	1	18,21,22	2.54	7 (38%)	26,30,33	1.24	4 (15%)
1	CFZ	A	90	1	18,21,22	2.46	7 (38%)	26,30,33	1.49	3 (11%)
1	CFZ	B	164	1	18,21,22	2.50	7 (38%)	26,30,33	1.25	2 (7%)
1	CFZ	A	417	1	18,21,22	2.49	7 (38%)	26,30,33	1.46	3 (11%)
1	UFT	A	689	1	18,21,22	2.60	10 (55%)	26,30,33	1.96	7 (26%)
1	CFZ	A	25	1	18,21,22	2.49	7 (38%)	26,30,33	1.41	3 (11%)
1	CFZ	B	411	1	18,21,22	2.51	7 (38%)	26,30,33	1.20	3 (11%)
1	CFZ	B	614	1	18,21,22	2.51	7 (38%)	26,30,33	1.20	3 (11%)
1	UFT	B	485	1	18,21,22	2.58	9 (50%)	26,30,33	1.99	7 (26%)
1	UFT	A	74	1	18,21,22	2.56	10 (55%)	26,30,33	2.03	8 (30%)
1	UFT	A	635	1	18,21,22	2.59	10 (55%)	26,30,33	2.00	8 (30%)
1	UFT	B	141	1	18,21,22	2.60	9 (50%)	26,30,33	1.95	7 (26%)
1	CFZ	B	667	1	18,21,22	2.49	7 (38%)	26,30,33	1.31	3 (11%)
1	UFT	A	347	1	18,21,22	2.58	10 (55%)	26,30,33	1.89	7 (26%)
1	CFZ	B	268	1	18,21,22	2.48	7 (38%)	26,30,33	1.46	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	UFT	A	366	1	18,21,22	2.58	10 (55%)	26,30,33	1.96	7 (26%)
1	UFT	B	302	1	18,21,22	2.62	9 (50%)	26,30,33	1.94	8 (30%)
1	UFT	B	94	1	18,21,22	2.58	10 (55%)	26,30,33	1.99	8 (30%)
1	UFT	B	635	1	18,21,22	2.59	9 (50%)	26,30,33	2.00	8 (30%)
1	CFZ	B	556	1	18,21,22	2.48	7 (38%)	26,30,33	1.36	3 (11%)
1	UFT	B	365	1	18,21,22	2.61	9 (50%)	26,30,33	1.88	6 (23%)
1	UFT	B	309	1	18,21,22	2.59	9 (50%)	26,30,33	1.93	8 (30%)
1	UFT	B	313	1	18,21,22	2.60	9 (50%)	26,30,33	1.90	8 (30%)
1	CFZ	B	76	1	18,21,22	2.52	7 (38%)	26,30,33	1.17	3 (11%)
1	CFZ	A	316	1	18,21,22	2.51	7 (38%)	26,30,33	1.13	2 (7%)
1	CFZ	A	79	1	18,21,22	2.51	7 (38%)	26,30,33	1.35	3 (11%)
1	CFZ	A	114	1	18,21,22	2.48	7 (38%)	26,30,33	1.44	4 (15%)
1	CFZ	B	151	1	18,21,22	2.51	7 (38%)	26,30,33	1.25	3 (11%)
1	CFZ	A	604	1	18,21,22	2.49	7 (38%)	26,30,33	1.24	4 (15%)
1	CFZ	A	165	1	18,21,22	2.52	7 (38%)	26,30,33	1.14	2 (7%)
1	UFT	A	695	1	18,21,22	2.61	9 (50%)	26,30,33	1.90	8 (30%)
1	CFZ	A	576	1	18,21,22	2.50	7 (38%)	26,30,33	1.28	3 (11%)
1	UFT	A	88	1	18,21,22	2.59	10 (55%)	26,30,33	1.93	8 (30%)
1	CFZ	B	21	1	18,21,22	2.54	7 (38%)	26,30,33	1.18	3 (11%)
1	UFT	A	633	1	18,21,22	2.61	10 (55%)	26,30,33	1.89	7 (26%)
1	CFZ	A	21	1	18,21,22	2.53	7 (38%)	26,30,33	1.23	3 (11%)
1	CFZ	B	404	1	18,21,22	2.49	7 (38%)	26,30,33	1.24	4 (15%)
1	CFZ	B	242	1	18,21,22	2.50	7 (38%)	26,30,33	1.30	3 (11%)
1	CFZ	B	565	1	18,21,22	2.53	7 (38%)	26,30,33	1.10	3 (11%)
1	CFZ	A	355	1	18,21,22	2.46	7 (38%)	26,30,33	1.15	2 (7%)
1	UFT	A	174	1	18,21,22	2.59	9 (50%)	26,30,33	2.00	6 (23%)
1	CFZ	A	387	1	18,21,22	2.52	7 (38%)	26,30,33	1.20	4 (15%)
1	CFZ	B	604	1	18,21,22	2.49	7 (38%)	26,30,33	1.26	3 (11%)
1	UFT	B	175	1	18,21,22	2.60	10 (55%)	26,30,33	1.92	7 (26%)
1	UFT	B	628	1	18,21,22	2.59	10 (55%)	26,30,33	1.98	7 (26%)
1	CFZ	B	498	1	18,21,22	2.47	7 (38%)	26,30,33	1.25	2 (7%)
1	UFT	B	489	1	18,21,22	2.60	9 (50%)	26,30,33	1.81	7 (26%)
1	CFZ	B	664	1	18,21,22	2.47	7 (38%)	26,30,33	1.53	3 (11%)
1	CFZ	B	651	1	18,21,22	2.51	7 (38%)	26,30,33	1.28	3 (11%)
1	CFZ	A	206	1	18,21,22	2.51	7 (38%)	26,30,33	1.27	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	UFT	B	11	1	18,21,22	2.60	9 (50%)	26,30,33	1.94	8 (30%)
1	CFZ	B	518	1	18,21,22	2.46	7 (38%)	26,30,33	1.37	3 (11%)
1	CFZ	B	161	1	18,21,22	2.48	7 (38%)	26,30,33	1.31	3 (11%)
1	UFT	A	229	1	18,21,22	2.62	9 (50%)	26,30,33	1.90	7 (26%)
1	UFT	A	663	1	18,21,22	2.56	9 (50%)	26,30,33	2.09	8 (30%)
1	CFZ	B	246	1	18,21,22	2.53	7 (38%)	26,30,33	1.21	2 (7%)
1	CFZ	B	25	1	18,21,22	2.50	7 (38%)	26,30,33	1.52	3 (11%)
1	UFT	B	182	1	18,21,22	2.57	9 (50%)	26,30,33	2.06	8 (30%)
1	UFT	B	154	1	18,21,22	2.59	10 (55%)	26,30,33	1.99	6 (23%)
1	UFT	B	44	1	18,21,22	2.64	9 (50%)	26,30,33	1.90	7 (26%)
1	UFT	B	431	1	18,21,22	2.58	10 (55%)	26,30,33	2.02	8 (30%)
1	UFT	B	602	1	18,21,22	2.61	9 (50%)	26,30,33	1.87	7 (26%)
1	CFZ	A	373	1	18,21,22	2.49	7 (38%)	26,30,33	1.24	3 (11%)
1	UFT	B	344	1	18,21,22	2.61	9 (50%)	26,30,33	1.88	7 (26%)
1	UFT	B	447	1	18,21,22	2.61	9 (50%)	26,30,33	1.87	7 (26%)
1	CFZ	A	540	1	18,21,22	2.52	7 (38%)	26,30,33	1.29	3 (11%)
1	UFT	A	169	1	18,21,22	2.58	10 (55%)	26,30,33	2.00	8 (30%)
1	CFZ	A	117	1	18,21,22	2.46	7 (38%)	26,30,33	1.50	4 (15%)
1	UFT	B	701	1	18,21,22	2.57	9 (50%)	26,30,33	1.97	7 (26%)
1	CFZ	B	110	1	18,21,22	2.51	7 (38%)	26,30,33	1.22	3 (11%)
1	UFT	B	170	1	18,21,22	2.56	10 (55%)	26,30,33	2.11	8 (30%)
1	CFZ	A	201	1	18,21,22	2.49	7 (38%)	26,30,33	1.27	3 (11%)
1	UFT	B	554	1	18,21,22	2.59	10 (55%)	26,30,33	2.00	8 (30%)
1	CFZ	A	103	1	18,21,22	2.49	7 (38%)	26,30,33	1.34	3 (11%)
1	UFT	B	106	1	18,21,22	2.58	9 (50%)	26,30,33	1.98	7 (26%)
1	UFT	B	153	1	18,21,22	2.62	9 (50%)	26,30,33	1.88	7 (26%)
1	CFZ	A	603	1	18,21,22	2.51	7 (38%)	26,30,33	1.17	2 (7%)
1	CFZ	A	439	1	18,21,22	2.50	7 (38%)	26,30,33	1.53	3 (11%)
1	CFZ	A	469	1	18,21,22	2.47	7 (38%)	26,30,33	1.41	3 (11%)
1	CFZ	B	381	1	18,21,22	2.52	7 (38%)	26,30,33	1.17	3 (11%)
1	CFZ	A	523	1	18,21,22	2.50	7 (38%)	26,30,33	1.22	3 (11%)
1	CFZ	B	637	1	18,21,22	2.47	7 (38%)	26,30,33	1.48	4 (15%)
1	CFZ	B	184	1	18,21,22	2.52	7 (38%)	26,30,33	1.19	2 (7%)
1	UFT	A	609	1	18,21,22	2.57	10 (55%)	26,30,33	2.04	8 (30%)
1	UFT	A	669	1	18,21,22	2.59	9 (50%)	26,30,33	1.88	7 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CFZ	A	353	1	18,21,22	2.47	7 (38%)	26,30,33	1.48	3 (11%)
1	UFT	A	196	1	18,21,22	2.58	9 (50%)	26,30,33	2.01	8 (30%)
1	CFZ	B	285	1	18,21,22	2.53	7 (38%)	26,30,33	1.13	3 (11%)
1	CFZ	A	363	1	18,21,22	2.51	7 (38%)	26,30,33	1.12	3 (11%)
1	UFT	A	155	1	18,21,22	2.58	9 (50%)	26,30,33	1.94	8 (30%)
1	UFT	B	334	1	18,21,22	2.59	9 (50%)	26,30,33	2.01	7 (26%)
1	UFT	A	216	1	18,21,22	2.62	9 (50%)	26,30,33	1.90	7 (26%)
1	UFT	A	84	1	18,21,22	2.59	10 (55%)	26,30,33	1.86	7 (26%)
1	UFT	B	571	1	18,21,22	2.60	9 (50%)	26,30,33	1.94	7 (26%)
1	CFZ	B	439	1	18,21,22	2.48	7 (38%)	26,30,33	1.49	3 (11%)
1	UFT	B	80	1	18,21,22	2.63	9 (50%)	26,30,33	1.86	7 (26%)
1	UFT	B	662	1	18,21,22	2.57	9 (50%)	26,30,33	1.97	8 (30%)
1	UFT	B	456	1	18,21,22	2.62	9 (50%)	26,30,33	1.86	5 (19%)
1	CFZ	A	96	1	18,21,22	2.49	7 (38%)	26,30,33	1.26	2 (7%)
1	CFZ	B	406	1	18,21,22	2.51	7 (38%)	26,30,33	1.27	3 (11%)
1	UFT	A	329	1	18,21,22	2.62	9 (50%)	26,30,33	1.87	7 (26%)
1	CFZ	A	325	1	18,21,22	2.52	7 (38%)	26,30,33	1.18	3 (11%)
1	UFT	A	163	1	18,21,22	2.60	9 (50%)	26,30,33	1.89	8 (30%)
1	CFZ	A	369	1	18,21,22	2.50	7 (38%)	26,30,33	1.31	3 (11%)
1	UFT	B	621	1	18,21,22	2.56	10 (55%)	26,30,33	2.07	8 (30%)
1	UFT	B	524	1	18,21,22	2.63	9 (50%)	26,30,33	1.87	7 (26%)
1	UFT	B	472	1	18,21,22	2.57	9 (50%)	26,30,33	2.06	6 (23%)
1	UFT	B	245	1	18,21,22	2.63	9 (50%)	26,30,33	1.84	6 (23%)
1	UFT	B	84	1	18,21,22	2.60	9 (50%)	26,30,33	1.94	7 (26%)
1	UFT	B	607	1	18,21,22	2.58	9 (50%)	26,30,33	2.01	7 (26%)
1	UFT	B	305	1	18,21,22	2.56	10 (55%)	26,30,33	1.93	6 (23%)
1	UFT	B	229	1	18,21,22	2.63	9 (50%)	26,30,33	1.85	5 (19%)
1	CFZ	A	600	1	18,21,22	2.52	7 (38%)	26,30,33	1.20	3 (11%)
1	UFT	A	214	1	18,21,22	2.60	9 (50%)	26,30,33	1.92	7 (26%)
1	UFT	B	555	1	18,21,22	2.57	9 (50%)	26,30,33	2.04	6 (23%)
1	CFZ	B	418	1	18,21,22	2.48	7 (38%)	26,30,33	1.29	3 (11%)
1	CFZ	B	698	1	18,21,22	2.52	7 (38%)	26,30,33	1.19	3 (11%)
1	CFZ	A	679	1	18,21,22	2.50	7 (38%)	26,30,33	1.22	3 (11%)
1	CFZ	B	506	1	18,21,22	2.50	7 (38%)	26,30,33	1.34	3 (11%)
1	CFZ	A	486	1	18,21,22	2.48	7 (38%)	26,30,33	1.29	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CFZ	A	378	1	18,21,22	2.49	7 (38%)	26,30,33	1.25	3 (11%)
1	UFT	A	690	1	18,21,22	2.60	9 (50%)	26,30,33	1.91	8 (30%)
1	UFT	A	504	1	18,21,22	2.59	10 (55%)	26,30,33	1.94	8 (30%)
1	UFT	B	60	1	18,21,22	2.56	9 (50%)	26,30,33	2.04	8 (30%)
1	CFZ	B	362	1	18,21,22	2.51	7 (38%)	26,30,33	1.43	2 (7%)
1	UFT	A	265	1	18,21,22	2.61	10 (55%)	26,30,33	1.94	7 (26%)
1	UFT	A	204	1	18,21,22	2.60	9 (50%)	26,30,33	1.90	6 (23%)
1	CFZ	A	704	1	18,21,22	2.49	7 (38%)	26,30,33	1.27	3 (11%)
1	UFT	A	430	1	18,21,22	2.58	10 (55%)	26,30,33	1.98	8 (30%)
1	UFT	B	535	1	18,21,22	2.64	9 (50%)	26,30,33	1.77	5 (19%)
1	CFZ	B	647	1	18,21,22	2.51	7 (38%)	26,30,33	1.20	3 (11%)
1	UFT	A	581	1	18,21,22	2.59	9 (50%)	26,30,33	1.97	7 (26%)
1	UFT	B	636	1	18,21,22	2.58	10 (55%)	26,30,33	2.08	8 (30%)
1	UFT	A	309	1	18,21,22	2.61	9 (50%)	26,30,33	1.93	8 (30%)
1	CFZ	A	518	1	18,21,22	2.51	7 (38%)	26,30,33	1.12	1 (3%)
1	CFZ	A	404	1	18,21,22	2.48	7 (38%)	26,30,33	1.25	4 (15%)
1	CFZ	B	104	1	18,21,22	2.52	7 (38%)	26,30,33	1.16	2 (7%)
1	UFT	A	296	1	18,21,22	2.58	10 (55%)	26,30,33	1.97	8 (30%)
1	UFT	A	179	1	18,21,22	2.63	9 (50%)	26,30,33	1.86	6 (23%)
1	CFZ	B	576	1	18,21,22	2.51	7 (38%)	26,30,33	1.29	3 (11%)
1	UFT	A	33	1	18,21,22	2.64	9 (50%)	26,30,33	1.84	7 (26%)
1	CFZ	B	218	1	18,21,22	2.47	7 (38%)	26,30,33	1.28	2 (7%)
1	CFZ	B	156	1	18,21,22	2.51	7 (38%)	26,30,33	1.28	3 (11%)
1	CFZ	A	551	1	18,21,22	2.52	7 (38%)	26,30,33	1.13	2 (7%)
1	UFT	B	71	1	18,21,22	2.58	9 (50%)	26,30,33	1.94	8 (30%)
1	UFT	A	202	1	18,21,22	2.58	10 (55%)	26,30,33	2.06	7 (26%)
1	UFT	A	86	1	18,21,22	2.60	10 (55%)	26,30,33	1.92	8 (30%)
1	CFZ	B	543	1	18,21,22	2.48	7 (38%)	26,30,33	1.30	3 (11%)
1	UFT	A	8	1	18,21,22	2.61	10 (55%)	26,30,33	1.86	7 (26%)
1	UFT	A	555	1	18,21,22	2.57	10 (55%)	26,30,33	2.06	7 (26%)
1	CFZ	A	383	1	18,21,22	2.50	7 (38%)	26,30,33	1.34	3 (11%)
1	UFT	A	471	1	18,21,22	2.60	9 (50%)	26,30,33	1.85	6 (23%)
1	UFT	A	14	1	18,21,22	2.60	10 (55%)	26,30,33	1.92	6 (23%)
1	UFT	A	481	1	18,21,22	2.59	9 (50%)	26,30,33	1.91	7 (26%)
1	UFT	A	582	1	18,21,22	2.57	10 (55%)	26,30,33	1.97	8 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CFZ	A	592	1	18,21,22	2.49	7 (38%)	26,30,33	1.30	3 (11%)
1	CFZ	A	323	1	18,21,22	2.50	7 (38%)	26,30,33	1.35	2 (7%)
1	CFZ	B	370	1	18,21,22	2.50	7 (38%)	26,30,33	1.26	3 (11%)
1	CFZ	A	28	1	18,21,22	2.49	7 (38%)	26,30,33	1.32	4 (15%)
1	UFT	B	687	1	18,21,22	2.60	9 (50%)	26,30,33	1.91	8 (30%)
1	UFT	A	141	1	18,21,22	2.59	9 (50%)	26,30,33	1.96	7 (26%)
1	CFZ	A	315	1	18,21,22	2.52	7 (38%)	26,30,33	1.30	2 (7%)
1	CFZ	B	39	1	18,21,22	2.56	7 (38%)	26,30,33	1.17	3 (11%)
1	CFZ	B	72	1	18,21,22	2.50	7 (38%)	26,30,33	1.22	2 (7%)
1	UFT	B	361	1	18,21,22	2.61	9 (50%)	26,30,33	2.10	7 (26%)
1	UFT	A	673	1	18,21,22	2.60	10 (55%)	26,30,33	2.05	6 (23%)
1	CFZ	A	140	1	18,21,22	2.47	7 (38%)	26,30,33	1.29	2 (7%)
1	CFZ	A	494	1	18,21,22	2.49	7 (38%)	26,30,33	1.29	3 (11%)
1	CFZ	A	131	1	18,21,22	2.50	7 (38%)	26,30,33	1.21	3 (11%)
1	UFT	A	302	1	18,21,22	2.62	9 (50%)	26,30,33	1.94	8 (30%)
1	UFT	B	466	1	18,21,22	2.58	10 (55%)	26,30,33	2.04	8 (30%)
1	UFT	B	437	1	18,21,22	2.56	9 (50%)	26,30,33	1.97	7 (26%)
1	UFT	B	629	1	18,21,22	2.60	9 (50%)	26,30,33	1.85	7 (26%)
1	UFT	A	621	1	18,21,22	2.57	9 (50%)	26,30,33	2.09	8 (30%)
1	CFZ	B	354	1	18,21,22	2.49	7 (38%)	26,30,33	1.35	3 (11%)
1	UFT	B	544	1	18,21,22	2.57	10 (55%)	26,30,33	2.00	6 (23%)
1	UFT	A	313	1	18,21,22	2.63	9 (50%)	26,30,33	1.85	6 (23%)
1	CFZ	A	76	1	18,21,22	2.49	7 (38%)	26,30,33	1.21	3 (11%)
1	UFT	A	350	1	18,21,22	2.62	9 (50%)	26,30,33	1.89	7 (26%)
1	CFZ	A	425	1	18,21,22	2.53	7 (38%)	26,30,33	1.21	3 (11%)
1	CFZ	B	120	1	18,21,22	2.53	7 (38%)	26,30,33	1.23	3 (11%)
1	CFZ	A	67	1	18,21,22	2.52	7 (38%)	26,30,33	1.19	3 (11%)
1	UFT	A	359	1	18,21,22	2.65	9 (50%)	26,30,33	1.93	8 (30%)
1	CFZ	A	335	1	18,21,22	2.49	7 (38%)	26,30,33	1.36	2 (7%)
1	UFT	A	549	1	18,21,22	2.61	10 (55%)	26,30,33	1.90	6 (23%)
1	CFZ	A	652	1	18,21,22	2.50	7 (38%)	26,30,33	1.23	3 (11%)
1	CFZ	A	657	1	18,21,22	2.43	7 (38%)	26,30,33	1.27	3 (11%)
1	CFZ	A	451	1	18,21,22	2.49	7 (38%)	26,30,33	1.28	3 (11%)
1	CFZ	B	130	1	18,21,22	2.50	7 (38%)	26,30,33	1.23	2 (7%)
1	CFZ	A	151	1	18,21,22	2.51	7 (38%)	26,30,33	1.25	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	UFT	A	97	1	18,21,22	2.59	9 (50%)	26,30,33	1.90	7 (26%)
1	CFZ	A	57	1	18,21,22	2.50	7 (38%)	26,30,33	1.14	3 (11%)
1	CFZ	B	438	1	18,21,22	2.48	7 (38%)	26,30,33	1.45	4 (15%)
1	CFZ	B	492	1	18,21,22	2.52	8 (44%)	26,30,33	1.14	2 (7%)
1	UFT	B	581	1	18,21,22	2.59	9 (50%)	26,30,33	1.97	7 (26%)
1	CFZ	A	579	1	18,21,22	2.50	7 (38%)	26,30,33	1.22	3 (11%)
1	UFT	A	719	1	18,21,22	2.58	10 (55%)	26,30,33	2.10	6 (23%)
1	CFZ	A	693	1	18,21,22	2.51	7 (38%)	26,30,33	1.19	2 (7%)
1	CFZ	A	583	1	18,21,22	2.47	7 (38%)	26,30,33	1.48	4 (15%)
1	CFZ	A	338	1	18,21,22	2.50	7 (38%)	26,30,33	1.41	2 (7%)
1	CFZ	A	585	1	18,21,22	2.51	7 (38%)	26,30,33	1.24	3 (11%)
1	UFT	B	669	1	18,21,22	2.61	9 (50%)	26,30,33	1.87	7 (26%)
1	UFT	A	112	1	18,21,22	2.59	10 (55%)	26,30,33	1.89	8 (30%)
1	CFZ	B	117	1	18,21,22	2.46	7 (38%)	26,30,33	1.50	4 (15%)
1	UFT	B	179	1	18,21,22	2.64	9 (50%)	26,30,33	1.88	6 (23%)
1	CFZ	A	370	1	18,21,22	2.51	7 (38%)	26,30,33	1.26	3 (11%)
1	CFZ	A	285	1	18,21,22	2.52	7 (38%)	26,30,33	1.13	3 (11%)
1	UFT	B	689	1	18,21,22	2.59	9 (50%)	26,30,33	1.96	7 (26%)
1	CFZ	B	338	1	18,21,22	2.47	7 (38%)	26,30,33	1.46	2 (7%)
1	CFZ	B	279	1	18,21,22	2.51	7 (38%)	26,30,33	1.15	2 (7%)
1	UFT	B	666	1	18,21,22	2.58	10 (55%)	26,30,33	1.95	8 (30%)
1	CFZ	A	171	1	18,21,22	2.47	7 (38%)	26,30,33	1.50	4 (15%)
1	UFT	B	174	1	18,21,22	2.59	9 (50%)	26,30,33	2.02	6 (23%)
1	CFZ	A	282	1	18,21,22	2.49	7 (38%)	26,30,33	1.40	3 (11%)
1	UFT	A	260	1	18,21,22	2.63	9 (50%)	26,30,33	1.85	6 (23%)
1	CFZ	A	528	1	18,21,22	2.54	7 (38%)	26,30,33	1.20	3 (11%)
1	CFZ	A	637	1	18,21,22	2.47	7 (38%)	26,30,33	1.49	4 (15%)
1	UFT	B	169	1	18,21,22	2.57	9 (50%)	26,30,33	2.01	8 (30%)
1	CFZ	A	625	1	18,21,22	2.50	7 (38%)	26,30,33	1.33	3 (11%)
1	UFT	A	608	1	18,21,22	2.57	9 (50%)	26,30,33	1.98	8 (30%)
1	CFZ	A	655	1	18,21,22	2.51	7 (38%)	26,30,33	1.47	3 (11%)
1	CFZ	B	600	1	18,21,22	2.52	7 (38%)	26,30,33	1.19	3 (11%)
1	CFZ	B	140	1	18,21,22	2.46	7 (38%)	26,30,33	1.29	2 (7%)
1	CFZ	B	131	1	18,21,22	2.50	7 (38%)	26,30,33	1.21	3 (11%)
1	UFT	B	377	1	18,21,22	2.61	9 (50%)	26,30,33	1.96	7 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CFZ	A	517	1	18,21,22	2.48	7 (38%)	26,30,33	1.55	3 (11%)
1	CFZ	A	63	1	18,21,22	2.46	7 (38%)	26,30,33	1.49	4 (15%)
1	UFT	B	197	1	18,21,22	2.57	10 (55%)	26,30,33	2.00	8 (30%)
1	UFT	B	135	1	18,21,22	2.62	9 (50%)	26,30,33	1.90	6 (23%)
1	UFT	A	500	1	18,21,22	2.57	10 (55%)	26,30,33	2.02	8 (30%)
1	UFT	B	74	1	18,21,22	2.56	9 (50%)	26,30,33	2.06	8 (30%)
1	CFZ	B	426	1	18,21,22	2.51	7 (38%)	26,30,33	1.26	3 (11%)
1	CFZ	A	418	1	18,21,22	2.47	7 (38%)	26,30,33	1.29	3 (11%)
1	CFZ	B	316	1	18,21,22	2.51	7 (38%)	26,30,33	1.15	2 (7%)
1	CFZ	A	492	1	18,21,22	2.49	7 (38%)	26,30,33	1.39	3 (11%)
1	UFT	A	653	1	18,21,22	2.60	9 (50%)	26,30,33	1.93	8 (30%)
1	UFT	B	389	1	18,21,22	2.62	9 (50%)	26,30,33	1.87	6 (23%)
1	CFZ	A	156	1	18,21,22	2.52	7 (38%)	26,30,33	1.27	3 (11%)
1	CFZ	A	498	1	18,21,22	2.48	7 (38%)	26,30,33	1.25	2 (7%)
1	CFZ	B	399	1	18,21,22	2.50	7 (38%)	26,30,33	1.30	3 (11%)
1	CFZ	A	667	1	18,21,22	2.49	7 (38%)	26,30,33	1.30	3 (11%)
1	UFT	B	423	1	18,21,22	2.62	10 (55%)	26,30,33	1.92	7 (26%)
1	UFT	B	606	1	18,21,22	2.55	10 (55%)	26,30,33	2.08	8 (30%)
1	UFT	B	633	1	18,21,22	2.60	10 (55%)	26,30,33	1.89	7 (26%)
1	CFZ	A	473	1	18,21,22	2.48	7 (38%)	26,30,33	1.25	3 (11%)
1	UFT	A	703	1	18,21,22	2.62	9 (50%)	26,30,33	1.84	5 (19%)
1	UFT	B	398	1	18,21,22	2.60	10 (55%)	26,30,33	1.94	8 (30%)
1	CFZ	A	459	1	18,21,22	2.47	7 (38%)	26,30,33	1.33	3 (11%)
1	CFZ	B	585	1	18,21,22	2.51	7 (38%)	26,30,33	1.22	3 (11%)
1	UFT	A	554	1	18,21,22	2.59	10 (55%)	26,30,33	1.95	8 (30%)
1	UFT	A	434	1	18,21,22	2.57	9 (50%)	26,30,33	1.99	8 (30%)
1	CFZ	A	49	1	18,21,22	2.50	7 (38%)	26,30,33	1.21	3 (11%)
1	CFZ	B	325	1	18,21,22	2.50	7 (38%)	26,30,33	1.27	3 (11%)
1	CFZ	B	511	1	18,21,22	2.52	7 (38%)	26,30,33	1.20	2 (7%)
1	UFT	A	105	1	18,21,22	2.58	9 (50%)	26,30,33	1.96	7 (26%)
1	CFZ	A	351	1	18,21,22	2.48	7 (38%)	26,30,33	1.19	3 (11%)
1	UFT	B	108	1	18,21,22	2.65	9 (50%)	26,30,33	1.81	5 (19%)
1	UFT	B	421	1	18,21,22	2.62	9 (50%)	26,30,33	1.89	7 (26%)
1	UFT	A	687	1	18,21,22	2.60	9 (50%)	26,30,33	1.90	8 (30%)
1	CFZ	A	444	1	18,21,22	2.47	7 (38%)	26,30,33	1.44	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	UFT	A	629	1	18,21,22	2.61	9 (50%)	26,30,33	1.85	7 (26%)
1	UFT	A	447	1	18,21,22	2.61	9 (50%)	26,30,33	1.87	7 (26%)
1	UFT	B	214	1	18,21,22	2.60	9 (50%)	26,30,33	1.91	8 (30%)
1	UFT	B	464	1	18,21,22	2.63	9 (50%)	26,30,33	1.92	7 (26%)
1	UFT	B	352	1	18,21,22	2.63	9 (50%)	26,30,33	1.92	7 (26%)
1	CFZ	B	407	1	18,21,22	2.49	7 (38%)	26,30,33	1.23	3 (11%)
1	CFZ	B	315	1	18,21,22	2.50	7 (38%)	26,30,33	1.32	2 (7%)
1	UFT	A	402	1	18,21,22	2.60	10 (55%)	26,30,33	1.90	7 (26%)
1	CFZ	A	130	1	18,21,22	2.51	7 (38%)	26,30,33	1.23	2 (7%)
1	CFZ	B	491	1	18,21,22	2.55	7 (38%)	26,30,33	1.16	4 (15%)
1	UFT	B	266	1	18,21,22	2.59	10 (55%)	26,30,33	1.96	8 (30%)
1	CFZ	A	15	1	18,21,22	2.45	7 (38%)	26,30,33	1.38	3 (11%)
1	UFT	B	673	1	18,21,22	2.59	9 (50%)	26,30,33	2.06	6 (23%)
1	CFZ	A	446	1	18,21,22	2.50	7 (38%)	26,30,33	1.43	3 (11%)
1	CFZ	B	424	1	18,21,22	2.51	7 (38%)	26,30,33	1.28	3 (11%)
1	UFT	A	503	1	18,21,22	2.58	10 (55%)	26,30,33	2.00	7 (26%)
1	CFZ	B	592	1	18,21,22	2.47	7 (38%)	26,30,33	1.27	2 (7%)
1	CFZ	B	512	1	18,21,22	2.52	7 (38%)	26,30,33	1.12	1 (3%)
1	CFZ	B	209	1	18,21,22	2.52	7 (38%)	26,30,33	1.16	2 (7%)
1	UFT	A	208	1	18,21,22	2.62	9 (50%)	26,30,33	1.89	8 (30%)
1	CFZ	A	440	1	18,21,22	2.47	7 (38%)	26,30,33	1.44	3 (11%)
1	UFT	B	43	1	18,21,22	2.62	9 (50%)	26,30,33	2.12	9 (34%)
1	UFT	B	32	1	18,21,22	2.61	9 (50%)	26,30,33	1.92	7 (26%)
1	UFT	B	703	1	18,21,22	2.62	9 (50%)	26,30,33	1.81	5 (19%)
1	UFT	B	33	1	18,21,22	2.62	9 (50%)	26,30,33	1.87	6 (23%)
1	CFZ	A	232	1	18,21,22	2.49	7 (38%)	26,30,33	1.28	4 (15%)
1	CFZ	A	234	1	18,21,22	2.48	7 (38%)	26,30,33	1.37	3 (11%)
1	UFT	A	32	1	18,21,22	2.60	11 (61%)	26,30,33	1.93	8 (30%)
1	CFZ	B	459	1	18,21,22	2.48	7 (38%)	26,30,33	1.33	3 (11%)
1	UFT	A	676	1	18,21,22	2.64	9 (50%)	26,30,33	1.94	7 (26%)
1	UFT	A	712	1	18,21,22	2.62	9 (50%)	26,30,33	1.87	7 (26%)
1	UFT	A	108	1	18,21,22	2.65	9 (50%)	26,30,33	1.81	5 (19%)
1	UFT	A	646	1	18,21,22	2.60	9 (50%)	26,30,33	1.99	6 (23%)
1	UFT	B	430	1	18,21,22	2.58	9 (50%)	26,30,33	1.98	7 (26%)
1	CFZ	B	129	1	18,21,22	2.53	7 (38%)	26,30,33	1.10	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CFZ	B	247	1	18,21,22	2.52	7 (38%)	26,30,33	1.15	2 (7%)
1	UFT	A	344	1	18,21,22	2.60	10 (55%)	26,30,33	1.98	7 (26%)
1	UFT	A	19	1	18,21,22	2.60	10 (55%)	26,30,33	1.95	8 (30%)
1	UFT	A	50	1	18,21,22	2.63	9 (50%)	26,30,33	1.86	6 (23%)
1	CFZ	B	378	1	18,21,22	2.50	7 (38%)	26,30,33	1.25	3 (11%)
1	UFT	B	471	1	18,21,22	2.60	9 (50%)	26,30,33	1.84	6 (23%)
1	UFT	B	481	1	18,21,22	2.58	9 (50%)	26,30,33	1.92	7 (26%)
1	CFZ	A	384	1	18,21,22	2.50	7 (38%)	26,30,33	1.32	3 (11%)
1	UFT	A	684	1	18,21,22	2.63	9 (50%)	26,30,33	1.82	6 (23%)
1	UFT	A	659	1	18,21,22	2.63	9 (50%)	26,30,33	1.85	7 (26%)
1	CFZ	A	241	1	18,21,22	2.47	7 (38%)	26,30,33	1.57	4 (15%)
1	CFZ	B	321	1	18,21,22	2.45	7 (38%)	26,30,33	1.43	3 (11%)
1	CFZ	A	568	1	18,21,22	2.53	7 (38%)	26,30,33	1.21	3 (11%)
1	CFZ	B	631	1	18,21,22	2.51	7 (38%)	26,30,33	1.35	3 (11%)
1	UFT	B	542	1	18,21,22	2.59	10 (55%)	26,30,33	1.93	7 (26%)
1	CFZ	A	321	1	18,21,22	2.49	7 (38%)	26,30,33	1.22	3 (11%)
1	CFZ	A	587	1	18,21,22	2.51	7 (38%)	26,30,33	1.18	3 (11%)
1	UFT	A	217	1	18,21,22	2.62	9 (50%)	26,30,33	1.89	7 (26%)
1	CFZ	B	568	1	18,21,22	2.52	7 (38%)	26,30,33	1.20	3 (11%)
1	UFT	A	398	1	18,21,22	2.59	10 (55%)	26,30,33	1.94	8 (30%)
1	CFZ	B	234	1	18,21,22	2.48	7 (38%)	26,30,33	1.31	3 (11%)
1	UFT	B	190	1	18,21,22	2.58	9 (50%)	26,30,33	2.00	8 (30%)
1	CFZ	B	536	1	18,21,22	2.47	7 (38%)	26,30,33	1.50	3 (11%)
1	CFZ	A	647	1	18,21,22	2.52	7 (38%)	26,30,33	1.21	3 (11%)
1	CFZ	B	639	1	18,21,22	2.49	7 (38%)	26,30,33	1.28	3 (11%)
1	CFZ	B	587	1	18,21,22	2.51	7 (38%)	26,30,33	1.17	3 (11%)
1	CFZ	A	73	1	18,21,22	2.51	7 (38%)	26,30,33	1.17	2 (7%)
1	UFT	B	359	1	18,21,22	2.60	10 (55%)	26,30,33	1.93	8 (30%)
1	UFT	B	283	1	18,21,22	2.62	9 (50%)	26,30,33	1.88	6 (23%)
1	UFT	B	366	1	18,21,22	2.57	9 (50%)	26,30,33	1.96	7 (26%)
1	CFZ	A	426	1	18,21,22	2.51	7 (38%)	26,30,33	1.27	3 (11%)
1	UFT	B	534	1	18,21,22	2.61	10 (55%)	26,30,33	1.88	7 (26%)
1	CFZ	B	657	1	18,21,22	2.42	7 (38%)	26,30,33	1.26	3 (11%)
1	UFT	B	55	1	18,21,22	2.60	9 (50%)	26,30,33	1.90	7 (26%)
1	UFT	A	192	1	18,21,22	2.62	10 (55%)	26,30,33	1.87	7 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CFZ	A	120	1	18,21,22	2.52	7 (38%)	26,30,33	1.22	3 (11%)
1	CFZ	B	124	1	18,21,22	2.51	7 (38%)	26,30,33	1.15	3 (11%)
1	CFZ	A	682	1	18,21,22	2.51	7 (38%)	26,30,33	1.21	2 (7%)
1	CFZ	B	383	1	18,21,22	2.48	7 (38%)	26,30,33	1.17	2 (7%)
1	UFT	A	618	1	18,21,22	2.57	9 (50%)	26,30,33	2.03	8 (30%)
1	UFT	A	666	1	18,21,22	2.58	9 (50%)	26,30,33	1.96	8 (30%)
1	CFZ	B	579	1	18,21,22	2.51	7 (38%)	26,30,33	1.22	3 (11%)
1	UFT	A	293	1	18,21,22	2.62	9 (50%)	26,30,33	1.85	6 (23%)
1	CFZ	B	441	1	18,21,22	2.53	7 (38%)	26,30,33	1.29	3 (11%)
1	CFZ	A	328	1	18,21,22	2.48	7 (38%)	26,30,33	1.46	2 (7%)
1	UFT	A	628	1	18,21,22	2.58	10 (55%)	26,30,33	1.98	7 (26%)
1	UFT	A	137	1	18,21,22	2.60	10 (55%)	26,30,33	1.91	8 (30%)
1	UFT	B	98	1	18,21,22	2.61	10 (55%)	26,30,33	1.94	8 (30%)
1	UFT	B	301	1	18,21,22	2.57	10 (55%)	26,30,33	1.99	8 (30%)
1	UFT	A	485	1	18,21,22	2.60	10 (55%)	26,30,33	1.94	6 (23%)
1	CFZ	B	548	1	18,21,22	2.50	7 (38%)	26,30,33	1.29	3 (11%)
1	CFZ	A	399	1	18,21,22	2.50	7 (38%)	26,30,33	1.31	3 (11%)
1	CFZ	B	332	1	18,21,22	2.49	7 (38%)	26,30,33	1.31	3 (11%)
1	UFT	B	530	1	18,21,22	2.59	9 (50%)	26,30,33	1.97	7 (26%)
1	UFT	B	656	1	18,21,22	2.58	10 (55%)	26,30,33	1.99	7 (26%)
1	UFT	B	48	1	18,21,22	2.59	10 (55%)	26,30,33	2.01	6 (23%)
1	UFT	A	44	1	18,21,22	2.63	9 (50%)	26,30,33	1.87	7 (26%)
1	CFZ	B	282	1	18,21,22	2.50	7 (38%)	26,30,33	1.38	3 (11%)
1	UFT	B	296	1	18,21,22	2.58	10 (55%)	26,30,33	1.97	8 (30%)
1	UFT	A	89	1	18,21,22	2.57	9 (50%)	26,30,33	2.04	8 (30%)
1	UFT	A	544	1	18,21,22	2.57	9 (50%)	26,30,33	2.00	6 (23%)
1	UFT	A	11	1	18,21,22	2.60	10 (55%)	26,30,33	1.86	8 (30%)
1	UFT	B	593	1	18,21,22	2.54	9 (50%)	26,30,33	1.93	8 (30%)
1	UFT	A	352	1	18,21,22	2.57	9 (50%)	26,30,33	2.00	8 (30%)
1	UFT	B	712	1	18,21,22	2.61	10 (55%)	26,30,33	1.84	6 (23%)
1	CFZ	A	46	1	18,21,22	2.52	7 (38%)	26,30,33	1.15	2 (7%)
1	UFT	A	432	1	18,21,22	2.61	10 (55%)	26,30,33	1.85	5 (19%)
1	CFZ	A	565	1	18,21,22	2.53	7 (38%)	26,30,33	1.10	3 (11%)
1	CFZ	B	655	1	18,21,22	2.51	7 (38%)	26,30,33	1.46	3 (11%)
1	UFT	A	365	1	18,21,22	2.63	9 (50%)	26,30,33	1.87	6 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CFZ	A	304	1	18,21,22	2.52	7 (38%)	26,30,33	1.14	3 (11%)
1	UFT	A	431	1	18,21,22	2.59	10 (55%)	26,30,33	2.02	8 (30%)
1	CFZ	A	124	1	18,21,22	2.51	7 (38%)	26,30,33	1.15	3 (11%)
1	CFZ	B	79	1	18,21,22	2.49	7 (38%)	26,30,33	1.35	3 (11%)
1	UFT	B	200	1	18,21,22	2.56	10 (55%)	26,30,33	2.01	7 (26%)
1	CFZ	B	198	1	18,21,22	2.49	7 (38%)	26,30,33	1.27	3 (11%)
1	UFT	A	43	1	18,21,22	2.62	9 (50%)	26,30,33	2.10	9 (34%)
1	CFZ	A	474	1	18,21,22	2.51	7 (38%)	26,30,33	1.25	3 (11%)
1	CFZ	B	75	1	18,21,22	2.49	7 (38%)	26,30,33	1.39	2 (7%)
1	UFT	B	347	1	18,21,22	2.58	9 (50%)	26,30,33	1.99	6 (23%)
1	UFT	A	182	1	18,21,22	2.56	9 (50%)	26,30,33	2.05	7 (26%)
1	UFT	B	653	1	18,21,22	2.57	9 (50%)	26,30,33	1.95	8 (30%)
1	UFT	B	367	1	18,21,22	2.62	9 (50%)	26,30,33	1.85	6 (23%)
1	UFT	B	590	1	18,21,22	2.60	9 (50%)	26,30,33	2.00	6 (23%)
1	UFT	B	251	1	18,21,22	2.62	10 (55%)	26,30,33	1.88	8 (30%)
1	UFT	A	175	1	18,21,22	2.60	9 (50%)	26,30,33	1.91	7 (26%)
1	UFT	B	322	1	18,21,22	2.61	9 (50%)	26,30,33	1.88	7 (26%)
1	CFZ	B	26	1	18,21,22	2.45	7 (38%)	26,30,33	1.33	3 (11%)
1	UFT	A	334	1	18,21,22	2.58	9 (50%)	26,30,33	2.01	7 (26%)
1	CFZ	A	691	1	18,21,22	2.48	7 (38%)	26,30,33	1.30	3 (11%)
1	UFT	B	493	1	18,21,22	2.66	9 (50%)	26,30,33	1.83	7 (26%)
1	CFZ	A	210	1	18,21,22	2.48	7 (38%)	26,30,33	1.37	3 (11%)
1	CFZ	A	184	1	18,21,22	2.52	7 (38%)	26,30,33	1.18	2 (7%)
1	UFT	A	456	1	18,21,22	2.62	9 (50%)	26,30,33	1.85	5 (19%)
1	CFZ	B	49	1	18,21,22	2.53	7 (38%)	26,30,33	1.16	4 (15%)
1	CFZ	A	436	1	18,21,22	2.52	7 (38%)	26,30,33	1.22	2 (7%)
1	UFT	B	577	1	18,21,22	2.61	10 (55%)	26,30,33	1.87	6 (23%)
1	CFZ	A	411	1	18,21,22	2.50	7 (38%)	26,30,33	1.20	3 (11%)
1	UFT	B	708	1	18,21,22	2.61	9 (50%)	26,30,33	1.88	7 (26%)
1	UFT	B	196	1	18,21,22	2.59	9 (50%)	26,30,33	2.01	8 (30%)
1	UFT	A	696	1	18,21,22	2.58	9 (50%)	26,30,33	1.96	8 (30%)
1	UFT	A	472	1	18,21,22	2.58	9 (50%)	26,30,33	2.02	6 (23%)
1	CFZ	A	279	1	18,21,22	2.53	7 (38%)	26,30,33	1.15	2 (7%)
1	UFT	A	116	1	18,21,22	2.58	9 (50%)	26,30,33	2.07	8 (30%)
1	UFT	B	115	1	18,21,22	2.58	9 (50%)	26,30,33	2.00	8 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CFZ	A	242	1	18,21,22	2.51	7 (38%)	26,30,33	1.29	3 (11%)
1	UFT	B	336	1	18,21,22	2.59	10 (55%)	26,30,33	1.98	8 (30%)
1	CFZ	A	556	1	18,21,22	2.48	7 (38%)	26,30,33	1.20	2 (7%)
1	UFT	B	86	1	18,21,22	2.60	10 (55%)	26,30,33	1.90	8 (30%)
1	UFT	A	336	1	18,21,22	2.58	9 (50%)	26,30,33	1.97	8 (30%)
1	CFZ	A	382	1	18,21,22	2.47	7 (38%)	26,30,33	1.38	2 (7%)
1	CFZ	B	171	1	18,21,22	2.46	7 (38%)	26,30,33	1.50	4 (15%)
1	UFT	B	502	1	18,21,22	2.60	10 (55%)	26,30,33	2.00	6 (23%)
1	UFT	B	545	1	18,21,22	2.61	9 (50%)	26,30,33	1.91	7 (26%)
1	UFT	B	163	1	18,21,22	2.61	9 (50%)	26,30,33	1.90	8 (30%)
1	CFZ	A	698	1	18,21,22	2.52	7 (38%)	26,30,33	1.18	3 (11%)
1	UFT	A	59	1	18,21,22	2.60	10 (55%)	26,30,33	1.92	7 (26%)
1	UFT	A	170	1	18,21,22	2.57	9 (50%)	26,30,33	2.11	8 (30%)
1	UFT	A	283	1	18,21,22	2.62	9 (50%)	26,30,33	1.89	6 (23%)
1	UFT	B	89	1	18,21,22	2.57	10 (55%)	26,30,33	2.04	8 (30%)
1	UFT	B	432	1	18,21,22	2.61	9 (50%)	26,30,33	1.87	5 (19%)
1	UFT	A	270	1	18,21,22	2.57	10 (55%)	26,30,33	2.03	7 (26%)
1	UFT	A	197	1	18,21,22	2.58	9 (50%)	26,30,33	2.00	8 (30%)
1	CFZ	B	63	1	18,21,22	2.47	7 (38%)	26,30,33	1.49	4 (15%)
1	CFZ	B	15	1	18,21,22	2.44	7 (38%)	26,30,33	1.39	3 (11%)
1	UFT	B	62	1	18,21,22	2.58	9 (50%)	26,30,33	2.05	8 (30%)
1	CFZ	B	212	1	18,21,22	2.49	7 (38%)	26,30,33	1.33	3 (11%)
1	CFZ	B	360	1	18,21,22	2.46	7 (38%)	26,30,33	1.40	3 (11%)
1	UFT	A	606	1	18,21,22	2.57	10 (55%)	26,30,33	2.07	7 (26%)
1	CFZ	A	188	1	18,21,22	2.52	7 (38%)	26,30,33	1.18	3 (11%)
1	CFZ	B	363	1	18,21,22	2.52	7 (38%)	26,30,33	1.11	2 (7%)
1	CFZ	A	212	1	18,21,22	2.48	7 (38%)	26,30,33	1.32	4 (15%)
1	CFZ	B	425	1	18,21,22	2.52	7 (38%)	26,30,33	1.22	3 (11%)
1	CFZ	B	351	1	18,21,22	2.51	7 (38%)	26,30,33	1.19	3 (11%)
1	UFT	B	97	1	18,21,22	2.60	9 (50%)	26,30,33	1.92	7 (26%)
1	UFT	B	265	1	18,21,22	2.61	9 (50%)	26,30,33	1.95	7 (26%)
1	UFT	A	656	1	18,21,22	2.57	9 (50%)	26,30,33	1.96	7 (26%)
1	CFZ	A	218	1	18,21,22	2.47	7 (38%)	26,30,33	1.28	2 (7%)
1	UFT	B	646	1	18,21,22	2.61	9 (50%)	26,30,33	1.98	6 (23%)
1	CFZ	B	34	1	18,21,22	2.48	7 (38%)	26,30,33	1.32	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CFZ	A	381	1	18,21,22	2.51	7 (38%)	26,30,33	1.31	2 (7%)
1	UFT	B	434	1	18,21,22	2.58	10 (55%)	26,30,33	2.01	8 (30%)
1	UFT	A	602	1	18,21,22	2.61	10 (55%)	26,30,33	1.88	7 (26%)
1	CFZ	B	693	1	18,21,22	2.51	7 (38%)	26,30,33	1.18	2 (7%)
1	CFZ	B	355	1	18,21,22	2.52	7 (38%)	26,30,33	1.17	4 (15%)
1	CFZ	B	405	1	18,21,22	2.50	7 (38%)	26,30,33	1.30	3 (11%)
1	UFT	A	60	1	18,21,22	2.55	9 (50%)	26,30,33	1.98	7 (26%)
1	UFT	A	464	1	18,21,22	2.63	9 (50%)	26,30,33	1.91	7 (26%)
1	CFZ	B	384	1	18,21,22	2.47	7 (38%)	26,30,33	1.41	2 (7%)
1	UFT	A	13	1	18,21,22	2.55	9 (50%)	26,30,33	2.04	7 (26%)
1	CFZ	A	268	1	18,21,22	2.48	7 (38%)	26,30,33	1.49	2 (7%)
1	UFT	B	329	1	18,21,22	2.60	10 (55%)	26,30,33	1.88	8 (30%)
1	CFZ	B	373	1	18,21,22	2.49	7 (38%)	26,30,33	1.24	3 (11%)
1	CFZ	A	72	1	18,21,22	2.50	7 (38%)	26,30,33	1.26	3 (11%)
1	CFZ	B	206	1	18,21,22	2.51	7 (38%)	26,30,33	1.26	3 (11%)
1	CFZ	A	506	1	18,21,22	2.50	7 (38%)	26,30,33	1.33	3 (11%)
1	UFT	B	582	1	18,21,22	2.58	9 (50%)	26,30,33	1.98	8 (30%)
1	UFT	B	233	1	18,21,22	2.63	10 (55%)	26,30,33	1.81	6 (23%)
1	CFZ	B	232	1	18,21,22	2.46	7 (38%)	26,30,33	1.37	4 (15%)
1	CFZ	A	149	1	18,21,22	2.50	7 (38%)	26,30,33	1.21	3 (11%)
1	UFT	A	61	1	18,21,22	2.58	9 (50%)	26,30,33	2.02	8 (30%)
1	CFZ	B	165	1	18,21,22	2.51	7 (38%)	26,30,33	1.15	2 (7%)
1	UFT	A	389	1	18,21,22	2.64	9 (50%)	26,30,33	1.85	7 (26%)
1	CFZ	A	354	1	18,21,22	2.46	7 (38%)	26,30,33	1.20	2 (7%)
1	UFT	A	266	1	18,21,22	2.61	10 (55%)	26,30,33	1.96	7 (26%)
1	UFT	A	499	1	18,21,22	2.61	9 (50%)	26,30,33	1.90	7 (26%)
1	CFZ	B	103	1	18,21,22	2.50	7 (38%)	26,30,33	1.32	3 (11%)
1	CFZ	A	104	1	18,21,22	2.53	7 (38%)	26,30,33	1.18	3 (11%)
1	CFZ	B	682	1	18,21,22	2.53	7 (38%)	26,30,33	1.20	2 (7%)
1	UFT	A	571	1	18,21,22	2.61	10 (55%)	26,30,33	1.94	7 (26%)
1	UFT	B	88	1	18,21,22	2.59	10 (55%)	26,30,33	1.94	8 (30%)
1	UFT	B	609	1	18,21,22	2.57	10 (55%)	26,30,33	2.07	8 (30%)
1	CFZ	A	651	1	18,21,22	2.49	7 (38%)	26,30,33	1.28	3 (11%)
1	UFT	A	361	1	18,21,22	2.59	9 (50%)	26,30,33	1.93	7 (26%)
1	CFZ	B	465	1	18,21,22	2.48	7 (38%)	26,30,33	1.30	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	UFT	B	69	1	18,21,22	2.57	9 (50%)	26,30,33	2.01	7 (26%)
1	UFT	B	676	1	18,21,22	2.63	9 (50%)	26,30,33	1.93	7 (26%)
1	UFT	A	154	1	18,21,22	2.59	9 (50%)	26,30,33	1.99	6 (23%)
1	CFZ	A	26	1	18,21,22	2.48	7 (38%)	26,30,33	1.29	3 (11%)
1	CFZ	A	491	1	18,21,22	2.50	7 (38%)	26,30,33	1.29	3 (11%)
1	CFZ	A	610	1	18,21,22	2.47	7 (38%)	26,30,33	1.45	4 (15%)
1	CFZ	B	323	1	18,21,22	2.51	7 (38%)	26,30,33	1.22	3 (11%)
1	CFZ	B	201	1	18,21,22	2.49	7 (38%)	26,30,33	1.29	3 (11%)
1	UFT	B	513	1	18,21,22	2.66	9 (50%)	26,30,33	1.79	6 (23%)
1	UFT	A	577	1	18,21,22	2.60	10 (55%)	26,30,33	1.88	7 (26%)
1	UFT	B	659	1	18,21,22	2.63	9 (50%)	26,30,33	1.86	7 (26%)
1	UFT	A	305	1	18,21,22	2.55	9 (50%)	26,30,33	1.95	6 (23%)
1	UFT	A	466	1	18,21,22	2.58	10 (55%)	26,30,33	2.04	7 (26%)
1	CFZ	B	111	1	18,21,22	2.49	7 (38%)	26,30,33	1.37	3 (11%)
1	CFZ	B	96	1	18,21,22	2.47	7 (38%)	26,30,33	1.40	3 (11%)
1	CFZ	A	39	1	18,21,22	2.56	7 (38%)	26,30,33	1.18	3 (11%)
1	CFZ	B	369	1	18,21,22	2.50	7 (38%)	26,30,33	1.31	3 (11%)
1	CFZ	A	512	1	18,21,22	2.50	7 (38%)	26,30,33	1.13	2 (7%)
1	CFZ	B	704	1	18,21,22	2.50	7 (38%)	26,30,33	1.27	3 (11%)
1	UFT	B	559	1	18,21,22	2.60	9 (50%)	26,30,33	1.96	7 (26%)
1	UFT	B	519	1	18,21,22	2.60	9 (50%)	26,30,33	1.99	8 (30%)
1	UFT	A	92	1	18,21,22	2.61	9 (50%)	26,30,33	1.85	7 (26%)
1	UFT	A	106	1	18,21,22	2.59	9 (50%)	26,30,33	1.99	7 (26%)
1	CFZ	B	304	1	18,21,22	2.51	7 (38%)	26,30,33	1.15	3 (11%)
1	CFZ	A	360	1	18,21,22	2.50	7 (38%)	26,30,33	1.28	3 (11%)
1	UFT	A	437	1	18,21,22	2.55	9 (50%)	26,30,33	1.97	7 (26%)
1	CFZ	B	469	1	18,21,22	2.47	7 (38%)	26,30,33	1.42	3 (11%)
1	CFZ	B	523	1	18,21,22	2.49	7 (38%)	26,30,33	1.20	2 (7%)
1	UFT	B	260	1	18,21,22	2.63	9 (50%)	26,30,33	1.85	6 (23%)
1	CFZ	A	558	1	18,21,22	2.51	7 (38%)	26,30,33	1.15	3 (11%)
1	CFZ	B	474	1	18,21,22	2.49	7 (38%)	26,30,33	1.25	3 (11%)
1	UFT	B	208	1	18,21,22	2.62	9 (50%)	26,30,33	1.88	6 (23%)
1	CFZ	B	46	1	18,21,22	2.53	7 (38%)	26,30,33	1.14	3 (11%)
1	UFT	B	608	1	18,21,22	2.56	10 (55%)	26,30,33	2.09	8 (30%)
1	CFZ	A	700	1	18,21,22	2.50	7 (38%)	26,30,33	1.28	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	UFT	B	192	1	18,21,22	2.62	10 (55%)	26,30,33	1.85	7 (26%)
1	UFT	A	69	1	18,21,22	2.57	10 (55%)	26,30,33	2.03	8 (30%)
1	CFZ	A	424	1	18,21,22	2.53	7 (38%)	26,30,33	1.28	3 (11%)
1	UFT	A	423	1	18,21,22	2.60	9 (50%)	26,30,33	1.92	7 (26%)
1	UFT	B	460	1	18,21,22	2.62	9 (50%)	26,30,33	1.85	7 (26%)
1	CFZ	B	517	1	18,21,22	2.51	7 (38%)	26,30,33	1.35	2 (7%)
1	CFZ	A	249	1	18,21,22	2.51	7 (38%)	26,30,33	1.17	3 (11%)
1	CFZ	A	406	1	18,21,22	2.52	7 (38%)	26,30,33	1.28	3 (11%)
1	CFZ	B	149	1	18,21,22	2.50	7 (38%)	26,30,33	1.22	3 (11%)
1	CFZ	B	528	1	18,21,22	2.52	7 (38%)	26,30,33	1.17	3 (11%)
1	CFZ	A	550	1	18,21,22	2.50	7 (38%)	26,30,33	1.21	2 (7%)
1	CFZ	B	353	1	18,21,22	2.47	7 (38%)	26,30,33	1.45	4 (15%)
1	CFZ	B	691	1	18,21,22	2.47	7 (38%)	26,30,33	1.30	3 (11%)
1	UFT	A	502	1	18,21,22	2.59	9 (50%)	26,30,33	1.99	6 (23%)
1	CFZ	B	550	1	18,21,22	2.52	7 (38%)	26,30,33	1.18	2 (7%)
1	UFT	B	216	1	18,21,22	2.65	9 (50%)	26,30,33	1.89	7 (26%)
1	CFZ	A	161	1	18,21,22	2.49	7 (38%)	26,30,33	1.31	3 (11%)
1	UFT	A	607	1	18,21,22	2.60	9 (50%)	26,30,33	1.90	8 (30%)
1	UFT	B	403	1	18,21,22	2.58	10 (55%)	26,30,33	1.98	8 (30%)
1	UFT	A	80	1	18,21,22	2.62	9 (50%)	26,30,33	1.85	7 (26%)
1	CFZ	A	362	1	18,21,22	2.46	7 (38%)	26,30,33	1.39	3 (11%)
1	CFZ	B	254	1	18,21,22	2.48	7 (38%)	26,30,33	1.21	3 (11%)
1	UFT	B	112	1	18,21,22	2.59	10 (55%)	26,30,33	1.91	8 (30%)
1	CFZ	A	34	1	18,21,22	2.51	7 (38%)	26,30,33	1.30	3 (11%)
1	CFZ	B	551	1	18,21,22	2.53	7 (38%)	26,30,33	1.12	2 (7%)
1	UFT	B	696	1	18,21,22	2.58	9 (50%)	26,30,33	1.96	8 (30%)
1	CFZ	B	473	1	18,21,22	2.46	7 (38%)	26,30,33	1.34	4 (15%)
1	CFZ	B	144	1	18,21,22	2.47	7 (38%)	26,30,33	1.52	3 (11%)
1	UFT	A	509	1	18,21,22	2.62	10 (55%)	26,30,33	1.93	7 (26%)
1	CFZ	A	477	1	18,21,22	2.51	7 (38%)	26,30,33	1.15	3 (11%)
1	UFT	A	534	1	18,21,22	2.62	10 (55%)	26,30,33	1.88	7 (26%)
1	UFT	A	535	1	18,21,22	2.65	9 (50%)	26,30,33	1.75	5 (19%)
1	UFT	B	8	1	18,21,22	2.63	9 (50%)	26,30,33	2.04	6 (23%)
1	UFT	B	101	1	18,21,22	2.58	10 (55%)	26,30,33	1.99	8 (30%)
1	CFZ	B	28	1	18,21,22	2.49	7 (38%)	26,30,33	1.95	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CFZ	A	574	1	18,21,22	2.49	7 (38%)	26,30,33	1.14	3 (11%)
1	UFT	B	160	1	18,21,22	2.57	10 (55%)	26,30,33	1.99	8 (30%)
1	CFZ	B	387	1	18,21,22	2.52	7 (38%)	26,30,33	1.11	1 (3%)
1	UFT	B	720	1	18,21,22	2.62	9 (50%)	26,30,33	1.79	4 (15%)
1	CFZ	A	209	1	18,21,22	2.52	7 (38%)	26,30,33	1.17	2 (7%)
1	UFT	A	708	1	18,21,22	2.59	9 (50%)	26,30,33	1.88	7 (26%)
1	CFZ	A	441	1	18,21,22	2.52	7 (38%)	26,30,33	1.17	3 (11%)
1	CFZ	B	188	1	18,21,22	2.51	7 (38%)	26,30,33	1.18	3 (11%)
1	CFZ	B	494	1	18,21,22	2.54	6 (33%)	26,30,33	1.27	2 (7%)
1	UFT	A	48	1	18,21,22	2.58	9 (50%)	26,30,33	2.02	6 (23%)
1	CFZ	A	219	1	18,21,22	2.52	7 (38%)	26,30,33	1.17	3 (11%)
1	CFZ	B	114	1	18,21,22	2.48	7 (38%)	26,30,33	1.45	4 (15%)
1	CFZ	B	73	1	18,21,22	2.51	7 (38%)	26,30,33	1.21	2 (7%)
1	UFT	A	590	1	18,21,22	2.56	9 (50%)	26,30,33	2.02	6 (23%)
1	CFZ	A	164	1	18,21,22	2.50	7 (38%)	26,30,33	1.22	3 (11%)
1	CFZ	B	574	1	18,21,22	2.51	7 (38%)	26,30,33	1.17	3 (11%)
1	CFZ	B	632	1	18,21,22	2.49	7 (38%)	26,30,33	1.25	2 (7%)
1	CFZ	A	139	1	18,21,22	2.50	7 (38%)	26,30,33	1.31	3 (11%)
1	UFT	A	519	1	18,21,22	2.51	9 (50%)	26,30,33	2.01	8 (30%)
1	CFZ	A	511	1	18,21,22	2.52	7 (38%)	26,30,33	1.20	2 (7%)
1	UFT	A	94	1	18,21,22	2.59	9 (50%)	26,30,33	2.00	7 (26%)
1	CFZ	A	620	1	18,21,22	2.49	7 (38%)	26,30,33	1.37	3 (11%)
1	UFT	A	720	1	18,21,22	2.59	9 (50%)	26,30,33	1.97	8 (30%)
1	CFZ	B	10	1	18,21,22	2.46	7 (38%)	26,30,33	1.28	2 (7%)
1	CFZ	A	129	1	18,21,22	2.53	7 (38%)	26,30,33	1.10	1 (3%)
1	UFT	A	421	1	18,21,22	2.61	10 (55%)	26,30,33	1.89	7 (26%)
1	CFZ	B	57	1	18,21,22	2.52	7 (38%)	26,30,33	1.16	3 (11%)
1	UFT	B	126	1	18,21,22	2.57	9 (50%)	26,30,33	2.01	7 (26%)
1	CFZ	B	440	1	18,21,22	2.50	7 (38%)	26,30,33	1.28	3 (11%)
1	UFT	B	13	1	18,21,22	2.58	9 (50%)	26,30,33	2.08	7 (26%)
1	CFZ	A	465	1	18,21,22	2.48	7 (38%)	26,30,33	1.30	2 (7%)
1	CFZ	B	298	1	18,21,22	2.53	7 (38%)	26,30,33	1.17	3 (11%)
1	UFT	A	460	1	18,21,22	2.61	9 (50%)	26,30,33	1.85	7 (26%)
1	CFZ	B	335	1	18,21,22	2.49	7 (38%)	26,30,33	1.36	2 (7%)
1	CFZ	B	620	1	18,21,22	2.48	7 (38%)	26,30,33	1.36	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CFZ	A	614	1	18,21,22	2.50	7 (38%)	26,30,33	1.20	3 (11%)
1	CFZ	B	679	1	18,21,22	2.49	7 (38%)	26,30,33	1.29	2 (7%)
1	UFT	B	358	1	18,21,22	2.64	9 (50%)	26,30,33	1.80	6 (23%)
1	UFT	A	135	1	18,21,22	2.63	9 (50%)	26,30,33	1.94	6 (23%)
1	UFT	B	14	1	18,21,22	2.60	9 (50%)	26,30,33	1.92	6 (23%)
1	UFT	A	126	1	18,21,22	2.58	9 (50%)	26,30,33	2.01	7 (26%)
1	UFT	B	270	1	18,21,22	2.57	10 (55%)	26,30,33	2.02	8 (30%)
1	UFT	B	217	1	18,21,22	2.61	10 (55%)	26,30,33	1.90	7 (26%)
1	UFT	B	499	1	18,21,22	2.62	9 (50%)	26,30,33	1.87	7 (26%)
1	UFT	B	500	1	18,21,22	2.56	10 (55%)	26,30,33	2.01	8 (30%)
1	CFZ	B	583	1	18,21,22	2.48	7 (38%)	26,30,33	1.48	4 (15%)
1	UFT	B	142	1	18,21,22	2.58	10 (55%)	26,30,33	1.99	8 (30%)
1	UFT	B	61	1	18,21,22	2.59	9 (50%)	26,30,33	2.01	8 (30%)
1	UFT	B	92	1	18,21,22	2.61	10 (55%)	26,30,33	1.87	7 (26%)
1	UFT	B	143	1	18,21,22	2.57	9 (50%)	26,30,33	2.10	8 (30%)
1	CFZ	B	652	1	18,21,22	2.50	7 (38%)	26,30,33	1.22	3 (11%)
1	UFT	B	215	1	18,21,22	2.58	10 (55%)	26,30,33	1.97	8 (30%)
1	UFT	A	403	1	18,21,22	2.58	10 (55%)	26,30,33	1.99	8 (30%)
1	UFT	A	524	1	18,21,22	2.68	9 (50%)	26,30,33	1.80	5 (19%)
1	UFT	A	190	1	18,21,22	2.58	10 (55%)	26,30,33	2.02	8 (30%)
1	CFZ	A	254	1	18,21,22	2.49	7 (38%)	26,30,33	1.21	3 (11%)
1	UFT	A	71	1	18,21,22	2.58	10 (55%)	26,30,33	1.99	7 (26%)
1	CFZ	B	417	1	18,21,22	2.49	7 (38%)	26,30,33	1.46	3 (11%)
1	CFZ	B	603	1	18,21,22	2.51	7 (38%)	26,30,33	1.20	3 (11%)
1	UFT	B	204	1	18,21,22	2.61	9 (50%)	26,30,33	1.89	6 (23%)
1	UFT	A	413	1	18,21,22	2.65	9 (50%)	26,30,33	1.80	6 (23%)
1	CFZ	B	139	1	18,21,22	2.49	7 (38%)	26,30,33	1.30	3 (11%)
1	CFZ	A	543	1	18,21,22	2.48	7 (38%)	26,30,33	1.31	4 (15%)
1	CFZ	B	700	1	18,21,22	2.51	7 (38%)	26,30,33	1.27	3 (11%)
1	CFZ	A	631	1	18,21,22	2.50	7 (38%)	26,30,33	1.35	3 (11%)
1	CFZ	A	332	1	18,21,22	2.49	7 (38%)	26,30,33	1.32	3 (11%)
1	CFZ	A	458	1	18,21,22	2.53	7 (38%)	26,30,33	1.25	2 (7%)
1	CFZ	B	610	1	18,21,22	2.48	7 (38%)	26,30,33	1.40	4 (15%)
1	UFT	A	377	1	18,21,22	2.62	9 (50%)	26,30,33	1.97	7 (26%)
1	UFT	A	489	1	18,21,22	2.58	9 (50%)	26,30,33	1.98	7 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CFZ	A	349	1	18,21,22	2.50	7 (38%)	26,30,33	1.19	3 (11%)
1	CFZ	A	664	1	18,21,22	2.47	7 (38%)	26,30,33	1.53	3 (11%)
1	CFZ	A	144	1	18,21,22	2.47	7 (38%)	26,30,33	1.52	3 (11%)
1	UFT	A	160	1	18,21,22	2.57	9 (50%)	26,30,33	1.99	8 (30%)
1	CFZ	B	157	1	18,21,22	2.51	7 (38%)	26,30,33	1.17	2 (7%)
1	CFZ	A	536	1	18,21,22	2.48	7 (38%)	26,30,33	1.50	2 (7%)
1	UFT	B	105	1	18,21,22	2.59	9 (50%)	26,30,33	1.95	7 (26%)
1	UFT	A	245	1	18,21,22	2.59	9 (50%)	26,30,33	1.94	8 (30%)
1	UFT	A	593	1	18,21,22	2.59	9 (50%)	26,30,33	1.95	8 (30%)
1	CFZ	A	157	1	18,21,22	2.51	7 (38%)	26,30,33	1.16	2 (7%)
1	UFT	B	663	1	18,21,22	2.56	10 (55%)	26,30,33	2.08	8 (30%)
1	UFT	B	137	1	18,21,22	2.59	9 (50%)	26,30,33	1.90	8 (30%)
1	UFT	A	98	1	18,21,22	2.60	10 (55%)	26,30,33	1.93	7 (26%)
1	UFT	A	301	1	18,21,22	2.57	9 (50%)	26,30,33	1.98	8 (30%)
1	UFT	B	50	1	18,21,22	2.58	9 (50%)	26,30,33	2.05	6 (23%)
1	UFT	A	101	1	18,21,22	2.57	10 (55%)	26,30,33	2.06	8 (30%)
1	CFZ	A	246	1	18,21,22	2.51	7 (38%)	26,30,33	1.19	3 (11%)
1	CFZ	A	639	1	18,21,22	2.49	7 (38%)	26,30,33	1.29	3 (11%)
1	UFT	A	153	1	18,21,22	2.63	9 (50%)	26,30,33	1.88	7 (26%)
1	UFT	B	19	1	18,21,22	2.59	9 (50%)	26,30,33	1.96	8 (30%)
1	UFT	A	62	1	18,21,22	2.56	10 (55%)	26,30,33	2.07	8 (30%)
1	CFZ	B	308	1	18,21,22	2.47	7 (38%)	26,30,33	1.51	4 (15%)
1	UFT	A	55	1	18,21,22	2.61	9 (50%)	26,30,33	1.89	7 (26%)
1	CFZ	A	247	1	18,21,22	2.50	7 (38%)	26,30,33	1.17	2 (7%)
1	CFZ	B	625	1	18,21,22	2.48	7 (38%)	26,30,33	1.33	3 (11%)
1	CFZ	A	632	1	18,21,22	2.49	7 (38%)	26,30,33	1.26	2 (7%)
1	CFZ	A	75	1	18,21,22	2.45	7 (38%)	26,30,33	1.46	3 (11%)
1	UFT	A	701	1	18,21,22	2.59	9 (50%)	26,30,33	1.98	7 (26%)
1	CFZ	A	298	1	18,21,22	2.53	7 (38%)	26,30,33	1.18	3 (11%)
1	CFZ	A	110	1	18,21,22	2.50	7 (38%)	26,30,33	1.21	3 (11%)
1	CFZ	B	643	1	18,21,22	2.51	7 (38%)	26,30,33	1.24	3 (11%)
1	CFZ	B	173	1	18,21,22	2.49	7 (38%)	26,30,33	1.20	2 (7%)
1	CFZ	A	173	1	18,21,22	2.49	7 (38%)	26,30,33	1.18	2 (7%)
1	CFZ	B	486	1	18,21,22	2.48	7 (38%)	26,30,33	1.29	2 (7%)
1	CFZ	B	249	1	18,21,22	2.51	7 (38%)	26,30,33	1.19	3 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UFT	B	155	1	-	0/7/25/26	0/2/2/2
1	UFT	A	530	1	-	2/7/25/26	0/2/2/2
1	UFT	A	143	1	-	2/7/25/26	0/2/2/2
1	UFT	A	200	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	446	1	-	0/7/25/26	0/2/2/2
1	UFT	B	504	1	-	2/7/25/26	0/2/2/2
1	UFT	A	358	1	-	0/7/25/26	0/2/2/2
1	UFT	B	402	1	-	0/7/25/26	0/2/2/2
1	UFT	B	695	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	328	1	-	3/7/25/26	0/2/2/2
1	UFT	B	42	1	-	0/7/25/26	0/2/2/2
1	UFT	A	662	1	-	2/7/25/26	0/2/2/2
1	UFT	A	542	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	407	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	458	1	-	0/7/25/26	0/2/2/2
1	UFT	A	115	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	372	1	-	0/7/25/26	0/2/2/2
1	UFT	A	559	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	540	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	10	1	-	2/7/25/26	0/2/2/2
1	UFT	A	322	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	111	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	477	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	198	1	-	0/7/25/26	0/2/2/2
1	UFT	B	116	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	643	1	-	0/7/25/26	0/2/2/2
1	UFT	A	233	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	372	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	241	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	438	1	-	0/7/25/26	0/2/2/2
1	UFT	A	367	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	564	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	462	1	-	0/7/25/26	0/2/2/2
1	UFT	A	251	1	-	2/7/25/26	0/2/2/2
1	UFT	A	636	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UFT	B	509	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	564	1	-	3/7/25/26	0/2/2/2
1	UFT	A	545	1	-	3/7/25/26	0/2/2/2
1	UFT	B	690	1	-	0/7/25/26	0/2/2/2
1	UFT	B	59	1	-	1/7/25/26	0/2/2/2
1	CFZ	B	558	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	90	1	-	0/7/25/26	0/2/2/2
1	UFT	A	142	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	219	1	-	2/7/25/26	0/2/2/2
1	UFT	A	493	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	548	1	-	1/7/25/26	0/2/2/2
1	UFT	A	513	1	-	2/7/25/26	0/2/2/2
1	UFT	B	293	1	-	2/7/25/26	0/2/2/2
1	UFT	A	42	1	-	0/7/25/26	0/2/2/2
1	UFT	B	549	1	-	2/7/25/26	0/2/2/2
1	UFT	B	719	1	-	2/7/25/26	0/2/2/2
1	UFT	B	684	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	308	1	-	0/7/25/26	0/2/2/2
1	UFT	B	618	1	-	0/7/25/26	0/2/2/2
1	UFT	B	202	1	-	2/7/25/26	0/2/2/2
1	UFT	A	215	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	210	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	405	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	67	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	455	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	90	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	164	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	417	1	-	0/7/25/26	0/2/2/2
1	UFT	A	689	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	25	1	-	3/7/25/26	0/2/2/2
1	CFZ	B	411	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	614	1	-	2/7/25/26	0/2/2/2
1	UFT	B	485	1	-	2/7/25/26	0/2/2/2
1	UFT	A	74	1	-	2/7/25/26	0/2/2/2
1	UFT	A	635	1	-	1/7/25/26	0/2/2/2
1	UFT	B	141	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	667	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UFT	A	347	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	268	1	-	0/7/25/26	0/2/2/2
1	UFT	A	366	1	-	0/7/25/26	0/2/2/2
1	UFT	B	302	1	-	2/7/25/26	0/2/2/2
1	UFT	B	94	1	-	1/7/25/26	0/2/2/2
1	UFT	B	635	1	-	1/7/25/26	0/2/2/2
1	CFZ	B	556	1	-	6/7/25/26	0/2/2/2
1	UFT	B	365	1	-	0/7/25/26	0/2/2/2
1	UFT	B	309	1	-	2/7/25/26	0/2/2/2
1	UFT	B	313	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	76	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	316	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	79	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	114	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	151	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	165	1	-	0/7/25/26	0/2/2/2
1	UFT	A	695	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	576	1	-	0/7/25/26	0/2/2/2
1	UFT	A	88	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	21	1	-	0/7/25/26	0/2/2/2
1	UFT	A	633	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	21	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	404	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	242	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	565	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	355	1	-	0/7/25/26	0/2/2/2
1	UFT	A	174	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	387	1	-	1/7/25/26	0/2/2/2
1	CFZ	B	604	1	-	0/7/25/26	0/2/2/2
1	UFT	B	175	1	-	2/7/25/26	0/2/2/2
1	UFT	B	628	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	498	1	-	0/7/25/26	0/2/2/2
1	UFT	B	489	1	-	1/7/25/26	0/2/2/2
1	CFZ	B	664	1	-	1/7/25/26	0/2/2/2
1	CFZ	B	651	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	206	1	-	2/7/25/26	0/2/2/2
1	UFT	B	11	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	518	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	161	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UFT	A	229	1	-	3/7/25/26	0/2/2/2
1	UFT	A	663	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	246	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	25	1	-	3/7/25/26	0/2/2/2
1	UFT	B	182	1	-	0/7/25/26	0/2/2/2
1	UFT	B	154	1	-	0/7/25/26	0/2/2/2
1	UFT	B	44	1	-	2/7/25/26	0/2/2/2
1	UFT	B	431	1	-	2/7/25/26	0/2/2/2
1	UFT	B	602	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	373	1	-	0/7/25/26	0/2/2/2
1	UFT	B	344	1	-	2/7/25/26	0/2/2/2
1	UFT	B	447	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	540	1	-	2/7/25/26	0/2/2/2
1	UFT	A	169	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	117	1	-	2/7/25/26	0/2/2/2
1	UFT	B	701	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	110	1	-	2/7/25/26	0/2/2/2
1	UFT	B	170	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	201	1	-	2/7/25/26	0/2/2/2
1	UFT	B	554	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	103	1	-	0/7/25/26	0/2/2/2
1	UFT	B	106	1	-	3/7/25/26	0/2/2/2
1	UFT	B	153	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	603	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	469	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	381	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	523	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	637	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	184	1	-	2/7/25/26	0/2/2/2
1	UFT	A	609	1	-	0/7/25/26	0/2/2/2
1	UFT	A	669	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	353	1	-	0/7/25/26	0/2/2/2
1	UFT	A	196	1	-	3/7/25/26	0/2/2/2
1	CFZ	B	285	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	363	1	-	2/7/25/26	0/2/2/2
1	UFT	A	155	1	-	0/7/25/26	0/2/2/2
1	UFT	B	334	1	-	3/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UFT	A	216	1	-	0/7/25/26	0/2/2/2
1	UFT	A	84	1	-	3/7/25/26	0/2/2/2
1	UFT	B	571	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	439	1	-	0/7/25/26	0/2/2/2
1	UFT	B	80	1	-	2/7/25/26	0/2/2/2
1	UFT	B	662	1	-	2/7/25/26	0/2/2/2
1	UFT	B	456	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	96	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	406	1	-	2/7/25/26	0/2/2/2
1	UFT	A	329	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	325	1	-	2/7/25/26	0/2/2/2
1	UFT	A	163	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	369	1	-	0/7/25/26	0/2/2/2
1	UFT	B	621	1	-	3/7/25/26	0/2/2/2
1	UFT	B	524	1	-	3/7/25/26	0/2/2/2
1	UFT	B	472	1	-	3/7/25/26	0/2/2/2
1	UFT	B	245	1	-	0/7/25/26	0/2/2/2
1	UFT	B	84	1	-	3/7/25/26	0/2/2/2
1	UFT	B	607	1	-	2/7/25/26	0/2/2/2
1	UFT	B	305	1	-	2/7/25/26	0/2/2/2
1	UFT	B	229	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	600	1	-	0/7/25/26	0/2/2/2
1	UFT	A	214	1	-	0/7/25/26	0/2/2/2
1	UFT	B	555	1	-	3/7/25/26	0/2/2/2
1	CFZ	B	418	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	698	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	679	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	506	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	486	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	690	1	-	0/7/25/26	0/2/2/2
1	UFT	A	504	1	-	2/7/25/26	0/2/2/2
1	UFT	B	60	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	362	1	-	0/7/25/26	0/2/2/2
1	UFT	A	265	1	-	0/7/25/26	0/2/2/2
1	UFT	A	204	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	704	1	-	2/7/25/26	0/2/2/2
1	UFT	A	430	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UFT	B	535	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	647	1	-	0/7/25/26	0/2/2/2
1	UFT	A	581	1	-	0/7/25/26	0/2/2/2
1	UFT	B	636	1	-	0/7/25/26	0/2/2/2
1	UFT	A	309	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	518	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	404	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	104	1	-	0/7/25/26	0/2/2/2
1	UFT	A	296	1	-	2/7/25/26	0/2/2/2
1	UFT	A	179	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	576	1	-	0/7/25/26	0/2/2/2
1	UFT	A	33	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	218	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	156	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	551	1	-	0/7/25/26	0/2/2/2
1	UFT	B	71	1	-	0/7/25/26	0/2/2/2
1	UFT	A	202	1	-	1/7/25/26	0/2/2/2
1	UFT	A	86	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	543	1	-	0/7/25/26	0/2/2/2
1	UFT	A	8	1	-	0/7/25/26	0/2/2/2
1	UFT	A	555	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	383	1	-	2/7/25/26	0/2/2/2
1	UFT	A	471	1	-	2/7/25/26	0/2/2/2
1	UFT	A	14	1	-	0/7/25/26	0/2/2/2
1	UFT	A	481	1	-	2/7/25/26	0/2/2/2
1	UFT	A	582	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	592	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	323	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	370	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	28	1	-	2/7/25/26	0/2/2/2
1	UFT	B	687	1	-	0/7/25/26	0/2/2/2
1	UFT	A	141	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	315	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	39	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	72	1	-	0/7/25/26	0/2/2/2
1	UFT	B	361	1	-	2/7/25/26	0/2/2/2
1	UFT	A	673	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	140	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	494	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CFZ	A	131	1	-	0/7/25/26	0/2/2/2
1	UFT	A	302	1	-	2/7/25/26	0/2/2/2
1	UFT	B	466	1	-	0/7/25/26	0/2/2/2
1	UFT	B	437	1	-	0/7/25/26	0/2/2/2
1	UFT	B	629	1	-	0/7/25/26	0/2/2/2
1	UFT	A	621	1	-	3/7/25/26	0/2/2/2
1	CFZ	B	354	1	-	2/7/25/26	0/2/2/2
1	UFT	B	544	1	-	2/7/25/26	0/2/2/2
1	UFT	A	313	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	76	1	-	2/7/25/26	0/2/2/2
1	UFT	A	350	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	425	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	120	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	67	1	-	2/7/25/26	0/2/2/2
1	UFT	A	359	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	335	1	-	2/7/25/26	0/2/2/2
1	UFT	A	549	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	652	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	657	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	451	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	130	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	151	1	-	2/7/25/26	0/2/2/2
1	UFT	A	97	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	57	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	438	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	492	1	-	0/7/25/26	0/2/2/2
1	UFT	B	581	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	579	1	-	0/7/25/26	0/2/2/2
1	UFT	A	719	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	693	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	583	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	338	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	585	1	-	0/7/25/26	0/2/2/2
1	UFT	B	669	1	-	2/7/25/26	0/2/2/2
1	UFT	A	112	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	117	1	-	2/7/25/26	0/2/2/2
1	UFT	B	179	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	370	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CFZ	A	285	1	-	0/7/25/26	0/2/2/2
1	UFT	B	689	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	338	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	279	1	-	0/7/25/26	0/2/2/2
1	UFT	B	666	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	171	1	-	2/7/25/26	0/2/2/2
1	UFT	B	174	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	282	1	-	0/7/25/26	0/2/2/2
1	UFT	A	260	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	528	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	637	1	-	2/7/25/26	0/2/2/2
1	UFT	B	169	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	625	1	-	1/7/25/26	0/2/2/2
1	UFT	A	608	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	655	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	600	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	140	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	131	1	-	0/7/25/26	0/2/2/2
1	UFT	B	377	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	517	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	63	1	-	2/7/25/26	0/2/2/2
1	UFT	B	197	1	-	0/7/25/26	0/2/2/2
1	UFT	B	135	1	-	0/7/25/26	0/2/2/2
1	UFT	A	500	1	-	0/7/25/26	0/2/2/2
1	UFT	B	74	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	426	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	418	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	316	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	492	1	-	0/7/25/26	0/2/2/2
1	UFT	A	653	1	-	0/7/25/26	0/2/2/2
1	UFT	B	389	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	156	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	498	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	399	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	667	1	-	2/7/25/26	0/2/2/2
1	UFT	B	423	1	-	2/7/25/26	0/2/2/2
1	UFT	B	606	1	-	0/7/25/26	0/2/2/2
1	UFT	B	633	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	473	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UFT	A	703	1	-	2/7/25/26	0/2/2/2
1	UFT	B	398	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	459	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	585	1	-	0/7/25/26	0/2/2/2
1	UFT	A	554	1	-	0/7/25/26	0/2/2/2
1	UFT	A	434	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	49	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	325	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	511	1	-	0/7/25/26	0/2/2/2
1	UFT	A	105	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	351	1	-	2/7/25/26	0/2/2/2
1	UFT	B	108	1	-	2/7/25/26	0/2/2/2
1	UFT	B	421	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	444	1	-	0/7/25/26	0/2/2/2
1	UFT	A	629	1	-	0/7/25/26	0/2/2/2
1	UFT	A	447	1	-	0/7/25/26	0/2/2/2
1	UFT	B	214	1	-	0/7/25/26	0/2/2/2
1	UFT	B	464	1	-	2/7/25/26	0/2/2/2
1	UFT	B	352	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	407	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	315	1	-	0/7/25/26	0/2/2/2
1	UFT	A	402	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	130	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	491	1	-	2/7/25/26	0/2/2/2
1	UFT	B	266	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	15	1	-	3/7/25/26	0/2/2/2
1	UFT	B	673	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	446	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	424	1	-	1/7/25/26	0/2/2/2
1	UFT	A	503	1	-	3/7/25/26	0/2/2/2
1	CFZ	B	592	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	512	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	209	1	-	0/7/25/26	0/2/2/2
1	UFT	A	208	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	440	1	-	2/7/25/26	0/2/2/2
1	UFT	B	43	1	-	4/7/25/26	0/2/2/2
1	UFT	B	32	1	-	2/7/25/26	0/2/2/2
1	UFT	B	703	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UFT	B	33	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	232	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	234	1	-	3/7/25/26	0/2/2/2
1	UFT	A	32	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	459	1	-	0/7/25/26	0/2/2/2
1	UFT	A	676	1	-	3/7/25/26	0/2/2/2
1	UFT	A	712	1	-	2/7/25/26	0/2/2/2
1	UFT	A	108	1	-	2/7/25/26	0/2/2/2
1	UFT	A	646	1	-	0/7/25/26	0/2/2/2
1	UFT	B	430	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	129	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	247	1	-	0/7/25/26	0/2/2/2
1	UFT	A	344	1	-	3/7/25/26	0/2/2/2
1	UFT	A	19	1	-	2/7/25/26	0/2/2/2
1	UFT	A	50	1	-	1/7/25/26	0/2/2/2
1	CFZ	B	378	1	-	0/7/25/26	0/2/2/2
1	UFT	B	471	1	-	0/7/25/26	0/2/2/2
1	UFT	B	481	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	384	1	-	0/7/25/26	0/2/2/2
1	UFT	A	684	1	-	2/7/25/26	0/2/2/2
1	UFT	A	659	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	241	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	321	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	568	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	631	1	-	0/7/25/26	0/2/2/2
1	UFT	B	542	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	321	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	587	1	-	2/7/25/26	0/2/2/2
1	UFT	A	217	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	568	1	-	0/7/25/26	0/2/2/2
1	UFT	A	398	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	234	1	-	3/7/25/26	0/2/2/2
1	UFT	B	190	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	536	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	647	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	639	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	587	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	73	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UFT	B	359	1	-	0/7/25/26	0/2/2/2
1	UFT	B	283	1	-	2/7/25/26	0/2/2/2
1	UFT	B	366	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	426	1	-	0/7/25/26	0/2/2/2
1	UFT	B	534	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	657	1	-	2/7/25/26	0/2/2/2
1	UFT	B	55	1	-	0/7/25/26	0/2/2/2
1	UFT	A	192	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	120	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	124	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	682	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	383	1	-	0/7/25/26	0/2/2/2
1	UFT	A	618	1	-	0/7/25/26	0/2/2/2
1	UFT	A	666	1	-	3/7/25/26	0/2/2/2
1	CFZ	B	579	1	-	0/7/25/26	0/2/2/2
1	UFT	A	293	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	441	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	328	1	-	3/7/25/26	0/2/2/2
1	UFT	A	628	1	-	0/7/25/26	0/2/2/2
1	UFT	A	137	1	-	0/7/25/26	0/2/2/2
1	UFT	B	98	1	-	0/7/25/26	0/2/2/2
1	UFT	B	301	1	-	2/7/25/26	0/2/2/2
1	UFT	A	485	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	548	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	399	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	332	1	-	2/7/25/26	0/2/2/2
1	UFT	B	530	1	-	2/7/25/26	0/2/2/2
1	UFT	B	656	1	-	0/7/25/26	0/2/2/2
1	UFT	B	48	1	-	0/7/25/26	0/2/2/2
1	UFT	A	44	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	282	1	-	0/7/25/26	0/2/2/2
1	UFT	B	296	1	-	2/7/25/26	0/2/2/2
1	UFT	A	89	1	-	0/7/25/26	0/2/2/2
1	UFT	A	544	1	-	2/7/25/26	0/2/2/2
1	UFT	A	11	1	-	0/7/25/26	0/2/2/2
1	UFT	B	593	1	-	3/7/25/26	0/2/2/2
1	UFT	A	352	1	-	2/7/25/26	0/2/2/2
1	UFT	B	712	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CFZ	A	46	1	-	2/7/25/26	0/2/2/2
1	UFT	A	432	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	565	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	655	1	-	2/7/25/26	0/2/2/2
1	UFT	A	365	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	304	1	-	0/7/25/26	0/2/2/2
1	UFT	A	431	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	124	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	79	1	-	0/7/25/26	0/2/2/2
1	UFT	B	200	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	198	1	-	0/7/25/26	0/2/2/2
1	UFT	A	43	1	-	4/7/25/26	0/2/2/2
1	CFZ	A	474	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	75	1	-	1/7/25/26	0/2/2/2
1	UFT	B	347	1	-	2/7/25/26	0/2/2/2
1	UFT	A	182	1	-	0/7/25/26	0/2/2/2
1	UFT	B	653	1	-	0/7/25/26	0/2/2/2
1	UFT	B	367	1	-	2/7/25/26	0/2/2/2
1	UFT	B	590	1	-	1/7/25/26	0/2/2/2
1	UFT	B	251	1	-	2/7/25/26	0/2/2/2
1	UFT	A	175	1	-	2/7/25/26	0/2/2/2
1	UFT	B	322	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	26	1	-	1/7/25/26	0/2/2/2
1	UFT	A	334	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	691	1	-	0/7/25/26	0/2/2/2
1	UFT	B	493	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	210	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	184	1	-	2/7/25/26	0/2/2/2
1	UFT	A	456	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	49	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	436	1	-	0/7/25/26	0/2/2/2
1	UFT	B	577	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	411	1	-	0/7/25/26	0/2/2/2
1	UFT	B	708	1	-	0/7/25/26	0/2/2/2
1	UFT	B	196	1	-	3/7/25/26	0/2/2/2
1	UFT	A	696	1	-	0/7/25/26	0/2/2/2
1	UFT	A	472	1	-	3/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CFZ	A	279	1	-	0/7/25/26	0/2/2/2
1	UFT	A	116	1	-	0/7/25/26	0/2/2/2
1	UFT	B	115	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	242	1	-	0/7/25/26	0/2/2/2
1	UFT	B	336	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	556	1	-	6/7/25/26	0/2/2/2
1	UFT	B	86	1	-	0/7/25/26	0/2/2/2
1	UFT	A	336	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	382	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	171	1	-	2/7/25/26	0/2/2/2
1	UFT	B	502	1	-	2/7/25/26	0/2/2/2
1	UFT	B	545	1	-	3/7/25/26	0/2/2/2
1	UFT	B	163	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	698	1	-	0/7/25/26	0/2/2/2
1	UFT	A	59	1	-	0/7/25/26	0/2/2/2
1	UFT	A	170	1	-	1/7/25/26	0/2/2/2
1	UFT	A	283	1	-	2/7/25/26	0/2/2/2
1	UFT	B	89	1	-	0/7/25/26	0/2/2/2
1	UFT	B	432	1	-	1/7/25/26	0/2/2/2
1	UFT	A	270	1	-	2/7/25/26	0/2/2/2
1	UFT	A	197	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	63	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	15	1	-	2/7/25/26	0/2/2/2
1	UFT	B	62	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	212	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	360	1	-	2/7/25/26	0/2/2/2
1	UFT	A	606	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	188	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	363	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	212	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	425	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	351	1	-	0/7/25/26	0/2/2/2
1	UFT	B	97	1	-	3/7/25/26	0/2/2/2
1	UFT	B	265	1	-	0/7/25/26	0/2/2/2
1	UFT	A	656	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	218	1	-	0/7/25/26	0/2/2/2
1	UFT	B	646	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	34	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CFZ	A	381	1	-	1/7/25/26	0/2/2/2
1	UFT	B	434	1	-	0/7/25/26	0/2/2/2
1	UFT	A	602	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	693	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	355	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	405	1	-	2/7/25/26	0/2/2/2
1	UFT	A	60	1	-	0/7/25/26	0/2/2/2
1	UFT	A	464	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	384	1	-	3/7/25/26	0/2/2/2
1	UFT	A	13	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	268	1	-	0/7/25/26	0/2/2/2
1	UFT	B	329	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	373	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	72	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	206	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	506	1	-	2/7/25/26	0/2/2/2
1	UFT	B	582	1	-	2/7/25/26	0/2/2/2
1	UFT	B	233	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	232	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	149	1	-	0/7/25/26	0/2/2/2
1	UFT	A	61	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	165	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	354	1	-	1/7/25/26	0/2/2/2
1	UFT	A	266	1	-	2/7/25/26	0/2/2/2
1	UFT	A	499	1	-	3/7/25/26	0/2/2/2
1	CFZ	B	103	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	104	1	-	1/7/25/26	0/2/2/2
1	CFZ	B	682	1	-	0/7/25/26	0/2/2/2
1	UFT	A	571	1	-	2/7/25/26	0/2/2/2
1	UFT	B	88	1	-	2/7/25/26	0/2/2/2
1	UFT	B	609	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	651	1	-	0/7/25/26	0/2/2/2
1	UFT	A	361	1	-	1/7/25/26	0/2/2/2
1	CFZ	B	465	1	-	0/7/25/26	0/2/2/2
1	UFT	B	69	1	-	0/7/25/26	0/2/2/2
1	UFT	B	676	1	-	3/7/25/26	0/2/2/2
1	UFT	A	154	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CFZ	A	26	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	491	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	610	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	323	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	201	1	-	2/7/25/26	0/2/2/2
1	UFT	B	513	1	-	1/7/25/26	0/2/2/2
1	UFT	A	577	1	-	0/7/25/26	0/2/2/2
1	UFT	B	659	1	-	3/7/25/26	0/2/2/2
1	UFT	A	305	1	-	2/7/25/26	0/2/2/2
1	UFT	A	466	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	111	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	96	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	39	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	369	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	512	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	704	1	-	2/7/25/26	0/2/2/2
1	UFT	B	559	1	-	1/7/25/26	0/2/2/2
1	UFT	B	519	1	-	2/7/25/26	0/2/2/2
1	UFT	A	92	1	-	2/7/25/26	0/2/2/2
1	UFT	A	106	1	-	3/7/25/26	0/2/2/2
1	CFZ	B	304	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	360	1	-	0/7/25/26	0/2/2/2
1	UFT	A	437	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	469	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	523	1	-	1/7/25/26	0/2/2/2
1	UFT	B	260	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	558	1	-	1/7/25/26	0/2/2/2
1	CFZ	B	474	1	-	2/7/25/26	0/2/2/2
1	UFT	B	208	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	46	1	-	2/7/25/26	0/2/2/2
1	UFT	B	608	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	700	1	-	2/7/25/26	0/2/2/2
1	UFT	B	192	1	-	3/7/25/26	0/2/2/2
1	UFT	A	69	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	424	1	-	1/7/25/26	0/2/2/2
1	UFT	A	423	1	-	2/7/25/26	0/2/2/2
1	UFT	B	460	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	517	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	249	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CFZ	A	406	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	149	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	528	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	550	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	353	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	691	1	-	0/7/25/26	0/2/2/2
1	UFT	A	502	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	550	1	-	0/7/25/26	0/2/2/2
1	UFT	B	216	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	161	1	-	0/7/25/26	0/2/2/2
1	UFT	A	607	1	-	2/7/25/26	0/2/2/2
1	UFT	B	403	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	362	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	254	1	-	0/7/25/26	0/2/2/2
1	UFT	B	112	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	34	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	551	1	-	0/7/25/26	0/2/2/2
1	UFT	B	696	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	473	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	144	1	-	2/7/25/26	0/2/2/2
1	UFT	A	509	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	477	1	-	3/7/25/26	0/2/2/2
1	UFT	A	534	1	-	2/7/25/26	0/2/2/2
1	UFT	A	535	1	-	0/7/25/26	0/2/2/2
1	UFT	B	8	1	-	2/7/25/26	0/2/2/2
1	UFT	B	101	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	28	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	574	1	-	0/7/25/26	0/2/2/2
1	UFT	B	160	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	387	1	-	2/7/25/26	0/2/2/2
1	UFT	B	720	1	1/1/5/5	3/7/25/26	0/2/2/2
1	CFZ	A	209	1	-	0/7/25/26	0/2/2/2
1	UFT	A	708	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	441	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	188	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	494	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	219	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CFZ	B	114	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	73	1	-	0/7/25/26	0/2/2/2
1	UFT	A	590	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	164	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	574	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	632	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	139	1	-	0/7/25/26	0/2/2/2
1	UFT	A	519	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	511	1	-	0/7/25/26	0/2/2/2
1	UFT	A	94	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	620	1	-	0/7/25/26	0/2/2/2
1	UFT	A	720	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	10	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	129	1	-	0/7/25/26	0/2/2/2
1	UFT	A	421	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	57	1	-	2/7/25/26	0/2/2/2
1	UFT	B	126	1	-	1/7/25/26	0/2/2/2
1	CFZ	B	440	1	-	1/7/25/26	0/2/2/2
1	UFT	B	13	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	465	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	298	1	-	2/7/25/26	0/2/2/2
1	UFT	A	460	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	335	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	620	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	614	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	679	1	-	0/7/25/26	0/2/2/2
1	UFT	B	358	1	-	0/7/25/26	0/2/2/2
1	UFT	A	135	1	-	0/7/25/26	0/2/2/2
1	UFT	B	14	1	-	0/7/25/26	0/2/2/2
1	UFT	A	126	1	-	1/7/25/26	0/2/2/2
1	UFT	B	270	1	-	2/7/25/26	0/2/2/2
1	UFT	B	217	1	-	0/7/25/26	0/2/2/2
1	UFT	B	499	1	-	3/7/25/26	0/2/2/2
1	UFT	B	500	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	583	1	-	2/7/25/26	0/2/2/2
1	UFT	B	142	1	-	0/7/25/26	0/2/2/2
1	UFT	B	61	1	-	2/7/25/26	0/2/2/2
1	UFT	B	92	1	-	2/7/25/26	0/2/2/2
1	UFT	B	143	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CFZ	B	652	1	-	0/7/25/26	0/2/2/2
1	UFT	B	215	1	-	0/7/25/26	0/2/2/2
1	UFT	A	403	1	-	0/7/25/26	0/2/2/2
1	UFT	A	524	1	-	0/7/25/26	0/2/2/2
1	UFT	A	190	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	254	1	-	0/7/25/26	0/2/2/2
1	UFT	A	71	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	417	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	603	1	-	0/7/25/26	0/2/2/2
1	UFT	B	204	1	-	0/7/25/26	0/2/2/2
1	UFT	A	413	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	139	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	543	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	700	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	631	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	332	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	458	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	610	1	-	1/7/25/26	0/2/2/2
1	UFT	A	377	1	-	3/7/25/26	0/2/2/2
1	UFT	A	489	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	349	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	664	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	144	1	-	2/7/25/26	0/2/2/2
1	UFT	A	160	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	157	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	536	1	-	0/7/25/26	0/2/2/2
1	UFT	B	105	1	-	1/7/25/26	0/2/2/2
1	UFT	A	245	1	-	0/7/25/26	0/2/2/2
1	UFT	A	593	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	157	1	-	0/7/25/26	0/2/2/2
1	UFT	B	663	1	-	0/7/25/26	0/2/2/2
1	UFT	B	137	1	-	0/7/25/26	0/2/2/2
1	UFT	A	98	1	-	0/7/25/26	0/2/2/2
1	UFT	A	301	1	-	2/7/25/26	0/2/2/2
1	UFT	B	50	1	-	1/7/25/26	0/2/2/2
1	UFT	A	101	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	246	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	639	1	-	2/7/25/26	0/2/2/2
1	UFT	A	153	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UFT	B	19	1	-	2/7/25/26	0/2/2/2
1	UFT	A	62	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	308	1	-	0/7/25/26	0/2/2/2
1	UFT	A	55	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	247	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	625	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	632	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	75	1	-	2/7/25/26	0/2/2/2
1	UFT	A	701	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	110	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	643	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	173	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	173	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	486	1	-	4/7/25/26	0/2/2/2
1	CFZ	B	249	1	-	0/7/25/26	0/2/2/2

The worst 5 of 5758 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	493	UFT	C2-N1	5.30	1.47	1.38
1	A	359	UFT	C2-N1	5.22	1.46	1.38
1	B	105	UFT	C2-N1	5.17	1.46	1.38
1	A	43	UFT	C2-N1	5.16	1.46	1.38
1	B	43	UFT	C2-N1	5.14	1.46	1.38

The worst 5 of 3511 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	28	CFZ	C2'-C1'-N1	-6.31	104.55	114.20
1	A	14	UFT	C4-N3-C2	-5.19	119.73	126.58
1	B	361	UFT	C4-N3-C2	-5.14	119.80	126.58
1	A	350	UFT	C4-N3-C2	-5.12	119.83	126.58
1	A	19	UFT	C4-N3-C2	-5.09	119.86	126.58

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	720	UFT	C2'

5 of 709 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	8	UFT	O4'-C4'-C5'-O5'
1	B	8	UFT	C3'-C4'-C5'-O5'
1	A	10	CFZ	C3'-C4'-C5'-O5'
1	A	15	CFZ	C3'-C4'-C5'-O5'
1	B	15	CFZ	C3'-C4'-C5'-O5'

There are no ring outliers.

294 monomers are involved in 386 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	200	UFT	1	0
1	B	446	CFZ	1	0
1	B	402	UFT	1	0
1	B	695	UFT	1	0
1	B	328	CFZ	2	0
1	B	458	CFZ	1	0
1	A	372	CFZ	1	0
1	A	10	CFZ	1	0
1	A	322	UFT	1	0
1	B	477	CFZ	1	0
1	A	643	CFZ	1	0
1	A	233	UFT	1	0
1	B	372	CFZ	2	0
1	B	509	UFT	2	0
1	B	558	CFZ	1	0
1	B	219	CFZ	2	0
1	A	548	CFZ	1	0
1	A	513	UFT	1	0
1	B	293	UFT	1	0
1	B	549	UFT	2	0
1	B	719	UFT	3	0
1	A	215	UFT	1	0
1	B	210	CFZ	1	0
1	A	417	CFZ	1	0
1	B	411	CFZ	2	0
1	B	485	UFT	1	0
1	A	347	UFT	1	0
1	A	366	UFT	1	0
1	B	94	UFT	1	0
1	B	556	CFZ	2	0
1	B	365	UFT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	316	CFZ	2	0
1	A	79	CFZ	2	0
1	A	165	CFZ	3	0
1	A	695	UFT	1	0
1	B	21	CFZ	3	0
1	A	633	UFT	2	0
1	A	21	CFZ	2	0
1	A	355	CFZ	3	0
1	A	387	CFZ	1	0
1	B	628	UFT	1	0
1	B	498	CFZ	1	0
1	B	489	UFT	1	0
1	B	518	CFZ	1	0
1	B	246	CFZ	2	0
1	B	25	CFZ	1	0
1	B	154	UFT	1	0
1	B	602	UFT	2	0
1	A	169	UFT	1	0
1	A	103	CFZ	1	0
1	B	106	UFT	2	0
1	B	153	UFT	1	0
1	B	637	CFZ	1	0
1	B	184	CFZ	1	0
1	A	609	UFT	1	0
1	A	669	UFT	2	0
1	A	216	UFT	1	0
1	A	84	UFT	1	0
1	B	571	UFT	1	0
1	B	80	UFT	2	0
1	A	96	CFZ	1	0
1	B	472	UFT	2	0
1	B	84	UFT	1	0
1	A	600	CFZ	2	0
1	A	214	UFT	1	0
1	B	555	UFT	1	0
1	B	418	CFZ	2	0
1	B	698	CFZ	3	0
1	A	486	CFZ	1	0
1	B	362	CFZ	1	0
1	A	265	UFT	1	0
1	A	204	UFT	1	0
1	A	430	UFT	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	535	UFT	1	0
1	B	647	CFZ	1	0
1	A	518	CFZ	1	0
1	A	179	UFT	2	0
1	A	33	UFT	2	0
1	B	218	CFZ	2	0
1	B	156	CFZ	1	0
1	A	551	CFZ	2	0
1	B	71	UFT	1	0
1	A	471	UFT	1	0
1	A	14	UFT	1	0
1	A	481	UFT	1	0
1	A	323	CFZ	1	0
1	B	687	UFT	2	0
1	A	315	CFZ	1	0
1	A	673	UFT	1	0
1	A	140	CFZ	1	0
1	B	437	UFT	1	0
1	B	629	UFT	3	0
1	A	313	UFT	3	0
1	A	350	UFT	1	0
1	A	425	CFZ	1	0
1	B	120	CFZ	2	0
1	A	359	UFT	1	0
1	A	549	UFT	4	0
1	A	57	CFZ	1	0
1	B	492	CFZ	5	0
1	A	693	CFZ	2	0
1	B	669	UFT	2	0
1	A	112	UFT	2	0
1	B	179	UFT	2	0
1	B	338	CFZ	1	0
1	B	279	CFZ	3	0
1	A	171	CFZ	1	0
1	A	260	UFT	3	0
1	A	637	CFZ	1	0
1	B	169	UFT	1	0
1	B	600	CFZ	2	0
1	B	140	CFZ	1	0
1	A	517	CFZ	1	0
1	B	197	UFT	1	0
1	B	135	UFT	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	74	UFT	1	0
1	A	418	CFZ	2	0
1	B	316	CFZ	2	0
1	A	492	CFZ	1	0
1	B	389	UFT	2	0
1	A	156	CFZ	1	0
1	A	498	CFZ	2	0
1	B	423	UFT	1	0
1	B	633	UFT	2	0
1	A	459	CFZ	1	0
1	B	511	CFZ	2	0
1	A	105	UFT	1	0
1	A	351	CFZ	2	0
1	B	421	UFT	1	0
1	A	687	UFT	2	0
1	A	444	CFZ	1	0
1	A	629	UFT	3	0
1	B	214	UFT	1	0
1	B	464	UFT	1	0
1	B	315	CFZ	1	0
1	A	402	UFT	1	0
1	B	491	CFZ	3	0
1	B	673	UFT	1	0
1	A	446	CFZ	1	0
1	B	424	CFZ	1	0
1	B	592	CFZ	1	0
1	B	512	CFZ	1	0
1	B	209	CFZ	4	0
1	A	208	UFT	2	0
1	B	32	UFT	2	0
1	B	33	UFT	2	0
1	A	234	CFZ	1	0
1	A	32	UFT	1	0
1	B	459	CFZ	1	0
1	A	108	UFT	1	0
1	A	646	UFT	2	0
1	B	430	UFT	1	0
1	B	247	CFZ	4	0
1	A	344	UFT	2	0
1	B	471	UFT	1	0
1	B	481	UFT	1	0
1	A	659	UFT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	631	CFZ	1	0
1	A	217	UFT	3	0
1	B	234	CFZ	2	0
1	B	536	CFZ	1	0
1	A	647	CFZ	1	0
1	B	587	CFZ	1	0
1	A	73	CFZ	1	0
1	B	366	UFT	1	0
1	B	55	UFT	3	0
1	A	120	CFZ	2	0
1	A	293	UFT	1	0
1	B	441	CFZ	2	0
1	A	328	CFZ	2	0
1	A	628	UFT	1	0
1	A	137	UFT	2	0
1	B	548	CFZ	1	0
1	B	282	CFZ	1	0
1	A	11	UFT	3	0
1	B	593	UFT	1	0
1	B	712	UFT	1	0
1	A	432	UFT	1	0
1	A	365	UFT	2	0
1	A	43	UFT	1	0
1	B	493	UFT	3	0
1	A	210	CFZ	1	0
1	A	184	CFZ	1	0
1	A	436	CFZ	1	0
1	B	577	UFT	2	0
1	A	411	CFZ	3	0
1	B	708	UFT	1	0
1	A	472	UFT	2	0
1	A	279	CFZ	3	0
1	A	242	CFZ	1	0
1	A	556	CFZ	3	0
1	A	336	UFT	1	0
1	B	171	CFZ	1	0
1	A	698	CFZ	3	0
1	A	59	UFT	1	0
1	B	432	UFT	1	0
1	A	197	UFT	1	0
1	B	363	CFZ	1	0
1	B	425	CFZ	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	351	CFZ	1	0
1	B	265	UFT	1	0
1	A	218	CFZ	2	0
1	B	646	UFT	2	0
1	B	34	CFZ	1	0
1	A	602	UFT	2	0
1	B	693	CFZ	2	0
1	A	60	UFT	1	0
1	A	464	UFT	1	0
1	A	72	CFZ	1	0
1	B	233	UFT	2	0
1	A	149	CFZ	1	0
1	B	165	CFZ	2	0
1	A	354	CFZ	2	0
1	A	571	UFT	1	0
1	B	465	CFZ	1	0
1	A	154	UFT	1	0
1	A	610	CFZ	1	0
1	B	323	CFZ	2	0
1	B	513	UFT	1	0
1	A	577	UFT	2	0
1	B	659	UFT	1	0
1	B	96	CFZ	1	0
1	A	512	CFZ	1	0
1	B	519	UFT	1	0
1	A	106	UFT	1	0
1	A	437	UFT	1	0
1	B	260	UFT	4	0
1	A	558	CFZ	1	0
1	B	208	UFT	2	0
1	A	424	CFZ	1	0
1	A	423	UFT	1	0
1	B	460	UFT	1	0
1	B	517	CFZ	1	0
1	A	249	CFZ	1	0
1	B	149	CFZ	1	0
1	A	550	CFZ	2	0
1	B	550	CFZ	3	0
1	B	216	UFT	1	0
1	B	403	UFT	1	0
1	A	80	UFT	3	0
1	B	112	UFT	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	34	CFZ	1	0
1	B	551	CFZ	4	0
1	A	509	UFT	2	0
1	A	477	CFZ	1	0
1	A	535	UFT	1	0
1	B	8	UFT	1	0
1	B	28	CFZ	2	0
1	A	574	CFZ	1	0
1	B	720	UFT	4	0
1	A	209	CFZ	4	0
1	A	708	UFT	1	0
1	A	441	CFZ	2	0
1	B	494	CFZ	2	0
1	A	590	UFT	2	0
1	A	164	CFZ	1	0
1	A	139	CFZ	1	0
1	A	519	UFT	3	0
1	A	511	CFZ	3	0
1	A	720	UFT	1	0
1	B	10	CFZ	2	0
1	A	421	UFT	1	0
1	B	13	UFT	1	0
1	A	465	CFZ	1	0
1	A	460	UFT	1	0
1	B	620	CFZ	1	0
1	B	679	CFZ	1	0
1	A	135	UFT	4	0
1	B	14	UFT	1	0
1	B	217	UFT	3	0
1	B	92	UFT	1	0
1	B	215	UFT	1	0
1	A	403	UFT	1	0
1	A	254	CFZ	1	0
1	A	71	UFT	1	0
1	B	417	CFZ	2	0
1	B	204	UFT	2	0
1	A	413	UFT	1	0
1	B	139	CFZ	1	0
1	A	631	CFZ	1	0
1	A	458	CFZ	2	0
1	A	144	CFZ	1	0
1	B	157	CFZ	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	105	UFT	1	0
1	A	593	UFT	1	0
1	A	157	CFZ	3	0
1	B	137	UFT	2	0
1	A	153	UFT	1	0
1	A	55	UFT	2	0
1	A	247	CFZ	1	0
1	B	643	CFZ	1	0
1	B	173	CFZ	1	0
1	A	173	CFZ	1	0
1	B	486	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-54779. 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](#)

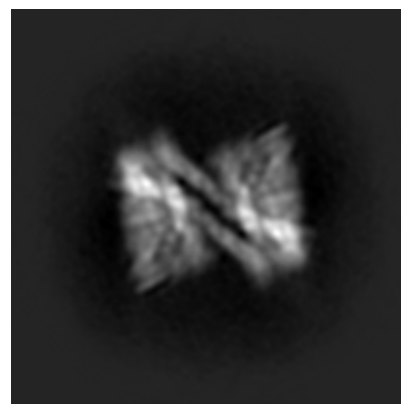
6.1.1 Primary map



X

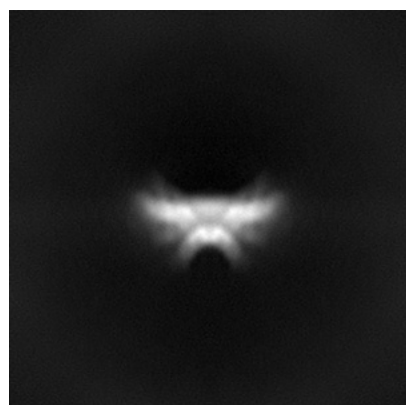


Y

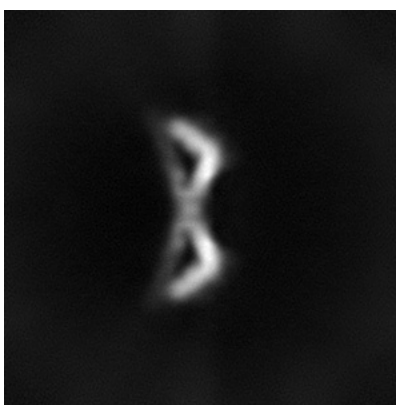


Z

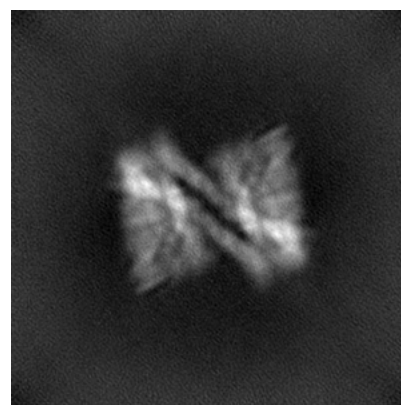
6.1.2 Raw map



X



Y

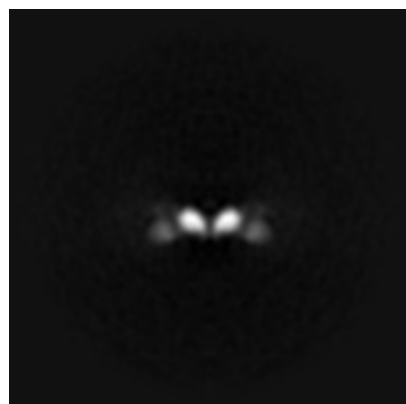


Z

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

6.2 Central slices [i](#)

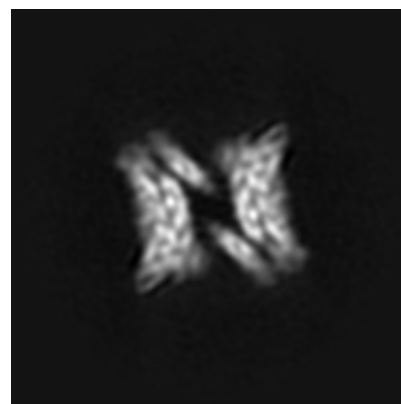
6.2.1 Primary map



X Index: 128

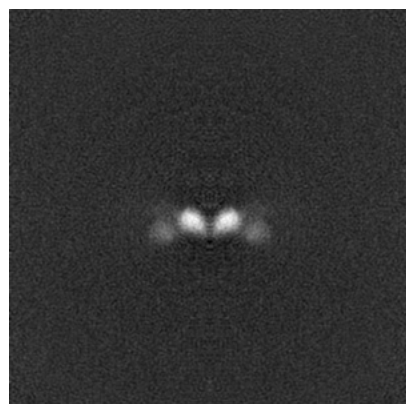


Y Index: 128

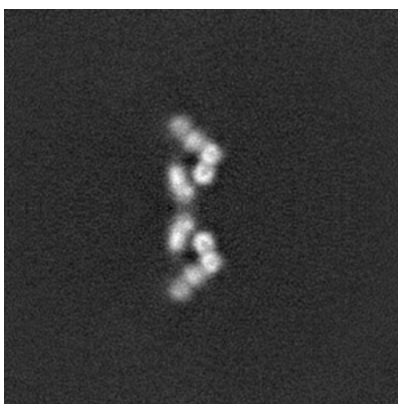


Z Index: 128

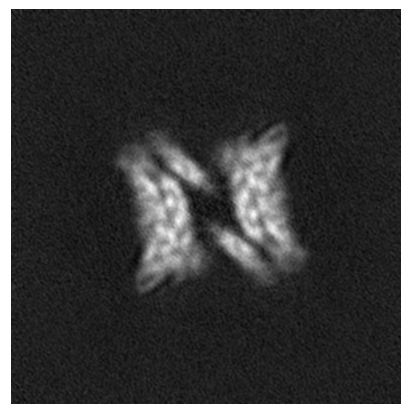
6.2.2 Raw map



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](#)

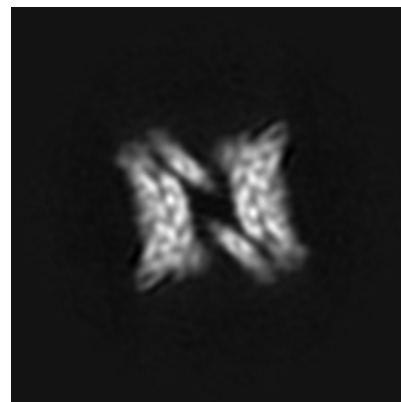
6.3.1 Primary map



X Index: 106



Y Index: 124

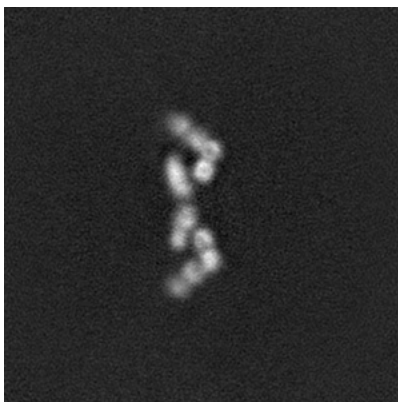


Z Index: 128

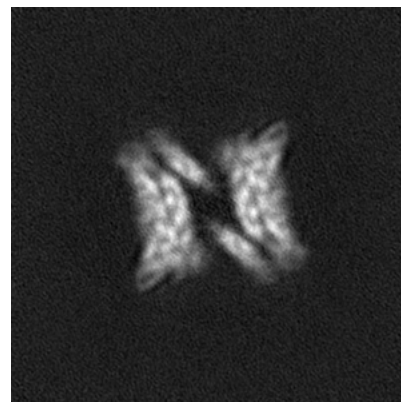
6.3.2 Raw map



X Index: 105



Y Index: 125



Z Index: 128

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

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

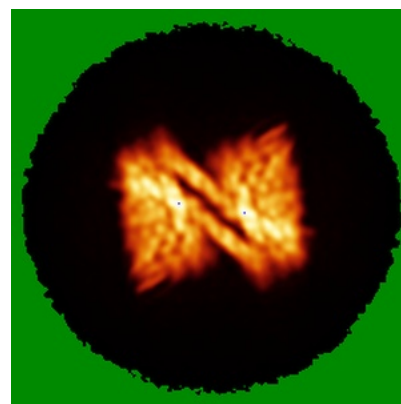
6.4.1 Primary map



X



Y

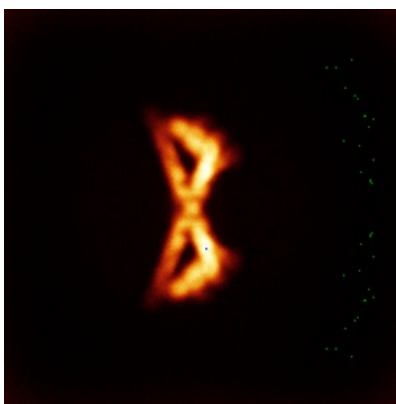


Z

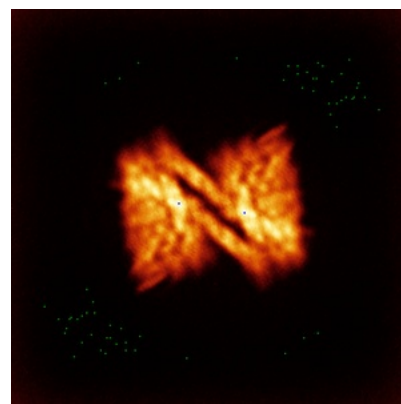
6.4.2 Raw map



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.

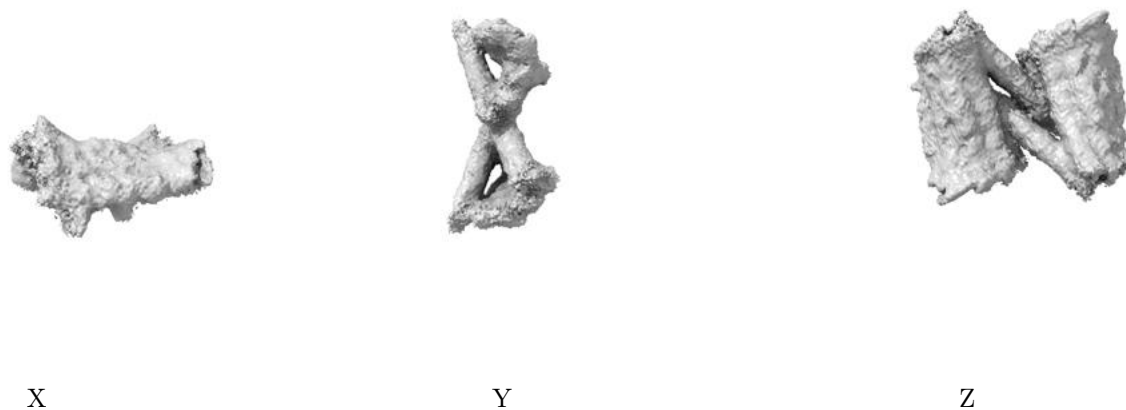
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.128. 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.

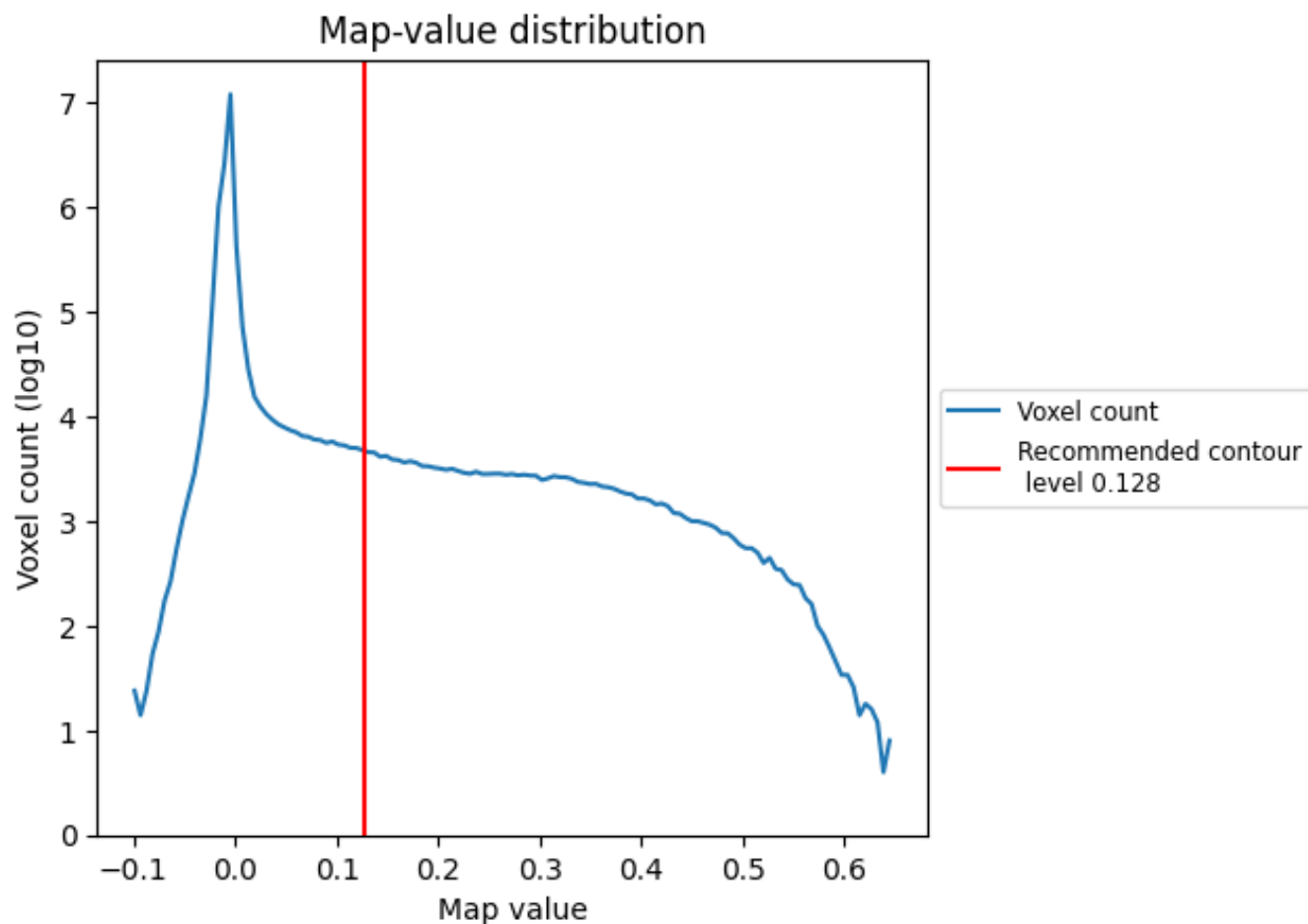
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

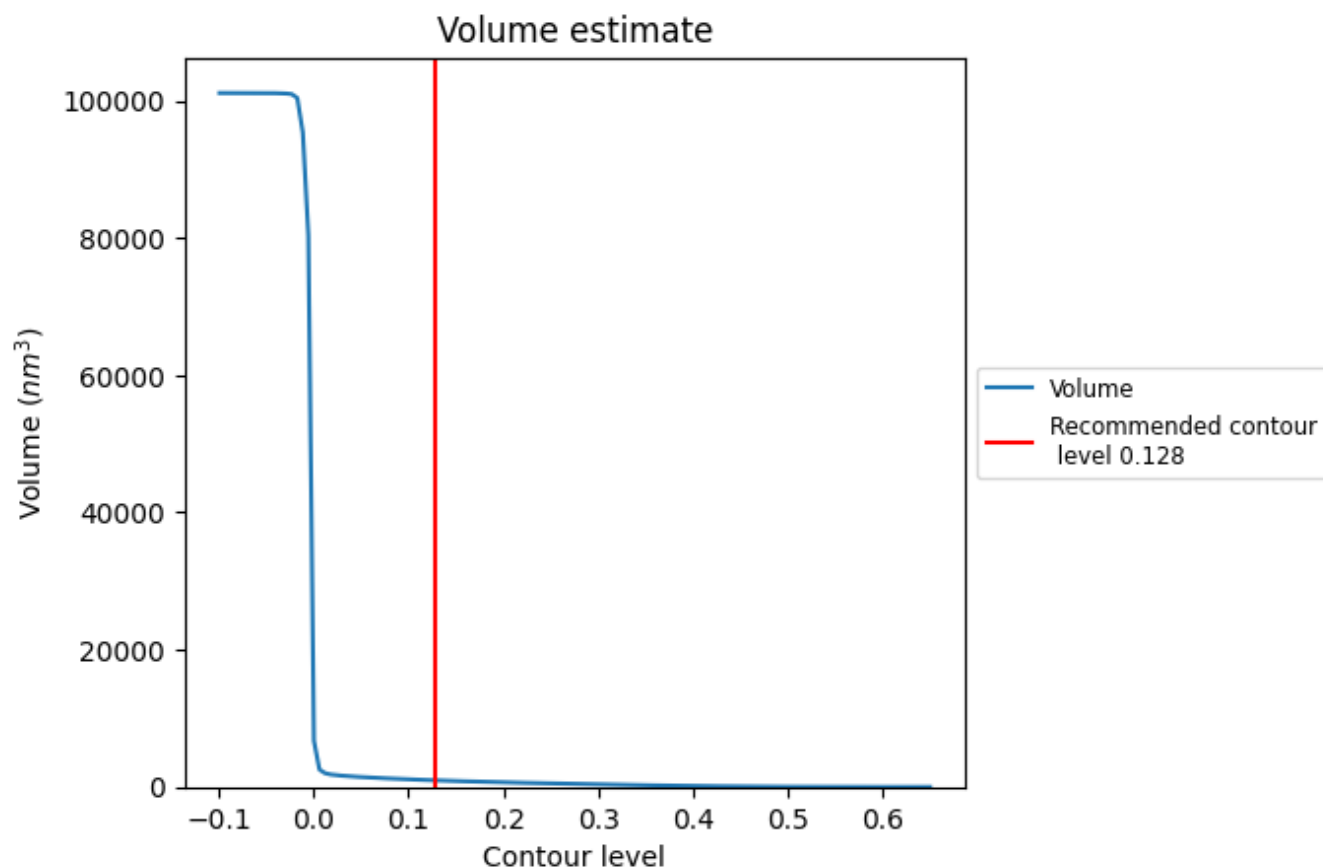
This section contains the results of statistical analysis of the map.

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.

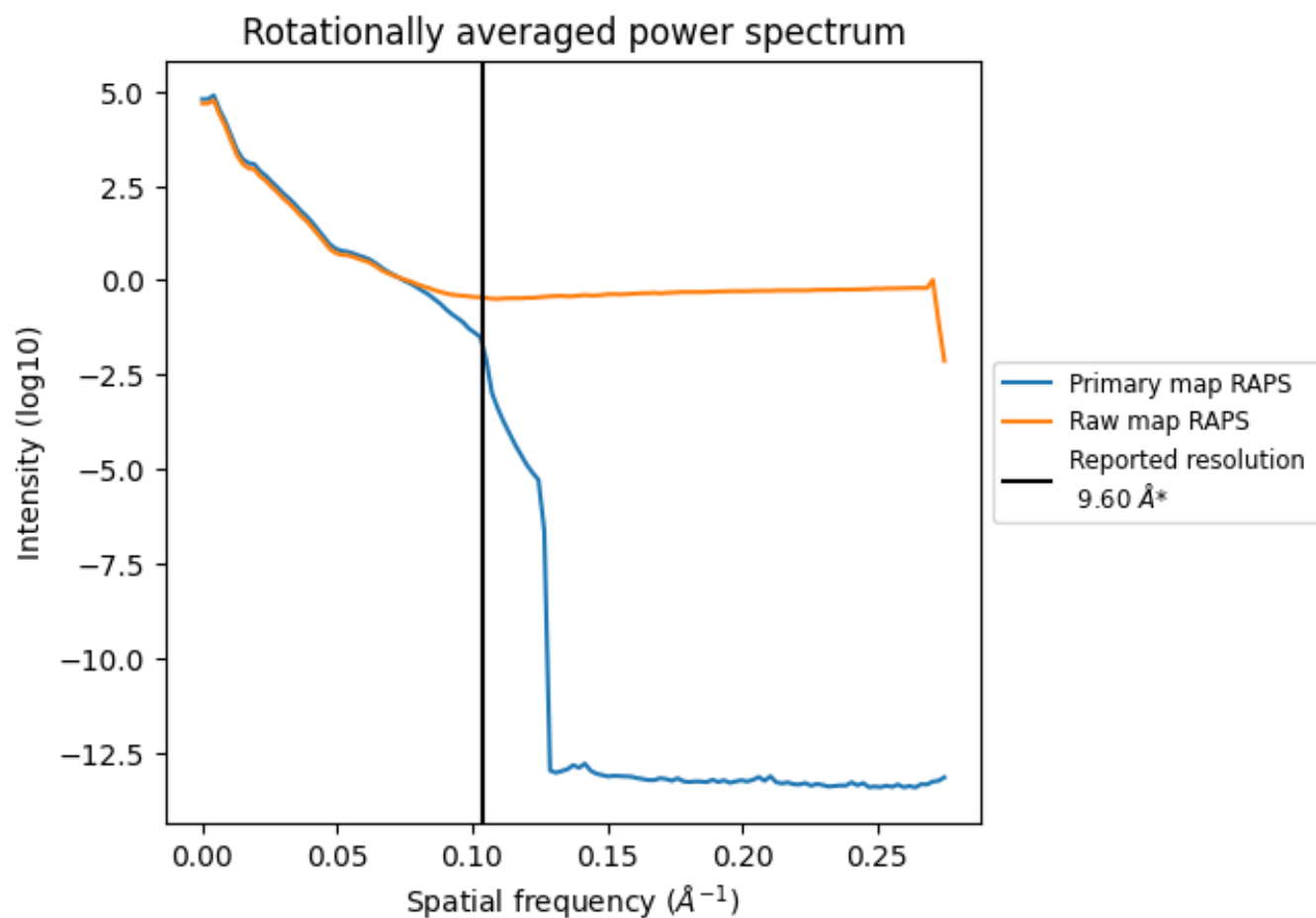
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 963 nm^3 ; this corresponds to an approximate mass of 870 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 ⓘ

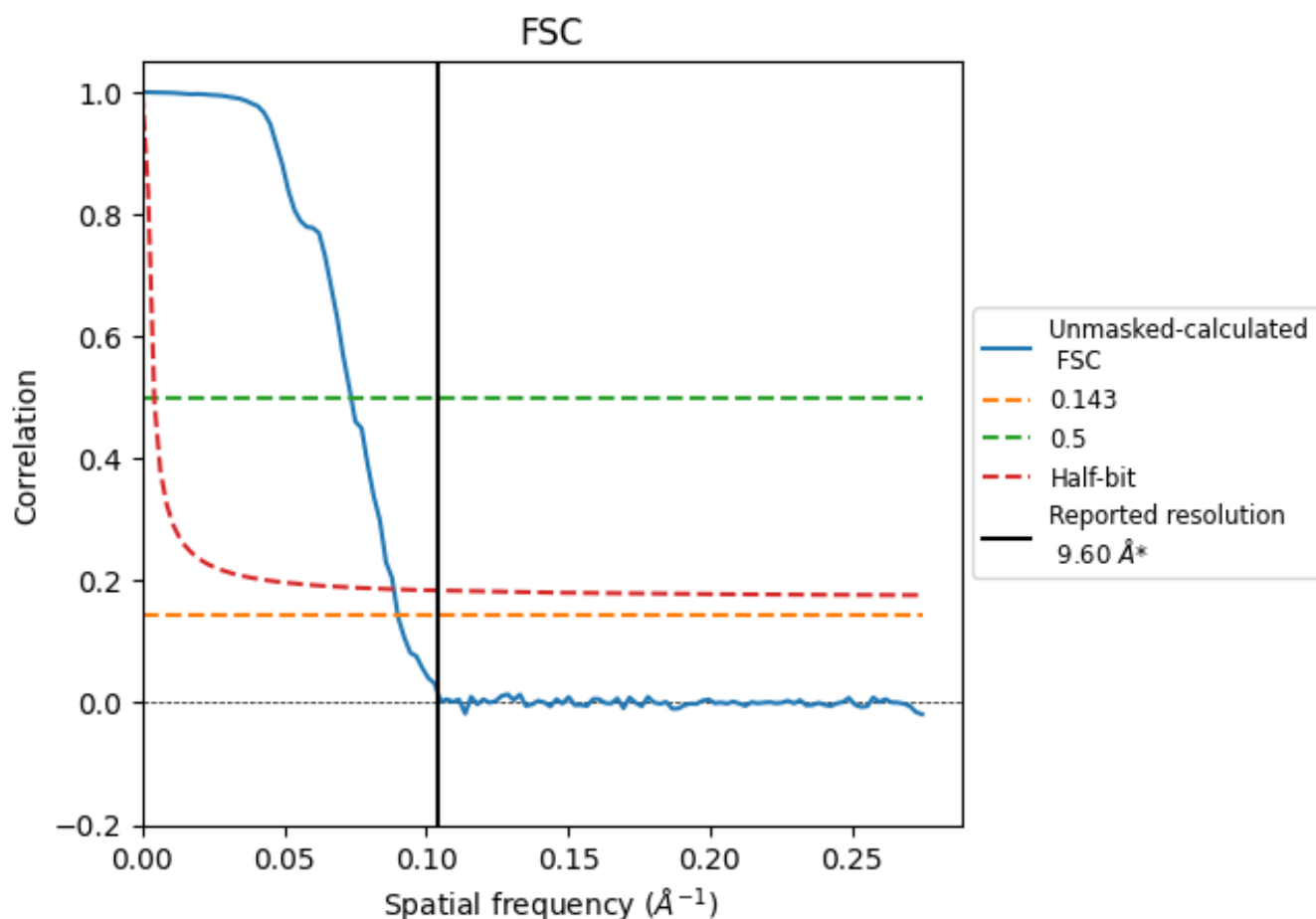


*Reported resolution corresponds to spatial frequency of 0.104 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.104 Å⁻¹

8.2 Resolution estimates [i](#)

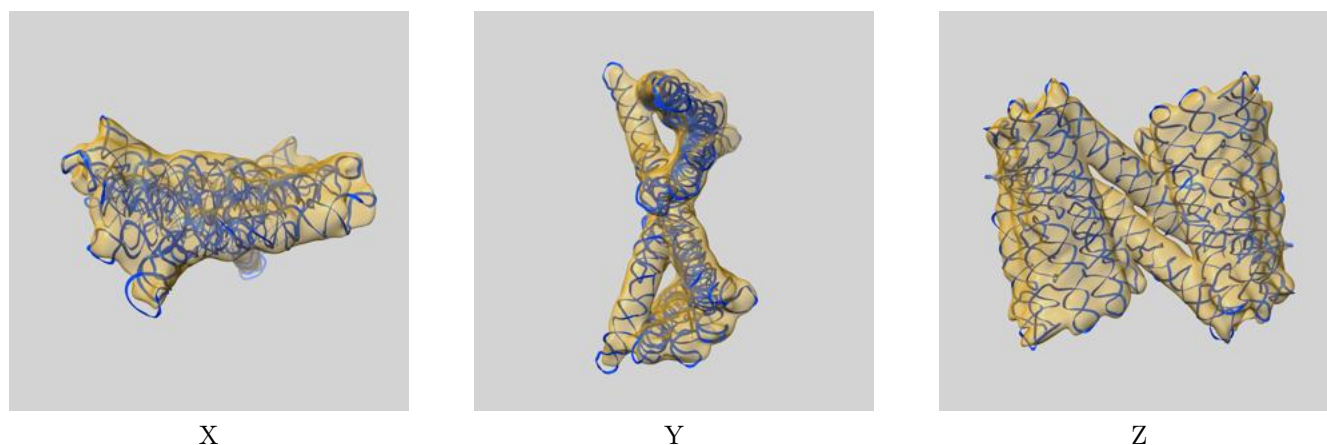
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	11.11	13.59	11.29

*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 11.11 differs from the reported value 9.6 by more than 10 %

9 Map-model fit [i](#)

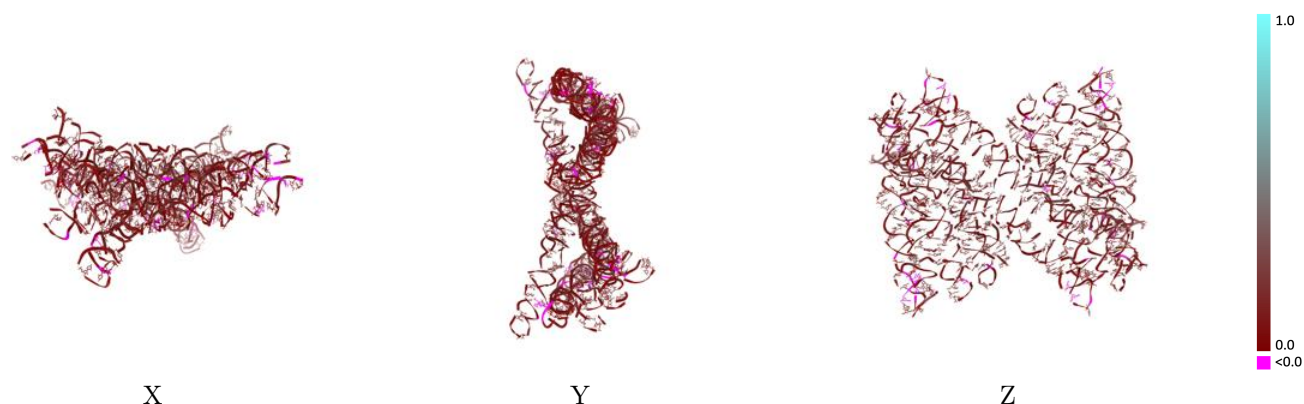
This section contains information regarding the fit between EMDB map EMD-54779 and PDB model 9SD9. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



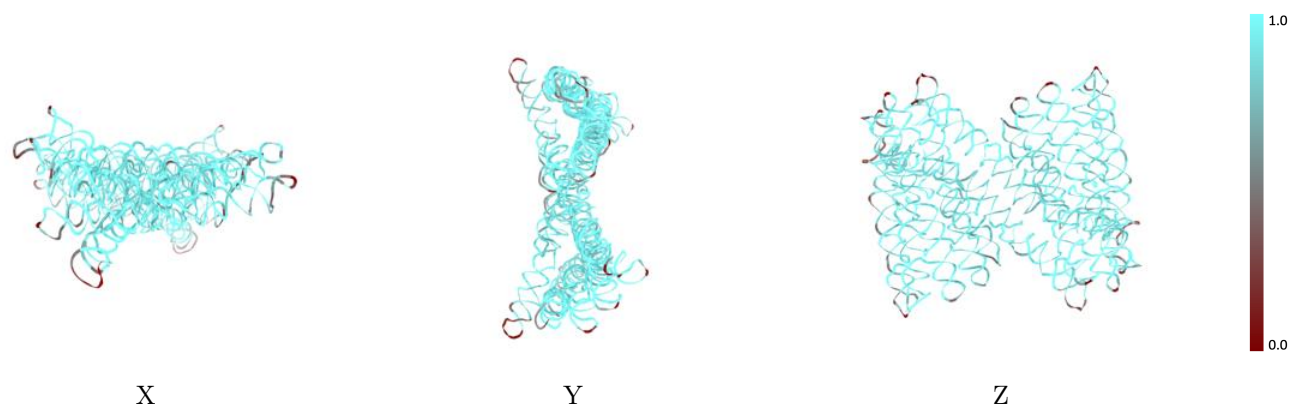
The images above show the 3D surface view of the map at the recommended contour level 0.128 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



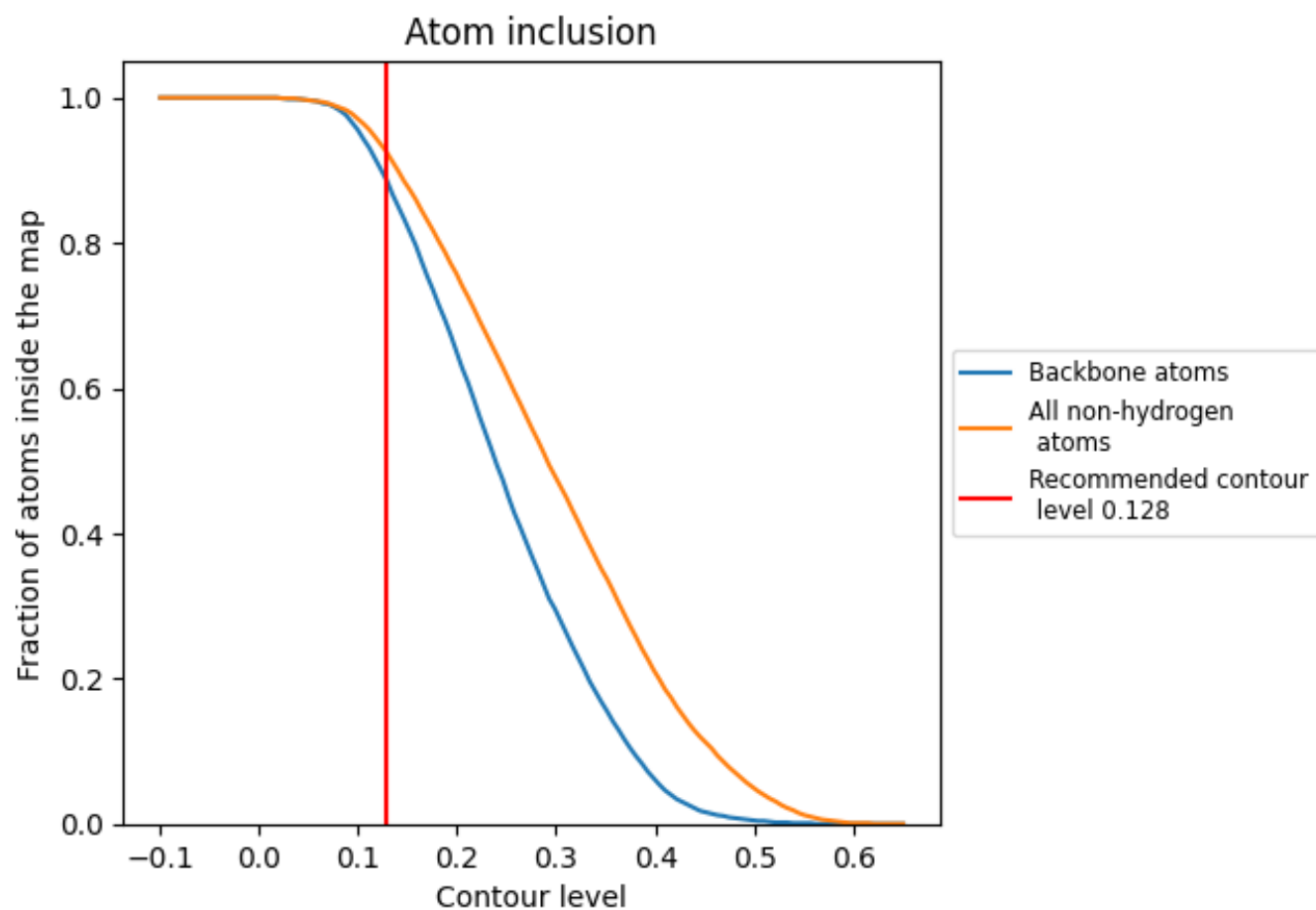
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.128).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 93% 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 (0.128) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9270	<div></div> 0.0950
A	<div></div> 0.9260	<div></div> 0.0940
B	<div></div> 0.9280	<div></div> 0.0950

