



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 12:12 PM UTC

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

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

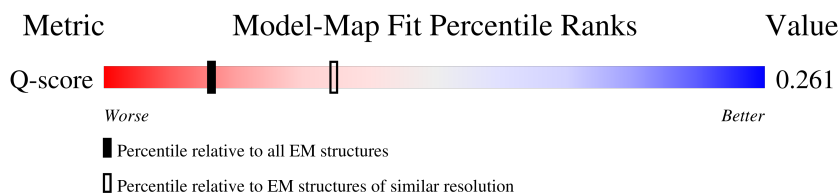
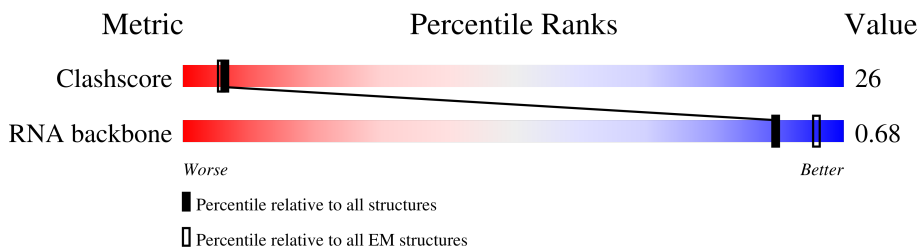
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

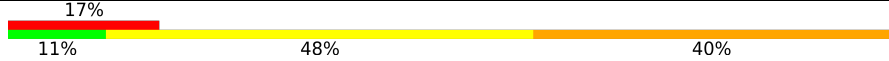
The reported resolution of this entry is 4.41 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
RNA backbone	8273	3508	-
Q-score	-	25397	3133 (3.91 - 4.91)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	238	

2 Entry composition

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

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

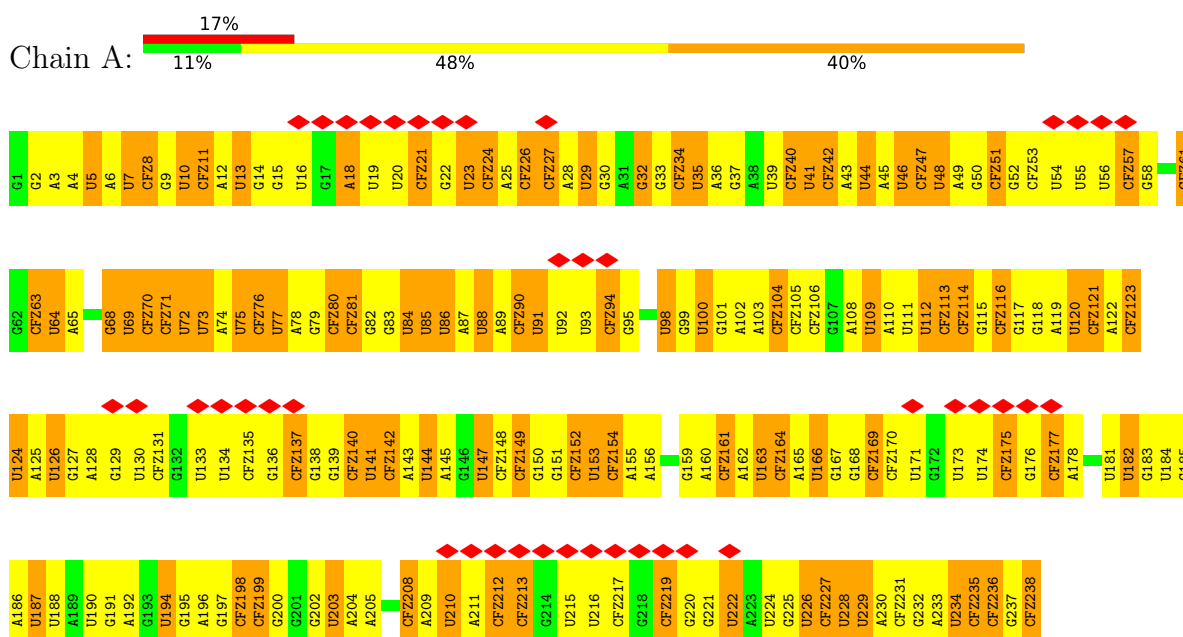
- Molecule 1 is a RNA chain called DNA/RNA (238-MER).

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

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DNA/RNA (238-MER)



4 Experimental information

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.54	17/2856 (0.6%)	0.29	0/4403

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	16	UFT	O3'-P	5.93	1.62	1.56
1	A	184	UFT	O3'-P	5.87	1.62	1.56
1	A	203	UFT	O3'-P	5.74	1.61	1.56
1	A	109	UFT	O3'-P	5.68	1.61	1.56
1	A	86	UFT	O3'-P	5.66	1.61	1.56
1	A	64	UFT	O3'-P	5.43	1.61	1.56
1	A	73	UFT	O3'-P	5.40	1.61	1.56
1	A	188	UFT	O3'-P	5.39	1.61	1.56
1	A	35	UFT	O3'-P	5.38	1.61	1.56
1	A	182	UFT	O3'-P	5.37	1.61	1.56
1	A	210	UFT	O3'-P	5.17	1.61	1.56
1	A	77	UFT	O3'-P	5.13	1.61	1.56
1	A	171	UFT	O3'-P	5.12	1.61	1.56
1	A	98	UFT	O3'-P	5.11	1.61	1.56
1	A	44	UFT	O3'-P	5.10	1.61	1.56
1	A	48	UFT	O3'-P	5.05	1.61	1.56
1	A	13	UFT	O3'-P	5.02	1.61	1.56

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5050	0	2426	191	0
All	All	5050	0	2426	191	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (191) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:A:H61	1:A:98:UFT:HN3	1.33	0.76
1:A:75:UFT:H2'	1:A:76:CFZ:H6	1.66	0.76
1:A:123:CFZ:H2'	1:A:124:UFT:H6	1.68	0.74
1:A:112:UFT:H2'	1:A:113:CFZ:H6	1.70	0.73
1:A:225:G:H3'	1:A:226:UFT:H6	1.71	0.73
1:A:162:A:H2'	1:A:163:UFT:H6	1.71	0.72
1:A:208:CFZ:N3	1:A:225:G:O6	2.24	0.70
1:A:3:A:H2'	1:A:4:A:C8	2.27	0.70
1:A:47:CFZ:H2'	1:A:48:UFT:H6	1.73	0.70
1:A:24:CFZ:H2'	1:A:25:A:H8	1.57	0.69
1:A:72:UFT:H2'	1:A:73:UFT:H6	1.74	0.69
1:A:18:A:N1	1:A:23:UFT:O4	2.26	0.68
1:A:69:UFT:H2'	1:A:70:CFZ:H6	1.75	0.67
1:A:122:A:N6	1:A:232:G:O6	2.27	0.67
1:A:108:A:H2'	1:A:109:UFT:H6	1.75	0.67
1:A:163:UFT:H2'	1:A:164:CFZ:H6	1.75	0.67
1:A:100:UFT:H2'	1:A:101:G:H8	1.59	0.67
1:A:166:UFT:C2	1:A:183:G:O6	2.44	0.65
1:A:2:G:O6	1:A:3:A:N6	2.29	0.65
1:A:229:UFT:H2'	1:A:230:A:H8	1.61	0.65
1:A:44:UFT:H2'	1:A:45:A:H8	1.60	0.65
1:A:137:CFZ:H6	1:A:137:CFZ:O5'	1.97	0.65
1:A:40:CFZ:H2'	1:A:41:UFT:H6	1.80	0.64
1:A:114:CFZ:H2'	1:A:115:G:C8	2.33	0.64
1:A:211:A:H61	1:A:222:UFT:HN3	1.46	0.64
1:A:213:CFZ:HN4	1:A:220:G:H1	1.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:G:H2'	1:A:118:G:C8	2.34	0.63
1:A:166:UFT:O2	1:A:183:G:C6	2.50	0.63
1:A:153:UFT:H2'	1:A:154:CFZ:H6	1.79	0.63
1:A:137:CFZ:H2'	1:A:138:G:C8	2.33	0.63
1:A:70:CFZ:H2'	1:A:71:CFZ:H6	1.79	0.63
1:A:41:UFT:H2'	1:A:42:CFZ:H6	1.80	0.63
1:A:68:G:H2'	1:A:69:UFT:H6	1.80	0.62
1:A:42:CFZ:H2'	1:A:43:A:H8	1.65	0.62
1:A:10:UFT:H2'	1:A:11:CFZ:H6	1.82	0.61
1:A:9:G:H2'	1:A:10:UFT:H6	1.81	0.61
1:A:89:A:H2'	1:A:90:CFZ:H6	1.82	0.61
1:A:68:G:H8	1:A:187:UFT:H2'	1.66	0.60
1:A:167:G:O6	1:A:182:UFT:O2	2.19	0.60
1:A:166:UFT:O2	1:A:183:G:O6	2.19	0.60
1:A:229:UFT:H2'	1:A:230:A:C8	2.37	0.60
1:A:80:CFZ:H2'	1:A:81:CFZ:H6	1.83	0.59
1:A:46:UFT:H2'	1:A:47:CFZ:H6	1.85	0.59
1:A:114:CFZ:H2'	1:A:115:G:H8	1.67	0.59
1:A:29:UFT:H2'	1:A:30:G:H8	1.69	0.58
1:A:5:UFT:H2'	1:A:6:A:C8	2.39	0.58
1:A:84:UFT:H2'	1:A:85:UFT:H6	1.84	0.58
1:A:147:UFT:H2'	1:A:232:G:H8	1.67	0.58
1:A:161:CFZ:H2'	1:A:162:A:C8	2.37	0.58
1:A:43:A:H2'	1:A:44:UFT:H6	1.85	0.58
1:A:144:UFT:H2'	1:A:145:A:C8	2.40	0.57
1:A:116:CFZ:H2'	1:A:117:G:C8	2.38	0.57
1:A:150:G:H2'	1:A:151:G:H8	1.69	0.57
1:A:88:UFT:H2'	1:A:89:A:H8	1.69	0.57
1:A:27:CFZ:H2'	1:A:28:A:C8	2.39	0.57
1:A:27:CFZ:H2'	1:A:28:A:H8	1.69	0.57
1:A:83:G:H2'	1:A:84:UFT:H6	1.87	0.57
1:A:57:CFZ:F2'	1:A:58:G:N2	2.26	0.56
1:A:82:G:H2'	1:A:83:G:H8	1.70	0.56
1:A:124:UFT:H2'	1:A:125:A:H8	1.70	0.56
1:A:159:G:H2'	1:A:160:A:C8	2.40	0.56
1:A:115:G:H2'	1:A:116:CFZ:H6	1.88	0.56
1:A:118:G:H2'	1:A:119:A:C8	2.41	0.56
1:A:12:A:H2'	1:A:13:UFT:H6	1.86	0.55
1:A:152:CFZ:H2'	1:A:153:UFT:H6	1.87	0.55
1:A:23:UFT:H2'	1:A:24:CFZ:H6	1.87	0.55
1:A:24:CFZ:H2'	1:A:25:A:C8	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:CFZ:H2'	1:A:35:UFT:H6	1.87	0.55
1:A:82:G:H2'	1:A:83:G:C8	2.42	0.55
1:A:150:G:H2'	1:A:151:G:C8	2.42	0.54
1:A:29:UFT:H2'	1:A:30:G:C8	2.42	0.54
1:A:137:CFZ:H2'	1:A:138:G:H8	1.71	0.54
1:A:18:A:H2	1:A:23:UFT:HN3	1.55	0.54
1:A:73:UFT:H2'	1:A:74:A:C8	2.42	0.54
1:A:185:G:H2'	1:A:186:A:C8	2.43	0.54
1:A:35:UFT:H2'	1:A:36:A:H8	1.73	0.53
1:A:227:CFZ:H2'	1:A:228:UFT:H6	1.89	0.53
1:A:25:A:H2'	1:A:26:CFZ:H6	1.90	0.53
1:A:14:G:H2'	1:A:15:G:C8	2.44	0.53
1:A:21:CFZ:O4'	1:A:22:G:N2	2.35	0.53
1:A:89:A:N6	1:A:98:UFT:HN3	2.04	0.53
1:A:122:A:H2'	1:A:123:CFZ:H6	1.91	0.53
1:A:177:CFZ:H2'	1:A:178:A:C8	2.45	0.53
1:A:74:A:H2'	1:A:75:UFT:H6	1.89	0.52
1:A:235:CFZ:F2'	1:A:236:CFZ:O4'	2.17	0.52
1:A:142:CFZ:H2'	1:A:143:A:C8	2.43	0.52
1:A:175:CFZ:F2'	1:A:176:G:OP2	2.17	0.52
1:A:219:CFZ:H2'	1:A:220:G:C8	2.44	0.52
1:A:35:UFT:H2'	1:A:36:A:C8	2.45	0.52
1:A:76:CFZ:H2'	1:A:77:UFT:H6	1.90	0.52
1:A:154:CFZ:H2'	1:A:155:A:C8	2.45	0.51
1:A:160:A:H2'	1:A:161:CFZ:H6	1.92	0.51
1:A:68:G:C8	1:A:187:UFT:H2'	2.45	0.51
1:A:51:CFZ:H2'	1:A:52:G:C8	2.46	0.51
1:A:167:G:C6	1:A:182:UFT:O2	2.63	0.51
1:A:238:CFZ:H6	1:A:238:CFZ:O5'	2.09	0.51
1:A:7:UFT:H2'	1:A:8:CFZ:H6	1.93	0.51
1:A:199:CFZ:H2'	1:A:200:G:C8	2.45	0.51
1:A:79:G:H2'	1:A:80:CFZ:H6	1.92	0.51
1:A:141:UFT:F2'	1:A:142:CFZ:O4'	2.19	0.51
1:A:144:UFT:H2'	1:A:145:A:H8	1.75	0.50
1:A:120:UFT:HN3	1:A:233:A:H61	1.58	0.50
1:A:151:G:H2'	1:A:152:CFZ:H6	1.93	0.50
1:A:51:CFZ:H2'	1:A:52:G:H8	1.76	0.50
1:A:81:CFZ:H2'	1:A:82:G:H8	1.77	0.50
1:A:197:G:H2'	1:A:198:CFZ:H6	1.94	0.50
1:A:136:G:H2'	1:A:137:CFZ:O4'	2.11	0.49
1:A:204:A:H2'	1:A:205:A:C8	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:A:H2'	1:A:104:CFZ:H6	1.94	0.49
1:A:209:A:H2'	1:A:210:UFT:H6	1.95	0.49
1:A:115:G:O2'	1:A:116:CFZ:O5'	2.25	0.49
1:A:142:CFZ:H2'	1:A:143:A:H8	1.78	0.49
1:A:220:G:H2'	1:A:221:G:H8	1.77	0.49
1:A:128:A:N6	1:A:141:UFT:HN3	2.11	0.49
1:A:88:UFT:H2'	1:A:89:A:C8	2.47	0.49
1:A:94:CFZ:F2'	1:A:95:G:OP2	2.21	0.49
1:A:161:CFZ:H2'	1:A:162:A:H8	1.77	0.48
1:A:61:CFZ:H6	1:A:61:CFZ:O5'	2.13	0.48
1:A:167:G:O6	1:A:182:UFT:C2	2.61	0.48
1:A:198:CFZ:H2'	1:A:199:CFZ:H6	1.95	0.48
1:A:115:G:H2'	1:A:116:CFZ:C6	2.43	0.48
1:A:32:G:O6	1:A:81:CFZ:N3	2.47	0.48
1:A:87:A:H2'	1:A:88:UFT:H6	1.96	0.48
1:A:126:UFT:H2'	1:A:127:G:C8	2.48	0.48
1:A:42:CFZ:H2'	1:A:43:A:C8	2.47	0.48
1:A:202:G:H2'	1:A:203:UFT:H6	1.96	0.47
1:A:85:UFT:H2'	1:A:86:UFT:H6	1.94	0.47
1:A:14:G:H2'	1:A:15:G:H8	1.79	0.47
1:A:128:A:H61	1:A:141:UFT:HN3	1.62	0.47
1:A:64:UFT:H2'	1:A:65:A:C8	2.49	0.47
1:A:74:A:H2'	1:A:75:UFT:C6	2.44	0.47
1:A:232:G:C2	1:A:233:A:N7	2.82	0.47
1:A:90:CFZ:H2'	1:A:91:UFT:H6	1.97	0.47
1:A:191:G:H2'	1:A:192:A:C8	2.49	0.47
1:A:22:G:H3'	1:A:23:UFT:H6	1.97	0.47
1:A:23:UFT:H6	1:A:23:UFT:O5'	2.15	0.46
1:A:233:A:H2'	1:A:234:UFT:H6	1.96	0.46
1:A:109:UFT:H2'	1:A:110:A:C8	2.51	0.46
1:A:100:UFT:H2'	1:A:101:G:C8	2.46	0.46
1:A:86:UFT:H2'	1:A:87:A:C8	2.50	0.46
1:A:159:G:H2'	1:A:160:A:H8	1.81	0.46
1:A:221:G:H2'	1:A:222:UFT:H6	1.98	0.46
1:A:6:A:H2'	1:A:7:UFT:O4'	2.16	0.46
1:A:126:UFT:H2'	1:A:127:G:H8	1.79	0.46
1:A:73:UFT:H2'	1:A:74:A:H8	1.81	0.45
1:A:5:UFT:O5'	1:A:5:UFT:H6	2.15	0.45
1:A:227:CFZ:H2'	1:A:228:UFT:C6	2.46	0.45
1:A:196:A:H2'	1:A:197:G:H8	1.80	0.45
1:A:102:A:H2'	1:A:103:A:C8	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:UFT:H2'	1:A:125:A:C8	2.49	0.45
1:A:234:UFT:H6	1:A:234:UFT:OP2	2.16	0.45
1:A:71:CFZ:H2'	1:A:72:UFT:H6	1.99	0.45
1:A:194:UFT:H2'	1:A:195:G:C8	2.52	0.45
1:A:112:UFT:C5	1:A:113:CFZ:H5	2.47	0.44
1:A:63:CFZ:H2'	1:A:64:UFT:H6	1.98	0.44
1:A:219:CFZ:H2'	1:A:220:G:H8	1.80	0.44
1:A:228:UFT:H2'	1:A:229:UFT:C6	2.48	0.44
1:A:44:UFT:H2'	1:A:45:A:C8	2.47	0.43
1:A:121:CFZ:H2'	1:A:122:A:C8	2.53	0.43
1:A:220:G:H2'	1:A:221:G:C8	2.52	0.43
1:A:77:UFT:H2'	1:A:78:A:H8	1.84	0.43
1:A:36:A:H2'	1:A:37:G:H8	1.84	0.43
1:A:186:A:H2'	1:A:187:UFT:O4'	2.19	0.43
1:A:138:G:H2'	1:A:139:G:H8	1.83	0.43
1:A:177:CFZ:H2'	1:A:178:A:H8	1.81	0.43
1:A:203:UFT:H2'	1:A:204:A:C8	2.55	0.42
1:A:2:G:C6	1:A:3:A:N6	2.87	0.42
1:A:36:A:H2'	1:A:37:G:C8	2.55	0.42
1:A:108:A:H2'	1:A:109:UFT:C6	2.48	0.42
1:A:237:G:H2'	1:A:238:CFZ:C6	2.49	0.42
1:A:98:UFT:H2'	1:A:99:G:C8	2.53	0.42
1:A:211:A:N6	1:A:222:UFT:HN3	2.15	0.42
1:A:102:A:H2'	1:A:103:A:H8	1.84	0.42
1:A:33:G:H2'	1:A:34:CFZ:H6	2.02	0.42
1:A:208:CFZ:C2	1:A:225:G:H1	2.32	0.42
1:A:40:CFZ:H2'	1:A:41:UFT:C6	2.48	0.41
1:A:211:A:H2'	1:A:212:CFZ:O4'	2.20	0.41
1:A:212:CFZ:H2'	1:A:213:CFZ:H6	2.02	0.41
1:A:129:G:O6	1:A:140:CFZ:N3	2.54	0.41
1:A:143:A:H2'	1:A:144:UFT:H6	2.02	0.41
1:A:168:G:H2'	1:A:169:CFZ:H6	2.03	0.41
1:A:4:A:H2'	1:A:5:UFT:C6	2.51	0.41
1:A:112:UFT:C6	1:A:113:CFZ:H5	2.50	0.41
1:A:149:CFZ:H2'	1:A:150:G:C8	2.56	0.41
1:A:175:CFZ:H6	1:A:175:CFZ:O5'	2.21	0.41
1:A:208:CFZ:O2	1:A:225:G:N1	2.44	0.41
1:A:196:A:H2'	1:A:197:G:C8	2.56	0.41
1:A:199:CFZ:H2'	1:A:200:G:H8	1.86	0.41
1:A:119:A:H2'	1:A:120:UFT:O4'	2.21	0.40
1:A:165:A:H2'	1:A:166:UFT:O4'	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:A:H2'	1:A:50:G:H8	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

5.3.3 RNA [i](#)

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

All (4) RNA backbone outliers are listed below:

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

There are no RNA pucker outliers to report.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	UFT	A	181	1	18,21,22	2.71	10 (55%)	25,30,33	2.07	7 (28%)
1	CFZ	A	123	1	18,21,22	2.54	7 (38%)	25,30,33	1.25	1 (4%)
1	CFZ	A	238	1	18,21,22	2.51	7 (38%)	25,30,33	1.38	3 (12%)
1	CFZ	A	106	1	18,21,22	2.55	7 (38%)	25,30,33	1.19	2 (8%)
1	UFT	A	124	1	18,21,22	2.64	9 (50%)	25,30,33	1.94	6 (24%)
1	UFT	A	194	1	18,21,22	2.67	10 (55%)	25,30,33	2.05	7 (28%)
1	UFT	A	73	1	18,21,22	2.67	10 (55%)	25,30,33	1.99	6 (24%)
1	UFT	A	229	1	18,21,22	2.69	10 (55%)	25,30,33	2.06	7 (28%)
1	UFT	A	111	1	18,21,22	2.62	10 (55%)	25,30,33	1.85	7 (28%)
1	UFT	A	190	1	18,21,22	2.64	10 (55%)	25,30,33	2.05	8 (32%)
1	UFT	A	84	1	18,21,22	2.67	10 (55%)	25,30,33	2.07	7 (28%)
1	CFZ	A	199	1	18,21,22	2.54	7 (38%)	25,30,33	1.24	3 (12%)
1	UFT	A	54	1	18,21,22	2.64	10 (55%)	25,30,33	2.15	7 (28%)
1	UFT	A	153	1	18,21,22	2.68	9 (50%)	25,30,33	2.01	7 (28%)
1	CFZ	A	114	1	18,21,22	2.54	6 (33%)	25,30,33	1.57	3 (12%)
1	CFZ	A	213	1	18,21,22	2.56	7 (38%)	25,30,33	1.42	4 (16%)
1	CFZ	A	104	1	18,21,22	2.54	7 (38%)	25,30,33	1.20	2 (8%)
1	CFZ	A	169	1	18,21,22	2.53	7 (38%)	25,30,33	1.35	2 (8%)
1	CFZ	A	137	1	18,21,22	2.53	6 (33%)	25,30,33	1.32	4 (16%)
1	UFT	A	228	1	18,21,22	2.68	10 (55%)	25,30,33	2.22	7 (28%)
1	CFZ	A	231	1	18,21,22	2.46	7 (38%)	25,30,33	1.38	4 (16%)
1	UFT	A	23	1	18,21,22	2.64	10 (55%)	25,30,33	1.95	7 (28%)
1	CFZ	A	140	1	18,21,22	2.46	7 (38%)	25,30,33	1.37	4 (16%)
1	CFZ	A	61	1	18,21,22	2.51	7 (38%)	25,30,33	1.39	3 (12%)
1	UFT	A	222	1	18,21,22	2.67	10 (55%)	25,30,33	2.10	7 (28%)
1	UFT	A	171	1	18,21,22	2.69	10 (55%)	25,30,33	2.10	6 (24%)
1	CFZ	A	227	1	18,21,22	2.56	6 (33%)	25,30,33	1.20	1 (4%)
1	CFZ	A	51	1	18,21,22	2.56	7 (38%)	25,30,33	1.44	2 (8%)
1	UFT	A	133	1	18,21,22	2.62	10 (55%)	25,30,33	2.07	8 (32%)
1	UFT	A	224	1	18,21,22	2.64	10 (55%)	25,30,33	2.18	8 (32%)
1	UFT	A	19	1	18,21,22	2.63	10 (55%)	25,30,33	2.11	8 (32%)
1	UFT	A	166	1	18,21,22	2.64	10 (55%)	25,30,33	2.01	6 (24%)
1	UFT	A	163	1	18,21,22	2.73	10 (55%)	25,30,33	2.18	8 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	UFT	A	92	1	18,21,22	2.60	10 (55%)	25,30,33	2.05	7 (28%)
1	UFT	A	72	1	18,21,22	2.67	10 (55%)	25,30,33	2.01	6 (24%)
1	CFZ	A	27	1	18,21,22	2.53	7 (38%)	25,30,33	1.23	2 (8%)
1	UFT	A	20	1	18,21,22	2.58	10 (55%)	25,30,33	2.20	8 (32%)
1	UFT	A	91	1	18,21,22	2.68	10 (55%)	25,30,33	2.12	8 (32%)
1	UFT	A	55	1	18,21,22	2.63	10 (55%)	25,30,33	2.05	8 (32%)
1	CFZ	A	217	1	18,21,22	2.49	7 (38%)	25,30,33	1.30	2 (8%)
1	UFT	A	234	1	18,21,22	2.64	10 (55%)	25,30,33	2.16	8 (32%)
1	UFT	A	86	1	18,21,22	2.69	10 (55%)	25,30,33	1.97	7 (28%)
1	CFZ	A	149	1	18,21,22	2.51	7 (38%)	25,30,33	1.34	3 (12%)
1	UFT	A	144	1	18,21,22	2.66	10 (55%)	25,30,33	2.05	7 (28%)
1	UFT	A	7	1	18,21,22	2.67	9 (50%)	25,30,33	2.04	5 (20%)
1	CFZ	A	154	1	18,21,22	2.52	7 (38%)	25,30,33	1.25	3 (12%)
1	UFT	A	46	1	18,21,22	2.68	9 (50%)	25,30,33	2.03	7 (28%)
1	UFT	A	88	1	18,21,22	2.66	10 (55%)	25,30,33	1.97	8 (32%)
1	UFT	A	216	1	18,21,22	2.62	10 (55%)	25,30,33	2.09	6 (24%)
1	CFZ	A	152	1	18,21,22	2.53	7 (38%)	25,30,33	1.21	2 (8%)
1	CFZ	A	76	1	18,21,22	2.52	6 (33%)	25,30,33	1.33	3 (12%)
1	CFZ	A	80	1	18,21,22	2.58	7 (38%)	25,30,33	1.25	2 (8%)
1	CFZ	A	70	1	18,21,22	2.56	7 (38%)	25,30,33	1.27	3 (12%)
1	UFT	A	44	1	18,21,22	2.68	10 (55%)	25,30,33	1.99	6 (24%)
1	UFT	A	56	1	18,21,22	2.59	10 (55%)	25,30,33	2.20	8 (32%)
1	CFZ	A	24	1	18,21,22	2.52	7 (38%)	25,30,33	1.44	2 (8%)
1	CFZ	A	105	1	18,21,22	2.49	7 (38%)	25,30,33	1.16	1 (4%)
1	UFT	A	141	1	18,21,22	2.63	10 (55%)	25,30,33	2.09	7 (28%)
1	UFT	A	215	1	18,21,22	2.63	10 (55%)	25,30,33	2.03	7 (28%)
1	CFZ	A	236	1	18,21,22	2.49	7 (38%)	25,30,33	1.29	3 (12%)
1	CFZ	A	90	1	18,21,22	2.55	7 (38%)	25,30,33	1.38	3 (12%)
1	CFZ	A	175	1	18,21,22	2.42	7 (38%)	25,30,33	1.56	4 (16%)
1	UFT	A	48	1	18,21,22	2.63	10 (55%)	25,30,33	2.10	7 (28%)
1	UFT	A	174	1	18,21,22	2.62	10 (55%)	25,30,33	2.14	7 (28%)
1	CFZ	A	40	1	18,21,22	2.53	7 (38%)	25,30,33	1.25	3 (12%)
1	CFZ	A	94	1	18,21,22	2.40	7 (38%)	25,30,33	1.51	3 (12%)
1	UFT	A	93	1	18,21,22	2.59	10 (55%)	25,30,33	2.08	7 (28%)
1	UFT	A	173	1	18,21,22	2.63	10 (55%)	25,30,33	2.00	6 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	UFT	A	109	1	18,21,22	2.69	10 (55%)	25,30,33	2.28	8 (32%)
1	CFZ	A	135	1	18,21,22	2.50	7 (38%)	25,30,33	1.18	1 (4%)
1	UFT	A	226	1	18,21,22	2.63	10 (55%)	25,30,33	2.18	7 (28%)
1	UFT	A	112	1	18,21,22	2.60	10 (55%)	25,30,33	1.98	7 (28%)
1	CFZ	A	42	1	18,21,22	2.55	7 (38%)	25,30,33	1.27	2 (8%)
1	CFZ	A	170	1	18,21,22	2.51	7 (38%)	25,30,33	1.53	2 (8%)
1	CFZ	A	235	1	18,21,22	2.51	7 (38%)	25,30,33	1.37	3 (12%)
1	UFT	A	39	1	18,21,22	2.64	10 (55%)	25,30,33	2.27	8 (32%)
1	UFT	A	85	1	18,21,22	2.63	10 (55%)	25,30,33	2.16	7 (28%)
1	CFZ	A	113	1	18,21,22	2.55	6 (33%)	25,30,33	1.35	3 (12%)
1	UFT	A	29	1	18,21,22	2.67	10 (55%)	25,30,33	2.07	7 (28%)
1	UFT	A	184	1	18,21,22	2.65	10 (55%)	25,30,33	2.24	8 (32%)
1	UFT	A	188	1	18,21,22	2.61	9 (50%)	25,30,33	2.11	8 (32%)
1	UFT	A	13	1	18,21,22	2.66	10 (55%)	25,30,33	2.02	6 (24%)
1	CFZ	A	161	1	18,21,22	2.56	7 (38%)	25,30,33	1.24	2 (8%)
1	UFT	A	120	1	18,21,22	2.67	9 (50%)	25,30,33	2.06	6 (24%)
1	UFT	A	41	1	18,21,22	2.67	10 (55%)	25,30,33	1.99	6 (24%)
1	UFT	A	16	1	18,21,22	2.62	9 (50%)	25,30,33	1.84	5 (20%)
1	CFZ	A	208	1	18,21,22	2.51	7 (38%)	25,30,33	1.34	2 (8%)
1	CFZ	A	8	1	18,21,22	2.52	7 (38%)	25,30,33	1.27	2 (8%)
1	UFT	A	35	1	18,21,22	2.65	9 (50%)	25,30,33	1.95	6 (24%)
1	CFZ	A	142	1	18,21,22	2.53	6 (33%)	25,30,33	1.21	2 (8%)
1	CFZ	A	26	1	18,21,22	2.53	7 (38%)	25,30,33	1.32	2 (8%)
1	CFZ	A	198	1	18,21,22	2.54	7 (38%)	25,30,33	1.22	2 (8%)
1	UFT	A	75	1	18,21,22	2.68	10 (55%)	25,30,33	2.11	7 (28%)
1	CFZ	A	116	1	18,21,22	2.54	7 (38%)	25,30,33	1.30	2 (8%)
1	CFZ	A	212	1	18,21,22	2.49	7 (38%)	25,30,33	1.38	2 (8%)
1	CFZ	A	81	1	18,21,22	2.54	7 (38%)	25,30,33	1.31	3 (12%)
1	CFZ	A	47	1	18,21,22	2.57	7 (38%)	25,30,33	1.25	3 (12%)
1	CFZ	A	164	1	18,21,22	2.54	7 (38%)	25,30,33	1.50	3 (12%)
1	UFT	A	130	1	18,21,22	2.62	10 (55%)	25,30,33	2.07	7 (28%)
1	UFT	A	10	1	18,21,22	2.71	10 (55%)	25,30,33	2.11	8 (32%)
1	CFZ	A	21	1	18,21,22	2.49	7 (38%)	25,30,33	1.49	3 (12%)
1	CFZ	A	219	1	18,21,22	2.52	7 (38%)	25,30,33	1.52	3 (12%)
1	CFZ	A	53	1	18,21,22	2.46	7 (38%)	25,30,33	1.49	3 (12%)

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UFT	A	181	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	123	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	238	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	106	1	-	0/7/25/26	0/2/2/2
1	UFT	A	124	1	-	0/7/25/26	0/2/2/2
1	UFT	A	194	1	-	0/7/25/26	0/2/2/2
1	UFT	A	73	1	-	0/7/25/26	0/2/2/2
1	UFT	A	229	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UFT	A	111	1	-	0/7/25/26	0/2/2/2
1	UFT	A	190	1	-	0/7/25/26	0/2/2/2
1	UFT	A	84	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	199	1	-	0/7/25/26	0/2/2/2
1	UFT	A	54	1	-	2/7/25/26	0/2/2/2
1	UFT	A	153	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	114	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	213	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	104	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	169	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	137	1	-	0/7/25/26	0/2/2/2
1	UFT	A	228	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	231	1	-	0/7/25/26	0/2/2/2
1	UFT	A	23	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	140	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	61	1	-	0/7/25/26	0/2/2/2
1	UFT	A	222	1	-	0/7/25/26	0/2/2/2
1	UFT	A	171	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	227	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	51	1	-	2/7/25/26	0/2/2/2
1	UFT	A	133	1	-	0/7/25/26	0/2/2/2
1	UFT	A	224	1	-	0/7/25/26	0/2/2/2
1	UFT	A	19	1	-	2/7/25/26	0/2/2/2
1	UFT	A	166	1	-	0/7/25/26	0/2/2/2
1	UFT	A	163	1	-	0/7/25/26	0/2/2/2
1	UFT	A	92	1	-	0/7/25/26	0/2/2/2
1	UFT	A	72	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	27	1	-	0/7/25/26	0/2/2/2
1	UFT	A	20	1	-	2/7/25/26	0/2/2/2
1	UFT	A	91	1	-	2/7/25/26	0/2/2/2
1	UFT	A	55	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	217	1	-	3/7/25/26	0/2/2/2
1	UFT	A	234	1	-	3/7/25/26	0/2/2/2
1	UFT	A	86	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	149	1	-	0/7/25/26	0/2/2/2
1	UFT	A	144	1	-	0/7/25/26	0/2/2/2
1	UFT	A	7	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	154	1	-	0/7/25/26	0/2/2/2
1	UFT	A	46	1	-	0/7/25/26	0/2/2/2
1	UFT	A	88	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UFT	A	216	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	152	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	76	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	80	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	70	1	-	0/7/25/26	0/2/2/2
1	UFT	A	44	1	-	0/7/25/26	0/2/2/2
1	UFT	A	56	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	24	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	105	1	-	0/7/25/26	0/2/2/2
1	UFT	A	141	1	-	0/7/25/26	0/2/2/2
1	UFT	A	215	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	236	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	90	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	175	1	-	2/7/25/26	0/2/2/2
1	UFT	A	48	1	-	0/7/25/26	0/2/2/2
1	UFT	A	174	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	40	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	94	1	-	2/7/25/26	0/2/2/2
1	UFT	A	93	1	-	2/7/25/26	0/2/2/2
1	UFT	A	173	1	-	0/7/25/26	0/2/2/2
1	UFT	A	109	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	135	1	-	2/7/25/26	0/2/2/2
1	UFT	A	226	1	-	3/7/25/26	0/2/2/2
1	UFT	A	112	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	42	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	170	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	235	1	-	3/7/25/26	0/2/2/2
1	UFT	A	39	1	-	0/7/25/26	0/2/2/2
1	UFT	A	85	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	113	1	-	0/7/25/26	0/2/2/2
1	UFT	A	29	1	-	0/7/25/26	0/2/2/2
1	UFT	A	184	1	-	3/7/25/26	0/2/2/2
1	UFT	A	188	1	-	0/7/25/26	0/2/2/2
1	UFT	A	13	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	161	1	-	0/7/25/26	0/2/2/2
1	UFT	A	120	1	-	0/7/25/26	0/2/2/2
1	UFT	A	41	1	-	0/7/25/26	0/2/2/2
1	UFT	A	16	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	208	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	8	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UFT	A	35	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	142	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	26	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	198	1	-	0/7/25/26	0/2/2/2
1	UFT	A	75	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	116	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	212	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	81	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	47	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	164	1	-	0/7/25/26	0/2/2/2
1	UFT	A	130	1	-	0/7/25/26	0/2/2/2
1	UFT	A	10	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	21	1	-	5/7/25/26	0/2/2/2
1	CFZ	A	219	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	53	1	-	0/7/25/26	0/2/2/2
1	UFT	A	126	1	-	0/7/25/26	0/2/2/2
1	UFT	A	203	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	63	1	-	0/7/25/26	0/2/2/2
1	UFT	A	187	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	34	1	-	0/7/25/26	0/2/2/2
1	UFT	A	64	1	-	0/7/25/26	0/2/2/2
1	UFT	A	98	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	121	1	-	0/7/25/26	0/2/2/2
1	UFT	A	210	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	71	1	-	0/7/25/26	0/2/2/2
1	UFT	A	147	1	-	2/7/25/26	0/2/2/2
1	UFT	A	77	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	57	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	177	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	11	1	-	0/7/25/26	0/2/2/2
1	UFT	A	69	1	-	0/7/25/26	0/2/2/2
1	UFT	A	100	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	148	1	-	2/7/25/26	0/2/2/2
1	UFT	A	134	1	-	2/7/25/26	0/2/2/2
1	UFT	A	5	1	-	0/7/25/26	0/2/2/2
1	UFT	A	182	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	131	1	-	0/7/25/26	0/2/2/2

All (1063) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	163	UFT	C2-N1	5.15	1.46	1.38
1	A	46	UFT	C2-N1	5.13	1.46	1.38
1	A	86	UFT	C2-N1	5.10	1.46	1.38
1	A	91	UFT	C2-N1	5.09	1.46	1.38
1	A	10	UFT	C2-N1	5.06	1.46	1.38
1	A	228	UFT	C2-N1	5.04	1.46	1.38
1	A	88	UFT	C2-N1	5.03	1.46	1.38
1	A	184	UFT	C2-N1	5.03	1.46	1.38
1	A	109	UFT	C2-N1	5.00	1.46	1.38
1	A	75	UFT	C2-N1	4.99	1.46	1.38
1	A	182	UFT	C2-N1	4.99	1.46	1.38
1	A	210	UFT	C2-N1	4.99	1.46	1.38
1	A	73	UFT	C2-N1	4.98	1.46	1.38
1	A	77	UFT	C2-N1	4.97	1.46	1.38
1	A	80	CFZ	C2'-C3'	-4.97	1.46	1.52
1	A	13	UFT	C2-N1	4.97	1.46	1.38
1	A	69	UFT	C2-N1	4.97	1.46	1.38
1	A	72	UFT	C2-N1	4.95	1.46	1.38
1	A	194	UFT	C2-N1	4.95	1.46	1.38
1	A	147	UFT	C2-N1	4.94	1.46	1.38
1	A	181	UFT	C2-N1	4.94	1.46	1.38
1	A	126	UFT	C2-N1	4.93	1.46	1.38
1	A	229	UFT	C2-N1	4.93	1.46	1.38
1	A	5	UFT	C2-N1	4.92	1.46	1.38
1	A	39	UFT	C2-N1	4.91	1.46	1.38
1	A	203	UFT	C2-N1	4.91	1.46	1.38
1	A	54	UFT	C2-N1	4.91	1.46	1.38
1	A	153	UFT	C2-N1	4.91	1.46	1.38
1	A	7	UFT	C2-N1	4.90	1.46	1.38
1	A	216	UFT	C2-N1	4.89	1.46	1.38
1	A	130	UFT	C2-N1	4.89	1.46	1.38
1	A	41	UFT	C2-N1	4.89	1.46	1.38
1	A	81	CFZ	C2'-C3'	-4.88	1.46	1.52
1	A	224	UFT	C2-N1	4.88	1.46	1.38
1	A	16	UFT	C2-N1	4.87	1.46	1.38
1	A	48	UFT	C2-N1	4.87	1.46	1.38
1	A	190	UFT	C2-N1	4.87	1.46	1.38
1	A	234	UFT	C2-N1	4.87	1.46	1.38
1	A	8	CFZ	C4-N4	4.86	1.45	1.33
1	A	213	CFZ	C4-N4	4.86	1.45	1.33
1	A	84	UFT	C2-N1	4.85	1.46	1.38
1	A	100	UFT	C2-N1	4.85	1.46	1.38
1	A	29	UFT	C2-N1	4.85	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	235	CFZ	C4-N4	4.84	1.45	1.33
1	A	24	CFZ	C4-N4	4.84	1.45	1.33
1	A	120	UFT	C2-N1	4.84	1.46	1.38
1	A	34	CFZ	C4-N4	4.84	1.45	1.33
1	A	144	UFT	C2-N1	4.83	1.46	1.38
1	A	21	CFZ	C4-N4	4.83	1.45	1.33
1	A	121	CFZ	C4-N4	4.83	1.45	1.33
1	A	64	UFT	C2-N1	4.83	1.46	1.38
1	A	173	UFT	C2-N1	4.83	1.46	1.38
1	A	140	CFZ	C4-N4	4.83	1.45	1.33
1	A	175	CFZ	C4-N4	4.83	1.45	1.33
1	A	171	UFT	C2-N1	4.82	1.46	1.38
1	A	114	CFZ	C2'-C3'	-4.82	1.46	1.52
1	A	222	UFT	C2-N1	4.82	1.46	1.38
1	A	212	CFZ	C4-N4	4.81	1.45	1.33
1	A	81	CFZ	C4-N4	4.81	1.45	1.33
1	A	53	CFZ	C4-N4	4.81	1.45	1.33
1	A	61	CFZ	C4-N4	4.81	1.45	1.33
1	A	23	UFT	C2-N1	4.81	1.46	1.38
1	A	187	UFT	C2-N1	4.81	1.46	1.38
1	A	219	CFZ	C4-N4	4.81	1.45	1.33
1	A	166	UFT	C2-N1	4.81	1.46	1.38
1	A	236	CFZ	C4-N4	4.81	1.45	1.33
1	A	57	CFZ	C4-N4	4.81	1.45	1.33
1	A	44	UFT	C2-N1	4.80	1.46	1.38
1	A	231	CFZ	C4-N4	4.80	1.45	1.33
1	A	217	CFZ	C4-N4	4.80	1.45	1.33
1	A	131	CFZ	C4-N4	4.80	1.45	1.33
1	A	71	CFZ	C2'-C3'	-4.80	1.46	1.52
1	A	148	CFZ	C2'-C3'	-4.80	1.46	1.52
1	A	106	CFZ	C4-N4	4.80	1.45	1.33
1	A	135	CFZ	C4-N4	4.80	1.45	1.33
1	A	42	CFZ	C4-N4	4.80	1.45	1.33
1	A	113	CFZ	C2'-C3'	-4.79	1.46	1.52
1	A	85	UFT	C2-N1	4.79	1.46	1.38
1	A	90	CFZ	C4-N4	4.79	1.45	1.33
1	A	161	CFZ	C4-N4	4.79	1.45	1.33
1	A	164	CFZ	C4-N4	4.79	1.45	1.33
1	A	19	UFT	C2-N1	4.79	1.46	1.38
1	A	56	UFT	C2-N1	4.79	1.46	1.38
1	A	198	CFZ	C4-N4	4.78	1.45	1.33
1	A	80	CFZ	C4-N4	4.77	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	121	CFZ	C2'-C3'	-4.77	1.46	1.52
1	A	188	UFT	C2-N1	4.77	1.45	1.38
1	A	238	CFZ	C4-N4	4.76	1.45	1.33
1	A	105	CFZ	C4-N4	4.76	1.45	1.33
1	A	213	CFZ	C2'-C3'	-4.76	1.46	1.52
1	A	174	UFT	C2-N1	4.75	1.45	1.38
1	A	63	CFZ	C4-N4	4.75	1.45	1.33
1	A	208	CFZ	C4-N4	4.75	1.45	1.33
1	A	148	CFZ	C4-N4	4.75	1.45	1.33
1	A	152	CFZ	C4-N4	4.75	1.45	1.33
1	A	170	CFZ	C4-N4	4.75	1.45	1.33
1	A	70	CFZ	C4-N4	4.75	1.45	1.33
1	A	27	CFZ	C4-N4	4.74	1.45	1.33
1	A	154	CFZ	C4-N4	4.74	1.45	1.33
1	A	98	UFT	C2-N1	4.74	1.45	1.38
1	A	104	CFZ	C4-N4	4.74	1.45	1.33
1	A	93	UFT	C2-N1	4.74	1.45	1.38
1	A	55	UFT	C2-N1	4.74	1.45	1.38
1	A	51	CFZ	C4-N4	4.74	1.45	1.33
1	A	40	CFZ	C4-N4	4.74	1.45	1.33
1	A	94	CFZ	C4-N4	4.73	1.45	1.33
1	A	208	CFZ	C2'-C3'	-4.73	1.46	1.52
1	A	35	UFT	C2-N1	4.73	1.45	1.38
1	A	20	UFT	C2-N1	4.73	1.45	1.38
1	A	169	CFZ	C4-N4	4.73	1.45	1.33
1	A	134	UFT	C2-N1	4.73	1.45	1.38
1	A	215	UFT	C2-N1	4.73	1.45	1.38
1	A	34	CFZ	C2'-C3'	-4.72	1.46	1.52
1	A	11	CFZ	C4-N4	4.72	1.45	1.33
1	A	51	CFZ	C2'-C3'	-4.71	1.46	1.52
1	A	177	CFZ	C2'-C3'	-4.71	1.46	1.52
1	A	106	CFZ	C2'-C3'	-4.71	1.46	1.52
1	A	199	CFZ	C4-N4	4.71	1.45	1.33
1	A	123	CFZ	C4-N4	4.71	1.45	1.33
1	A	26	CFZ	C4-N4	4.70	1.45	1.33
1	A	71	CFZ	C4-N4	4.70	1.45	1.33
1	A	226	UFT	C2-N1	4.70	1.45	1.38
1	A	92	UFT	C2-N1	4.70	1.45	1.38
1	A	47	CFZ	C2'-C3'	-4.70	1.46	1.52
1	A	116	CFZ	C4-N4	4.70	1.45	1.33
1	A	133	UFT	C2-N1	4.70	1.45	1.38
1	A	198	CFZ	C2'-C3'	-4.69	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	141	UFT	C2-N1	4.69	1.45	1.38
1	A	227	CFZ	C2'-C3'	-4.69	1.46	1.52
1	A	227	CFZ	C4-N4	4.69	1.45	1.33
1	A	142	CFZ	C4-N4	4.69	1.45	1.33
1	A	177	CFZ	C4-N4	4.69	1.45	1.33
1	A	124	UFT	C2-N1	4.69	1.45	1.38
1	A	76	CFZ	C4-N4	4.68	1.45	1.33
1	A	113	CFZ	C4-N4	4.68	1.45	1.33
1	A	16	UFT	C6-N1	4.68	1.49	1.38
1	A	63	CFZ	C2'-C3'	-4.67	1.46	1.52
1	A	137	CFZ	C4-N4	4.67	1.45	1.33
1	A	47	CFZ	C4-N4	4.67	1.45	1.33
1	A	219	CFZ	C2'-C3'	-4.66	1.46	1.52
1	A	161	CFZ	C2'-C3'	-4.66	1.46	1.52
1	A	70	CFZ	C2'-C3'	-4.66	1.46	1.52
1	A	111	UFT	C2-N1	4.65	1.45	1.38
1	A	199	CFZ	C2'-C3'	-4.64	1.46	1.52
1	A	120	UFT	C6-N1	4.64	1.49	1.38
1	A	111	UFT	C6-N1	4.63	1.49	1.38
1	A	116	CFZ	C2'-C3'	-4.63	1.46	1.52
1	A	90	CFZ	C2'-C3'	-4.63	1.46	1.52
1	A	112	UFT	C6-N1	4.63	1.49	1.38
1	A	166	UFT	C6-N1	4.62	1.49	1.38
1	A	86	UFT	C6-N1	4.62	1.49	1.38
1	A	149	CFZ	C4-N4	4.62	1.45	1.33
1	A	173	UFT	C6-N1	4.61	1.49	1.38
1	A	149	CFZ	C2'-C3'	-4.61	1.46	1.52
1	A	27	CFZ	C2'-C3'	-4.60	1.46	1.52
1	A	7	UFT	C6-N1	4.60	1.49	1.38
1	A	8	CFZ	C2'-C3'	-4.60	1.46	1.52
1	A	187	UFT	C6-N1	4.60	1.49	1.38
1	A	42	CFZ	C2'-C3'	-4.59	1.46	1.52
1	A	46	UFT	C6-N1	4.59	1.49	1.38
1	A	134	UFT	C6-N1	4.59	1.49	1.38
1	A	124	UFT	C6-N1	4.59	1.49	1.38
1	A	20	UFT	C6-N1	4.59	1.49	1.38
1	A	188	UFT	C6-N1	4.59	1.49	1.38
1	A	203	UFT	C6-N1	4.59	1.49	1.38
1	A	40	CFZ	C2'-C3'	-4.58	1.46	1.52
1	A	181	UFT	C6-N1	4.58	1.49	1.38
1	A	174	UFT	C6-N1	4.58	1.49	1.38
1	A	98	UFT	C6-N1	4.58	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	152	CFZ	C2'-C3'	-4.58	1.46	1.52
1	A	104	CFZ	C2'-C3'	-4.58	1.46	1.52
1	A	114	CFZ	C4-N4	4.57	1.45	1.33
1	A	133	UFT	C6-N1	4.57	1.49	1.38
1	A	229	UFT	C6-N1	4.57	1.49	1.38
1	A	29	UFT	C6-N1	4.57	1.49	1.38
1	A	56	UFT	C6-N1	4.57	1.49	1.38
1	A	144	UFT	C6-N1	4.57	1.49	1.38
1	A	210	UFT	C6-N1	4.57	1.49	1.38
1	A	137	CFZ	C2-N3	4.57	1.45	1.36
1	A	215	UFT	C6-N1	4.57	1.49	1.38
1	A	135	CFZ	C2'-C3'	-4.57	1.46	1.52
1	A	88	UFT	C6-N1	4.57	1.49	1.38
1	A	47	CFZ	C2-N3	4.57	1.45	1.36
1	A	77	UFT	C6-N1	4.57	1.49	1.38
1	A	222	UFT	C6-N1	4.57	1.49	1.38
1	A	190	UFT	C6-N1	4.56	1.49	1.38
1	A	93	UFT	C6-N1	4.56	1.49	1.38
1	A	123	CFZ	C2-N3	4.56	1.45	1.36
1	A	112	UFT	C2-N1	4.56	1.45	1.38
1	A	19	UFT	C6-N1	4.56	1.49	1.38
1	A	55	UFT	C6-N1	4.56	1.49	1.38
1	A	169	CFZ	C2-N3	4.56	1.45	1.36
1	A	92	UFT	C6-N1	4.56	1.48	1.38
1	A	35	UFT	C6-N1	4.55	1.48	1.38
1	A	142	CFZ	C2'-C3'	-4.55	1.46	1.52
1	A	226	UFT	C6-N1	4.55	1.48	1.38
1	A	182	UFT	C6-N1	4.54	1.48	1.38
1	A	194	UFT	C6-N1	4.54	1.48	1.38
1	A	123	CFZ	C2'-C3'	-4.54	1.46	1.52
1	A	51	CFZ	C2-N3	4.54	1.45	1.36
1	A	44	UFT	C6-N1	4.54	1.48	1.38
1	A	153	UFT	C6-N1	4.53	1.48	1.38
1	A	116	CFZ	C2-N3	4.53	1.45	1.36
1	A	224	UFT	C6-N1	4.53	1.48	1.38
1	A	142	CFZ	C2-N3	4.53	1.45	1.36
1	A	170	CFZ	C2'-C3'	-4.53	1.46	1.52
1	A	171	UFT	C6-N1	4.53	1.48	1.38
1	A	13	UFT	C6-N1	4.53	1.48	1.38
1	A	141	UFT	C6-N1	4.53	1.48	1.38
1	A	137	CFZ	C2'-C3'	-4.52	1.46	1.52
1	A	54	UFT	C6-N1	4.52	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	21	CFZ	C2'-C3'	-4.52	1.46	1.52
1	A	169	CFZ	C2'-C3'	-4.52	1.46	1.52
1	A	24	CFZ	C2-N3	4.52	1.45	1.36
1	A	100	UFT	C6-N1	4.52	1.48	1.38
1	A	64	UFT	C6-N1	4.52	1.48	1.38
1	A	73	UFT	C6-N1	4.52	1.48	1.38
1	A	130	UFT	C6-N1	4.52	1.48	1.38
1	A	26	CFZ	C2'-C3'	-4.52	1.46	1.52
1	A	114	CFZ	C2-N3	4.52	1.45	1.36
1	A	216	UFT	C6-N1	4.52	1.48	1.38
1	A	76	CFZ	C2'-C3'	-4.51	1.46	1.52
1	A	72	UFT	C6-N1	4.51	1.48	1.38
1	A	164	CFZ	C2'-C3'	-4.51	1.46	1.52
1	A	23	UFT	C6-N1	4.51	1.48	1.38
1	A	126	UFT	C6-N1	4.50	1.48	1.38
1	A	147	UFT	C6-N1	4.50	1.48	1.38
1	A	212	CFZ	C2'-C3'	-4.50	1.46	1.52
1	A	61	CFZ	C2'-C3'	-4.49	1.46	1.52
1	A	39	UFT	C6-N1	4.49	1.48	1.38
1	A	10	UFT	C6-N1	4.49	1.48	1.38
1	A	85	UFT	C6-N1	4.49	1.48	1.38
1	A	76	CFZ	C2-N3	4.49	1.45	1.36
1	A	91	UFT	C6-N1	4.49	1.48	1.38
1	A	84	UFT	C6-N1	4.48	1.48	1.38
1	A	227	CFZ	C2-N3	4.48	1.45	1.36
1	A	177	CFZ	C2-N3	4.48	1.45	1.36
1	A	5	UFT	C6-N1	4.47	1.48	1.38
1	A	231	CFZ	C2'-C3'	-4.47	1.46	1.52
1	A	164	CFZ	C2-N3	4.47	1.45	1.36
1	A	217	CFZ	C2'-C3'	-4.47	1.46	1.52
1	A	236	CFZ	C2'-C3'	-4.47	1.46	1.52
1	A	69	UFT	C6-N1	4.47	1.48	1.38
1	A	75	UFT	C6-N1	4.46	1.48	1.38
1	A	228	UFT	C6-N1	4.46	1.48	1.38
1	A	163	UFT	C6-N1	4.46	1.48	1.38
1	A	71	CFZ	C2-N3	4.46	1.45	1.36
1	A	234	UFT	C6-N1	4.45	1.48	1.38
1	A	161	CFZ	C2-N3	4.45	1.45	1.36
1	A	154	CFZ	C2-N3	4.45	1.45	1.36
1	A	41	UFT	C6-N1	4.44	1.48	1.38
1	A	48	UFT	C6-N1	4.44	1.48	1.38
1	A	24	CFZ	C2'-C3'	-4.44	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	40	CFZ	C2-N3	4.44	1.45	1.36
1	A	113	CFZ	C2-N3	4.44	1.45	1.36
1	A	184	UFT	C6-N1	4.43	1.48	1.38
1	A	104	CFZ	C2-N3	4.42	1.45	1.36
1	A	34	CFZ	C2-N3	4.42	1.45	1.36
1	A	109	UFT	C6-N1	4.42	1.48	1.38
1	A	80	CFZ	C2-N3	4.42	1.45	1.36
1	A	90	CFZ	C2-N3	4.42	1.45	1.36
1	A	238	CFZ	C2'-C3'	-4.42	1.46	1.52
1	A	42	CFZ	C2-N3	4.41	1.45	1.36
1	A	11	CFZ	C2'-C3'	-4.41	1.46	1.52
1	A	199	CFZ	C2-N3	4.41	1.45	1.36
1	A	238	CFZ	C2-N3	4.40	1.45	1.36
1	A	152	CFZ	C2-N3	4.40	1.45	1.36
1	A	70	CFZ	C2-N3	4.40	1.45	1.36
1	A	16	UFT	C5-C4	4.40	1.53	1.43
1	A	26	CFZ	C2-N3	4.39	1.45	1.36
1	A	105	CFZ	C2-N3	4.39	1.45	1.36
1	A	149	CFZ	C2-N3	4.39	1.45	1.36
1	A	11	CFZ	C2-N3	4.38	1.45	1.36
1	A	198	CFZ	C2-N3	4.38	1.45	1.36
1	A	148	CFZ	C2-N3	4.37	1.45	1.36
1	A	27	CFZ	C2-N3	4.37	1.45	1.36
1	A	235	CFZ	C2'-C3'	-4.36	1.46	1.52
1	A	226	UFT	C5-C4	4.35	1.53	1.43
1	A	170	CFZ	C2-N3	4.35	1.45	1.36
1	A	77	UFT	C2'-C3'	-4.35	1.46	1.52
1	A	61	CFZ	C2-N3	4.34	1.45	1.36
1	A	112	UFT	C5-C4	4.33	1.53	1.43
1	A	181	UFT	C2'-C3'	-4.33	1.47	1.52
1	A	236	CFZ	C2-N3	4.33	1.44	1.36
1	A	144	UFT	C5-C4	4.33	1.53	1.43
1	A	181	UFT	C5-C4	4.33	1.53	1.43
1	A	140	CFZ	C2'-C3'	-4.32	1.47	1.52
1	A	63	CFZ	C2-N3	4.32	1.44	1.36
1	A	7	UFT	C5-C4	4.32	1.53	1.43
1	A	141	UFT	C5-C4	4.31	1.53	1.43
1	A	100	UFT	C5-C4	4.31	1.53	1.43
1	A	188	UFT	C5-C4	4.31	1.53	1.43
1	A	53	CFZ	C2-N3	4.31	1.44	1.36
1	A	131	CFZ	C2'-C3'	-4.31	1.47	1.52
1	A	106	CFZ	C2-N3	4.31	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	153	UFT	C5-C4	4.31	1.53	1.43
1	A	29	UFT	C5-C4	4.30	1.53	1.43
1	A	120	UFT	C5-C4	4.30	1.53	1.43
1	A	92	UFT	C5-C4	4.30	1.53	1.43
1	A	153	UFT	C2'-C3'	-4.29	1.47	1.52
1	A	229	UFT	C5-C4	4.29	1.53	1.43
1	A	133	UFT	C5-C4	4.29	1.53	1.43
1	A	210	UFT	C5-C4	4.29	1.53	1.43
1	A	171	UFT	C2'-C3'	-4.29	1.47	1.52
1	A	187	UFT	C5-C4	4.28	1.53	1.43
1	A	174	UFT	C5-C4	4.28	1.53	1.43
1	A	39	UFT	C5-C4	4.28	1.53	1.43
1	A	124	UFT	C2'-C3'	-4.28	1.47	1.52
1	A	194	UFT	C5-C4	4.28	1.53	1.43
1	A	173	UFT	C5-C4	4.27	1.53	1.43
1	A	203	UFT	C5-C4	4.27	1.53	1.43
1	A	190	UFT	C5-C4	4.27	1.53	1.43
1	A	44	UFT	C2'-C3'	-4.27	1.47	1.52
1	A	131	CFZ	C2-N3	4.27	1.44	1.36
1	A	134	UFT	C5-C4	4.26	1.53	1.43
1	A	46	UFT	C2'-C3'	-4.26	1.47	1.52
1	A	124	UFT	C5-C4	4.26	1.53	1.43
1	A	182	UFT	C5-C4	4.26	1.53	1.43
1	A	55	UFT	C5-C4	4.26	1.53	1.43
1	A	56	UFT	C5-C4	4.26	1.53	1.43
1	A	111	UFT	C5-C4	4.26	1.53	1.43
1	A	23	UFT	C2'-C3'	-4.26	1.47	1.52
1	A	19	UFT	C5-C4	4.26	1.53	1.43
1	A	163	UFT	C2'-C3'	-4.26	1.47	1.52
1	A	72	UFT	C2'-C3'	-4.26	1.47	1.52
1	A	105	CFZ	C2'-C3'	-4.26	1.47	1.52
1	A	98	UFT	C5-C4	4.26	1.52	1.43
1	A	126	UFT	C5-C4	4.26	1.52	1.43
1	A	93	UFT	C5-C4	4.25	1.52	1.43
1	A	212	CFZ	C2-N3	4.25	1.44	1.36
1	A	213	CFZ	C2-N3	4.25	1.44	1.36
1	A	184	UFT	C5-C4	4.25	1.52	1.43
1	A	48	UFT	C5-C4	4.25	1.52	1.43
1	A	234	UFT	C5-C4	4.24	1.52	1.43
1	A	215	UFT	C5-C4	4.24	1.52	1.43
1	A	20	UFT	C5-C4	4.24	1.52	1.43
1	A	120	UFT	C2'-C3'	-4.24	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	35	UFT	C5-C4	4.23	1.52	1.43
1	A	210	UFT	C2'-C3'	-4.23	1.47	1.52
1	A	86	UFT	C5-C4	4.23	1.52	1.43
1	A	23	UFT	C5-C4	4.23	1.52	1.43
1	A	64	UFT	C5-C4	4.23	1.52	1.43
1	A	77	UFT	C5-C4	4.23	1.52	1.43
1	A	35	UFT	C2'-C3'	-4.23	1.47	1.52
1	A	224	UFT	C5-C4	4.23	1.52	1.43
1	A	216	UFT	C5-C4	4.23	1.52	1.43
1	A	130	UFT	C5-C4	4.22	1.52	1.43
1	A	91	UFT	C5-C4	4.22	1.52	1.43
1	A	222	UFT	C5-C4	4.22	1.52	1.43
1	A	235	CFZ	C2-N3	4.21	1.44	1.36
1	A	41	UFT	C2'-C3'	-4.21	1.47	1.52
1	A	147	UFT	C5-C4	4.21	1.52	1.43
1	A	219	CFZ	C2-N3	4.21	1.44	1.36
1	A	10	UFT	C5-C4	4.21	1.52	1.43
1	A	73	UFT	C5-C4	4.21	1.52	1.43
1	A	8	CFZ	C2-N3	4.21	1.44	1.36
1	A	121	CFZ	C2-N3	4.20	1.44	1.36
1	A	69	UFT	C5-C4	4.20	1.52	1.43
1	A	166	UFT	C5-C4	4.20	1.52	1.43
1	A	44	UFT	C5-C4	4.20	1.52	1.43
1	A	84	UFT	C5-C4	4.20	1.52	1.43
1	A	72	UFT	C5-C4	4.19	1.52	1.43
1	A	7	UFT	C2'-C3'	-4.18	1.47	1.52
1	A	53	CFZ	C2'-C3'	-4.18	1.47	1.52
1	A	46	UFT	C5-C4	4.18	1.52	1.43
1	A	10	UFT	C2'-C3'	-4.18	1.47	1.52
1	A	88	UFT	C5-C4	4.17	1.52	1.43
1	A	229	UFT	C2'-C3'	-4.17	1.47	1.52
1	A	13	UFT	C5-C4	4.16	1.52	1.43
1	A	41	UFT	C5-C4	4.16	1.52	1.43
1	A	75	UFT	C5-C4	4.16	1.52	1.43
1	A	228	UFT	C5-C4	4.15	1.52	1.43
1	A	85	UFT	C5-C4	4.15	1.52	1.43
1	A	100	UFT	C2'-C3'	-4.15	1.47	1.52
1	A	171	UFT	C5-C4	4.15	1.52	1.43
1	A	109	UFT	C5-C4	4.15	1.52	1.43
1	A	86	UFT	C2'-C3'	-4.14	1.47	1.52
1	A	69	UFT	C2'-C3'	-4.14	1.47	1.52
1	A	29	UFT	C2'-C3'	-4.14	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	88	UFT	C2'-C3'	-4.14	1.47	1.52
1	A	163	UFT	C5-C4	4.14	1.52	1.43
1	A	73	UFT	C2'-C3'	-4.13	1.47	1.52
1	A	91	UFT	C2'-C3'	-4.13	1.47	1.52
1	A	144	UFT	C2'-C3'	-4.12	1.47	1.52
1	A	5	UFT	C5-C4	4.12	1.52	1.43
1	A	226	UFT	C2'-C3'	-4.12	1.47	1.52
1	A	81	CFZ	C2-N3	4.12	1.44	1.36
1	A	13	UFT	C2'-C3'	-4.11	1.47	1.52
1	A	194	UFT	C2'-C3'	-4.10	1.47	1.52
1	A	64	UFT	C2'-C3'	-4.10	1.47	1.52
1	A	21	CFZ	C2-N3	4.10	1.44	1.36
1	A	84	UFT	C2'-C3'	-4.09	1.47	1.52
1	A	54	UFT	C5-C4	4.09	1.52	1.43
1	A	57	CFZ	C2'-C3'	-4.08	1.47	1.52
1	A	109	UFT	C2'-C3'	-4.08	1.47	1.52
1	A	217	CFZ	C2-N3	4.08	1.44	1.36
1	A	57	CFZ	C2-N3	4.06	1.44	1.36
1	A	215	UFT	C2'-C3'	-4.06	1.47	1.52
1	A	222	UFT	C2'-C3'	-4.06	1.47	1.52
1	A	175	CFZ	C2-N3	4.06	1.44	1.36
1	A	75	UFT	C2'-C3'	-4.05	1.47	1.52
1	A	135	CFZ	C2-N3	4.05	1.44	1.36
1	A	5	UFT	C2'-C3'	-4.05	1.47	1.52
1	A	94	CFZ	C2-N3	4.04	1.44	1.36
1	A	208	CFZ	C2-N3	4.04	1.44	1.36
1	A	231	CFZ	C2-N3	4.04	1.44	1.36
1	A	166	UFT	C2'-C3'	-4.04	1.47	1.52
1	A	19	UFT	C2'-C3'	-4.03	1.47	1.52
1	A	98	UFT	C2'-C3'	-4.01	1.47	1.52
1	A	111	UFT	C2'-C3'	-4.01	1.47	1.52
1	A	154	CFZ	C2'-C3'	-4.00	1.47	1.52
1	A	190	UFT	C2'-C3'	-4.00	1.47	1.52
1	A	203	UFT	C2'-C3'	-3.99	1.47	1.52
1	A	85	UFT	C2'-C3'	-3.98	1.47	1.52
1	A	174	UFT	C2'-C3'	-3.98	1.47	1.52
1	A	16	UFT	C2'-C3'	-3.98	1.47	1.52
1	A	133	UFT	C2'-C3'	-3.96	1.47	1.52
1	A	55	UFT	C2'-C3'	-3.96	1.47	1.52
1	A	141	UFT	C2'-C3'	-3.95	1.47	1.52
1	A	216	UFT	C2'-C3'	-3.95	1.47	1.52
1	A	228	UFT	C2'-C3'	-3.93	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	140	CFZ	C2-N3	3.93	1.44	1.36
1	A	48	UFT	C2'-C3'	-3.92	1.47	1.52
1	A	112	UFT	C2'-C3'	-3.90	1.47	1.52
1	A	93	UFT	C2'-C3'	-3.89	1.47	1.52
1	A	126	UFT	C2'-C3'	-3.87	1.47	1.52
1	A	54	UFT	C2'-C3'	-3.86	1.47	1.52
1	A	130	UFT	C2'-C3'	-3.86	1.47	1.52
1	A	173	UFT	C2'-C3'	-3.85	1.47	1.52
1	A	224	UFT	C2'-C3'	-3.82	1.47	1.52
1	A	188	UFT	C2'-C3'	-3.80	1.47	1.52
1	A	39	UFT	C2'-C3'	-3.79	1.47	1.52
1	A	92	UFT	C2'-C3'	-3.76	1.47	1.52
1	A	234	UFT	C2'-C3'	-3.75	1.47	1.52
1	A	187	UFT	C2'-C3'	-3.72	1.47	1.52
1	A	184	UFT	C2'-C3'	-3.69	1.47	1.52
1	A	164	CFZ	O2-C2	3.66	1.30	1.23
1	A	114	CFZ	O2-C2	3.65	1.30	1.23
1	A	182	UFT	C2'-C3'	-3.64	1.47	1.52
1	A	20	UFT	C2'-C3'	-3.63	1.47	1.52
1	A	219	CFZ	O2-C2	3.63	1.30	1.23
1	A	90	CFZ	O2-C2	3.62	1.30	1.23
1	A	56	UFT	C2'-C3'	-3.62	1.47	1.52
1	A	94	CFZ	O2-C2	3.60	1.30	1.23
1	A	177	CFZ	O2-C2	3.60	1.30	1.23
1	A	106	CFZ	O2-C2	3.59	1.30	1.23
1	A	121	CFZ	O2-C2	3.59	1.30	1.23
1	A	147	UFT	C2'-C3'	-3.59	1.48	1.52
1	A	71	CFZ	O2-C2	3.59	1.30	1.23
1	A	148	CFZ	O2-C2	3.59	1.30	1.23
1	A	26	CFZ	O2-C2	3.58	1.30	1.23
1	A	169	CFZ	O2-C2	3.58	1.30	1.23
1	A	94	CFZ	C2'-C3'	-3.58	1.48	1.52
1	A	113	CFZ	O2-C2	3.58	1.30	1.23
1	A	47	CFZ	O2-C2	3.57	1.30	1.23
1	A	76	CFZ	O2-C2	3.57	1.30	1.23
1	A	42	CFZ	O2-C2	3.57	1.30	1.23
1	A	21	CFZ	O2-C2	3.56	1.30	1.23
1	A	123	CFZ	O2-C2	3.56	1.30	1.23
1	A	170	CFZ	O2-C2	3.56	1.30	1.23
1	A	175	CFZ	O2-C2	3.56	1.30	1.23
1	A	161	CFZ	O2-C2	3.56	1.30	1.23
1	A	217	CFZ	O2-C2	3.55	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	CFZ	O2-C2	3.55	1.30	1.23
1	A	105	CFZ	O2-C2	3.55	1.30	1.23
1	A	208	CFZ	O2-C2	3.55	1.30	1.23
1	A	198	CFZ	O2-C2	3.54	1.30	1.23
1	A	57	CFZ	O2-C2	3.54	1.30	1.23
1	A	154	CFZ	O2-C2	3.54	1.30	1.23
1	A	199	CFZ	O2-C2	3.54	1.30	1.23
1	A	135	CFZ	O2-C2	3.54	1.30	1.23
1	A	142	CFZ	O2-C2	3.54	1.30	1.23
1	A	24	CFZ	O2-C2	3.53	1.30	1.23
1	A	63	CFZ	O2-C2	3.53	1.30	1.23
1	A	8	CFZ	O2-C2	3.52	1.30	1.23
1	A	104	CFZ	O2-C2	3.52	1.30	1.23
1	A	137	CFZ	O2-C2	3.52	1.30	1.23
1	A	238	CFZ	O2-C2	3.52	1.30	1.23
1	A	149	CFZ	O2-C2	3.52	1.30	1.23
1	A	235	CFZ	O2-C2	3.52	1.30	1.23
1	A	227	CFZ	C2'-C1'	-3.51	1.48	1.53
1	A	70	CFZ	O2-C2	3.51	1.30	1.23
1	A	80	CFZ	O2-C2	3.51	1.30	1.23
1	A	40	CFZ	O2-C2	3.50	1.30	1.23
1	A	227	CFZ	O2-C2	3.50	1.30	1.23
1	A	152	CFZ	O2-C2	3.50	1.30	1.23
1	A	34	CFZ	O2-C2	3.49	1.30	1.23
1	A	61	CFZ	O2-C2	3.49	1.30	1.23
1	A	134	UFT	C2'-C3'	-3.49	1.48	1.52
1	A	212	CFZ	O2-C2	3.49	1.30	1.23
1	A	140	CFZ	O2-C2	3.48	1.30	1.23
1	A	11	CFZ	O2-C2	3.48	1.30	1.23
1	A	27	CFZ	O2-C2	3.48	1.30	1.23
1	A	213	CFZ	O2-C2	3.48	1.30	1.23
1	A	116	CFZ	O2-C2	3.47	1.30	1.23
1	A	116	CFZ	O4'-C1'	3.47	1.50	1.42
1	A	81	CFZ	O2-C2	3.47	1.30	1.23
1	A	131	CFZ	O2-C2	3.44	1.30	1.23
1	A	236	CFZ	O2-C2	3.44	1.30	1.23
1	A	53	CFZ	O2-C2	3.42	1.30	1.23
1	A	154	CFZ	O4'-C1'	3.41	1.49	1.42
1	A	175	CFZ	C2'-C1'	-3.40	1.49	1.53
1	A	123	CFZ	O4'-C1'	3.38	1.49	1.42
1	A	70	CFZ	O4'-C1'	3.38	1.49	1.42
1	A	227	CFZ	O4'-C1'	3.36	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	42	CFZ	O4'-C1'	3.34	1.49	1.42
1	A	231	CFZ	O2-C2	3.33	1.29	1.23
1	A	175	CFZ	C2'-C3'	-3.33	1.48	1.52
1	A	148	CFZ	O4'-C1'	3.33	1.49	1.42
1	A	80	CFZ	O4'-C1'	3.33	1.49	1.42
1	A	47	CFZ	O4'-C1'	3.32	1.49	1.42
1	A	121	CFZ	O4'-C1'	3.32	1.49	1.42
1	A	142	CFZ	O4'-C1'	3.32	1.49	1.42
1	A	47	CFZ	C2'-C1'	-3.31	1.49	1.53
1	A	208	CFZ	O4'-C1'	3.31	1.49	1.42
1	A	161	CFZ	O4'-C1'	3.31	1.49	1.42
1	A	199	CFZ	O4'-C1'	3.30	1.49	1.42
1	A	63	CFZ	O4'-C1'	3.29	1.49	1.42
1	A	24	CFZ	O4'-C1'	3.29	1.49	1.42
1	A	213	CFZ	O4'-C1'	3.29	1.49	1.42
1	A	137	CFZ	C2'-C1'	-3.29	1.49	1.53
1	A	26	CFZ	O4'-C1'	3.29	1.49	1.42
1	A	106	CFZ	O4'-C1'	3.28	1.49	1.42
1	A	34	CFZ	O4'-C1'	3.28	1.49	1.42
1	A	217	CFZ	C2'-C1'	-3.28	1.49	1.53
1	A	164	CFZ	O4'-C1'	3.28	1.49	1.42
1	A	104	CFZ	O4'-C1'	3.27	1.49	1.42
1	A	51	CFZ	O4'-C1'	3.27	1.49	1.42
1	A	76	CFZ	O4'-C1'	3.27	1.49	1.42
1	A	235	CFZ	C2'-C1'	-3.27	1.49	1.53
1	A	71	CFZ	O4'-C1'	3.27	1.49	1.42
1	A	213	CFZ	C2'-C1'	-3.26	1.49	1.53
1	A	114	CFZ	O4'-C1'	3.26	1.49	1.42
1	A	27	CFZ	O4'-C1'	3.26	1.49	1.42
1	A	137	CFZ	O4'-C1'	3.26	1.49	1.42
1	A	152	CFZ	O4'-C1'	3.26	1.49	1.42
1	A	235	CFZ	O4'-C1'	3.25	1.49	1.42
1	A	140	CFZ	C2'-C1'	-3.25	1.49	1.53
1	A	198	CFZ	O4'-C1'	3.24	1.49	1.42
1	A	105	CFZ	O4'-C1'	3.24	1.49	1.42
1	A	90	CFZ	O4'-C1'	3.23	1.49	1.42
1	A	113	CFZ	O4'-C1'	3.23	1.49	1.42
1	A	219	CFZ	O4'-C1'	3.22	1.49	1.42
1	A	54	UFT	O4-C4	-3.22	1.18	1.24
1	A	169	CFZ	O4'-C1'	3.22	1.49	1.42
1	A	8	CFZ	O4'-C1'	3.21	1.49	1.42
1	A	81	CFZ	O4'-C1'	3.21	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	70	CFZ	C2'-C1'	-3.20	1.49	1.53
1	A	149	CFZ	C2'-C1'	-3.20	1.49	1.53
1	A	238	CFZ	C2'-C1'	-3.20	1.49	1.53
1	A	238	CFZ	O4'-C1'	3.20	1.49	1.42
1	A	154	CFZ	C2'-C1'	-3.20	1.49	1.53
1	A	26	CFZ	C2'-C1'	-3.19	1.49	1.53
1	A	163	UFT	O4-C4	-3.19	1.18	1.24
1	A	177	CFZ	O4'-C1'	3.19	1.49	1.42
1	A	236	CFZ	O4'-C1'	3.19	1.49	1.42
1	A	149	CFZ	O4'-C1'	3.19	1.49	1.42
1	A	212	CFZ	O4'-C1'	3.18	1.49	1.42
1	A	135	CFZ	C2'-C1'	-3.18	1.49	1.53
1	A	106	CFZ	C2'-C1'	-3.18	1.49	1.53
1	A	40	CFZ	C2'-C1'	-3.18	1.49	1.53
1	A	11	CFZ	O4'-C1'	3.17	1.49	1.42
1	A	113	CFZ	C2'-C1'	-3.17	1.49	1.53
1	A	131	CFZ	C2'-C1'	-3.17	1.49	1.53
1	A	81	CFZ	C2'-C1'	-3.16	1.49	1.53
1	A	170	CFZ	C2'-C1'	-3.15	1.49	1.53
1	A	104	CFZ	C2'-C1'	-3.15	1.49	1.53
1	A	61	CFZ	O4'-C1'	3.14	1.49	1.42
1	A	34	CFZ	C2'-C1'	-3.13	1.49	1.53
1	A	40	CFZ	O4'-C1'	3.13	1.49	1.42
1	A	231	CFZ	O4'-C1'	3.13	1.49	1.42
1	A	42	CFZ	C2'-C1'	-3.13	1.49	1.53
1	A	109	UFT	C2'-C1'	-3.12	1.49	1.53
1	A	53	CFZ	O4'-C1'	3.12	1.49	1.42
1	A	5	UFT	O4-C4	-3.12	1.18	1.24
1	A	63	CFZ	C2'-C1'	-3.12	1.49	1.53
1	A	161	CFZ	C2'-C1'	-3.12	1.49	1.53
1	A	131	CFZ	O4'-C1'	3.11	1.49	1.42
1	A	90	CFZ	C2'-C1'	-3.11	1.49	1.53
1	A	140	CFZ	O4'-C1'	3.10	1.49	1.42
1	A	234	UFT	C2'-C1'	-3.10	1.49	1.53
1	A	94	CFZ	O4'-C1'	3.09	1.49	1.42
1	A	80	CFZ	C2'-C1'	-3.08	1.49	1.53
1	A	147	UFT	O4-C4	-3.07	1.18	1.24
1	A	21	CFZ	O4'-C1'	3.06	1.49	1.42
1	A	177	CFZ	C2'-C1'	-3.06	1.49	1.53
1	A	57	CFZ	C2'-C1'	-3.06	1.49	1.53
1	A	199	CFZ	C2'-C1'	-3.05	1.49	1.53
1	A	135	CFZ	O4'-C1'	3.05	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61	CFZ	C2'-C1'	-3.04	1.49	1.53
1	A	228	UFT	O4-C4	-3.04	1.18	1.24
1	A	198	CFZ	C2'-C1'	-3.04	1.49	1.53
1	A	170	CFZ	O4'-C1'	3.03	1.49	1.42
1	A	51	CFZ	C2'-C1'	-3.03	1.49	1.53
1	A	84	UFT	O4-C4	-3.03	1.18	1.24
1	A	53	CFZ	C2'-C1'	-3.02	1.49	1.53
1	A	142	CFZ	C2'-C1'	-3.02	1.49	1.53
1	A	10	UFT	O4-C4	-3.02	1.18	1.24
1	A	169	CFZ	C2'-C1'	-3.01	1.49	1.53
1	A	152	CFZ	C2'-C1'	-3.01	1.49	1.53
1	A	27	CFZ	C2'-C1'	-3.01	1.49	1.53
1	A	10	UFT	C2'-C1'	-3.00	1.49	1.53
1	A	41	UFT	C2'-C1'	-3.00	1.49	1.53
1	A	217	CFZ	O4'-C1'	3.00	1.48	1.42
1	A	71	CFZ	C2'-C1'	-3.00	1.49	1.53
1	A	13	UFT	O4-C4	-3.00	1.18	1.24
1	A	75	UFT	O4-C4	-2.99	1.18	1.24
1	A	76	CFZ	C2'-C1'	-2.99	1.49	1.53
1	A	224	UFT	O4-C4	-2.98	1.18	1.24
1	A	175	CFZ	O4'-C1'	2.98	1.48	1.42
1	A	41	UFT	O4-C4	-2.98	1.18	1.24
1	A	116	CFZ	C2'-C1'	-2.98	1.49	1.53
1	A	69	UFT	C2'-C1'	-2.98	1.49	1.53
1	A	69	UFT	O4-C4	-2.98	1.18	1.24
1	A	94	CFZ	C2'-C1'	-2.98	1.49	1.53
1	A	114	CFZ	C2'-C1'	-2.97	1.49	1.53
1	A	21	CFZ	C2'-C1'	-2.97	1.49	1.53
1	A	85	UFT	O4-C4	-2.97	1.18	1.24
1	A	184	UFT	O4-C4	-2.97	1.18	1.24
1	A	187	UFT	O4-C4	-2.97	1.18	1.24
1	A	123	CFZ	C2'-C1'	-2.97	1.49	1.53
1	A	171	UFT	O4-C4	-2.96	1.18	1.24
1	A	86	UFT	O4-C4	-2.96	1.18	1.24
1	A	194	UFT	O4-C4	-2.95	1.18	1.24
1	A	164	CFZ	C2'-C1'	-2.95	1.49	1.53
1	A	236	CFZ	C2'-C1'	-2.95	1.49	1.53
1	A	72	UFT	O4-C4	-2.94	1.18	1.24
1	A	109	UFT	O4-C4	-2.93	1.18	1.24
1	A	57	CFZ	O4'-C1'	2.93	1.48	1.42
1	A	8	CFZ	C2'-C1'	-2.93	1.49	1.53
1	A	44	UFT	O4-C4	-2.93	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	133	UFT	O4-C4	-2.93	1.18	1.24
1	A	39	UFT	O4-C4	-2.93	1.18	1.24
1	A	91	UFT	O4-C4	-2.92	1.18	1.24
1	A	126	UFT	O4-C4	-2.92	1.18	1.24
1	A	88	UFT	O4-C4	-2.92	1.18	1.24
1	A	134	UFT	O4-C4	-2.92	1.18	1.24
1	A	234	UFT	O4-C4	-2.92	1.18	1.24
1	A	130	UFT	O4-C4	-2.92	1.18	1.24
1	A	181	UFT	O4-C4	-2.92	1.18	1.24
1	A	141	UFT	C2'-C1'	-2.92	1.49	1.53
1	A	48	UFT	O4-C4	-2.92	1.18	1.24
1	A	166	UFT	O4-C4	-2.92	1.18	1.24
1	A	215	UFT	O4-C4	-2.91	1.18	1.24
1	A	64	UFT	O4-C4	-2.91	1.18	1.24
1	A	222	UFT	O4-C4	-2.91	1.18	1.24
1	A	19	UFT	O4-C4	-2.91	1.18	1.24
1	A	5	UFT	C2-N3	2.91	1.43	1.38
1	A	182	UFT	O4-C4	-2.91	1.18	1.24
1	A	55	UFT	O4-C4	-2.91	1.18	1.24
1	A	229	UFT	O4-C4	-2.91	1.18	1.24
1	A	35	UFT	O4-C4	-2.90	1.18	1.24
1	A	173	UFT	O4-C4	-2.90	1.18	1.24
1	A	226	UFT	O4-C4	-2.90	1.18	1.24
1	A	163	UFT	C2-N3	2.90	1.43	1.38
1	A	174	UFT	O4-C4	-2.90	1.18	1.24
1	A	29	UFT	O4-C4	-2.90	1.18	1.24
1	A	216	UFT	O4-C4	-2.89	1.18	1.24
1	A	46	UFT	O4-C4	-2.89	1.18	1.24
1	A	100	UFT	O4-C4	-2.88	1.18	1.24
1	A	93	UFT	O4-C4	-2.88	1.18	1.24
1	A	228	UFT	C2'-C1'	-2.88	1.49	1.53
1	A	188	UFT	O4-C4	-2.87	1.18	1.24
1	A	92	UFT	O4-C4	-2.87	1.18	1.24
1	A	73	UFT	O4-C4	-2.87	1.18	1.24
1	A	112	UFT	O4-C4	-2.87	1.18	1.24
1	A	190	UFT	O4-C4	-2.87	1.18	1.24
1	A	20	UFT	O4-C4	-2.87	1.18	1.24
1	A	141	UFT	O4-C4	-2.87	1.18	1.24
1	A	7	UFT	O4-C4	-2.87	1.18	1.24
1	A	98	UFT	O4-C4	-2.87	1.18	1.24
1	A	84	UFT	C2'-C1'	-2.86	1.49	1.53
1	A	228	UFT	C2-N3	2.86	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	120	UFT	O4-C4	-2.86	1.18	1.24
1	A	144	UFT	O4-C4	-2.86	1.18	1.24
1	A	56	UFT	O4-C4	-2.86	1.18	1.24
1	A	111	UFT	O4-C4	-2.86	1.18	1.24
1	A	11	CFZ	C2'-C1'	-2.85	1.49	1.53
1	A	77	UFT	O4-C4	-2.85	1.18	1.24
1	A	184	UFT	C2-N3	2.85	1.42	1.38
1	A	153	UFT	O4-C4	-2.84	1.19	1.24
1	A	10	UFT	C2-N3	2.83	1.42	1.38
1	A	109	UFT	C2-N3	2.83	1.42	1.38
1	A	147	UFT	C2-N3	2.83	1.42	1.38
1	A	219	CFZ	C2'-C1'	-2.83	1.49	1.53
1	A	231	CFZ	C2'-C1'	-2.83	1.49	1.53
1	A	75	UFT	C2-N3	2.82	1.42	1.38
1	A	111	UFT	C2'-C1'	-2.82	1.49	1.53
1	A	171	UFT	O4'-C1'	2.82	1.48	1.42
1	A	121	CFZ	C2'-C1'	-2.81	1.49	1.53
1	A	124	UFT	O4-C4	-2.81	1.19	1.24
1	A	163	UFT	C2'-C1'	-2.80	1.49	1.53
1	A	148	CFZ	C2'-C1'	-2.79	1.49	1.53
1	A	126	UFT	C2-N3	2.79	1.42	1.38
1	A	210	UFT	O4-C4	-2.79	1.19	1.24
1	A	75	UFT	C2'-C1'	-2.78	1.49	1.53
1	A	39	UFT	C2-N3	2.78	1.42	1.38
1	A	212	CFZ	C2'-C1'	-2.78	1.49	1.53
1	A	105	CFZ	C2'-C1'	-2.78	1.49	1.53
1	A	173	UFT	C2'-C1'	-2.77	1.49	1.53
1	A	229	UFT	O4'-C1'	2.77	1.48	1.42
1	A	88	UFT	C2'-C1'	-2.77	1.49	1.53
1	A	203	UFT	O4-C4	-2.76	1.19	1.24
1	A	171	UFT	C2'-C1'	-2.76	1.49	1.53
1	A	187	UFT	C2'-C1'	-2.76	1.49	1.53
1	A	229	UFT	C2-N3	2.76	1.42	1.38
1	A	55	UFT	C2'-C1'	-2.75	1.49	1.53
1	A	153	UFT	C2'-C1'	-2.75	1.49	1.53
1	A	73	UFT	C2'-C1'	-2.75	1.49	1.53
1	A	222	UFT	C2-N3	2.75	1.42	1.38
1	A	44	UFT	C2'-C1'	-2.75	1.49	1.53
1	A	19	UFT	C2'-C1'	-2.74	1.49	1.53
1	A	23	UFT	O4-C4	-2.74	1.19	1.24
1	A	91	UFT	C2-N3	2.74	1.42	1.38
1	A	5	UFT	C2'-C1'	-2.73	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	35	UFT	C2'-C1'	-2.72	1.49	1.53
1	A	184	UFT	C2'-C1'	-2.72	1.49	1.53
1	A	69	UFT	C2-N3	2.72	1.42	1.38
1	A	208	CFZ	C2'-C1'	-2.72	1.49	1.53
1	A	98	UFT	C2'-C1'	-2.71	1.49	1.53
1	A	23	UFT	C2-N3	2.71	1.42	1.38
1	A	224	UFT	C2-N3	2.71	1.42	1.38
1	A	16	UFT	O4-C4	-2.71	1.19	1.24
1	A	144	UFT	C2-N3	2.71	1.42	1.38
1	A	100	UFT	C2'-C1'	-2.71	1.49	1.53
1	A	229	UFT	C2'-C1'	-2.71	1.49	1.53
1	A	166	UFT	C2-N3	2.70	1.42	1.38
1	A	64	UFT	C2-N3	2.70	1.42	1.38
1	A	203	UFT	C2-N3	2.70	1.42	1.38
1	A	84	UFT	C2-N3	2.70	1.42	1.38
1	A	54	UFT	C2-N3	2.70	1.42	1.38
1	A	120	UFT	O4'-C1'	2.70	1.48	1.42
1	A	234	UFT	C2-N3	2.70	1.42	1.38
1	A	48	UFT	C2'-C1'	-2.69	1.49	1.53
1	A	174	UFT	C2'-C1'	-2.69	1.49	1.53
1	A	24	CFZ	C2'-C1'	-2.69	1.49	1.53
1	A	48	UFT	C2-N3	2.69	1.42	1.38
1	A	171	UFT	C2-N3	2.69	1.42	1.38
1	A	91	UFT	O4'-C1'	2.69	1.48	1.42
1	A	64	UFT	C2'-C1'	-2.69	1.49	1.53
1	A	5	UFT	O4'-C1'	2.69	1.48	1.42
1	A	228	UFT	O4'-C1'	2.68	1.48	1.42
1	A	182	UFT	C2'-C1'	-2.68	1.49	1.53
1	A	163	UFT	O4'-C1'	2.68	1.48	1.42
1	A	187	UFT	C2-N3	2.68	1.42	1.38
1	A	181	UFT	C2-N3	2.68	1.42	1.38
1	A	194	UFT	C2-N3	2.68	1.42	1.38
1	A	29	UFT	C2-N3	2.67	1.42	1.38
1	A	44	UFT	O4'-C1'	2.67	1.48	1.42
1	A	181	UFT	C2'-C1'	-2.67	1.49	1.53
1	A	216	UFT	C2-N3	2.67	1.42	1.38
1	A	222	UFT	O4'-C1'	2.67	1.48	1.42
1	A	44	UFT	C2-N3	2.66	1.42	1.38
1	A	88	UFT	O4'-C1'	2.66	1.48	1.42
1	A	73	UFT	O4'-C1'	2.66	1.48	1.42
1	A	29	UFT	O4'-C1'	2.66	1.48	1.42
1	A	194	UFT	O4'-C1'	2.66	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	85	UFT	C2'-C1'	-2.66	1.49	1.53
1	A	181	UFT	O4'-C1'	2.66	1.48	1.42
1	A	7	UFT	O4'-C1'	2.66	1.48	1.42
1	A	13	UFT	O4'-C1'	2.66	1.48	1.42
1	A	153	UFT	O4'-C1'	2.65	1.48	1.42
1	A	35	UFT	O4'-C1'	2.65	1.48	1.42
1	A	73	UFT	C2-N3	2.65	1.42	1.38
1	A	72	UFT	O4'-C1'	2.65	1.48	1.42
1	A	124	UFT	C2'-C1'	-2.65	1.49	1.53
1	A	84	UFT	O4'-C1'	2.65	1.48	1.42
1	A	222	UFT	C2'-C1'	-2.65	1.49	1.53
1	A	69	UFT	O4'-C1'	2.65	1.48	1.42
1	A	124	UFT	O4'-C1'	2.64	1.48	1.42
1	A	144	UFT	O4'-C1'	2.64	1.48	1.42
1	A	41	UFT	C2-N3	2.64	1.42	1.38
1	A	75	UFT	O4'-C1'	2.64	1.48	1.42
1	A	226	UFT	C2-N3	2.64	1.42	1.38
1	A	72	UFT	C2-N3	2.64	1.42	1.38
1	A	54	UFT	O4'-C1'	2.64	1.48	1.42
1	A	86	UFT	C2-N3	2.64	1.42	1.38
1	A	46	UFT	C2-N3	2.64	1.42	1.38
1	A	184	UFT	O4'-C1'	2.63	1.48	1.42
1	A	190	UFT	O4'-C1'	2.63	1.48	1.42
1	A	153	UFT	C2-N3	2.63	1.42	1.38
1	A	10	UFT	O4'-C1'	2.63	1.48	1.42
1	A	86	UFT	O4'-C1'	2.63	1.48	1.42
1	A	7	UFT	C2'-C1'	-2.63	1.49	1.53
1	A	64	UFT	O4'-C1'	2.63	1.48	1.42
1	A	130	UFT	C2'-C1'	-2.63	1.49	1.53
1	A	173	UFT	O4'-C1'	2.62	1.48	1.42
1	A	56	UFT	C2-N3	2.62	1.42	1.38
1	A	77	UFT	C2'-C1'	-2.62	1.49	1.53
1	A	98	UFT	C2-N3	2.62	1.42	1.38
1	A	144	UFT	C2'-C1'	-2.62	1.49	1.53
1	A	41	UFT	O4'-C1'	2.62	1.48	1.42
1	A	188	UFT	C2'-C1'	-2.62	1.49	1.53
1	A	215	UFT	O4'-C1'	2.62	1.48	1.42
1	A	13	UFT	C2-N3	2.62	1.42	1.38
1	A	224	UFT	O4'-C1'	2.61	1.48	1.42
1	A	20	UFT	C2'-C1'	-2.61	1.49	1.53
1	A	77	UFT	O4'-C1'	2.61	1.48	1.42
1	A	46	UFT	O4'-C1'	2.61	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	210	UFT	O4'-C1'	2.61	1.48	1.42
1	A	141	UFT	O4'-C1'	2.61	1.48	1.42
1	A	130	UFT	C2-N3	2.61	1.42	1.38
1	A	226	UFT	C2'-C1'	-2.60	1.49	1.53
1	A	100	UFT	C2-N3	2.60	1.42	1.38
1	A	109	UFT	O4'-C1'	2.60	1.48	1.42
1	A	173	UFT	C2-N3	2.60	1.42	1.38
1	A	133	UFT	C2'-C1'	-2.60	1.50	1.53
1	A	134	UFT	C2-N3	2.60	1.42	1.38
1	A	190	UFT	C2-N3	2.60	1.42	1.38
1	A	93	UFT	C2-N3	2.59	1.42	1.38
1	A	190	UFT	C2'-C1'	-2.59	1.50	1.53
1	A	16	UFT	O4'-C1'	2.59	1.48	1.42
1	A	39	UFT	C2'-C1'	-2.59	1.50	1.53
1	A	92	UFT	C2-N3	2.59	1.42	1.38
1	A	100	UFT	O4'-C1'	2.59	1.48	1.42
1	A	85	UFT	O4'-C1'	2.59	1.48	1.42
1	A	55	UFT	O4'-C1'	2.59	1.48	1.42
1	A	215	UFT	C2'-C1'	-2.59	1.50	1.53
1	A	141	UFT	C2-N3	2.58	1.42	1.38
1	A	216	UFT	C2'-C1'	-2.58	1.50	1.53
1	A	19	UFT	C2-N3	2.58	1.42	1.38
1	A	48	UFT	O4'-C1'	2.58	1.48	1.42
1	A	174	UFT	C2-N3	2.58	1.42	1.38
1	A	20	UFT	C2-N3	2.58	1.42	1.38
1	A	55	UFT	C2-N3	2.58	1.42	1.38
1	A	133	UFT	C2-N3	2.58	1.42	1.38
1	A	92	UFT	O4'-C1'	2.58	1.48	1.42
1	A	98	UFT	O4'-C1'	2.58	1.48	1.42
1	A	166	UFT	O4'-C1'	2.58	1.48	1.42
1	A	16	UFT	C2-N3	2.58	1.42	1.38
1	A	234	UFT	O4'-C1'	2.58	1.48	1.42
1	A	54	UFT	C2'-C1'	-2.57	1.50	1.53
1	A	85	UFT	C2-N3	2.57	1.42	1.38
1	A	224	UFT	C2'-C1'	-2.57	1.50	1.53
1	A	93	UFT	C2'-C1'	-2.57	1.50	1.53
1	A	35	UFT	C2-N3	2.57	1.42	1.38
1	A	7	UFT	C2-N3	2.57	1.42	1.38
1	A	112	UFT	O4'-C1'	2.57	1.47	1.42
1	A	56	UFT	C2'-C1'	-2.56	1.50	1.53
1	A	77	UFT	C2-N3	2.56	1.42	1.38
1	A	120	UFT	C2-N3	2.56	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	188	UFT	C2-N3	2.56	1.42	1.38
1	A	29	UFT	C2'-C1'	-2.56	1.50	1.53
1	A	23	UFT	O4'-C1'	2.56	1.47	1.42
1	A	72	UFT	C2'-C1'	-2.56	1.50	1.53
1	A	39	UFT	O4'-C1'	2.55	1.47	1.42
1	A	126	UFT	O4'-C1'	2.55	1.47	1.42
1	A	210	UFT	C2-N3	2.55	1.42	1.38
1	A	203	UFT	O4'-C1'	2.55	1.47	1.42
1	A	226	UFT	O4'-C1'	2.54	1.47	1.42
1	A	23	UFT	C2'-C1'	-2.54	1.50	1.53
1	A	13	UFT	C2'-C1'	-2.54	1.50	1.53
1	A	19	UFT	O4'-C1'	2.53	1.47	1.42
1	A	92	UFT	C2'-C1'	-2.53	1.50	1.53
1	A	166	UFT	C2'-C1'	-2.53	1.50	1.53
1	A	88	UFT	C2-N3	2.52	1.42	1.38
1	A	215	UFT	C2-N3	2.52	1.42	1.38
1	A	194	UFT	C2'-C1'	-2.52	1.50	1.53
1	A	91	UFT	C2'-C1'	-2.52	1.50	1.53
1	A	130	UFT	O4'-C1'	2.52	1.47	1.42
1	A	112	UFT	C2'-C1'	-2.52	1.50	1.53
1	A	112	UFT	C2-N3	2.52	1.42	1.38
1	A	126	UFT	C2'-C1'	-2.51	1.50	1.53
1	A	134	UFT	O4'-C1'	2.51	1.47	1.42
1	A	134	UFT	C2'-C1'	-2.51	1.50	1.53
1	A	210	UFT	C2'-C1'	-2.50	1.50	1.53
1	A	56	UFT	O4'-C1'	2.50	1.47	1.42
1	A	133	UFT	O4'-C1'	2.50	1.47	1.42
1	A	46	UFT	C2'-C1'	-2.50	1.50	1.53
1	A	147	UFT	C2'-C1'	-2.49	1.50	1.53
1	A	86	UFT	C2'-C1'	-2.49	1.50	1.53
1	A	111	UFT	O4'-C1'	2.49	1.47	1.42
1	A	216	UFT	O4'-C1'	2.49	1.47	1.42
1	A	120	UFT	C2'-C1'	-2.48	1.50	1.53
1	A	111	UFT	C2-N3	2.48	1.42	1.38
1	A	124	UFT	C2-N3	2.48	1.42	1.38
1	A	181	UFT	O2-C2	-2.48	1.18	1.23
1	A	182	UFT	O2-C2	-2.47	1.18	1.23
1	A	188	UFT	O4'-C1'	2.46	1.47	1.42
1	A	20	UFT	O4'-C1'	2.45	1.47	1.42
1	A	182	UFT	C2-N3	2.43	1.42	1.38
1	A	182	UFT	O4'-C1'	2.43	1.47	1.42
1	A	174	UFT	O4'-C1'	2.41	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	203	UFT	C2'-C1'	-2.41	1.50	1.53
1	A	140	CFZ	C6-C5	2.39	1.40	1.35
1	A	147	UFT	C4-N3	2.39	1.42	1.38
1	A	171	UFT	O2-C2	-2.38	1.18	1.23
1	A	55	UFT	O2-C2	-2.38	1.18	1.23
1	A	194	UFT	O2-C2	-2.37	1.18	1.23
1	A	147	UFT	O4'-C1'	2.37	1.47	1.42
1	A	5	UFT	O2-C2	-2.37	1.18	1.23
1	A	75	UFT	O2-C2	-2.37	1.18	1.23
1	A	144	UFT	O2-C2	-2.36	1.18	1.23
1	A	112	UFT	O2-C2	-2.36	1.18	1.23
1	A	16	UFT	O2-C2	-2.36	1.18	1.23
1	A	190	UFT	O2-C2	-2.36	1.18	1.23
1	A	141	UFT	O2-C2	-2.36	1.18	1.23
1	A	187	UFT	O2-C2	-2.36	1.18	1.23
1	A	64	UFT	O2-C2	-2.35	1.18	1.23
1	A	126	UFT	O2-C2	-2.35	1.18	1.23
1	A	188	UFT	O2-C2	-2.35	1.18	1.23
1	A	109	UFT	O2-C2	-2.35	1.18	1.23
1	A	234	UFT	O2-C2	-2.35	1.18	1.23
1	A	84	UFT	O2-C2	-2.34	1.18	1.23
1	A	29	UFT	O2-C2	-2.34	1.18	1.23
1	A	93	UFT	O4'-C1'	2.34	1.47	1.42
1	A	72	UFT	O2-C2	-2.34	1.18	1.23
1	A	215	UFT	O2-C2	-2.34	1.18	1.23
1	A	226	UFT	O2-C2	-2.34	1.18	1.23
1	A	35	UFT	O2-C2	-2.34	1.18	1.23
1	A	120	UFT	O2-C2	-2.34	1.18	1.23
1	A	153	UFT	O2-C2	-2.33	1.18	1.23
1	A	216	UFT	O2-C2	-2.33	1.18	1.23
1	A	224	UFT	O2-C2	-2.33	1.18	1.23
1	A	222	UFT	C4-N3	2.33	1.42	1.38
1	A	147	UFT	O2-C2	-2.33	1.18	1.23
1	A	134	UFT	O2-C2	-2.33	1.18	1.23
1	A	92	UFT	O2-C2	-2.33	1.18	1.23
1	A	98	UFT	O2-C2	-2.33	1.18	1.23
1	A	229	UFT	O2-C2	-2.33	1.18	1.23
1	A	41	UFT	O2-C2	-2.32	1.18	1.23
1	A	163	UFT	O2-C2	-2.32	1.19	1.23
1	A	10	UFT	O2-C2	-2.32	1.19	1.23
1	A	222	UFT	O2-C2	-2.32	1.19	1.23
1	A	39	UFT	O2-C2	-2.32	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	UFT	O2-C2	-2.32	1.19	1.23
1	A	133	UFT	O2-C2	-2.31	1.19	1.23
1	A	173	UFT	O2-C2	-2.31	1.19	1.23
1	A	48	UFT	O2-C2	-2.31	1.19	1.23
1	A	73	UFT	O2-C2	-2.31	1.19	1.23
1	A	228	UFT	O2-C2	-2.31	1.19	1.23
1	A	100	UFT	O2-C2	-2.31	1.19	1.23
1	A	69	UFT	O2-C2	-2.31	1.19	1.23
1	A	174	UFT	O2-C2	-2.31	1.19	1.23
1	A	54	UFT	O2-C2	-2.31	1.19	1.23
1	A	184	UFT	O2-C2	-2.31	1.19	1.23
1	A	44	UFT	O2-C2	-2.31	1.19	1.23
1	A	77	UFT	O2-C2	-2.30	1.19	1.23
1	A	13	UFT	O2-C2	-2.30	1.19	1.23
1	A	5	UFT	C4-N3	2.30	1.42	1.38
1	A	19	UFT	O2-C2	-2.30	1.19	1.23
1	A	85	UFT	O2-C2	-2.30	1.19	1.23
1	A	20	UFT	O2-C2	-2.29	1.19	1.23
1	A	93	UFT	O2-C2	-2.29	1.19	1.23
1	A	23	UFT	O2-C2	-2.28	1.19	1.23
1	A	46	UFT	O2-C2	-2.28	1.19	1.23
1	A	91	UFT	O2-C2	-2.28	1.19	1.23
1	A	130	UFT	O2-C2	-2.27	1.19	1.23
1	A	210	UFT	O2-C2	-2.27	1.19	1.23
1	A	124	UFT	O2-C2	-2.27	1.19	1.23
1	A	7	UFT	O2-C2	-2.27	1.19	1.23
1	A	111	UFT	O2-C2	-2.26	1.19	1.23
1	A	184	UFT	C4-N3	2.26	1.42	1.38
1	A	231	CFZ	C6-C5	2.25	1.40	1.35
1	A	86	UFT	O2-C2	-2.25	1.19	1.23
1	A	166	UFT	O2-C2	-2.24	1.19	1.23
1	A	75	UFT	C4-N3	2.24	1.42	1.38
1	A	135	CFZ	C6-C5	2.24	1.40	1.35
1	A	21	CFZ	C6-C5	2.23	1.40	1.35
1	A	187	UFT	O4'-C1'	2.23	1.47	1.42
1	A	163	UFT	C4-N3	2.23	1.42	1.38
1	A	24	CFZ	C6-C5	2.23	1.40	1.35
1	A	203	UFT	O2-C2	-2.23	1.19	1.23
1	A	88	UFT	O2-C2	-2.22	1.19	1.23
1	A	39	UFT	C4-N3	2.22	1.42	1.38
1	A	109	UFT	C4-N3	2.22	1.42	1.38
1	A	53	CFZ	C6-C5	2.21	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	91	UFT	C4-N3	2.21	1.42	1.38
1	A	228	UFT	C4-N3	2.21	1.42	1.38
1	A	16	UFT	C2'-C1'	-2.21	1.50	1.53
1	A	217	CFZ	C6-C5	2.20	1.40	1.35
1	A	57	CFZ	C6-C5	2.20	1.40	1.35
1	A	64	UFT	C4-N3	2.18	1.42	1.38
1	A	212	CFZ	C6-C5	2.18	1.40	1.35
1	A	213	CFZ	C6-C5	2.18	1.40	1.35
1	A	234	UFT	C4-N3	2.18	1.42	1.38
1	A	29	UFT	C4-N3	2.17	1.42	1.38
1	A	171	UFT	C4-N3	2.17	1.42	1.38
1	A	121	CFZ	C6-C5	2.17	1.40	1.35
1	A	219	CFZ	C6-C5	2.16	1.40	1.35
1	A	23	UFT	C4-N3	2.16	1.42	1.38
1	A	61	CFZ	C6-C5	2.16	1.40	1.35
1	A	81	CFZ	C6-C5	2.15	1.40	1.35
1	A	94	CFZ	C6-C5	2.15	1.40	1.35
1	A	44	UFT	C4-N3	2.14	1.42	1.38
1	A	175	CFZ	C6-C5	2.14	1.40	1.35
1	A	224	UFT	C4-N3	2.14	1.42	1.38
1	A	34	CFZ	C6-C5	2.14	1.40	1.35
1	A	85	UFT	C4-N3	2.14	1.42	1.38
1	A	8	CFZ	C6-C5	2.14	1.40	1.35
1	A	70	CFZ	C6-C5	2.14	1.40	1.35
1	A	84	UFT	C4-N3	2.14	1.42	1.38
1	A	13	UFT	C4-N3	2.13	1.42	1.38
1	A	194	UFT	C4-N3	2.13	1.42	1.38
1	A	11	CFZ	C6-C5	2.12	1.40	1.35
1	A	154	CFZ	C6-C5	2.12	1.40	1.35
1	A	235	CFZ	C6-C5	2.12	1.40	1.35
1	A	236	CFZ	C6-C5	2.12	1.40	1.35
1	A	90	CFZ	C6-C5	2.12	1.40	1.35
1	A	131	CFZ	C6-C5	2.12	1.40	1.35
1	A	187	UFT	C4-N3	2.11	1.42	1.38
1	A	27	CFZ	C6-C5	2.11	1.40	1.35
1	A	208	CFZ	C6-C5	2.11	1.40	1.35
1	A	100	UFT	C4-N3	2.11	1.42	1.38
1	A	177	CFZ	C6-C5	2.11	1.40	1.35
1	A	181	UFT	C4-N3	2.10	1.42	1.38
1	A	69	UFT	C4-N3	2.10	1.42	1.38
1	A	55	UFT	C4-N3	2.10	1.42	1.38
1	A	199	CFZ	C6-C5	2.10	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	130	UFT	C4-N3	2.10	1.42	1.38
1	A	144	UFT	C4-N3	2.10	1.42	1.38
1	A	203	UFT	C4-N3	2.09	1.42	1.38
1	A	73	UFT	C4-N3	2.08	1.42	1.38
1	A	80	CFZ	C6-C5	2.08	1.39	1.35
1	A	86	UFT	C4-N3	2.07	1.42	1.38
1	A	54	UFT	C4-N3	2.07	1.42	1.38
1	A	152	CFZ	C6-C5	2.07	1.39	1.35
1	A	10	UFT	C4-N3	2.07	1.42	1.38
1	A	226	UFT	C4-N3	2.07	1.42	1.38
1	A	20	UFT	C4-N3	2.06	1.42	1.38
1	A	106	CFZ	C6-C5	2.06	1.39	1.35
1	A	48	UFT	C4-N3	2.06	1.42	1.38
1	A	198	CFZ	C6-C5	2.06	1.39	1.35
1	A	126	UFT	C4-N3	2.06	1.42	1.38
1	A	40	CFZ	C6-C5	2.06	1.39	1.35
1	A	215	UFT	C4-N3	2.06	1.42	1.38
1	A	47	CFZ	C6-C5	2.06	1.39	1.35
1	A	42	CFZ	C6-C5	2.06	1.39	1.35
1	A	93	UFT	C4-N3	2.06	1.42	1.38
1	A	56	UFT	C4-N3	2.06	1.42	1.38
1	A	104	CFZ	C6-C5	2.06	1.39	1.35
1	A	41	UFT	C4-N3	2.06	1.42	1.38
1	A	72	UFT	C4-N3	2.06	1.42	1.38
1	A	238	CFZ	C6-C5	2.06	1.39	1.35
1	A	164	CFZ	C6-C5	2.05	1.39	1.35
1	A	182	UFT	C4-N3	2.05	1.42	1.38
1	A	71	CFZ	C6-C5	2.05	1.39	1.35
1	A	123	CFZ	C6-C5	2.05	1.39	1.35
1	A	63	CFZ	C6-C5	2.05	1.39	1.35
1	A	105	CFZ	C6-C5	2.05	1.39	1.35
1	A	19	UFT	C4-N3	2.05	1.42	1.38
1	A	169	CFZ	C6-C5	2.04	1.39	1.35
1	A	88	UFT	C4-N3	2.04	1.42	1.38
1	A	161	CFZ	C6-C5	2.04	1.39	1.35
1	A	141	UFT	C4-N3	2.04	1.42	1.38
1	A	116	CFZ	C6-C5	2.04	1.39	1.35
1	A	173	UFT	C4-N3	2.04	1.42	1.38
1	A	26	CFZ	C6-C5	2.04	1.39	1.35
1	A	133	UFT	C4-N3	2.03	1.42	1.38
1	A	216	UFT	C4-N3	2.03	1.42	1.38
1	A	166	UFT	C4-N3	2.03	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	190	UFT	C4-N3	2.03	1.42	1.38
1	A	111	UFT	C4-N3	2.03	1.42	1.38
1	A	148	CFZ	C6-C5	2.02	1.39	1.35
1	A	229	UFT	C4-N3	2.02	1.42	1.38
1	A	51	CFZ	C6-C5	2.02	1.39	1.35
1	A	112	UFT	C4-N3	2.02	1.42	1.38
1	A	92	UFT	C4-N3	2.02	1.42	1.38
1	A	149	CFZ	C6-C5	2.01	1.39	1.35
1	A	134	UFT	C4-N3	2.01	1.42	1.38
1	A	174	UFT	C4-N3	2.01	1.42	1.38
1	A	98	UFT	C4-N3	2.01	1.42	1.38
1	A	170	CFZ	C6-C5	2.00	1.39	1.35

All (621) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	UFT	C4-N3-C2	-6.31	118.77	126.61
1	A	147	UFT	C4-N3-C2	-6.19	118.93	126.61
1	A	184	UFT	C4-N3-C2	-6.12	119.02	126.61
1	A	228	UFT	C4-N3-C2	-6.09	119.05	126.61
1	A	163	UFT	C4-N3-C2	-6.07	119.07	126.61
1	A	39	UFT	C4-N3-C2	-5.98	119.19	126.61
1	A	54	UFT	C4-N3-C2	-5.97	119.20	126.61
1	A	75	UFT	C4-N3-C2	-5.93	119.25	126.61
1	A	226	UFT	C4-N3-C2	-5.90	119.28	126.61
1	A	224	UFT	C4-N3-C2	-5.85	119.35	126.61
1	A	109	UFT	C4-N3-C2	-5.85	119.35	126.61
1	A	10	UFT	C4-N3-C2	-5.85	119.35	126.61
1	A	126	UFT	C4-N3-C2	-5.83	119.38	126.61
1	A	181	UFT	C4-N3-C2	-5.77	119.44	126.61
1	A	222	UFT	C4-N3-C2	-5.75	119.48	126.61
1	A	234	UFT	C4-N3-C2	-5.74	119.48	126.61
1	A	91	UFT	C4-N3-C2	-5.72	119.50	126.61
1	A	29	UFT	C4-N3-C2	-5.68	119.56	126.61
1	A	64	UFT	C4-N3-C2	-5.68	119.56	126.61
1	A	144	UFT	C4-N3-C2	-5.67	119.58	126.61
1	A	84	UFT	C4-N3-C2	-5.66	119.58	126.61
1	A	194	UFT	C4-N3-C2	-5.63	119.63	126.61
1	A	44	UFT	C4-N3-C2	-5.61	119.65	126.61
1	A	229	UFT	C4-N3-C2	-5.60	119.65	126.61
1	A	100	UFT	C4-N3-C2	-5.60	119.66	126.61
1	A	182	UFT	C4-N3-C2	-5.58	119.68	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	UFT	C4-N3-C2	-5.57	119.70	126.61
1	A	171	UFT	C4-N3-C2	-5.54	119.73	126.61
1	A	69	UFT	C4-N3-C2	-5.52	119.76	126.61
1	A	72	UFT	C4-N3-C2	-5.50	119.78	126.61
1	A	48	UFT	C4-N3-C2	-5.49	119.80	126.61
1	A	187	UFT	C4-N3-C2	-5.48	119.81	126.61
1	A	112	UFT	C4-N3-C2	-5.44	119.85	126.61
1	A	133	UFT	C4-N3-C2	-5.44	119.86	126.61
1	A	166	UFT	C4-N3-C2	-5.43	119.87	126.61
1	A	13	UFT	C4-N3-C2	-5.43	119.87	126.61
1	A	41	UFT	C4-N3-C2	-5.43	119.88	126.61
1	A	153	UFT	C4-N3-C2	-5.43	119.88	126.61
1	A	141	UFT	C4-N3-C2	-5.42	119.89	126.61
1	A	173	UFT	C4-N3-C2	-5.42	119.89	126.61
1	A	215	UFT	C4-N3-C2	-5.41	119.90	126.61
1	A	174	UFT	C4-N3-C2	-5.40	119.91	126.61
1	A	19	UFT	C4-N3-C2	-5.38	119.93	126.61
1	A	92	UFT	C4-N3-C2	-5.37	119.94	126.61
1	A	190	UFT	C4-N3-C2	-5.36	119.96	126.61
1	A	7	UFT	C4-N3-C2	-5.36	119.96	126.61
1	A	134	UFT	C4-N3-C2	-5.35	119.97	126.61
1	A	130	UFT	C4-N3-C2	-5.34	119.98	126.61
1	A	93	UFT	C4-N3-C2	-5.29	120.04	126.61
1	A	20	UFT	C4-N3-C2	-5.29	120.05	126.61
1	A	188	UFT	C4-N3-C2	-5.29	120.05	126.61
1	A	56	UFT	C4-N3-C2	-5.29	120.05	126.61
1	A	86	UFT	C4-N3-C2	-5.29	120.05	126.61
1	A	55	UFT	C4-N3-C2	-5.28	120.05	126.61
1	A	73	UFT	C4-N3-C2	-5.28	120.06	126.61
1	A	98	UFT	C4-N3-C2	-5.27	120.07	126.61
1	A	216	UFT	C4-N3-C2	-5.24	120.10	126.61
1	A	35	UFT	C4-N3-C2	-5.18	120.18	126.61
1	A	210	UFT	C4-N3-C2	-5.16	120.20	126.61
1	A	120	UFT	C4-N3-C2	-5.16	120.21	126.61
1	A	77	UFT	C4-N3-C2	-5.14	120.23	126.61
1	A	46	UFT	C4-N3-C2	-5.13	120.24	126.61
1	A	23	UFT	C4-N3-C2	-5.10	120.28	126.61
1	A	88	UFT	C4-N3-C2	-5.08	120.31	126.61
1	A	203	UFT	C4-N3-C2	-5.03	120.37	126.61
1	A	124	UFT	C4-N3-C2	-5.00	120.40	126.61
1	A	111	UFT	C4-N3-C2	-5.00	120.41	126.61
1	A	16	UFT	C4-N3-C2	-4.73	120.74	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	UFT	C2'-C1'-N1	-4.72	107.01	114.27
1	A	208	CFZ	C2'-C1'-N1	-4.67	107.09	114.27
1	A	226	UFT	N3-C2-N1	4.67	120.97	114.89
1	A	219	CFZ	C3'-C2'-C1'	4.63	108.47	103.10
1	A	114	CFZ	C3'-C2'-C1'	4.57	108.41	103.10
1	A	121	CFZ	C2'-C1'-N1	-4.53	107.31	114.27
1	A	53	CFZ	C2'-C3'-C4'	4.43	108.27	102.43
1	A	213	CFZ	C2'-C1'-N1	-4.42	107.48	114.27
1	A	229	UFT	N3-C2-N1	4.40	120.62	114.89
1	A	164	CFZ	C3'-C2'-C1'	4.40	108.21	103.10
1	A	39	UFT	N3-C2-N1	4.35	120.55	114.89
1	A	228	UFT	N3-C2-N1	4.34	120.54	114.89
1	A	5	UFT	N3-C2-N1	4.33	120.53	114.89
1	A	144	UFT	N3-C2-N1	4.32	120.52	114.89
1	A	109	UFT	C3'-C2'-C1'	4.31	108.10	103.10
1	A	181	UFT	N3-C2-N1	4.30	120.50	114.89
1	A	184	UFT	N3-C2-N1	4.28	120.46	114.89
1	A	29	UFT	N3-C2-N1	4.26	120.44	114.89
1	A	20	UFT	C3'-C2'-C1'	4.26	108.04	103.10
1	A	109	UFT	N3-C2-N1	4.24	120.41	114.89
1	A	16	UFT	N3-C2-N1	4.24	120.41	114.89
1	A	100	UFT	N3-C2-N1	4.23	120.39	114.89
1	A	54	UFT	C5-C4-N3	4.22	120.71	114.80
1	A	126	UFT	N3-C2-N1	4.22	120.38	114.89
1	A	10	UFT	N3-C2-N1	4.21	120.37	114.89
1	A	5	UFT	C5-C4-N3	4.20	120.69	114.80
1	A	147	UFT	C5-C4-N3	4.19	120.68	114.80
1	A	210	UFT	N3-C2-N1	4.19	120.34	114.89
1	A	7	UFT	C2'-C1'-N1	-4.18	107.84	114.27
1	A	234	UFT	N3-C2-N1	4.18	120.33	114.89
1	A	163	UFT	C5-C4-N3	4.17	120.64	114.80
1	A	171	UFT	N3-C2-N1	4.16	120.30	114.89
1	A	182	UFT	N3-C2-N1	4.13	120.27	114.89
1	A	91	UFT	N3-C2-N1	4.13	120.27	114.89
1	A	147	UFT	N3-C2-N1	4.13	120.26	114.89
1	A	141	UFT	N3-C2-N1	4.13	120.26	114.89
1	A	194	UFT	N3-C2-N1	4.12	120.26	114.89
1	A	124	UFT	N3-C2-N1	4.12	120.25	114.89
1	A	75	UFT	N3-C2-N1	4.12	120.25	114.89
1	A	190	UFT	N3-C2-N1	4.11	120.24	114.89
1	A	94	CFZ	C2'-C3'-C4'	4.11	107.84	102.43
1	A	222	UFT	N3-C2-N1	4.10	120.23	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	UFT	N3-C2-N1	4.10	120.23	114.89
1	A	120	UFT	N3-C2-N1	4.09	120.22	114.89
1	A	224	UFT	N3-C2-N1	4.08	120.21	114.89
1	A	153	UFT	N3-C2-N1	4.08	120.20	114.89
1	A	56	UFT	C3'-C2'-C1'	4.08	107.83	103.10
1	A	7	UFT	N3-C2-N1	4.08	120.20	114.89
1	A	163	UFT	N3-C2-N1	4.08	120.20	114.89
1	A	48	UFT	N3-C2-N1	4.07	120.20	114.89
1	A	54	UFT	N3-C2-N1	4.07	120.19	114.89
1	A	188	UFT	N3-C2-N1	4.07	120.19	114.89
1	A	92	UFT	N3-C2-N1	4.06	120.17	114.89
1	A	44	UFT	N3-C2-N1	4.06	120.17	114.89
1	A	173	UFT	N3-C2-N1	4.05	120.17	114.89
1	A	112	UFT	N3-C2-N1	4.05	120.16	114.89
1	A	170	CFZ	C3'-C2'-C1'	4.05	107.80	103.10
1	A	166	UFT	N3-C2-N1	4.04	120.15	114.89
1	A	24	CFZ	C3'-C2'-C1'	4.04	107.79	103.10
1	A	56	UFT	C2'-C3'-C4'	4.04	107.75	102.43
1	A	147	UFT	C3'-C2'-C1'	4.03	107.78	103.10
1	A	64	UFT	N3-C2-N1	4.03	120.14	114.89
1	A	75	UFT	C5-C4-N3	4.01	120.42	114.80
1	A	85	UFT	C2'-C1'-N1	-4.01	108.11	114.27
1	A	46	UFT	N3-C2-N1	4.01	120.11	114.89
1	A	228	UFT	C5-C4-N3	4.00	120.40	114.80
1	A	187	UFT	N3-C2-N1	3.99	120.09	114.89
1	A	184	UFT	C5-C4-N3	3.99	120.39	114.80
1	A	23	UFT	N3-C2-N1	3.99	120.08	114.89
1	A	56	UFT	N3-C2-N1	3.98	120.07	114.89
1	A	69	UFT	N3-C2-N1	3.98	120.07	114.89
1	A	73	UFT	N3-C2-N1	3.97	120.05	114.89
1	A	84	UFT	N3-C2-N1	3.96	120.05	114.89
1	A	215	UFT	N3-C2-N1	3.96	120.05	114.89
1	A	77	UFT	N3-C2-N1	3.96	120.04	114.89
1	A	19	UFT	N3-C2-N1	3.96	120.04	114.89
1	A	20	UFT	N3-C2-N1	3.96	120.04	114.89
1	A	224	UFT	C5-C4-N3	3.96	120.34	114.80
1	A	85	UFT	C5-C4-N3	3.95	120.33	114.80
1	A	134	UFT	N3-C2-N1	3.94	120.02	114.89
1	A	13	UFT	N3-C2-N1	3.93	120.01	114.89
1	A	86	UFT	N3-C2-N1	3.93	120.00	114.89
1	A	131	CFZ	C3'-C2'-C1'	3.92	107.65	103.10
1	A	133	UFT	N3-C2-N1	3.92	120.00	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	UFT	N3-C2-N1	3.92	119.99	114.89
1	A	41	UFT	N3-C2-N1	3.92	119.99	114.89
1	A	35	UFT	N3-C2-N1	3.91	119.98	114.89
1	A	55	UFT	N3-C2-N1	3.91	119.98	114.89
1	A	188	UFT	C3'-C2'-C1'	3.90	107.63	103.10
1	A	84	UFT	C5-C4-N3	3.90	120.26	114.80
1	A	21	CFZ	C2'-C3'-C4'	3.89	107.56	102.43
1	A	10	UFT	C5-C4-N3	3.89	120.25	114.80
1	A	93	UFT	N3-C2-N1	3.89	119.95	114.89
1	A	174	UFT	N3-C2-N1	3.88	119.94	114.89
1	A	134	UFT	C2'-C3'-C4'	3.88	107.54	102.43
1	A	170	CFZ	C2'-C3'-C4'	3.87	107.53	102.43
1	A	216	UFT	N3-C2-N1	3.86	119.92	114.89
1	A	8	CFZ	C2'-C1'-N1	-3.85	108.35	114.27
1	A	5	UFT	O4-C4-C5	-3.85	118.52	125.16
1	A	175	CFZ	F2'-C2'-C3'	3.85	116.74	109.14
1	A	169	CFZ	C3'-C2'-C1'	3.85	107.56	103.10
1	A	39	UFT	C5-C4-N3	3.82	120.16	114.80
1	A	88	UFT	N3-C2-N1	3.82	119.87	114.89
1	A	21	CFZ	C3'-C2'-C1'	3.82	107.53	103.10
1	A	126	UFT	C5-C4-N3	3.82	120.14	114.80
1	A	235	CFZ	C3'-C2'-C1'	3.81	107.53	103.10
1	A	147	UFT	O4-C4-C5	-3.81	118.58	125.16
1	A	217	CFZ	C2'-C3'-C4'	3.81	107.45	102.43
1	A	203	UFT	N3-C2-N1	3.81	119.85	114.89
1	A	64	UFT	C5-C4-N3	3.81	120.13	114.80
1	A	44	UFT	C5-C4-N3	3.81	120.13	114.80
1	A	222	UFT	C5-C4-N3	3.81	120.13	114.80
1	A	181	UFT	C5-C4-N3	3.81	120.13	114.80
1	A	131	CFZ	C2'-C3'-C4'	3.80	107.44	102.43
1	A	91	UFT	C5-C4-N3	3.80	120.12	114.80
1	A	130	UFT	C5-C4-N3	3.79	120.11	114.80
1	A	111	UFT	N3-C2-N1	3.79	119.83	114.89
1	A	90	CFZ	C3'-C2'-C1'	3.79	107.50	103.10
1	A	182	UFT	C5-C4-N3	3.78	120.09	114.80
1	A	184	UFT	C3'-C2'-C1'	3.78	107.48	103.10
1	A	13	UFT	C5-C4-N3	3.77	120.08	114.80
1	A	174	UFT	C5-C4-N3	3.77	120.08	114.80
1	A	133	UFT	C5-C4-N3	3.77	120.08	114.80
1	A	194	UFT	C5-C4-N3	3.77	120.07	114.80
1	A	234	UFT	C5-C4-N3	3.76	120.07	114.80
1	A	171	UFT	C2'-C1'-N1	-3.76	108.50	114.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	UFT	C5-C4-N3	3.75	120.05	114.80
1	A	85	UFT	N3-C2-N1	3.75	119.77	114.89
1	A	72	UFT	C5-C4-N3	3.75	120.05	114.80
1	A	141	UFT	C3'-C2'-C1'	3.75	107.45	103.10
1	A	20	UFT	C2'-C3'-C4'	3.74	107.37	102.43
1	A	130	UFT	N3-C2-N1	3.74	119.76	114.89
1	A	166	UFT	C5-C4-N3	3.74	120.03	114.80
1	A	187	UFT	C5-C4-N3	3.73	120.02	114.80
1	A	177	CFZ	C3'-C2'-C1'	3.73	107.43	103.10
1	A	112	UFT	C5-C4-N3	3.72	120.02	114.80
1	A	226	UFT	C5-C4-N3	3.71	120.00	114.80
1	A	29	UFT	C5-C4-N3	3.71	119.99	114.80
1	A	51	CFZ	C3'-C2'-C1'	3.71	107.40	103.10
1	A	86	UFT	C5-C4-N3	3.70	119.98	114.80
1	A	215	UFT	C5-C4-N3	3.69	119.97	114.80
1	A	69	UFT	C5-C4-N3	3.69	119.97	114.80
1	A	171	UFT	C5-C4-N3	3.69	119.97	114.80
1	A	41	UFT	C5-C4-N3	3.69	119.96	114.80
1	A	19	UFT	C5-C4-N3	3.68	119.96	114.80
1	A	187	UFT	C3'-C2'-C1'	3.68	107.37	103.10
1	A	238	CFZ	C3'-C2'-C1'	3.67	107.36	103.10
1	A	173	UFT	C5-C4-N3	3.67	119.94	114.80
1	A	182	UFT	C3'-C2'-C1'	3.67	107.36	103.10
1	A	174	UFT	C2'-C3'-C4'	3.66	107.26	102.43
1	A	100	UFT	C5-C4-N3	3.66	119.93	114.80
1	A	144	UFT	C5-C4-N3	3.66	119.93	114.80
1	A	134	UFT	C5-C4-N3	3.66	119.93	114.80
1	A	216	UFT	C3'-C2'-C1'	3.66	107.35	103.10
1	A	130	UFT	C3'-C2'-C1'	3.65	107.34	103.10
1	A	39	UFT	C3'-C2'-C1'	3.65	107.33	103.10
1	A	48	UFT	C5-C4-N3	3.64	119.91	114.80
1	A	93	UFT	C5-C4-N3	3.64	119.90	114.80
1	A	216	UFT	C5-C4-N3	3.64	119.90	114.80
1	A	163	UFT	O4-C4-C5	-3.63	118.90	125.16
1	A	7	UFT	C5-C4-N3	3.63	119.89	114.80
1	A	229	UFT	C5-C4-N3	3.62	119.87	114.80
1	A	212	CFZ	C3'-C2'-C1'	3.62	107.30	103.10
1	A	153	UFT	C5-C4-N3	3.62	119.87	114.80
1	A	88	UFT	C5-C4-N3	3.61	119.86	114.80
1	A	174	UFT	C3'-C2'-C1'	3.61	107.29	103.10
1	A	92	UFT	C5-C4-N3	3.61	119.85	114.80
1	A	141	UFT	C5-C4-N3	3.61	119.85	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	UFT	O4-C4-C5	-3.60	118.95	125.16
1	A	20	UFT	C5-C4-N3	3.60	119.84	114.80
1	A	55	UFT	C5-C4-N3	3.60	119.84	114.80
1	A	73	UFT	C5-C4-N3	3.60	119.84	114.80
1	A	19	UFT	C3'-C2'-C1'	3.59	107.27	103.10
1	A	11	CFZ	C3'-C2'-C1'	3.58	107.25	103.10
1	A	75	UFT	O4-C4-C5	-3.58	118.99	125.16
1	A	24	CFZ	C2'-C1'-N1	-3.57	108.78	114.27
1	A	54	UFT	O4-C4-C5	-3.57	119.01	125.16
1	A	190	UFT	C5-C4-N3	3.56	119.79	114.80
1	A	35	UFT	C5-C4-N3	3.56	119.78	114.80
1	A	56	UFT	C5-C4-N3	3.56	119.78	114.80
1	A	188	UFT	C5-C4-N3	3.55	119.77	114.80
1	A	226	UFT	C3'-C2'-C1'	3.55	107.22	103.10
1	A	77	UFT	C5-C4-N3	3.54	119.76	114.80
1	A	134	UFT	C3'-C2'-C1'	3.54	107.20	103.10
1	A	57	CFZ	C3'-C2'-C1'	3.54	107.20	103.10
1	A	35	UFT	C2'-C1'-N1	-3.53	108.84	114.27
1	A	93	UFT	C3'-C2'-C1'	3.53	107.20	103.10
1	A	80	CFZ	C2'-C1'-N1	-3.52	108.86	114.27
1	A	46	UFT	C5-C4-N3	3.51	119.71	114.80
1	A	137	CFZ	C3'-C2'-C1'	3.50	107.16	103.10
1	A	111	UFT	C5-C4-N3	3.50	119.70	114.80
1	A	48	UFT	C3'-C2'-C1'	3.49	107.15	103.10
1	A	98	UFT	C5-C4-N3	3.49	119.68	114.80
1	A	61	CFZ	C3'-C2'-C1'	3.48	107.14	103.10
1	A	187	UFT	C2'-C3'-C4'	3.48	107.01	102.43
1	A	222	UFT	O4-C4-C5	-3.47	119.18	125.16
1	A	120	UFT	C5-C4-N3	3.46	119.65	114.80
1	A	184	UFT	O4-C4-C5	-3.44	119.23	125.16
1	A	203	UFT	C5-C4-N3	3.42	119.60	114.80
1	A	203	UFT	C3'-C2'-C1'	3.40	107.05	103.10
1	A	109	UFT	C2'-C3'-C4'	3.39	106.90	102.43
1	A	231	CFZ	C3'-C2'-C1'	3.39	107.03	103.10
1	A	64	UFT	O4-C4-C5	-3.39	119.32	125.16
1	A	224	UFT	O4-C4-C5	-3.39	119.32	125.16
1	A	126	UFT	C3'-C2'-C1'	3.38	107.03	103.10
1	A	85	UFT	O4-C4-C5	-3.38	119.33	125.16
1	A	140	CFZ	C3'-C2'-C1'	3.37	107.02	103.10
1	A	109	UFT	O4-C4-C5	-3.37	119.34	125.16
1	A	84	UFT	O4-C4-C5	-3.37	119.35	125.16
1	A	91	UFT	O4-C4-C5	-3.37	119.35	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	UFT	O4-C4-C5	-3.36	119.37	125.16
1	A	81	CFZ	C3'-C2'-C1'	3.36	107.00	103.10
1	A	210	UFT	C5-C4-N3	3.36	119.50	114.80
1	A	23	UFT	C5-C4-N3	3.35	119.49	114.80
1	A	53	CFZ	C3'-C2'-C1'	3.35	106.98	103.10
1	A	234	UFT	O4-C4-C5	-3.35	119.39	125.16
1	A	228	UFT	C3'-C2'-C1'	3.34	106.98	103.10
1	A	94	CFZ	C3'-C2'-C1'	3.33	106.97	103.10
1	A	182	UFT	C2'-C3'-C4'	3.33	106.82	102.43
1	A	39	UFT	O4-C4-C5	-3.33	119.42	125.16
1	A	76	CFZ	C3'-C2'-C1'	3.32	106.95	103.10
1	A	114	CFZ	C2'-C3'-C4'	3.31	106.80	102.43
1	A	124	UFT	C5-C4-N3	3.31	119.44	114.80
1	A	188	UFT	C2'-C3'-C4'	3.30	106.78	102.43
1	A	46	UFT	C3'-C2'-C1'	3.30	106.93	103.10
1	A	135	CFZ	C2'-C3'-C4'	3.29	106.77	102.43
1	A	26	CFZ	C3'-C2'-C1'	3.27	106.90	103.10
1	A	227	CFZ	C3'-C2'-C1'	3.26	106.89	103.10
1	A	10	UFT	O4-C4-C5	-3.24	119.57	125.16
1	A	140	CFZ	C2'-C3'-C4'	3.24	106.70	102.43
1	A	235	CFZ	C2'-C3'-C4'	3.24	106.70	102.43
1	A	147	UFT	C2'-C3'-C4'	3.24	106.69	102.43
1	A	234	UFT	C2'-C3'-C4'	3.23	106.69	102.43
1	A	61	CFZ	C2'-C3'-C4'	3.23	106.69	102.43
1	A	44	UFT	O4-C4-C5	-3.23	119.60	125.16
1	A	133	UFT	C3'-C2'-C1'	3.22	106.83	103.10
1	A	126	UFT	O4-C4-C5	-3.21	119.62	125.16
1	A	55	UFT	C3'-C2'-C1'	3.20	106.81	103.10
1	A	93	UFT	C2'-C3'-C4'	3.19	106.64	102.43
1	A	236	CFZ	C3'-C2'-C1'	3.19	106.81	103.10
1	A	163	UFT	C3'-C2'-C1'	3.19	106.80	103.10
1	A	216	UFT	C2'-C3'-C4'	3.19	106.63	102.43
1	A	113	CFZ	C2'-C1'-N1	-3.17	109.40	114.27
1	A	166	UFT	C2'-C1'-N1	-3.15	109.42	114.27
1	A	187	UFT	O4-C4-C5	-3.14	119.74	125.16
1	A	70	CFZ	C2'-C1'-N1	-3.14	109.45	114.27
1	A	13	UFT	O4-C4-C5	-3.14	119.75	125.16
1	A	199	CFZ	C2'-C1'-N1	-3.13	109.46	114.27
1	A	238	CFZ	C2'-C3'-C4'	3.12	106.54	102.43
1	A	194	UFT	O4-C4-C5	-3.12	119.79	125.16
1	A	69	UFT	C3'-C2'-C1'	3.11	106.72	103.10
1	A	63	CFZ	C2'-C1'-N1	-3.11	109.49	114.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	210	UFT	C3'-C2'-C1'	3.11	106.71	103.10
1	A	73	UFT	C3'-C2'-C1'	3.10	106.70	103.10
1	A	64	UFT	C2'-C1'-N1	-3.10	109.51	114.27
1	A	141	UFT	C2'-C3'-C4'	3.10	106.51	102.43
1	A	29	UFT	O4-C4-C5	-3.09	119.83	125.16
1	A	92	UFT	C2'-C1'-N1	-3.09	109.52	114.27
1	A	41	UFT	O4-C4-C5	-3.09	119.84	125.16
1	A	69	UFT	O4-C4-C5	-3.08	119.85	125.16
1	A	126	UFT	C2'-C3'-C4'	3.08	106.49	102.43
1	A	86	UFT	O4-C4-C5	-3.08	119.86	125.16
1	A	181	UFT	O4-C4-C5	-3.07	119.86	125.16
1	A	57	CFZ	C4'-O4'-C1'	-3.06	102.70	109.47
1	A	224	UFT	C3'-C2'-C1'	3.06	106.65	103.10
1	A	16	UFT	C3'-C2'-C1'	3.06	106.65	103.10
1	A	113	CFZ	C3'-C2'-C1'	3.05	106.65	103.10
1	A	174	UFT	O4-C4-C5	-3.05	119.90	125.16
1	A	173	UFT	C3'-C2'-C1'	3.05	106.64	103.10
1	A	47	CFZ	C3'-C2'-C1'	3.05	106.64	103.10
1	A	152	CFZ	C2'-C1'-N1	-3.05	109.59	114.27
1	A	229	UFT	O4-C4-C5	-3.04	119.91	125.16
1	A	98	UFT	C2'-C1'-N1	-3.04	109.60	114.27
1	A	166	UFT	O4-C4-C5	-3.04	119.93	125.16
1	A	182	UFT	O4-C4-C5	-3.03	119.93	125.16
1	A	48	UFT	O4-C4-C5	-3.03	119.93	125.16
1	A	153	UFT	C2'-C1'-N1	-3.03	109.61	114.27
1	A	100	UFT	O4-C4-C5	-3.03	119.94	125.16
1	A	149	CFZ	C3'-C2'-C1'	3.03	106.61	103.10
1	A	130	UFT	O4-C4-C5	-3.03	119.94	125.16
1	A	51	CFZ	C2'-C3'-C4'	3.02	106.41	102.43
1	A	216	UFT	O4-C4-C5	-3.02	119.95	125.16
1	A	133	UFT	O4-C4-C5	-3.02	119.96	125.16
1	A	16	UFT	C5-C4-N3	3.02	119.03	114.80
1	A	72	UFT	O4-C4-C5	-3.01	119.97	125.16
1	A	215	UFT	C2'-C1'-N1	-3.01	109.65	114.27
1	A	34	CFZ	C2'-C1'-N1	-3.01	109.65	114.27
1	A	123	CFZ	C3'-C2'-C1'	3.01	106.59	103.10
1	A	90	CFZ	C2'-C3'-C4'	3.00	106.39	102.43
1	A	100	UFT	C2'-C1'-N1	-3.00	109.66	114.27
1	A	173	UFT	O4-C4-C5	-2.98	120.02	125.16
1	A	41	UFT	C3'-C2'-C1'	2.98	106.56	103.10
1	A	39	UFT	C2'-C3'-C4'	2.97	106.35	102.43
1	A	73	UFT	O4-C4-C5	-2.97	120.04	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	UFT	O4-C4-C5	-2.97	120.05	125.16
1	A	144	UFT	O4-C4-C5	-2.96	120.05	125.16
1	A	215	UFT	O4-C4-C5	-2.96	120.06	125.16
1	A	19	UFT	O4-C4-C5	-2.95	120.07	125.16
1	A	93	UFT	O4-C4-C5	-2.95	120.08	125.16
1	A	175	CFZ	C2'-C1'-N1	-2.95	109.74	114.27
1	A	56	UFT	O4-C4-C5	-2.94	120.09	125.16
1	A	190	UFT	O4-C4-C5	-2.93	120.11	125.16
1	A	84	UFT	C2'-C1'-N1	-2.93	109.77	114.27
1	A	20	UFT	O4-C4-C5	-2.92	120.12	125.16
1	A	71	CFZ	C2'-C1'-N1	-2.92	109.78	114.27
1	A	88	UFT	O4-C4-C5	-2.92	120.13	125.16
1	A	13	UFT	C2'-C1'-N1	-2.92	109.79	114.27
1	A	88	UFT	C3'-C2'-C1'	2.92	106.48	103.10
1	A	10	UFT	C3'-C2'-C1'	2.91	106.48	103.10
1	A	55	UFT	O4-C4-C5	-2.91	120.15	125.16
1	A	175	CFZ	C3'-C2'-C1'	2.90	106.47	103.10
1	A	92	UFT	O4-C4-C5	-2.90	120.16	125.16
1	A	116	CFZ	C3'-C2'-C1'	2.90	106.46	103.10
1	A	23	UFT	O4-C4-C5	-2.89	120.19	125.16
1	A	46	UFT	O4-C4-C5	-2.88	120.19	125.16
1	A	106	CFZ	C2'-C1'-N1	-2.88	109.84	114.27
1	A	42	CFZ	C2'-C1'-N1	-2.88	109.85	114.27
1	A	23	UFT	C3'-C2'-C1'	2.88	106.44	103.10
1	A	19	UFT	C2'-C3'-C4'	2.87	106.22	102.43
1	A	164	CFZ	C2'-C3'-C4'	2.86	106.20	102.43
1	A	29	UFT	C2'-C1'-N1	-2.86	109.87	114.27
1	A	222	UFT	C2'-C1'-N1	-2.86	109.88	114.27
1	A	226	UFT	O4-C4-C5	-2.85	120.24	125.16
1	A	112	UFT	O4-C4-C5	-2.85	120.25	125.16
1	A	124	UFT	C2'-C1'-N1	-2.84	109.90	114.27
1	A	161	CFZ	C3'-C2'-C1'	2.84	106.40	103.10
1	A	198	CFZ	C3'-C2'-C1'	2.84	106.39	103.10
1	A	72	UFT	C2'-C1'-N1	-2.84	109.91	114.27
1	A	153	UFT	O4-C4-C5	-2.82	120.29	125.16
1	A	7	UFT	O4-C4-C5	-2.82	120.29	125.16
1	A	194	UFT	C2'-C1'-N1	-2.82	109.94	114.27
1	A	98	UFT	O4-C4-C5	-2.81	120.31	125.16
1	A	190	UFT	C2'-C1'-N1	-2.81	109.95	114.27
1	A	35	UFT	O4-C4-C5	-2.81	120.31	125.16
1	A	92	UFT	C3'-C2'-C1'	2.80	106.35	103.10
1	A	77	UFT	O4-C4-C5	-2.80	120.33	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	UFT	C2'-C1'-N1	-2.80	109.97	114.27
1	A	190	UFT	C3'-C2'-C1'	2.79	106.34	103.10
1	A	55	UFT	C2'-C3'-C4'	2.79	106.10	102.43
1	A	134	UFT	C2'-C1'-N1	-2.79	109.99	114.27
1	A	212	CFZ	C2'-C1'-N1	-2.78	109.99	114.27
1	A	219	CFZ	C2'-C3'-C4'	2.78	106.10	102.43
1	A	203	UFT	O4-C4-C5	-2.78	120.37	125.16
1	A	141	UFT	O4-C4-C5	-2.78	120.38	125.16
1	A	40	CFZ	C3'-C2'-C1'	2.77	106.32	103.10
1	A	215	UFT	C3'-C2'-C1'	2.77	106.31	103.10
1	A	85	UFT	C3'-C2'-C1'	2.77	106.31	103.10
1	A	26	CFZ	C2'-C3'-C4'	2.76	106.06	102.43
1	A	111	UFT	O4-C4-C5	-2.75	120.42	125.16
1	A	54	UFT	C2'-C1'-N1	-2.75	110.04	114.27
1	A	140	CFZ	C4'-O4'-C1'	-2.75	103.40	109.47
1	A	81	CFZ	C2'-C1'-N1	-2.74	110.05	114.27
1	A	226	UFT	O2-C2-N1	-2.74	119.23	122.80
1	A	72	UFT	C3'-C2'-C1'	2.73	106.27	103.10
1	A	120	UFT	O4-C4-C5	-2.73	120.46	125.16
1	A	217	CFZ	C3'-C2'-C1'	2.72	106.26	103.10
1	A	234	UFT	C4'-O4'-C1'	-2.72	103.47	109.47
1	A	40	CFZ	C2'-C1'-N1	-2.72	110.10	114.27
1	A	44	UFT	C2'-C1'-N1	-2.71	110.10	114.27
1	A	77	UFT	C2'-C1'-N1	-2.71	110.10	114.27
1	A	19	UFT	C2'-C1'-N1	-2.71	110.10	114.27
1	A	27	CFZ	C3'-C2'-C1'	2.71	106.25	103.10
1	A	54	UFT	C3'-C2'-C1'	2.70	106.24	103.10
1	A	91	UFT	C2'-C1'-N1	-2.70	110.13	114.27
1	A	124	UFT	C3'-C2'-C1'	2.69	106.22	103.10
1	A	219	CFZ	O2-C2-N3	-2.68	118.10	122.33
1	A	76	CFZ	C2'-C1'-N1	-2.68	110.15	114.27
1	A	149	CFZ	C2'-C1'-N1	-2.68	110.15	114.27
1	A	181	UFT	C3'-C2'-C1'	2.68	106.20	103.10
1	A	188	UFT	O4-C4-C5	-2.67	120.56	125.16
1	A	144	UFT	C2'-C1'-N1	-2.65	110.20	114.27
1	A	133	UFT	C2'-C1'-N1	-2.65	110.20	114.27
1	A	224	UFT	C2'-C3'-C4'	2.64	105.92	102.43
1	A	130	UFT	C2'-C3'-C4'	2.64	105.91	102.43
1	A	46	UFT	C1'-N1-C2	2.64	122.33	117.59
1	A	55	UFT	C2'-C1'-N1	-2.64	110.22	114.27
1	A	34	CFZ	C3'-C2'-C1'	2.62	106.14	103.10
1	A	48	UFT	C2'-C3'-C4'	2.62	105.88	102.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	UFT	C2'-C1'-N1	-2.61	110.26	114.27
1	A	153	UFT	C3'-C2'-C1'	2.61	106.13	103.10
1	A	11	CFZ	C2'-C3'-C4'	2.61	105.87	102.43
1	A	111	UFT	C2'-C1'-N1	-2.60	110.28	114.27
1	A	210	UFT	O4-C4-C5	-2.60	120.69	125.16
1	A	42	CFZ	C3'-C2'-C1'	2.59	106.11	103.10
1	A	199	CFZ	C3'-C2'-C1'	2.59	106.11	103.10
1	A	27	CFZ	C2'-C1'-N1	-2.59	110.30	114.27
1	A	98	UFT	C3'-C2'-C1'	2.59	106.10	103.10
1	A	5	UFT	O2-C2-N1	-2.58	119.44	122.80
1	A	46	UFT	C2'-C3'-C4'	2.57	105.82	102.43
1	A	229	UFT	C2'-C1'-N1	-2.57	110.32	114.27
1	A	57	CFZ	C2'-C3'-C4'	2.56	105.81	102.43
1	A	91	UFT	C3'-C2'-C1'	2.55	106.06	103.10
1	A	142	CFZ	C3'-C2'-C1'	2.55	106.06	103.10
1	A	86	UFT	C2'-C1'-N1	-2.55	110.36	114.27
1	A	236	CFZ	C2'-C3'-C4'	2.54	105.78	102.43
1	A	112	UFT	O2-C2-N1	-2.53	119.50	122.80
1	A	104	CFZ	C2'-C1'-N1	-2.53	110.38	114.27
1	A	231	CFZ	C4'-O4'-C1'	-2.53	103.89	109.47
1	A	177	CFZ	C2'-C3'-C4'	2.52	105.76	102.43
1	A	238	CFZ	C2'-C1'-N1	-2.52	110.40	114.27
1	A	203	UFT	C2'-C1'-N1	-2.52	110.41	114.27
1	A	124	UFT	O4-C4-C5	-2.51	120.83	125.16
1	A	77	UFT	C3'-C2'-C1'	2.51	106.01	103.10
1	A	161	CFZ	C2'-C1'-N1	-2.51	110.42	114.27
1	A	71	CFZ	C3'-C2'-C1'	2.50	106.00	103.10
1	A	61	CFZ	C2'-C1'-N1	-2.48	110.45	114.27
1	A	198	CFZ	C2'-C1'-N1	-2.48	110.47	114.27
1	A	142	CFZ	C2'-C1'-N1	-2.47	110.48	114.27
1	A	148	CFZ	O2-C2-N3	-2.46	118.44	122.33
1	A	39	UFT	O2-C2-N1	-2.46	119.60	122.80
1	A	75	UFT	C2'-C1'-N1	-2.45	110.50	114.27
1	A	210	UFT	C2'-C1'-N1	-2.45	110.50	114.27
1	A	234	UFT	O2-C2-N1	-2.45	119.61	122.80
1	A	184	UFT	C2'-C3'-C4'	2.44	105.65	102.43
1	A	175	CFZ	O3'-C3'-C2'	2.44	120.82	111.85
1	A	130	UFT	C2'-C1'-N1	-2.44	110.53	114.27
1	A	234	UFT	C3'-C2'-C1'	2.43	105.92	103.10
1	A	133	UFT	C2'-C3'-C4'	2.42	105.62	102.43
1	A	231	CFZ	C2'-C3'-C4'	2.40	105.60	102.43
1	A	171	UFT	O2-C2-N1	-2.40	119.67	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	CFZ	C3'-C2'-C1'	2.39	105.87	103.10
1	A	229	UFT	O2-C2-N1	-2.37	119.71	122.80
1	A	100	UFT	C3'-C2'-C1'	2.37	105.85	103.10
1	A	8	CFZ	C3'-C2'-C1'	2.37	105.85	103.10
1	A	144	UFT	O2-C2-N1	-2.36	119.72	122.80
1	A	228	UFT	O2-C2-N1	-2.36	119.72	122.80
1	A	137	CFZ	C2'-C1'-N1	-2.36	110.65	114.27
1	A	29	UFT	O2-C2-N1	-2.36	119.73	122.80
1	A	104	CFZ	C3'-C2'-C1'	2.36	105.83	103.10
1	A	10	UFT	C2'-C3'-C4'	2.36	105.53	102.43
1	A	190	UFT	C2'-C3'-C4'	2.35	105.52	102.43
1	A	48	UFT	C2'-C1'-N1	-2.34	110.67	114.27
1	A	141	UFT	O2-C2-N1	-2.34	119.75	122.80
1	A	40	CFZ	C2'-C3'-C4'	2.34	105.51	102.43
1	A	163	UFT	C2'-C3'-C4'	2.33	105.50	102.43
1	A	100	UFT	O2-C2-N1	-2.33	119.77	122.80
1	A	88	UFT	C2'-C3'-C4'	2.33	105.50	102.43
1	A	39	UFT	C2'-C1'-N1	-2.33	110.69	114.27
1	A	222	UFT	O2-C2-N1	-2.32	119.78	122.80
1	A	144	UFT	C3'-C2'-C1'	2.31	105.78	103.10
1	A	166	UFT	O2-C2-N1	-2.31	119.79	122.80
1	A	64	UFT	C3'-C2'-C1'	2.31	105.78	103.10
1	A	163	UFT	C1'-N1-C2	2.28	121.69	117.59
1	A	63	CFZ	C3'-C2'-C1'	2.28	105.75	103.10
1	A	86	UFT	C3'-C2'-C1'	2.28	105.75	103.10
1	A	75	UFT	O2-C2-N1	-2.28	119.83	122.80
1	A	169	CFZ	C2'-C3'-C4'	2.27	105.43	102.43
1	A	126	UFT	O2-C2-N1	-2.27	119.84	122.80
1	A	88	UFT	C2'-C1'-N1	-2.27	110.79	114.27
1	A	154	CFZ	F2'-C2'-C1'	-2.26	104.34	108.88
1	A	147	UFT	O2-C2-N1	-2.26	119.86	122.80
1	A	84	UFT	C3'-C2'-C1'	2.26	105.72	103.10
1	A	64	UFT	O2-C2-N1	-2.25	119.86	122.80
1	A	21	CFZ	O4'-C1'-C2'	2.25	108.22	105.84
1	A	112	UFT	C2'-C1'-N1	-2.25	110.82	114.27
1	A	184	UFT	O2-C2-N1	-2.24	119.88	122.80
1	A	80	CFZ	C3'-C2'-C1'	2.24	105.70	103.10
1	A	131	CFZ	C2'-C1'-N1	-2.24	110.83	114.27
1	A	106	CFZ	C3'-C2'-C1'	2.23	105.69	103.10
1	A	5	UFT	C2'-C3'-C4'	2.23	105.37	102.43
1	A	105	CFZ	C3'-C2'-C1'	2.22	105.68	103.10
1	A	224	UFT	O2-C2-N1	-2.21	119.92	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	CFZ	C2'-C3'-C4'	2.21	105.34	102.43
1	A	13	UFT	C3'-C2'-C1'	2.21	105.66	103.10
1	A	75	UFT	C3'-C2'-C1'	2.21	105.66	103.10
1	A	112	UFT	C3'-C2'-C1'	2.21	105.66	103.10
1	A	98	UFT	O2-C2-N1	-2.21	119.92	122.80
1	A	181	UFT	O2-C2-N1	-2.20	119.93	122.80
1	A	147	UFT	C1'-N1-C2	2.20	121.54	117.59
1	A	236	CFZ	C2'-C1'-N1	-2.20	110.90	114.27
1	A	224	UFT	C2'-C1'-N1	-2.19	110.91	114.27
1	A	121	CFZ	C4'-O4'-C1'	-2.19	104.64	109.47
1	A	54	UFT	O2-C2-N1	-2.18	119.95	122.80
1	A	109	UFT	O2-C2-N1	-2.18	119.96	122.80
1	A	133	UFT	O2-C2-N1	-2.18	119.96	122.80
1	A	213	CFZ	C6-C5-C4	2.17	121.09	117.53
1	A	90	CFZ	C2'-C1'-N1	-2.16	110.95	114.27
1	A	10	UFT	O2-C2-N1	-2.16	119.98	122.80
1	A	47	CFZ	C2'-C1'-N1	-2.15	110.97	114.27
1	A	35	UFT	C3'-C2'-C1'	2.15	105.59	103.10
1	A	194	UFT	O2-C2-N1	-2.15	120.00	122.80
1	A	190	UFT	O2-C2-N1	-2.15	120.00	122.80
1	A	231	CFZ	C2'-C1'-N1	-2.14	110.98	114.27
1	A	29	UFT	C3'-C2'-C1'	2.14	105.59	103.10
1	A	184	UFT	C2'-C1'-N1	-2.14	110.98	114.27
1	A	5	UFT	C3'-C2'-C1'	2.14	105.58	103.10
1	A	23	UFT	O2-C2-N1	-2.14	120.01	122.80
1	A	56	UFT	C2'-C1'-N1	-2.14	110.99	114.27
1	A	53	CFZ	O4'-C1'-C2'	2.13	108.10	105.84
1	A	131	CFZ	O4'-C1'-C2'	2.13	108.10	105.84
1	A	152	CFZ	C3'-C2'-C1'	2.13	105.57	103.10
1	A	194	UFT	C3'-C2'-C1'	2.12	105.56	103.10
1	A	134	UFT	O2-C2-N1	-2.12	120.03	122.80
1	A	109	UFT	C1'-N1-C2	2.12	121.41	117.59
1	A	94	CFZ	C2'-C1'-N1	-2.12	111.01	114.27
1	A	154	CFZ	F2'-C2'-C3'	2.12	113.33	109.14
1	A	92	UFT	O2-C2-N1	-2.12	120.04	122.80
1	A	187	UFT	O2-C2-N1	-2.12	120.04	122.80
1	A	229	UFT	C3'-C2'-C1'	2.12	105.56	103.10
1	A	44	UFT	O2-C2-N1	-2.11	120.05	122.80
1	A	85	UFT	O2-C2-N1	-2.11	120.05	122.80
1	A	93	UFT	O2-C2-N1	-2.11	120.05	122.80
1	A	226	UFT	C4'-O4'-C1'	-2.11	104.81	109.47
1	A	213	CFZ	C4'-O4'-C1'	-2.11	104.81	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11	CFZ	C2'-C1'-N1	-2.11	111.03	114.27
1	A	76	CFZ	C2'-C3'-C4'	2.11	105.21	102.43
1	A	164	CFZ	O2-C2-N3	-2.10	119.02	122.33
1	A	213	CFZ	C3'-C2'-C1'	2.10	105.53	103.10
1	A	215	UFT	O2-C2-N1	-2.10	120.07	122.80
1	A	69	UFT	C2'-C1'-N1	-2.09	111.06	114.27
1	A	188	UFT	C2'-C1'-N1	-2.09	111.06	114.27
1	A	111	UFT	C3'-C2'-C1'	2.09	105.53	103.10
1	A	120	UFT	O2-C2-N1	-2.09	120.08	122.80
1	A	73	UFT	C2'-C1'-N1	-2.09	111.07	114.27
1	A	20	UFT	O2-C2-N1	-2.08	120.08	122.80
1	A	10	UFT	C1'-N1-C2	2.08	121.33	117.59
1	A	19	UFT	O2-C2-N1	-2.08	120.09	122.80
1	A	188	UFT	O2-C2-N1	-2.08	120.09	122.80
1	A	154	CFZ	O3'-C3'-C2'	2.07	119.48	111.85
1	A	86	UFT	C1'-N1-C2	2.07	121.31	117.59
1	A	77	UFT	C1'-N1-C2	2.07	121.31	117.59
1	A	140	CFZ	O2-C2-N3	-2.07	119.07	122.33
1	A	81	CFZ	O2-C2-N3	-2.07	119.07	122.33
1	A	173	UFT	C2'-C1'-N1	-2.07	111.10	114.27
1	A	235	CFZ	C4'-O4'-C1'	-2.06	104.91	109.47
1	A	98	UFT	C2'-C3'-C4'	2.05	105.14	102.43
1	A	41	UFT	C2'-C1'-N1	-2.05	111.12	114.27
1	A	55	UFT	O2-C2-N1	-2.05	120.13	122.80
1	A	199	CFZ	C4'-O4'-C1'	-2.05	104.94	109.47
1	A	208	CFZ	C4'-O4'-C1'	-2.05	104.94	109.47
1	A	137	CFZ	N4-C4-N3	2.05	121.57	117.91
1	A	116	CFZ	C4'-O4'-C1'	-2.04	104.96	109.47
1	A	114	CFZ	O2-C2-N3	-2.04	119.12	122.33
1	A	149	CFZ	C4'-O4'-C1'	-2.04	104.97	109.47
1	A	174	UFT	O2-C2-N1	-2.03	120.15	122.80
1	A	84	UFT	O2-C2-N1	-2.03	120.15	122.80
1	A	222	UFT	C3'-C2'-C1'	2.03	105.46	103.10
1	A	163	UFT	O2-C2-N1	-2.03	120.15	122.80
1	A	69	UFT	C1'-N1-C2	2.03	121.23	117.59
1	A	228	UFT	C2'-C3'-C4'	2.03	105.10	102.43
1	A	70	CFZ	C4'-O4'-C1'	-2.03	104.99	109.47
1	A	91	UFT	C1'-N1-C2	2.02	121.22	117.59
1	A	111	UFT	O2-C2-N1	-2.02	120.17	122.80
1	A	177	CFZ	C2'-C1'-N1	-2.02	111.17	114.27
1	A	20	UFT	C2'-C1'-N1	-2.02	111.17	114.27
1	A	153	UFT	O2-C2-N1	-2.02	120.17	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	UFT	O4-C4-C5	-2.01	121.69	125.16
1	A	47	CFZ	C2'-C3'-C4'	2.01	105.08	102.43
1	A	91	UFT	C2'-C3'-C4'	2.01	105.08	102.43
1	A	148	CFZ	C1'-N1-C2	2.00	122.87	118.44
1	A	88	UFT	C1'-N1-C2	2.00	121.19	117.59
1	A	113	CFZ	C2'-C3'-C4'	2.00	105.07	102.43
1	A	56	UFT	O2-C2-N1	-2.00	120.19	122.80

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	19	UFT	O4'-C4'-C5'-O5'
1	A	21	CFZ	C2'-C1'-N1-C6
1	A	21	CFZ	O4'-C4'-C5'-O5'
1	A	57	CFZ	C4'-C5'-O5'-P
1	A	91	UFT	O4'-C4'-C5'-O5'
1	A	116	CFZ	O4'-C4'-C5'-O5'
1	A	147	UFT	O4'-C4'-C5'-O5'
1	A	174	UFT	O4'-C4'-C5'-O5'
1	A	177	CFZ	O4'-C4'-C5'-O5'
1	A	182	UFT	O4'-C4'-C5'-O5'
1	A	187	UFT	O4'-C4'-C5'-O5'
1	A	219	CFZ	O4'-C4'-C5'-O5'
1	A	234	UFT	O4'-C4'-C5'-O5'
1	A	21	CFZ	C3'-C4'-C5'-O5'
1	A	91	UFT	C3'-C4'-C5'-O5'
1	A	93	UFT	O4'-C4'-C5'-O5'
1	A	116	CFZ	C3'-C4'-C5'-O5'
1	A	134	UFT	C3'-C4'-C5'-O5'
1	A	171	UFT	O4'-C4'-C5'-O5'
1	A	175	CFZ	O4'-C4'-C5'-O5'
1	A	177	CFZ	C3'-C4'-C5'-O5'
1	A	187	UFT	C3'-C4'-C5'-O5'
1	A	219	CFZ	C3'-C4'-C5'-O5'
1	A	234	UFT	C3'-C4'-C5'-O5'
1	A	55	UFT	O4'-C4'-C5'-O5'
1	A	134	UFT	O4'-C4'-C5'-O5'
1	A	147	UFT	C3'-C4'-C5'-O5'
1	A	184	UFT	O4'-C4'-C5'-O5'
1	A	184	UFT	C3'-C4'-C5'-O5'
1	A	217	CFZ	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	19	UFT	C3'-C4'-C5'-O5'
1	A	55	UFT	C3'-C4'-C5'-O5'
1	A	94	CFZ	O4'-C4'-C5'-O5'
1	A	174	UFT	C3'-C4'-C5'-O5'
1	A	182	UFT	C3'-C4'-C5'-O5'
1	A	51	CFZ	C3'-C4'-C5'-O5'
1	A	94	CFZ	C3'-C4'-C5'-O5'
1	A	148	CFZ	C3'-C4'-C5'-O5'
1	A	93	UFT	C3'-C4'-C5'-O5'
1	A	171	UFT	C3'-C4'-C5'-O5'
1	A	175	CFZ	C3'-C4'-C5'-O5'
1	A	226	UFT	O4'-C4'-C5'-O5'
1	A	226	UFT	C3'-C4'-C5'-O5'
1	A	51	CFZ	O4'-C4'-C5'-O5'
1	A	217	CFZ	C3'-C4'-C5'-O5'
1	A	54	UFT	O4'-C4'-C5'-O5'
1	A	54	UFT	C3'-C4'-C5'-O5'
1	A	135	CFZ	C3'-C4'-C5'-O5'
1	A	148	CFZ	O4'-C4'-C5'-O5'
1	A	21	CFZ	C2'-C1'-N1-C2
1	A	216	UFT	C3'-C4'-C5'-O5'
1	A	226	UFT	C4'-C5'-O5'-P
1	A	170	CFZ	C4'-C5'-O5'-P
1	A	234	UFT	C4'-C5'-O5'-P
1	A	235	CFZ	C3'-C4'-C5'-O5'
1	A	55	UFT	C4'-C5'-O5'-P
1	A	135	CFZ	C4'-C5'-O5'-P
1	A	77	UFT	C3'-C4'-C5'-O5'
1	A	21	CFZ	O4'-C1'-N1-C6
1	A	216	UFT	O4'-C4'-C5'-O5'
1	A	235	CFZ	O4'-C4'-C5'-O5'
1	A	20	UFT	C3'-C4'-C5'-O5'
1	A	184	UFT	C2'-C1'-N1-C2
1	A	217	CFZ	C2'-C1'-N1-C2
1	A	235	CFZ	C2'-C1'-N1-C2
1	A	20	UFT	O4'-C4'-C5'-O5'
1	A	116	CFZ	C4'-C5'-O5'-P
1	A	56	UFT	C3'-C4'-C5'-O5'

There are no ring outliers.

93 monomers are involved in 163 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	123	CFZ	2	0
1	A	238	CFZ	2	0
1	A	124	UFT	3	0
1	A	194	UFT	1	0
1	A	73	UFT	3	0
1	A	229	UFT	3	0
1	A	84	UFT	2	0
1	A	199	CFZ	3	0
1	A	153	UFT	2	0
1	A	114	CFZ	2	0
1	A	213	CFZ	2	0
1	A	104	CFZ	1	0
1	A	169	CFZ	1	0
1	A	137	CFZ	4	0
1	A	228	UFT	3	0
1	A	23	UFT	5	0
1	A	140	CFZ	1	0
1	A	61	CFZ	1	0
1	A	222	UFT	3	0
1	A	227	CFZ	2	0
1	A	51	CFZ	2	0
1	A	166	UFT	4	0
1	A	163	UFT	2	0
1	A	72	UFT	2	0
1	A	27	CFZ	2	0
1	A	91	UFT	1	0
1	A	234	UFT	2	0
1	A	86	UFT	2	0
1	A	149	CFZ	1	0
1	A	144	UFT	3	0
1	A	7	UFT	2	0
1	A	154	CFZ	2	0
1	A	46	UFT	1	0
1	A	88	UFT	3	0
1	A	152	CFZ	2	0
1	A	76	CFZ	2	0
1	A	80	CFZ	2	0
1	A	70	CFZ	2	0
1	A	44	UFT	3	0
1	A	24	CFZ	3	0
1	A	141	UFT	3	0
1	A	236	CFZ	1	0
1	A	90	CFZ	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	175	CFZ	2	0
1	A	48	UFT	1	0
1	A	40	CFZ	2	0
1	A	94	CFZ	1	0
1	A	109	UFT	3	0
1	A	226	UFT	1	0
1	A	112	UFT	3	0
1	A	42	CFZ	3	0
1	A	235	CFZ	1	0
1	A	85	UFT	2	0
1	A	113	CFZ	3	0
1	A	29	UFT	2	0
1	A	13	UFT	1	0
1	A	161	CFZ	3	0
1	A	120	UFT	2	0
1	A	41	UFT	3	0
1	A	208	CFZ	3	0
1	A	8	CFZ	1	0
1	A	35	UFT	3	0
1	A	142	CFZ	3	0
1	A	26	CFZ	1	0
1	A	198	CFZ	2	0
1	A	75	UFT	3	0
1	A	116	CFZ	4	0
1	A	212	CFZ	2	0
1	A	81	CFZ	3	0
1	A	47	CFZ	2	0
1	A	164	CFZ	1	0
1	A	10	UFT	2	0
1	A	21	CFZ	1	0
1	A	219	CFZ	2	0
1	A	126	UFT	2	0
1	A	203	UFT	2	0
1	A	63	CFZ	1	0
1	A	187	UFT	3	0
1	A	34	CFZ	2	0
1	A	64	UFT	2	0
1	A	98	UFT	3	0
1	A	121	CFZ	1	0
1	A	210	UFT	1	0
1	A	71	CFZ	2	0
1	A	147	UFT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	77	UFT	2	0
1	A	57	CFZ	1	0
1	A	177	CFZ	2	0
1	A	11	CFZ	1	0
1	A	69	UFT	2	0
1	A	100	UFT	2	0
1	A	5	UFT	3	0
1	A	182	UFT	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

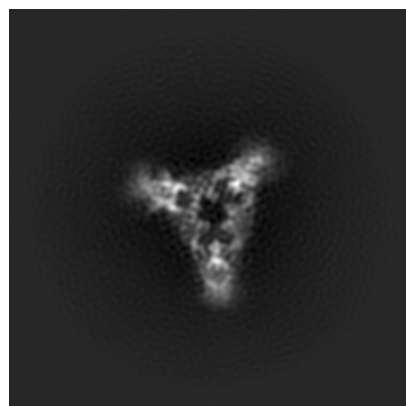
6 Map visualisation [i](#)

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

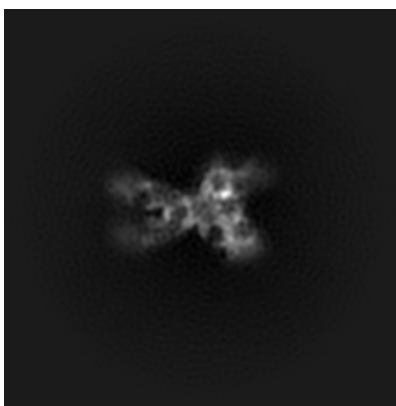
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

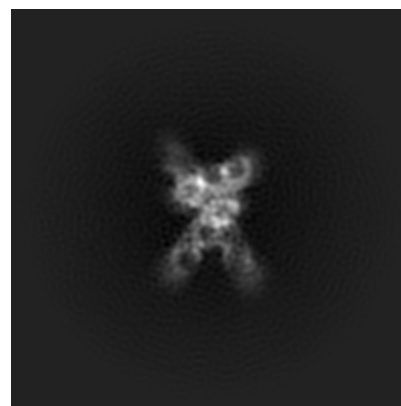
6.1.1 Primary map



X

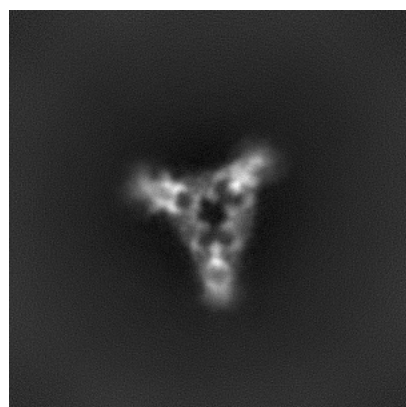


Y

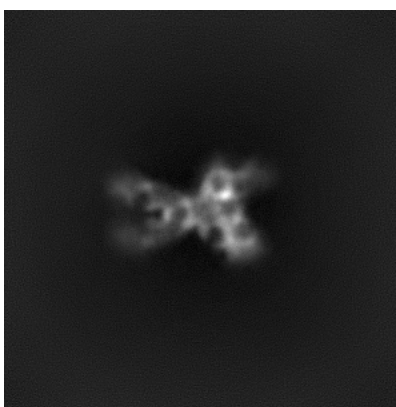


Z

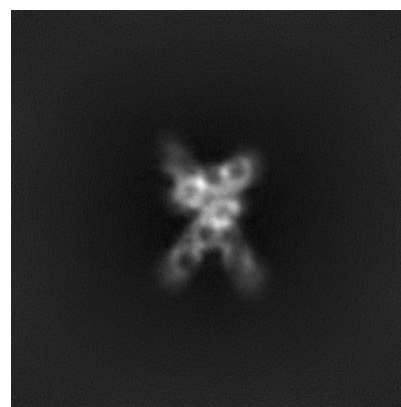
6.1.2 Raw map



X



Y

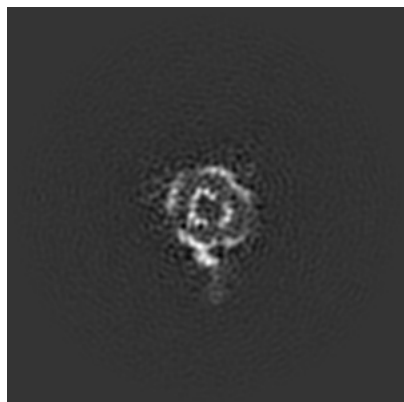


Z

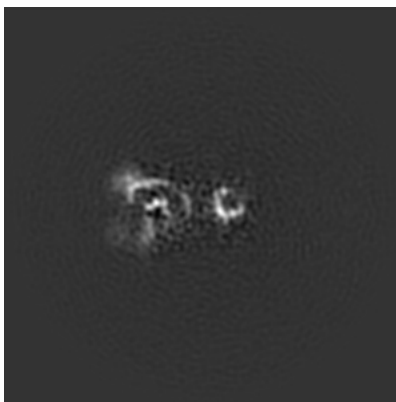
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

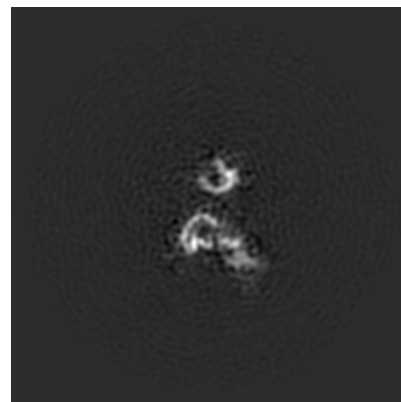
6.2.1 Primary map



X Index: 200

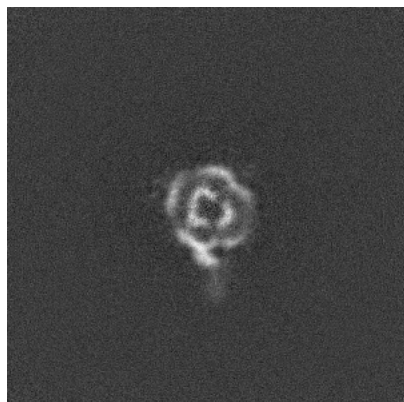


Y Index: 200

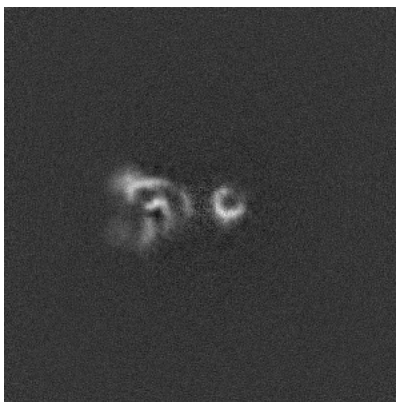


Z Index: 200

6.2.2 Raw map



X Index: 200



Y Index: 200

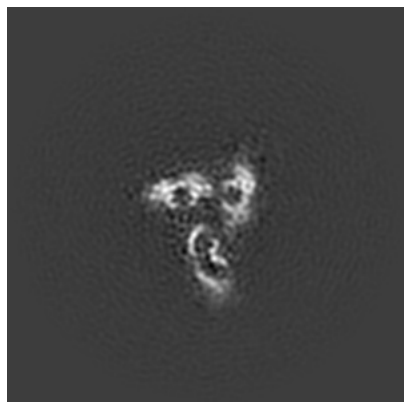


Z Index: 200

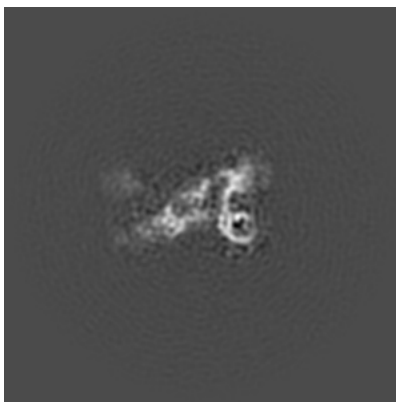
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

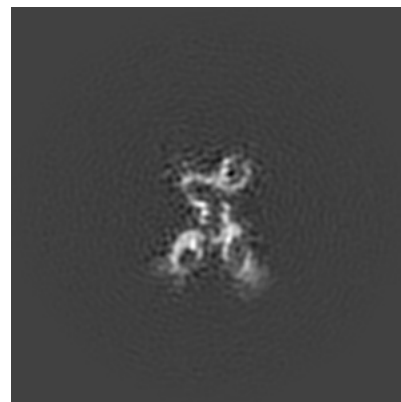
6.3.1 Primary map



X Index: 214

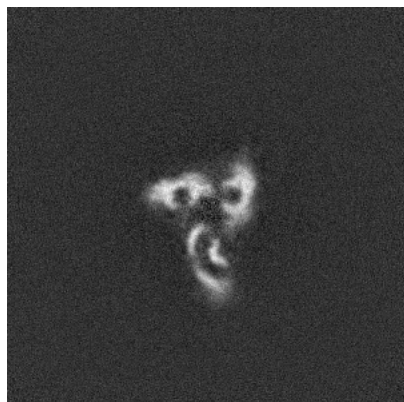


Y Index: 227

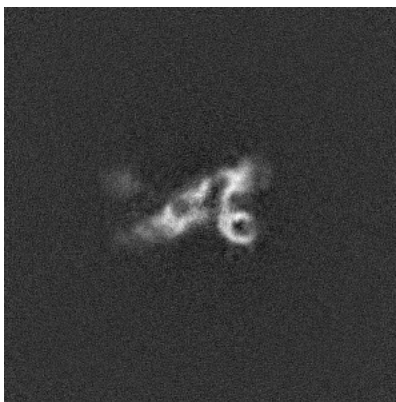


Z Index: 221

6.3.2 Raw map



X Index: 214



Y Index: 227

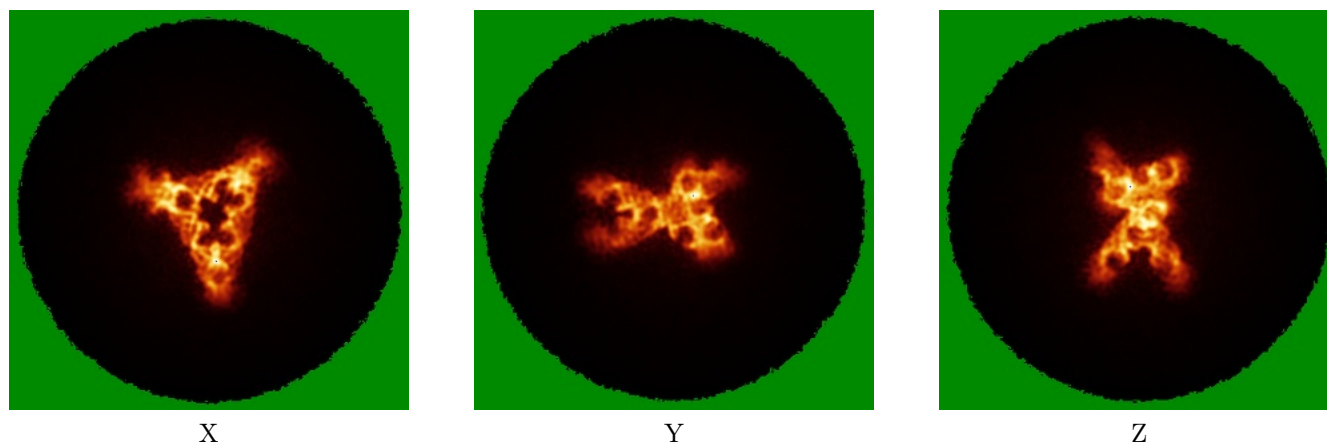


Z Index: 223

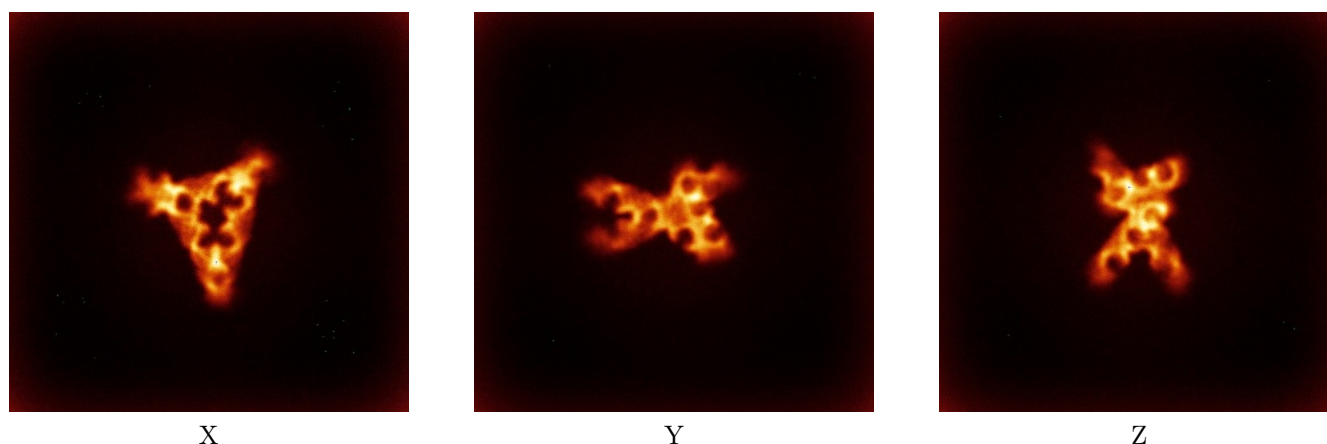
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

This section was not generated.

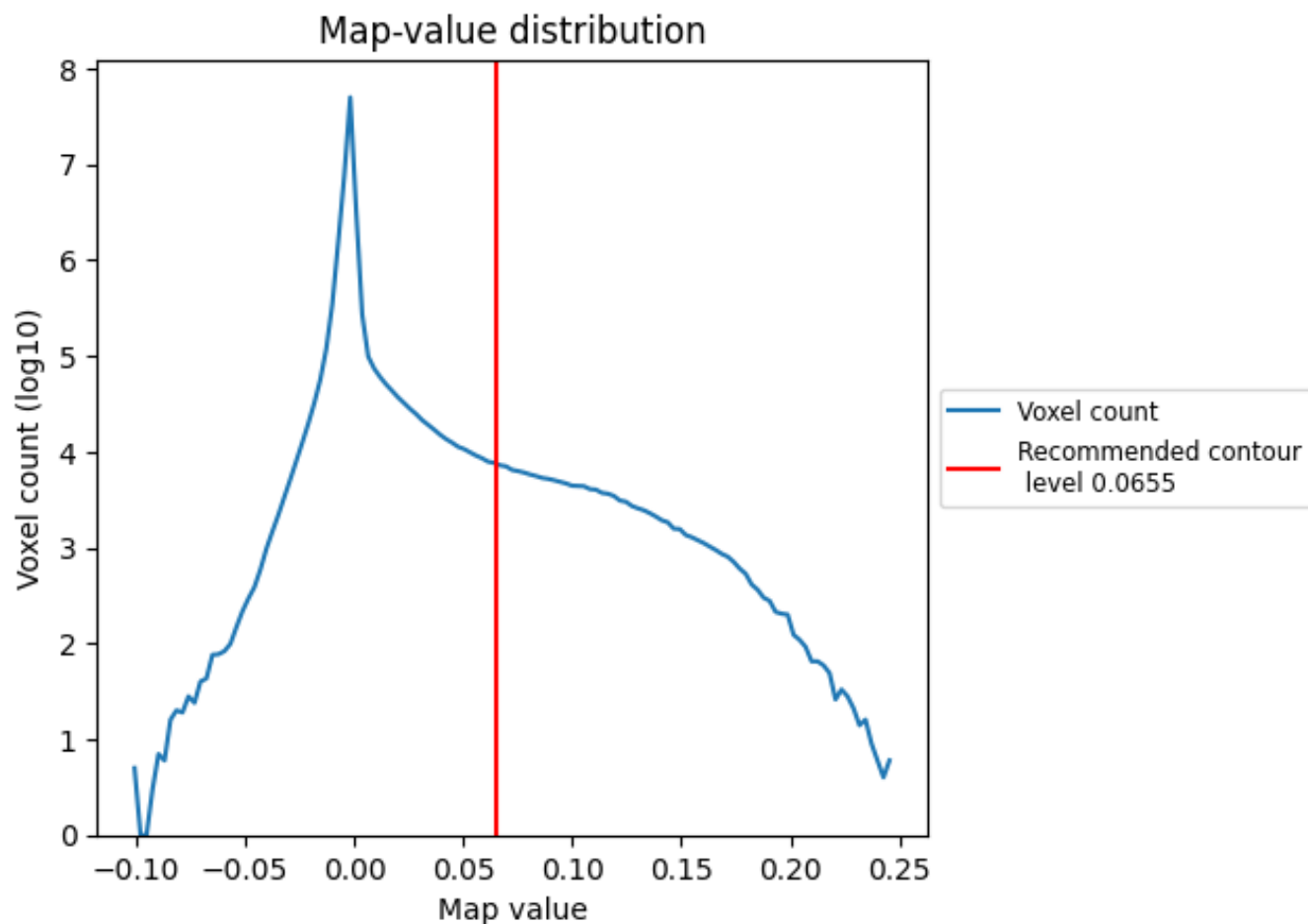
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

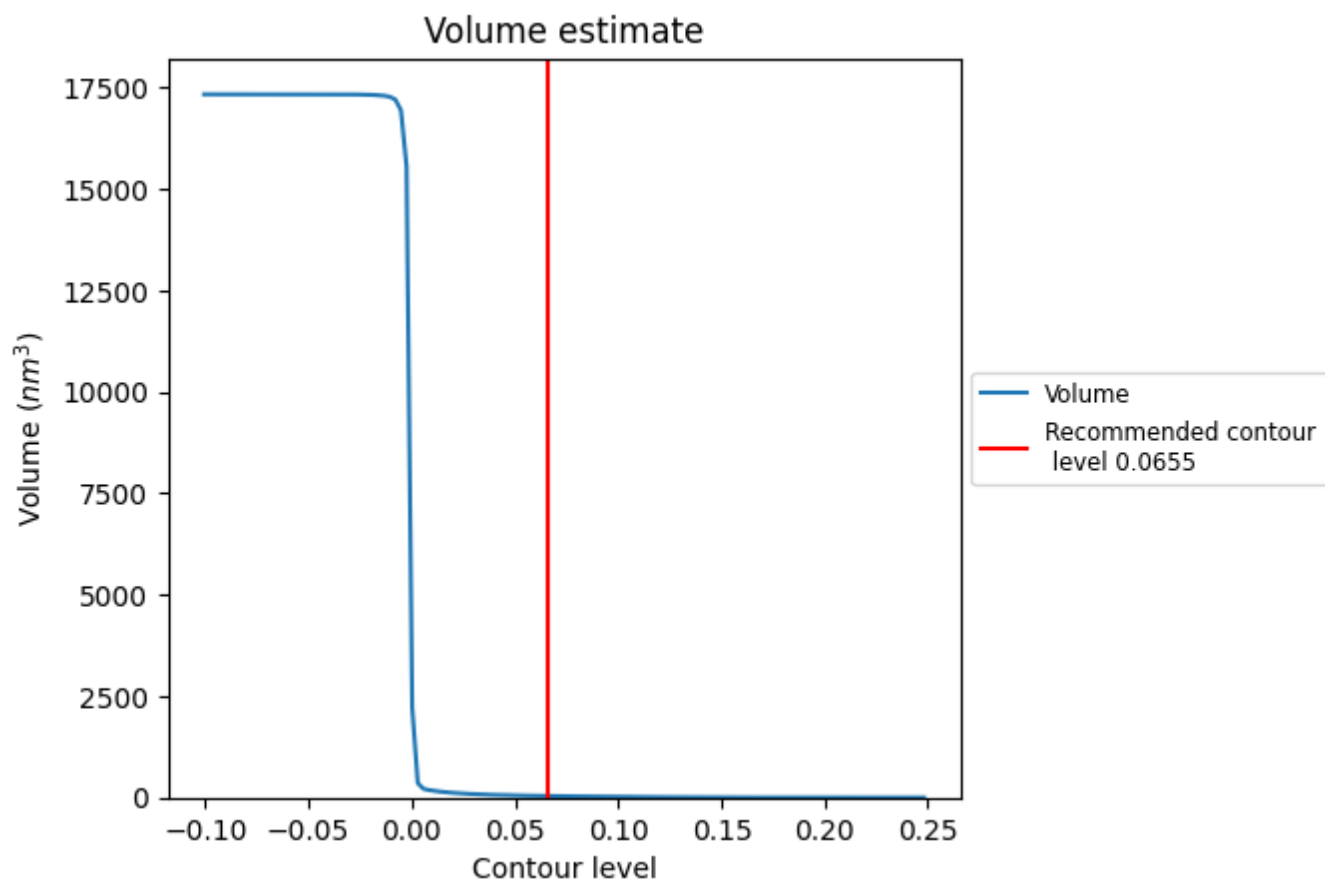
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

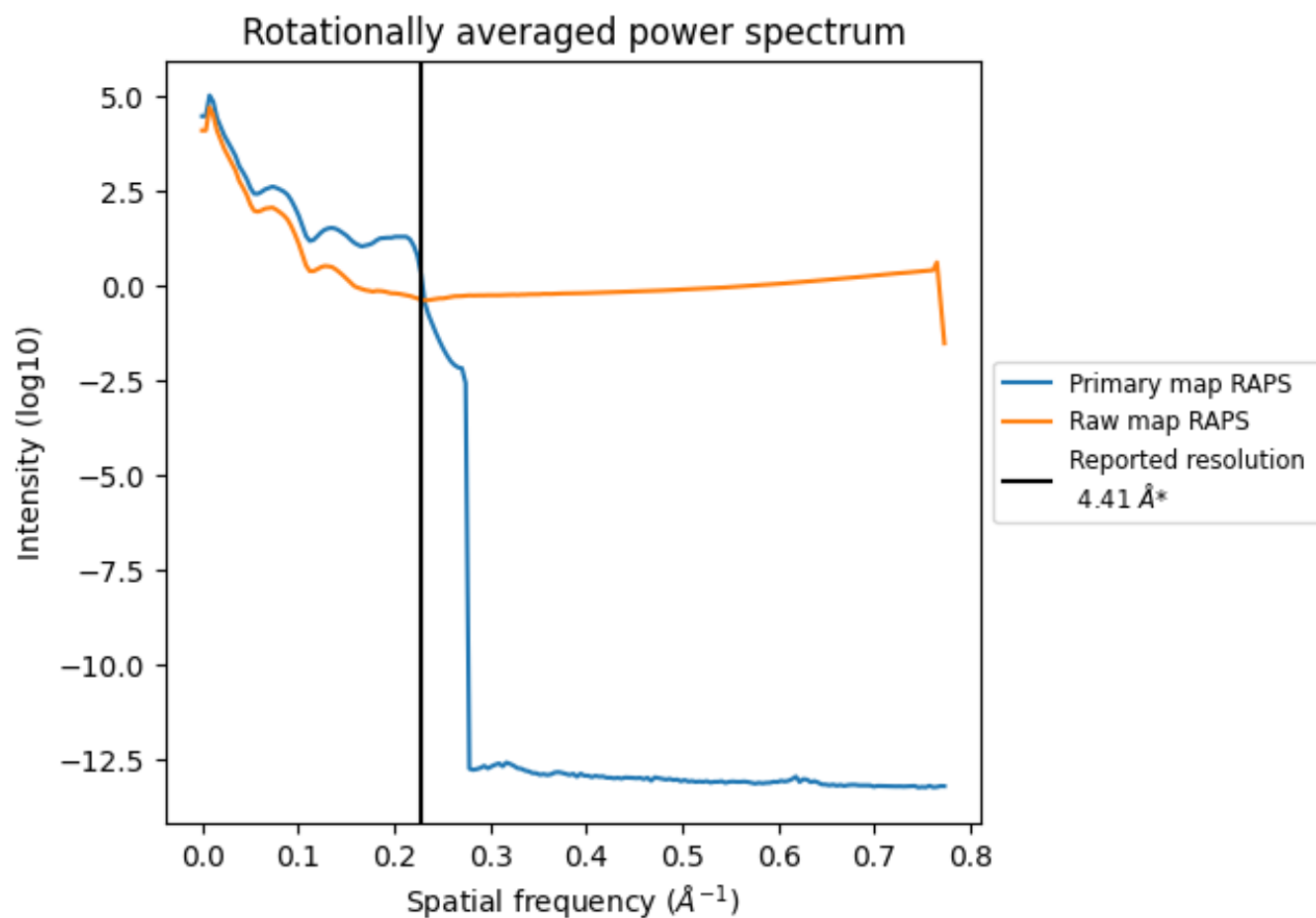
7.2 Volume estimate [i](#)



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

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

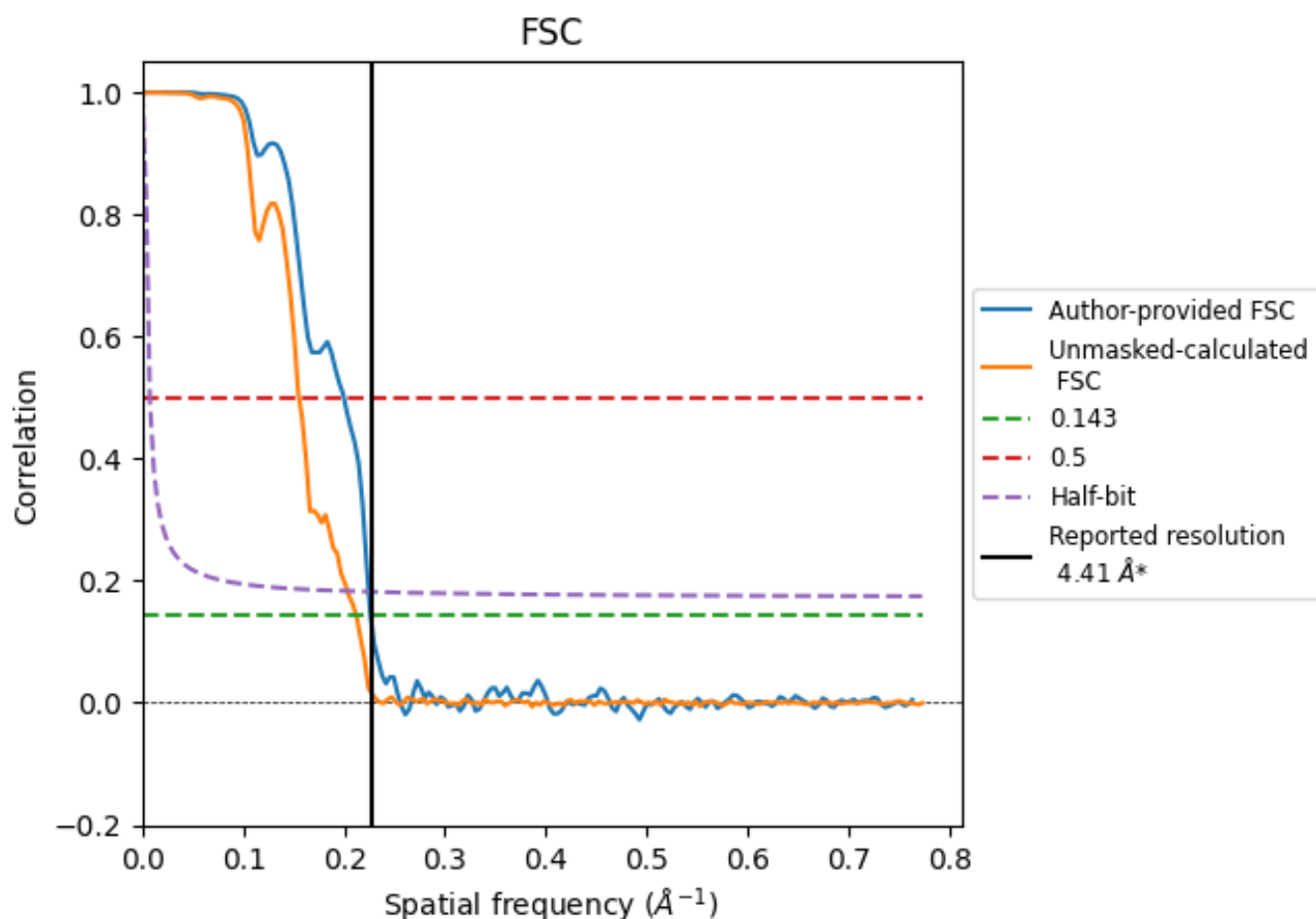


*Reported resolution corresponds to spatial frequency of 0.227 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

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

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

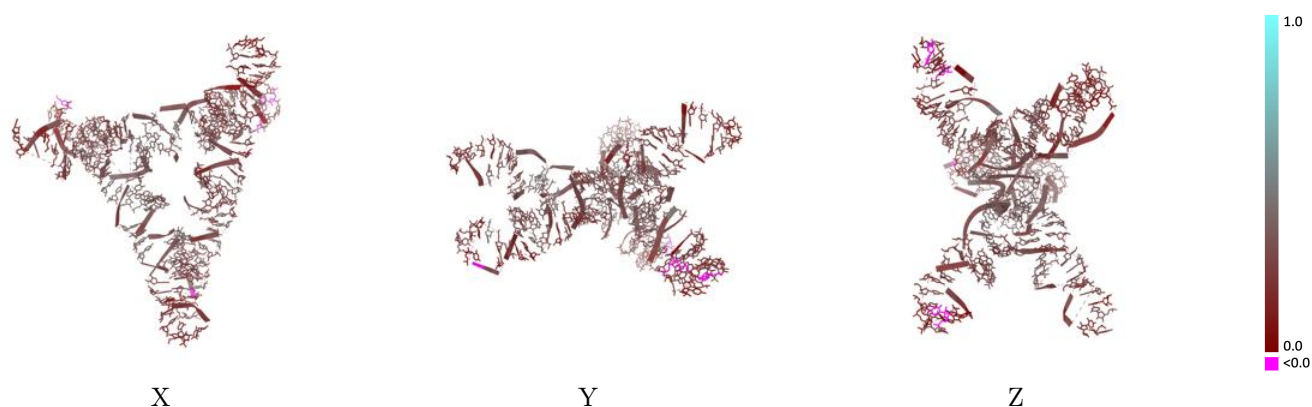
9 Map-model fit [i](#)

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

9.1 Map-model overlay [i](#)

This section was not generated.

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

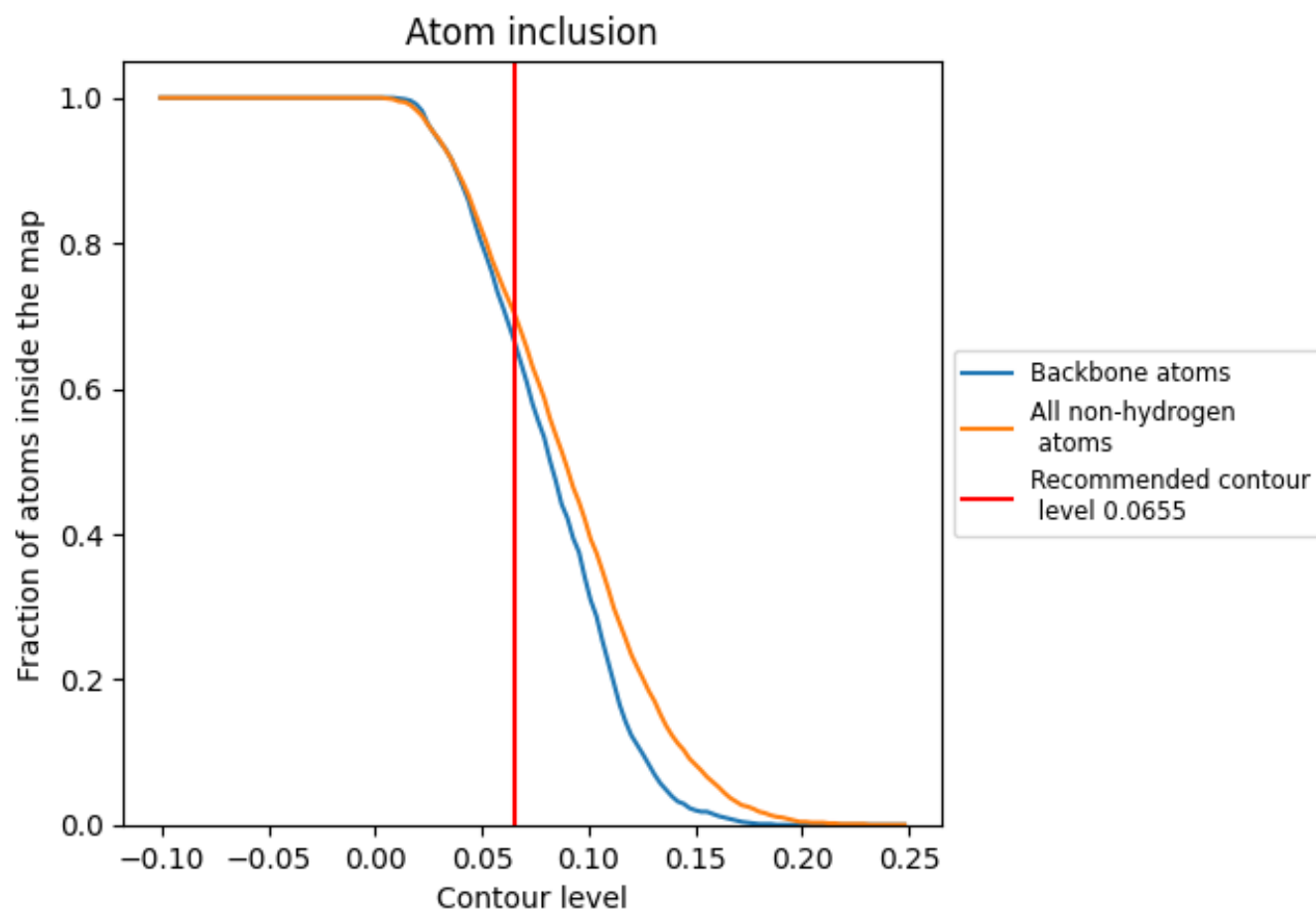


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0655) and Q-score for the entire model and for each chain.

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

