Integrative Structure Validation Report

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The following software was used in the production of this report:

Python-IHM Version 1.3
MolProbity Version 4.5.2
Integrative Modeling Validation Version 1.2

PDB ID	8ZZJ
PDB-Dev ID	PDBDEV_00000019
Structure Title	Multiple co-existing states of an RNA four-way junction resolved by FRET, SAXS, and integrative modeling: major state
Structure Authors	Hanke, C.A.; Vardanyan, H.; Sindbert, S.; Kalinin, S.; Barth, A.; Dimura, M.; Soltysinski, T.; Lach, G.; Springstubbe, D.; Apel, B.; Snell, E.; Grant, T.D.; Lipfert, J.; Mueller, S.; Bujnicki, J.M.; Gohlke, H.; Seidel, C.A.M.

This is a PDB-Dev IM Structure Validation Report for a publicly released PDB-Dev entry.

We welcome your comments at pdb-dev@mail.wwpdb.org

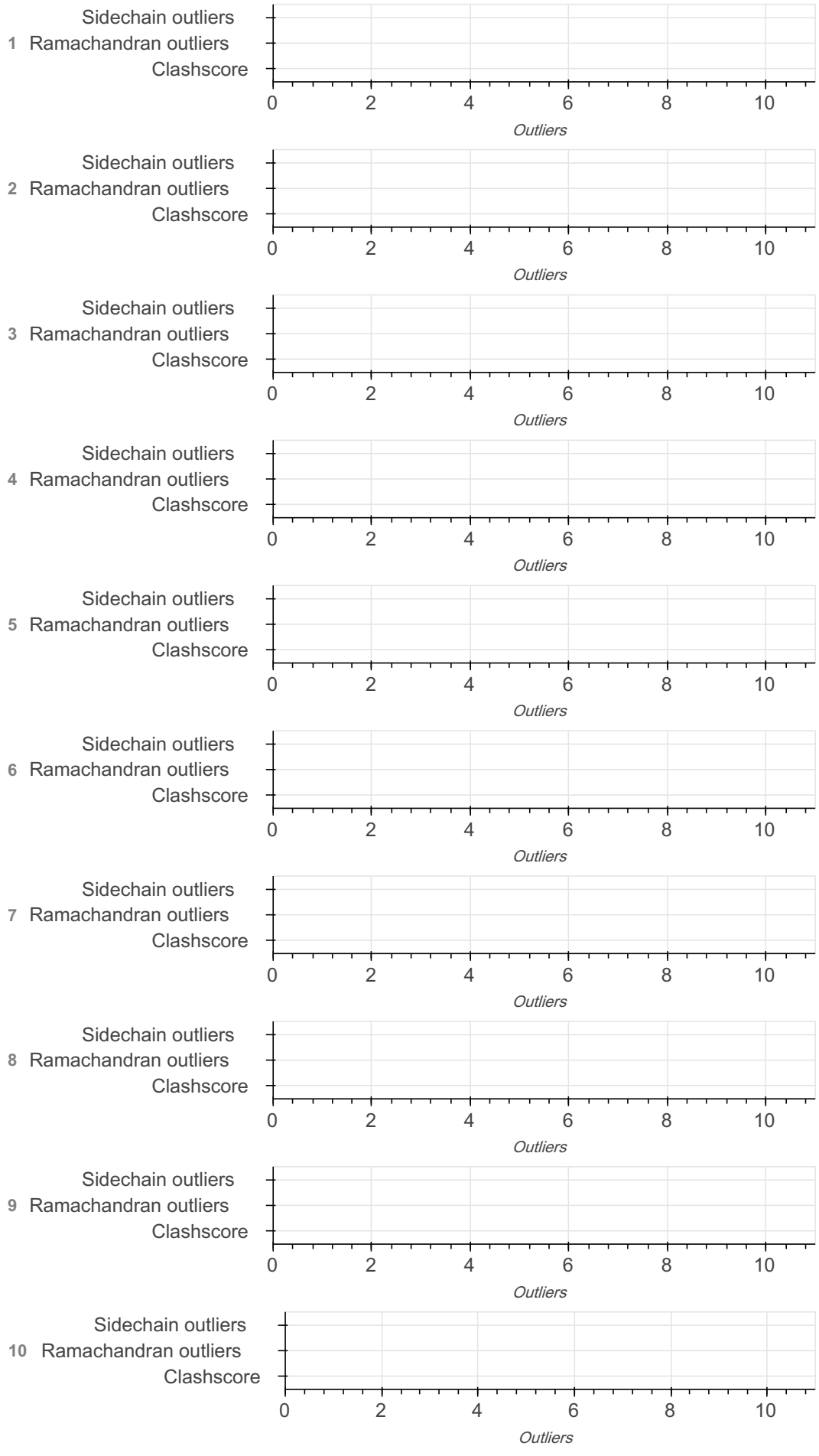
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

List of references used to build this report is available here.

Overall quality

This validation report contains model quality assessments for all structures, data quality assessment for SAS datasets and fit to model assessments for SAS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to 256.

Model Quality: MolProbity Analysis


1
2
3
4
5
6
7
8
9
10
Sidechain outliers
Ramachandran outliers
Clashscore
0
2
4
6
8
10
Outliers

Ensemble information

This entry consists of 2 distinct ensemble(s).

Summary

This entry consists of 10 unique models, with 4 subunits in each model. A total of 54 datasets or restraints were used to build this entry. Each model is represented by 8 rigid bodies and 0 flexible or non-rigid units.

Entry composition

There are 10 unique types of models in this entry.These models are titled Best RBD model for (ad)_a, Cluster representative from RBD error estimation for (ad)_a, Cluster representative from RBD error estimation for (ad)_a, Cluster representative from RBD error estimation for (ad)_a, Cluster representative from RBD error estimation for (ad)_a, Cluster representative from RBD error estimation for (ad)_a, Cluster representative from RBD error estimation for (ad)_a, MD model for (ad)_a best describing the experimental data, Ensemble member from MD for (ad)_a describing the experimental data, Ensemble member from MD for (ad)_a describing the experimental data respectively.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	RNA (37-MER) - strand a	A	A	37
1	2	2	RNA (37-MER) - strand b	B	B	37
1	3	3	RNA (32-MER) - strand c	C	C	32
1	4	4	RNA (32-MER) - strand d	D	D	32
2	1	1	RNA (37-MER) - strand a	A	A	37
2	2	2	RNA (37-MER) - strand b	B	B	37
2	3	3	RNA (32-MER) - strand c	C	C	32

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
2	4	4	RNA (32-MER) - strand d	D	D	32
3	1	1	RNA (37-MER) - strand a	A	A	37
3	2	2	RNA (37-MER) - strand b	B	B	37
3	3	3	RNA (32-MER) - strand c	C	C	32
3	4	4	RNA (32-MER) - strand d	D	D	32
4	1	1	RNA (37-MER) - strand a	A	A	37
4	2	2	RNA (37-MER) - strand b	B	B	37
4	3	3	RNA (32-MER) - strand c	C	C	32
4	4	4	RNA (32-MER) - strand d	D	D	32
5	1	1	RNA (37-MER) - strand a	A	A	37
5	2	2	RNA (37-MER) - strand b	B	B	37
5	3	3	RNA (32-MER) - strand c	C	C	32
5	4	4	RNA (32-MER) - strand d	D	D	32
6	1	1	RNA (37-MER) - strand a	A	A	37
6	2	2	RNA (37-MER) - strand b	B	B	37

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
6	3	3	RNA (32-MER) - strand c	C	C	32
6	4	4	RNA (32-MER) - strand d	D	D	32
7	1	1	RNA (37-MER) - strand a	A	A	37
7	2	2	RNA (37-MER) - strand b	B	B	37
7	3	3	RNA (32-MER) - strand c	C	C	32
7	4	4	RNA (32-MER) - strand d	D	D	32
8	1	1	RNA (37-MER) - strand a	A	A	37
8	2	2	RNA (37-MER) - strand b	B	B	37
8	3	3	RNA (32-MER) - strand c	C	C	32
8	4	4	RNA (32-MER) - strand d	D	D	32
9	1	1	RNA (37-MER) - strand a	A	A	37
9	2	2	RNA (37-MER) - strand b	B	B	37
9	3	3	RNA (32-MER) - strand c	C	C	32
9	4	4	RNA (32-MER) - strand d	D	D	32
10	1	1	RNA (37-MER) - strand a	A	A	37

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
10	2	2	RNA (37-MER) - strand b	B	B	37
10	3	3	RNA (32-MER) - strand c	C	C	32
10	4	4	RNA (32-MER) - strand d	D	D	32

Datasets used for modeling

There are 54 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Single molecule FRET data	File	10.5281/zenodo.6640962
2	Single molecule FRET data	File	10.5281/zenodo.6640962
3	Single molecule FRET data	File	10.5281/zenodo.6640962
4	Single molecule FRET data	File	10.5281/zenodo.6640962
5	Single molecule FRET data	File	10.5281/zenodo.6640962
6	Single molecule FRET data	File	10.5281/zenodo.6640962
7	Single molecule FRET data	File	10.5281/zenodo.6640962
8	Single molecule FRET data	File	10.5281/zenodo.6640962
9	Single molecule FRET data	File	10.5281/zenodo.6640962
10	Single molecule FRET data	File	10.5281/zenodo.6640962
11	Single molecule FRET data	File	10.5281/zenodo.6640962
12	Single molecule FRET data	File	10.5281/zenodo.6640962
13	Single molecule FRET data	File	10.5281/zenodo.6640962
14	Single molecule FRET data	File	10.5281/zenodo.6640962

ID	Dataset type	Database name	Data access code
15	Single molecule FRET data	File	10.5281/zenodo.6640962
16	Single molecule FRET data	File	10.5281/zenodo.6640962
17	Single molecule FRET data	File	10.5281/zenodo.6640962
18	Single molecule FRET data	File	10.5281/zenodo.6640962
19	Single molecule FRET data	File	10.5281/zenodo.6640962
20	Single molecule FRET data	File	10.5281/zenodo.6640962
21	Single molecule FRET data	File	10.5281/zenodo.6640962
22	Single molecule FRET data	File	10.5281/zenodo.6640962
23	Single molecule FRET data	File	10.5281/zenodo.6640962
24	Single molecule FRET data	File	10.5281/zenodo.6640962
25	Single molecule FRET data	File	10.5281/zenodo.6640962
26	Single molecule FRET data	File	10.5281/zenodo.6640962
27	Single molecule FRET data	File	10.5281/zenodo.6640962
28	Single molecule FRET data	File	10.5281/zenodo.6640962
29	Single molecule FRET data	File	10.5281/zenodo.6640962
30	Single molecule FRET data	File	10.5281/zenodo.6640962
31	Single molecule FRET data	File	10.5281/zenodo.6640962
32	Single molecule FRET data	File	10.5281/zenodo.6640962
33	Single molecule FRET data	File	10.5281/zenodo.6640962
34	Single molecule FRET data	File	10.5281/zenodo.6640962
35	Single molecule FRET data	File	10.5281/zenodo.6640962
36	Single molecule FRET data	File	10.5281/zenodo.6640962
37	Single molecule FRET data	File	10.5281/zenodo.6640962

ID	Dataset type	Database name	Data access code
38	Single molecule FRET data	File	10.5281/zenodo.6640962
39	Single molecule FRET data	File	10.5281/zenodo.6640962
40	Single molecule FRET data	File	10.5281/zenodo.6640962
41	Single molecule FRET data	File	10.5281/zenodo.6640962
42	Single molecule FRET data	File	10.5281/zenodo.6640962
43	Single molecule FRET data	File	10.5281/zenodo.6640962
44	Single molecule FRET data	File	10.5281/zenodo.6640962
45	Single molecule FRET data	File	10.5281/zenodo.6640962
46	Single molecule FRET data	File	10.5281/zenodo.6640962
47	Single molecule FRET data	File	10.5281/zenodo.6640962
48	Single molecule FRET data	File	10.5281/zenodo.6640962
49	Single molecule FRET data	File	10.5281/zenodo.6640962
50	Single molecule FRET data	File	10.5281/zenodo.6640962
51	De Novo model	File	10.5281/zenodo.6640962
52	De Novo model	File	10.5281/zenodo.6640962
53	De Novo model	File	10.5281/zenodo.6640962
54	De Novo model	File	10.5281/zenodo.6640962

Representation

This entry has only one representation and includes 8 rigid bodies and 0 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	1-16, 17-37	-
B	1-21, 22-37	-

Chain ID	Rigid bodies	Non-rigid segments
C	1-16, 17-32	-
D	1-16, 17-32	-

Methodology and software

This entry is a result of 3 distinct protocol(s).

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	1	None	Rigid body docking	None	1000	True	False
2	1	None	Refinement	None	1000	True	False
3	1	None	Error estimation (Bootstrapping)	None	100	True	False
1	2	None	Rigid body docking	None	1000	True	False
2	2	None	Refinement	None	1000	True	False
3	2	None	Error estimation (Bootstrapping)	None	100	True	False
4	2	MD simulations	Refinement by restrained MD	None	10000	True	False

There are 5 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	FPS (FRET Positioning and Screening)	1.100	model building and validation	http://www.mpc.hhu.de/software/fps.html
2	Paris	Not available	Burst selection	http://www.mpc.hhu.de/software/software-package.html

ID	Software name	Software version	Software classification	Software location
3	Tatiana	Not available	Photon distribution analysis (PDA)	http://www.mpc.hhu.de/software/software-package.html
4	Python_clustering_script	Not available	Clustering	Not available
5	Amber 11	Not available	model building	http://ambermd.org/

Data quality

Single molecule FRET

Validation for this section is under development.

Model quality

For models with atomic structures, molprobity analysis is performed. For models with coarse-grained or multi-scale structures, excluded volume analysis is performed.

Standard geometry: bond outliers

There are 14920 bond outliers in this entry. A summary is provided below, and a detailed list of outliers can be found here.

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
C3'--H3'	1.09	0.97	1380
C4'--H4'	1.09	0.97	1380
O2'--HO2'	0.96	0.84	1380
C5'--H5''	1.09	0.97	1380
C2'--H2'	1.09	0.97	1380
C5'--H5'	1.09	0.97	1380
C1'--H1'	1.09	0.97	1380
N1--H1	1.00	0.86	301

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
C6--H6	1.08	0.93	690
N2--H21	1.01	0.86	430
C8--H8	1.08	0.93	690
N2--H22	1.01	0.86	430
N3--H3	1.01	0.86	78
C5--H5	1.08	0.93	207
C2--H2	1.08	0.93	260
N4--H42	1.01	0.86	430
N6--H62	1.01	0.86	260
N1--H1	1.01	0.86	129
N6--H61	1.01	0.86	260
N4--H41	1.01	0.86	430
C5--H5	1.09	0.93	483
N3--H3	1.09	0.86	182

Standard geometry: angle outliers

There are 3994 angle outliers in this entry. A summary is provided below, and a detailed list of outliers can be found here.

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O3'-P-O5'	104.00	48.60	1
O3'-P-O5'	104.00	49.18	1
C3'-O3'-P	120.20	166.65	1
O3'-P-O5'	104.00	147.39	1
O3'-P-O5'	104.00	75.86	1
C3'-O3'-P	120.20	145.62	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O3'-P-O5'	104.00	128.46	1
O3'-P-O5'	104.00	84.13	1
C3'-O3'-P	120.20	138.30	1
C4'-C3'-C2'	102.60	90.95	1
O3'-P-O5'	104.00	87.20	1
O5'-C5'-C4'	111.50	127.45	1
O4'-C4'-C3'	104.00	114.43	1
C4'-O4'-C1'	109.90	100.42	1
C4'-C3'-C2'	102.60	93.18	1
C4'-C3'-C2'	102.60	93.23	1
C3'-C2'-C1'	101.30	110.61	1
O4'-C4'-C3'	104.00	113.30	1
O4'-C4'-C3'	104.00	113.28	1
C4'-C3'-C2'	102.60	93.39	1
C4'-C3'-C2'	102.60	93.56	1
C3'-C2'-C1'	101.30	92.38	1
O4'-C4'-C3'	104.00	112.76	1
C4'-C3'-C2'	102.60	93.86	1
O3'-P-OP2	108.00	81.94	1
O4'-C4'-C3'	104.00	112.51	1
C5'-C4'-C3'	116.00	103.28	1
C4'-C3'-C2'	102.60	94.17	1
O4'-C4'-C3'	104.00	112.32	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C4'-C3'-C2'	102.60	94.33	1
C4'-O4'-C1'	109.90	118.16	1
C5'-C4'-C3'	116.00	128.32	1
C3'-C2'-C1'	101.30	109.46	1
C4'-C3'-C2'	102.60	94.50	1
C3'-O3'-P	120.20	132.24	1
O3'-P-O5'	104.00	116.01	1
C5'-C4'-O4'	109.80	121.79	1
O4'-C1'-N1	108.50	120.42	1
C4'-C3'-C2'	102.60	94.68	1
O4'-C1'-C2'	107.60	99.74	1
O5'-C5'-C4'	111.50	123.28	1
C4'-C3'-C2'	102.60	94.77	1
O4'-C1'-N1	108.50	120.24	1
C4'-O4'-C1'	109.90	102.11	1
C3'-C2'-C1'	101.30	93.52	1
O3'-P-O5'	104.00	115.66	1
C4'-C3'-C2'	102.60	94.84	1
C4'-C3'-C2'	102.60	94.86	1
C4'-C3'-C2'	102.60	94.87	1
C4'-C3'-C2'	102.60	94.89	1
O3'-P-O5'	104.00	115.54	1
O4'-C1'-N1	108.50	120.03	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C4'-C3'-O3'	113.00	101.52	1
C4'-C3'-C2'	102.60	94.96	1
C5'-C4'-C3'	116.00	104.54	1
C4'-C3'-C2'	102.60	94.99	1
C3'-C2'-C1'	101.30	108.90	1
C4'-O4'-C1'	109.90	117.49	1
C4'-C3'-C2'	102.60	95.03	1
C4'-C3'-C2'	102.60	95.04	2
O4'-C4'-C3'	104.00	111.56	1
C3'-C2'-C1'	101.30	93.75	1
O4'-C1'-C2'	107.60	100.07	1
O3'-P-O5'	104.00	115.26	1
O4'-C4'-C3'	104.00	96.49	1
C5'-C4'-C3'	116.00	104.76	1
C5'-C4'-O4'	109.80	120.97	1
C3'-C2'-C1'	101.30	108.74	1
C4'-C3'-C2'	102.60	95.17	1
C4'-O4'-C1'	109.90	102.47	1
C4'-C3'-C2'	102.60	95.18	1
C5'-C4'-O4'	109.80	120.86	1
O4'-C4'-C3'	104.00	111.37	1
O4'-C1'-N1	108.50	119.55	1
O3'-P-O5'	104.00	115.04	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C5'-C4'-O4'	109.80	120.81	1
O4'-C4'-C3'	104.00	111.34	1
C4'-C3'-C2'	102.60	95.26	1
C3'-C2'-C1'	101.30	108.64	1
O4'-C4'-C3'	104.00	111.33	1
C4'-C3'-C2'	102.60	95.27	1
C4'-O4'-C1'	109.90	102.57	1
O4'-C1'-C2'	107.60	100.28	1
C4'-C3'-C2'	102.60	95.30	1
C3'-C2'-C1'	101.30	108.59	1
C4'-C3'-C2'	102.60	95.33	1
C5'-C4'-C3'	116.00	105.09	1
O4'-C1'-N1	108.50	119.37	1
C3'-O3'-P	120.20	131.06	1
C4'-O4'-C1'	109.90	102.71	1
O4'-C1'-N9	108.50	119.29	1
C4'-C3'-C2'	102.60	95.42	1
C3'-C2'-C1'	101.30	108.48	1
C5'-C4'-C3'	116.00	105.23	1
O4'-C1'-C2'	107.60	100.44	1
C3'-C2'-O2'	110.70	121.42	1
O5'-C5'-C4'	111.50	122.13	1
C4'-O4'-C1'	109.90	116.98	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O4'-C1'-C2'	107.60	100.54	1
C4'-C3'-C2'	102.60	95.58	1
O4'-C4'-C3'	104.00	111.01	1
O3'-P-O5'	104.00	93.50	1
O5'-C5'-C4'	111.50	122.00	1
C5'-C4'-C3'	116.00	105.50	1
C4'-C3'-O3'	113.00	102.53	1
C4'-C3'-C2'	102.60	95.62	1
C4'-C3'-O3'	113.00	123.45	1
C5'-C4'-O4'	109.80	120.23	1
C5'-C4'-C3'	116.00	105.59	1
O3'-P-O5'	104.00	114.36	1
C4'-C3'-C2'	102.60	95.70	1
O3'-C3'-C2'	113.70	103.36	1
O4'-C1'-C2'	107.60	100.71	1
O3'-P-O5'	104.00	93.68	1
C3'-C2'-O2'	110.70	121.01	1
O4'-C1'-C2'	107.60	100.73	1
O3'-P-O5'	104.00	114.30	1
C4'-C3'-C2'	102.60	95.74	1
C2'-C1'-N1	112.00	101.74	1
C3'-C2'-O2'	110.70	120.96	1
C5'-C4'-O4'	109.80	120.06	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C4'-O4'-C1'	109.90	116.74	1
C5'-C4'-C3'	116.00	105.75	1
C4'-C3'-C2'	102.60	95.77	1
C5'-C4'-C3'	116.00	105.77	1
O3'-P-O5'	104.00	114.18	1
C4'-C3'-C2'	102.60	95.81	1
O4'-C4'-C3'	104.00	110.79	1
C5'-C4'-C3'	116.00	105.83	1
C4'-C3'-C2'	102.60	95.85	1
C3'-C2'-C1'	101.30	94.58	1
C3'-C2'-C1'	101.30	108.01	1
C4'-C3'-C2'	102.60	95.89	1
O3'-P-O5'	104.00	114.04	1
O5'-C5'-C4'	111.50	101.46	1
O2'-C2'-C1'	108.40	98.37	1
O4'-C4'-C3'	104.00	110.68	1
C4'-C3'-O3'	113.00	103.02	1
O4'-C1'-N1	108.50	118.48	1
O3'-P-O5'	104.00	94.03	1
O4'-C4'-C3'	104.00	110.65	1
O4'-C1'-N1	108.50	118.47	1
C3'-C2'-C1'	101.30	107.95	1
C3'-C2'-C1'	101.30	94.66	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O4'-C1'-N9	108.50	118.45	1
O3'-C3'-C2'	113.70	103.75	1
C4'-C3'-C2'	102.60	95.97	1
O3'-P-O5'	104.00	113.93	1
O4'-C4'-C3'	104.00	110.61	1
C5'-C4'-O4'	109.80	119.71	1
O5'-C5'-C4'	111.50	121.40	1
O3'-C3'-C2'	113.70	103.80	1
O4'-C1'-N1	108.50	118.38	1
C3'-C2'-O2'	110.70	120.57	1
O3'-P-O5'	104.00	113.85	1
C4'-O4'-C1'	109.90	103.34	1
O3'-C3'-C2'	113.70	103.86	1
C5'-C4'-O4'	109.80	119.64	1
O3'-P-O5'	104.00	113.84	1
O5'-C5'-C4'	111.50	121.34	1
C3'-O3'-P	120.20	130.04	1
C5'-C4'-O4'	109.80	119.63	1
O4'-C4'-C3'	104.00	110.55	1
C4'-C3'-C2'	102.60	96.06	1
C4'-C3'-O3'	113.00	122.81	1
C4'-C3'-C2'	102.60	96.07	1
C3'-C2'-O2'	110.70	120.49	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C3'-C2'-O2'	110.70	120.48	1
C3'-C2'-C1'	101.30	107.82	1
O5'-C5'-C4'	111.50	121.26	1
C5'-C4'-O4'	109.80	119.55	1
C4'-C3'-C2'	102.60	96.10	1
O4'-C1'-N1	108.50	118.22	1
C4'-C3'-C2'	102.60	96.12	1
O2'-C2'-C1'	108.40	118.10	1
C5'-C4'-O4'	109.80	119.50	1
C2'-C1'-N1	112.00	102.30	1
O4'-C1'-C2'	107.60	101.14	1
C4'-O4'-C1'	109.90	103.44	1
O4'-C1'-N1	108.50	118.19	1
C4'-C3'-O3'	113.00	103.32	1
O3'-P-O5'	104.00	94.33	1
C4'-O4'-C1'	109.90	103.45	1
C4'-C3'-C2'	102.60	96.16	1
C4'-C3'-O3'	113.00	122.65	1
O4'-C4'-C3'	104.00	110.43	1
O4'-C1'-N9	108.50	118.14	1
C3'-C2'-O2'	110.70	120.33	1
O4'-C1'-C2'	107.60	101.19	1
P-O5'-C5'	120.90	130.50	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O4'-C1'-C2'	107.60	101.21	2
C5'-C4'-O4'	109.80	119.38	1
O4'-C1'-N9	108.50	118.07	1
C4'-C3'-O3'	113.00	103.43	1
O4'-C4'-C3'	104.00	110.38	1
O4'-C1'-N1	108.50	118.06	1
O4'-C1'-N9	108.50	118.03	1
O4'-C4'-C3'	104.00	110.36	1
O4'-C1'-N1	108.50	118.03	1
C4'-C3'-C2'	102.60	96.25	1
C5'-C4'-O4'	109.80	119.31	1
C4'-C3'-C2'	102.60	96.26	1
O4'-C1'-C2'	107.60	101.26	1
O4'-C1'-N1	108.50	117.99	1
C4'-C3'-C2'	102.60	96.27	1
O4'-C1'-N1	108.50	117.98	1
C4'-C3'-C2'	102.60	96.28	1
O3'-P-O5'	104.00	94.54	2
C2'-C1'-N9	112.00	102.55	1
C3'-C2'-C1'	101.30	95.01	1
O4'-C4'-C3'	106.10	112.39	1
O5'-C5'-C4'	111.50	120.93	1
C3'-C2'-C1'	101.30	107.56	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O4'-C1'-N1	108.50	117.88	1
C5'-C4'-C3'	116.00	106.66	1
O3'-P-O5'	104.00	94.66	1
C4'-O4'-C1'	109.90	103.67	1
O4'-C1'-N9	108.50	117.84	1
O3'-P-O5'	104.00	113.33	2
C4'-O4'-C1'	109.90	103.69	1
C4'-C3'-C2'	102.60	96.40	1
O3'-P-O5'	104.00	113.30	1
C5'-C4'-O4'	109.80	119.09	1
C3'-C2'-C1'	101.30	107.48	1
C3'-C2'-C1'	101.30	95.13	1
C5'-C4'-C3'	116.00	106.78	1
C4'-C3'-C2'	102.60	96.46	1
O4'-C1'-C2'	107.60	101.46	1
C4'-C3'-C2'	102.60	96.47	1
C3'-C2'-C1'	101.30	107.42	1
C3'-C2'-C1'	101.30	95.18	1
O4'-C1'-N1	108.50	117.68	1
C4'-C3'-C2'	102.60	96.49	1
O4'-C1'-C2'	107.60	101.49	1
O3'-P-O5'	104.00	113.15	1
C3'-C2'-C1'	101.30	95.21	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C4'-C3'-C2'	102.60	96.51	1
C4'-C3'-C2'	102.60	96.52	1
C4'-C3'-C2'	102.60	96.53	1
O4'-C1'-N1	108.50	117.61	1
C3'-C2'-C1'	101.30	95.23	1
C5'-C4'-C3'	116.00	125.09	1
O4'-C1'-C2'	107.60	113.66	1
C4'-C3'-O3'	113.00	103.92	1
C3'-O3'-P	120.20	129.28	1
C4'-O4'-C1'	109.90	103.88	1
O4'-C4'-C3'	104.00	110.00	1
O4'-C4'-C3'	104.00	109.99	1
C4'-C3'-O3'	109.40	118.39	1
C4'-C3'-C2'	102.60	96.61	1
O3'-P-O5'	104.00	112.98	1
C5'-C4'-O4'	109.80	118.78	1
O4'-C1'-C2'	107.60	101.62	1
C2'-C1'-N9	112.00	103.05	1
C4'-O4'-C1'	109.90	103.94	1
O2'-C2'-C1'	108.40	99.46	1
C3'-C2'-C1'	101.30	107.25	1
C4'-C3'-C2'	102.60	96.66	1
P-O5'-C5'	120.90	129.80	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C3'-C2'-C1'	101.30	107.23	1
O3'-P-O5'	104.00	112.89	1
O4'-C1'-N1	108.50	117.38	1
C5'-C4'-O4'	109.80	118.68	1
C2'-C1'-N1	112.00	120.87	1
C5'-C4'-C3'	116.00	107.13	1
C4'-C3'-O3'	113.00	104.13	1
C2'-C1'-N9	112.00	103.14	1
C4'-C3'-C2'	102.60	96.69	1
O4'-C1'-N9	108.50	117.35	1
C3'-C2'-C1'	101.30	107.19	1
C5'-C4'-C3'	116.00	107.16	1
C3'-C2'-C1'	101.30	95.41	1
O4'-C1'-C2'	107.60	101.73	1
C2'-C1'-N9	112.00	103.19	1
C5'-C4'-C3'	116.00	107.19	1
C3'-C2'-O2'	110.70	119.49	1
C4'-C3'-C2'	102.60	96.74	1
O4'-C1'-N1	108.50	117.28	1
C4'-C3'-C2'	102.60	96.75	1
C4'-C3'-C2'	102.60	96.77	1
O4'-C4'-C3'	104.00	109.83	1
O3'-P-O5'	104.00	112.74	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O4'-C1'-N9	108.50	117.23	1
C5'-C4'-C3'	116.00	107.27	1
O4'-C1'-N1	108.50	117.21	1
C5'-C4'-O4'	109.80	118.51	1
O4'-C4'-C3'	104.00	109.81	1
C3'-C2'-O2'	110.70	119.41	1
C4'-O4'-C1'	109.90	115.70	1
C3'-C2'-O2'	110.70	119.39	1
C4'-C3'-O3'	113.00	104.31	1
O4'-C4'-C3'	104.00	109.79	1
O4'-C1'-N9	108.50	117.19	1
C3'-C2'-O2'	110.70	119.38	1
O4'-C1'-N1	108.50	117.17	2
C4'-C3'-O3'	113.00	121.67	1
C2'-C1'-N9	112.00	103.34	1
C4'-C3'-O3'	113.00	121.65	1
C5'-C4'-O4'	109.80	118.45	1
O4'-C4'-C3'	104.00	98.23	1
O4'-C1'-N9	108.50	117.14	1
O4'-C1'-N1	108.50	117.13	1
C3'-C2'-C1'	101.30	95.54	1
O5'-C5'-C4'	111.50	120.12	1
C4'-C3'-C2'	102.60	96.86	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O4'-C4'-C3'	104.00	109.73	1
C4'-C3'-C2'	102.60	108.33	1
O3'-P-O5'	104.00	112.59	1
C2'-C1'-N9	112.00	103.41	1
C4'-O4'-C1'	109.90	115.62	1
C4'-C3'-C2'	102.60	96.89	2
C5'-C4'-O4'	109.80	101.24	1
O3'-P-O5'	104.00	112.55	1
C4'-C3'-C2'	102.60	96.90	2
C4'-O4'-C1'	109.90	115.60	1
O4'-C1'-N1	108.50	117.04	1
C4'-O4'-C1'	109.90	115.59	1
O3'-P-O5'	104.00	112.52	2
O2'-C2'-C1'	108.40	116.91	1
C4'-C3'-C2'	102.60	96.93	2
O4'-C4'-C3'	104.00	109.67	1
C2'-C1'-N9	112.00	103.50	1
P-O5'-C5'	120.90	129.40	1
O3'-P-O5'	104.00	112.50	1
C3'-C2'-O2'	110.70	119.19	1
C4'-C3'-C2'	102.60	96.94	1
O4'-C1'-C2'	107.60	101.94	1
O3'-C3'-C2'	113.70	122.17	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C4'-C3'-C2'	102.60	96.96	1
O4'-C4'-C3'	104.00	109.64	1
C4'-C3'-O3'	113.00	104.55	1
C4'-O4'-C1'	109.90	115.53	1
O4'-C1'-C2'	107.60	113.23	1
C4'-C3'-C2'	102.60	96.97	1
O3'-P-O5'	104.00	112.44	1
O4'-C1'-N1	108.50	116.94	1
O4'-C4'-C3'	104.00	109.62	2
C3'-C2'-O2'	110.70	119.12	1
C5'-C4'-C3'	116.00	107.58	1
O4'-C1'-N1	108.50	116.91	1
O4'-C1'-C2'	107.60	101.99	1
O3'-P-O5'	104.00	112.41	1
P-O5'-C5'	120.90	129.29	1
C4'-O4'-C1'	109.90	115.49	1
O2'-C2'-C1'	108.40	116.78	1
C3'-C2'-O2'	110.70	119.07	1
O4'-C4'-C3'	104.00	98.43	1
O4'-C1'-N9	108.50	116.86	1
C4'-C3'-C2'	102.60	97.03	1
C3'-C2'-O2'	110.70	102.35	1
O5'-C5'-C4'	111.50	103.16	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C2'-C1'-N9	112.00	103.66	1
C3'-C2'-O2'	110.70	119.03	1
C4'-C3'-C2'	102.60	97.05	2
C3'-C2'-C1'	101.30	106.85	1
O3'-C3'-C2'	113.70	105.37	1
O4'-C4'-C3'	104.00	109.55	1
C2'-C1'-N1	112.00	103.68	1
O4'-C4'-C3'	104.00	109.54	1
O4'-C1'-N9	108.50	116.81	1
P-O5'-C5'	120.90	129.21	1
O2'-C2'-C1'	108.40	100.09	1
O3'-C3'-C2'	113.70	105.41	1
O4'-C4'-C3'	104.00	109.52	1
C3'-C2'-O2'	110.70	118.97	1
O5'-C5'-C4'	111.50	119.77	1
O3'-P-O5'	104.00	112.27	1
O3'-P-OP2	108.00	91.47	1
C5'-C4'-O4'	109.80	118.07	1
O4'-C1'-N9	108.50	116.77	1
O4'-C1'-C2'	107.60	102.09	1
O3'-C3'-C2'	113.70	105.44	1
C3'-C2'-C1'	101.30	106.80	1
C4'-C3'-C2'	102.60	97.10	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C3'-C2'-O2'	110.70	118.95	1
C4'-C3'-O3'	113.00	104.75	1
C4'-C3'-O3'	113.00	104.76	1
O3'-C3'-C2'	113.70	105.48	1
C4'-C3'-C2'	102.60	97.14	1
O5'-C5'-C4'	111.50	119.69	1
C5'-C4'-O4'	109.80	117.99	1
O3'-P-O5'	104.00	112.18	1
O4'-C1'-N1	108.50	116.68	1
C2'-C1'-N1	112.00	103.82	1
C5'-C4'-C3'	115.20	107.03	1
O5'-C5'-C4'	111.50	103.33	1
O3'-P-O5'	104.00	112.16	1
O4'-C4'-C3'	104.00	109.44	1
C4'-C3'-C2'	102.60	97.16	1
O2'-C2'-C1'	108.40	116.55	1
C3'-C2'-O2'	110.70	118.85	1
C3'-O3'-P	120.20	128.34	1
C4'-C3'-C2'	102.60	97.18	2
C5'-C4'-C3'	116.00	107.87	1
C2'-C1'-N9	112.00	103.88	1
C4'-O4'-C1'	109.90	104.49	1
O2'-C2'-C1'	108.40	116.51	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O4'-C1'-N1	108.50	116.59	1
C4'-C3'-C2'	102.60	97.21	2
C4'-C3'-O3'	113.00	121.08	1
C5'-C4'-O4'	109.80	117.88	1
O3'-P-O5'	104.00	112.07	1
O4'-C1'-N9	108.50	116.57	1
O4'-C1'-N1	108.50	116.56	1
O4'-C4'-C3'	104.00	109.36	1
O4'-C4'-C3'	104.00	98.64	1
O4'-C1'-N9	108.50	116.53	3
O4'-C1'-C2'	107.60	102.25	1
P-O5'-C5'	120.90	128.93	1
C5'-C4'-C3'	116.00	107.99	2
C3'-C2'-O2'	110.70	118.70	1
C4'-C3'-C2'	102.60	97.26	1
C2'-C1'-N1	112.00	104.00	1
O3'-P-O5'	104.00	111.99	1
C4'-C3'-C2'	102.60	97.27	1
O2'-C2'-C1'	108.40	116.39	1
C4'-C3'-C2'	102.60	97.28	1
O3'-P-O5'	104.00	111.97	1
O3'-P-OP1	108.00	92.05	1
P-O5'-C5'	120.90	112.93	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O4'-C1'-N9	108.50	116.47	1
C2'-C1'-N9	112.00	104.04	1
C3'-C2'-C1'	101.30	106.60	1
C3'-C2'-O2'	110.70	118.66	1
C4'-O4'-C1'	109.90	104.60	1
C5'-C4'-C3'	116.00	108.05	1
O5'-C5'-C4'	111.50	103.55	1
O2'-C2'-C1'	108.40	100.45	1
C5'-C4'-O4'	109.80	117.74	1
O4'-C4'-C3'	104.00	109.29	1
O5'-C5'-C4'	111.50	119.43	1
O4'-C1'-N9	108.50	116.43	1
O3'-P-O5'	104.00	96.08	1
O2'-C2'-C1'	108.40	100.48	1
C5'-C4'-C3'	116.00	108.08	1
C5'-C4'-O4'	109.80	117.71	1
C4'-C3'-O3'	113.00	105.09	1
O4'-C1'-C2'	107.60	102.33	1
O4'-C4'-C3'	104.00	109.26	1
C2'-C1'-N9	112.00	104.12	1
C3'-C2'-O2'	110.70	118.58	1
O4'-C1'-N1	108.50	116.37	1
C4'-O4'-C1'	109.90	104.66	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C3'-C2'-O2'	110.70	118.56	2
O4'-C1'-C2'	107.60	102.36	1
C4'-C3'-C2'	102.60	97.36	1
C2'-C1'-N9	112.00	104.15	1
O4'-C4'-C3'	104.00	109.23	1
O4'-C1'-N1	108.50	116.34	1
O2'-C2'-C1'	108.40	116.23	1
O4'-C1'-C2'	107.60	102.39	1
O3'-C3'-C2'	113.70	121.52	1
O3'-C3'-C2'	113.70	105.89	1
C4'-C3'-C2'	102.60	97.40	2
C4'-O4'-C1'	109.90	115.10	1
O4'-C4'-C3'	104.00	98.80	1
C3'-C2'-O2'	110.70	118.49	1
C2'-C1'-N1	112.00	119.79	1
C4'-C3'-C2'	102.60	97.41	1
O4'-C4'-C3'	104.00	109.19	1
C5'-C4'-C3'	115.20	107.42	1
C4'-O4'-C1'	109.90	115.08	1
O4'-C1'-N1	108.50	116.27	2
C4'-C3'-C2'	102.60	97.42	1
C3'-C2'-C1'	101.30	106.48	1
O5'-C5'-C4'	111.50	103.74	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C4'-O4'-C1'	109.90	104.72	1
O5'-C5'-C4'	111.50	119.26	1
C2'-C1'-N1	112.00	104.24	1
C3'-C2'-O2'	110.70	118.46	1
C4'-C3'-O3'	113.00	120.76	1
O4'-C1'-C2'	107.60	102.43	1
C5'-C4'-C3'	116.00	108.25	1
C4'-C3'-C2'	102.60	97.44	1
O3'-P-O5'	104.00	111.74	1
O2'-C2'-C1'	108.40	100.66	1
O3'-P-O5'	104.00	96.27	1
C3'-C2'-C1'	101.30	106.45	1
C4'-C3'-O3'	113.00	105.28	1
C2'-C1'-N9	112.00	104.29	1
C5'-C4'-C3'	116.00	108.29	1
O2'-C2'-C1'	108.40	116.10	1
O3'-P-O5'	104.00	111.68	1
C4'-C3'-O3'	113.00	105.32	1
O4'-C1'-N9	108.50	116.18	1
O5'-C5'-C4'	111.50	119.18	1
C4'-O4'-C1'	109.90	104.78	1
O2'-C2'-C1'	108.40	100.73	1
O3'-P-O5'	104.00	111.66	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C3'-C2'-C1'	101.30	96.20	1
O4'-C4'-C3'	104.00	109.09	2
C3'-C2'-O2'	110.70	118.33	1
C4'-C3'-C2'	102.60	107.69	1
O3'-P-O5'	104.00	111.63	1
C2'-C1'-N1	112.00	104.38	1
C3'-C2'-C1'	101.30	106.37	1
C4'-C3'-C2'	102.60	97.53	1
O3'-P-O5'	104.00	111.61	1
C3'-C2'-O2'	110.70	118.30	1
C4'-C3'-O3'	113.00	120.59	1
C4'-C3'-C2'	102.60	97.54	1
C3'-C2'-O2'	110.70	118.29	1
O3'-P-O5'	104.00	111.59	1
C4'-O4'-C1'	109.90	104.84	1
O2'-C2'-C1'	108.40	100.82	1
O3'-C3'-C2'	113.70	106.12	1
C4'-C3'-C2'	102.60	97.55	1
C3'-C2'-O2'	110.70	118.27	1
C3'-C2'-C1'	101.30	96.26	1
O2'-C2'-C1'	108.40	115.95	1
O4'-C1'-C2'	107.60	102.56	1
C4'-C3'-C2'	102.60	97.57	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C3'-C2'-C1'	101.30	106.33	1
O4'-C1'-C2'	107.60	102.58	1
C4'-O4'-C1'	109.90	114.91	1
C4'-C3'-O3'	113.00	120.51	1
C4'-C3'-C2'	102.60	97.59	1
O3'-C3'-C2'	113.70	106.19	1
C4'-O4'-C1'	109.90	104.90	1
C3'-C2'-O2'	110.70	118.20	1
C4'-O4'-C1'	109.90	114.90	1
O4'-C4'-C3'	104.00	109.00	1
O3'-P-O5'	104.00	111.49	1
C4'-C3'-O3'	113.00	105.51	1
O4'-C4'-C3'	104.00	108.99	1
O4'-C1'-N9	108.50	115.98	1
C4'-C3'-C2'	102.60	97.61	1
O3'-P-O5'	104.00	111.48	1
C3'-C2'-C1'	101.30	96.32	1
C3'-C2'-C1'	101.30	106.28	1
O2'-C2'-C1'	108.40	115.87	1
C3'-C2'-C1'	101.30	106.27	1
C5'-C4'-O4'	109.80	117.25	1
O3'-C3'-C2'	113.70	106.26	1
C4'-C3'-O3'	113.00	120.44	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O3'-P-O5'	104.00	111.43	1
O3'-C3'-C2'	113.70	121.13	1
C3'-O3'-P	120.20	127.63	1
C4'-C3'-C2'	102.60	97.65	1
O4'-C1'-N1	108.50	115.92	1
C5'-C4'-C3'	116.00	108.58	1
C2'-C1'-N1	112.00	104.58	1
O5'-C5'-C4'	111.50	118.92	1
O4'-C1'-C2'	107.60	102.66	1
C4'-O4'-C1'	109.90	114.84	1
C4'-C3'-C2'	102.60	107.54	1
O2'-C2'-C1'	108.40	115.79	1
O2'-C2'-C1'	108.40	115.78	1
C3'-C2'-O2'	110.70	118.08	1
C4'-C3'-O3'	113.00	120.37	1
C4'-C3'-O3'	113.00	105.63	1
C3'-O3'-P	120.20	127.57	1
C3'-C2'-O2'	110.70	118.06	1
C4'-C3'-C2'	102.60	97.70	1
C3'-C2'-O2'	110.70	118.05	1
C3'-C2'-O2'	110.70	118.04	1
C3'-C2'-C1'	101.30	106.19	1
C4'-C3'-C2'	102.60	97.71	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C3'-C2'-O2'	110.70	118.03	1
P-O5'-C5'	120.90	128.23	1
C5'-C4'-C3'	116.00	108.67	1
O3'-P-O5'	104.00	111.33	1
O4'-C1'-C2'	107.60	102.71	1
O3'-C3'-C2'	113.70	106.38	1
C2'-C1'-N9	112.00	104.68	1
C4'-C3'-C2'	102.60	97.73	1
O4'-C1'-C2'	107.60	102.73	1
C5'-C4'-C3'	116.00	108.70	1
O3'-C3'-C2'	113.70	106.40	1
C5'-C4'-C3'	116.00	108.71	1
O3'-P-OP1	108.00	122.58	1
C2'-C1'-N9	112.00	104.71	1
O4'-C1'-N1	108.50	115.79	1
O4'-C1'-N9	108.50	115.79	1
O4'-C4'-C3'	104.00	99.14	1
O4'-C1'-C2'	107.60	112.45	2
O4'-C1'-N1	108.50	115.77	1
C5'-C4'-O4'	109.80	117.07	2
O3'-P-O5'	104.00	111.27	1
O3'-C3'-C2'	113.70	120.97	1
O3'-C3'-C2'	113.70	106.44	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O3'-P-OP1	108.00	122.53	1
O4'-C1'-C2'	107.60	102.76	2
O4'-C4'-C3'	104.00	108.84	1
C4'-C3'-C2'	102.60	97.76	1
O5'-C5'-C4'	111.50	118.75	1
O3'-P-O5'	104.00	111.25	1
P-O5'-C5'	120.90	128.14	1
O3'-C3'-C2'	113.70	106.46	1
O4'-C1'-C2'	107.60	102.77	1
C5'-C4'-O4'	109.80	117.04	1
O2'-C2'-C1'	108.40	101.17	1
C3'-C2'-C1'	101.30	96.48	1
C3'-C2'-O2'	110.70	117.93	1
C3'-C2'-C1'	101.30	106.11	1
O4'-C4'-C3'	104.00	108.81	1
C4'-C3'-C2'	102.60	97.80	1
C3'-C2'-C1'	101.30	106.09	1
C2'-C1'-N1	112.00	104.81	1
O2'-C2'-C1'	108.40	115.58	1
C4'-C3'-O3'	113.00	105.83	1
C3'-C2'-C1'	101.30	106.08	1
C4'-O4'-C1'	109.90	114.68	1
O3'-P-O5'	104.00	111.17	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C4'-O4'-C1'	109.90	105.12	1
C4'-C3'-O3'	113.00	120.15	2
C4'-C3'-C2'	102.60	97.84	1
O4'-C1'-N1	108.50	115.64	1
O4'-C1'-N9	108.50	115.63	1
C3'-C2'-O2'	110.70	117.83	1
C4'-O4'-C1'	109.90	105.15	1
C5'-C4'-C3'	116.00	108.88	1
C3'-C2'-C1'	101.30	106.05	1
O3'-C3'-C2'	113.70	106.58	1
O4'-C4'-C3'	104.00	108.75	1
C4'-C3'-C2'	102.60	97.86	1
O4'-C4'-C3'	104.00	108.74	1
O4'-C1'-N1	108.50	115.60	1
O2'-C2'-C1'	108.40	115.50	1
O3'-P-O5'	104.00	111.09	1
O5'-C5'-C4'	111.50	118.59	1
O4'-C1'-N9	108.50	115.59	2
C5'-C4'-C3'	116.00	123.09	1
C5'-C4'-C3'	116.00	108.91	1
O3'-C3'-C2'	113.70	106.61	1
O4'-C1'-C2'	107.60	112.32	1
O3'-P-O5'	104.00	96.92	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O4'-C1'-N1	108.50	115.57	1
O3'-P-OP1	108.00	122.14	1
O3'-P-O5'	104.00	111.07	2
O5'-C5'-C4'	111.50	104.43	1
C3'-C2'-O2'	110.70	117.77	1
C4'-C3'-C2'	102.60	107.31	1
C3'-C2'-C1'	101.30	106.01	1
C5'-C4'-C3'	116.00	108.94	1
O3'-P-O5'	104.00	111.06	1
O3'-C3'-C2'	113.70	106.65	1
C2'-C1'-N9	112.00	104.95	1
O4'-C1'-N1	108.50	115.55	1
O4'-C1'-N9	108.50	115.55	1
C4'-C3'-O3'	113.00	120.04	1
O4'-C4'-C3'	104.00	108.69	1
C5'-C4'-O4'	109.80	116.83	1
C2'-C1'-N1	112.00	119.03	1
C2'-C1'-N9	112.00	104.97	1
C4'-O4'-C1'	109.90	114.59	1
C4'-O4'-C1'	109.90	114.58	1
O3'-P-O5'	104.00	111.01	1
C2'-C1'-N9	112.00	104.99	1
O2'-C2'-C1'	108.40	101.40	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C5'-C4'-O4'	109.80	116.80	1
C3'-C2'-O2'	110.70	117.70	1
C3'-C2'-C1'	101.30	96.63	1
O4'-C1'-N1	108.50	115.49	2
O4'-C4'-C3'	104.00	108.66	2
C3'-C2'-O2'	110.70	117.68	1
C4'-O4'-C1'	109.90	114.56	1
C4'-O4'-C1'	109.90	105.24	1
O3'-C3'-C2'	113.70	120.68	1
O4'-C1'-N1	108.50	115.48	1
C2'-C1'-N9	112.00	105.02	1
C4'-C3'-C2'	102.60	97.95	1
O3'-P-O5'	104.00	110.97	1
C2'-C1'-N1	112.00	105.03	1
C5'-C4'-C3'	116.00	109.03	1
O5'-C5'-C4'	111.50	104.53	1
C3'-C2'-O2'	110.70	117.66	1
O2'-C2'-C1'	108.40	115.35	1
C3'-C2'-C1'	101.30	105.93	1
O3'-C3'-C2'	113.70	106.77	1
C4'-C3'-C2'	102.60	97.98	1
C5'-C4'-O4'	109.80	116.72	1
C5'-C4'-C3'	116.00	109.08	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O4'-C1'-N1	108.50	115.42	1
C4'-C3'-O3'	113.00	119.91	1
O4'-C4'-C3'	104.00	108.61	1
O3'-P-O5'	104.00	110.91	1
O4'-C4'-C3'	104.00	108.60	1
C4'-C3'-O3'	113.00	106.10	1
C4'-O4'-C1'	109.90	114.50	1
C5'-C4'-C3'	116.00	109.11	1
C4'-C3'-O3'	113.00	106.11	1
C3'-O3'-P	120.20	127.09	1
O4'-C1'-C2'	107.60	103.01	2
C4'-C3'-C2'	102.60	98.01	1
O4'-C1'-N9	108.50	115.38	1
O4'-C1'-N1	108.50	115.38	1
C2'-C1'-N9	112.00	118.87	1
O4'-C1'-C2'	105.80	110.38	1
O4'-C1'-N1	108.50	115.36	2
C4'-O4'-C1'	109.90	105.33	1
O4'-C1'-C2'	107.60	112.17	1
C3'-C2'-C1'	101.30	96.73	1
O4'-C1'-N9	108.50	115.35	1
C3'-C2'-C1'	101.30	105.87	1
O4'-C1'-N1	108.50	115.35	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C3'-C2'-O2'	110.70	103.85	1
C3'-C2'-C1'	101.30	105.86	1
O4'-C1'-N9	108.50	115.34	1
O4'-C4'-C3'	104.00	99.44	1
O4'-C4'-C3'	104.00	108.56	1
O4'-C1'-C2'	107.60	112.15	1
C4'-O4'-C1'	109.90	105.35	1
C2'-C1'-N9	114.00	107.18	1
C5'-C4'-O4'	109.80	116.62	2
C5'-C4'-C3'	116.00	109.18	1
P-O5'-C5'	120.90	127.71	1
O4'-C4'-C3'	104.00	108.54	1
C5'-C4'-O4'	109.80	102.99	1
C5'-C4'-C3'	116.00	109.20	1
C4'-C3'-C2'	102.60	98.07	1
C3'-C2'-C1'	101.30	105.83	1
O4'-C1'-C2'	107.60	112.13	1
P-O5'-C5'	120.90	127.69	1
C4'-O4'-C1'	109.90	105.37	1
O5'-C5'-C4'	111.50	104.72	1
C4'-C3'-O3'	113.00	119.78	1
O4'-C1'-C2'	107.60	112.12	1
C5'-C4'-C3'	116.00	109.22	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O4'-C1'-N1	108.50	115.28	1
O3'-P-O5'	104.00	110.76	1
O4'-C1'-C2'	107.60	103.09	1
O3'-C3'-C2'	113.70	106.94	1
C3'-C2'-C1'	101.30	96.79	1
C2'-C1'-N9	112.00	105.24	1
C3'-O3'-P	120.20	113.45	1
O3'-P-O5'	104.00	110.75	1
C5'-C4'-O4'	109.80	116.54	2
C5'-C4'-C3'	116.00	109.26	1
O4'-C1'-C2'	107.60	103.11	1
C3'-C2'-C1'	101.30	105.79	1
O3'-C3'-C2'	113.70	106.97	1
O3'-P-O5'	104.00	110.73	1
O4'-C1'-N9	108.50	101.77	1
C4'-C3'-C2'	102.60	98.11	1
C5'-C4'-C3'	116.00	109.28	1
O2'-C2'-C1'	108.40	101.69	1
C3'-C2'-O2'	110.70	103.99	1
C2'-C1'-N9	112.00	105.29	1
C3'-C2'-C1'	101.30	105.77	2
O4'-C1'-N9	108.50	115.20	1
O4'-C1'-N9	108.50	115.19	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O3'-C3'-C2'	113.70	107.01	1
O5'-C5'-C4'	111.50	104.81	1
C5'-C4'-O4'	109.80	116.48	1
O4'-C1'-C2'	107.60	103.15	1
C4'-C3'-C2'	102.60	98.15	1
O3'-C3'-C2'	113.70	107.02	1
O3'-P-O5'	104.00	97.32	1
O3'-P-O5'	104.00	110.68	1
C2'-C1'-N1	112.00	105.33	1
O3'-P-O5'	104.00	110.67	1
C3'-C2'-O2'	110.70	117.37	2
C3'-C2'-C1'	101.30	105.74	2
O4'-C4'-C3'	104.00	108.44	1
O2'-C2'-C1'	108.40	115.06	1
O3'-C3'-C2'	113.70	107.04	2
N6-C6-N1	118.60	105.29	1
P-O5'-C5'	120.90	127.55	1
C5'-C4'-O4'	109.80	116.45	1
O2'-C2'-C1'	108.40	101.75	1
C3'-C2'-C1'	101.30	96.87	1
C4'-C3'-C2'	102.60	107.03	1
C4'-O4'-C1'	109.90	105.47	1
O4'-C4'-C3'	104.00	108.42	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C3'-C2'-C1'	101.30	105.72	1
C4'-C3'-O3'	113.00	119.63	1
C2'-C1'-N9	112.00	105.37	1
C5'-C4'-O4'	109.80	116.42	1
C3'-C2'-C1'	101.30	96.88	1
C4'-C3'-O3'	113.00	119.62	1
O4'-C4'-C3'	104.00	108.41	2
C4'-C3'-C2'	102.60	107.01	1
P-O5'-C5'	120.90	127.51	1
C5'-C4'-O4'	109.80	103.19	1
O4'-C1'-N1	108.50	115.11	1
C3'-C2'-O2'	110.70	117.31	1
C4'-C3'-C2'	102.60	98.20	1
O2'-C2'-C1'	108.40	114.99	1
C4'-C3'-O3'	113.00	106.41	1
C4'-O4'-C1'	109.90	105.51	2
O4'-C1'-N1	108.50	115.09	1
O3'-P-O5'	104.00	110.59	1
C2'-C1'-N9	112.00	105.42	1
O4'-C4'-C3'	104.00	108.39	1
O5'-C5'-C4'	111.50	104.92	1
P-O5'-C5'	120.90	127.48	1
O5'-C5'-C4'	111.50	118.08	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C2'-C1'-N9	112.00	105.43	1
C3'-C2'-C1'	101.30	96.92	1
P-O5'-C5'	120.90	114.33	1
O4'-C4'-C3'	104.00	99.62	1
O4'-C1'-C2'	107.60	111.97	1
C4'-O4'-C1'	109.90	114.27	1
O5'-C5'-C4'	111.50	118.05	1
P-O5'-C5'	120.90	114.35	1
C4'-C3'-O3'	113.00	106.45	1
O3'-C3'-C2'	113.70	120.25	1
C3'-O3'-P	120.20	126.75	1
O4'-C1'-C2'	107.60	103.23	1
C3'-C2'-O2'	110.70	117.25	1
O4'-C4'-C3'	104.00	108.36	1
C4'-C3'-O3'	113.00	106.46	1
O3'-C3'-C2'	113.70	107.18	1
O4'-C4'-C3'	104.00	108.35	2
O4'-C1'-C2'	105.80	110.15	1
O5'-C5'-C4'	111.50	104.98	1
O4'-C1'-N1	108.50	115.01	1
O2'-C2'-C1'	108.40	114.91	1
C4'-C3'-C2'	102.60	98.27	1
O4'-C1'-N1	108.50	115.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O3'-P-O5'	104.00	110.50	1
C3'-C2'-O2'	110.70	117.19	1
C3'-C2'-O2'	110.70	104.22	1
O4'-C4'-C3'	104.00	108.32	1
O4'-C1'-C2'	107.60	111.92	1
C3'-C2'-O2'	110.70	117.17	1
C3'-C2'-C1'	101.30	96.99	1
P-O5'-C5'	120.90	127.37	1
N6-C6-N1	118.60	105.66	1
O4'-C1'-N1	108.50	114.97	1
O3'-C3'-C2'	113.70	107.24	1
O4'-C1'-C2'	107.60	103.29	1
O2'-C2'-C1'	108.40	101.94	1
C4'-C3'-C2'	102.60	98.30	1
O3'-C3'-C2'	113.70	120.15	1
C5'-C4'-C3'	116.00	109.55	1
C2'-C1'-N9	112.00	105.55	1
O4'-C1'-C2'	107.60	103.30	1
C3'-C2'-C1'	101.30	105.60	2
O5'-C5'-C4'	111.50	117.94	1
O4'-C4'-C3'	104.00	108.29	1
C3'-C2'-C1'	101.30	97.01	1
C5'-C4'-C3'	116.00	109.56	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
P-O5'-C5'	120.90	127.34	1
C4'-C3'-C2'	102.60	98.31	1
C5'-C4'-C3'	116.00	109.57	1
O5'-C5'-C4'	111.50	105.07	1
C5'-C4'-C3'	116.00	109.58	1
O3'-P-O5'	104.00	110.42	1
O4'-C4'-C3'	104.00	99.72	1
C2'-C1'-N1	112.00	105.58	1
C3'-C2'-O2'	110.70	117.12	1
O5'-C5'-C4'	111.70	105.28	1
O4'-C1'-C2'	107.60	103.32	1
O4'-C4'-C3'	106.10	110.37	1
O4'-C1'-N1	108.50	114.91	1
O5'-C5'-C4'	111.50	117.90	1
C5'-C4'-O4'	109.80	116.20	1
C3'-O3'-P	120.20	126.60	1
O3'-C3'-C2'	113.70	120.10	1
O4'-C1'-C2'	107.60	111.86	1
O4'-C4'-C3'	104.00	108.26	2
C3'-C2'-O2'	110.70	117.09	1
C3'-C2'-O2'	110.70	117.08	2
C4'-O4'-C1'	109.90	105.65	1
C5'-C4'-C3'	116.00	109.63	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
P-O5'-C5'	120.90	127.27	1
O4'-C1'-C2'	107.60	103.35	1
O4'-C1'-N1	108.50	114.87	1
C3'-O3'-P	120.20	126.57	1
C3'-O3'-P	120.20	126.56	1
C4'-O4'-C1'	109.90	105.66	1
C4'-C3'-O3'	113.00	119.36	1
O3'-P-O5'	104.00	110.36	1
C4'-C3'-O3'	113.00	106.65	1
P-O5'-C5'	120.90	127.25	1
O4'-C1'-N1	108.50	114.85	1
O5'-C5'-C4'	111.50	117.85	1
C5'-C4'-C3'	115.20	108.85	1
C4'-O4'-C1'	109.90	105.67	1
O4'-C1'-C2'	107.60	103.37	1
O4'-C1'-N1	108.50	114.84	1
C5'-C4'-O4'	109.10	115.43	1
O3'-P-O5'	104.00	110.33	1
C3'-C2'-O2'	110.70	117.03	2
C2'-C1'-N1	112.00	105.68	1
C3'-C2'-O2'	110.70	117.02	2
C4'-C3'-C2'	102.60	98.39	1
C5'-C4'-C3'	116.00	109.68	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O3'-P-O5'	104.00	110.32	1
O5'-C5'-C4'	111.50	117.81	1
O4'-C4'-C3'	104.00	108.21	1
O4'-C1'-N1	108.50	114.80	1
O4'-C1'-N9	108.50	114.80	1
C4'-O4'-C1'	109.90	105.70	1
C2'-C1'-N9	112.00	105.70	1
O3'-C3'-C2'	113.70	120.00	1
O5'-C5'-C4'	111.50	105.21	1
C5'-C4'-C3'	116.00	109.71	1
O4'-C4'-C3'	104.00	108.19	1
O5'-C5'-C4'	111.50	117.79	1
C4'-C3'-C2'	102.60	98.41	1
C4'-C3'-O3'	113.00	106.72	1
C4'-C3'-O3'	113.00	119.28	1
C4'-C3'-C2'	102.60	98.42	1
O4'-C4'-C3'	104.00	99.82	1
C5'-C4'-C3'	116.00	109.74	2
C5'-C4'-O4'	109.80	103.54	1
O4'-C1'-N1	108.50	114.76	1
O4'-C4'-C3'	104.00	108.17	1
C5'-C4'-O4'	109.80	116.05	1
C4'-O4'-C1'	109.90	105.73	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O4'-C1'-N9	108.50	114.75	1
C4'-C3'-C2'	102.60	106.77	1
O3'-P-O5'	104.00	110.25	1
O4'-C1'-C2'	107.60	103.44	2
C2'-C1'-N1	112.00	105.76	1
C3'-C2'-C1'	101.30	97.14	1
C5'-C4'-O4'	109.80	103.56	1
O2'-C2'-C1'	108.40	102.16	1
O4'-C4'-C3'	104.00	99.84	1
C3'-C2'-O2'	110.70	116.93	1
C5'-C4'-O4'	109.80	116.03	2
C5'-C4'-O4'	109.80	116.02	1
C4'-O4'-C1'	109.90	105.76	1
O4'-C4'-C3'	104.00	99.86	1
C5'-C4'-C3'	116.00	109.79	1
C4'-C3'-C2'	102.60	106.74	1
O4'-C1'-C2'	107.60	103.46	1
C2'-C1'-N9	112.00	105.79	1
C3'-C2'-O2'	110.70	116.91	1
C3'-O3'-P	120.20	126.41	1
O5'-C5'-C4'	111.50	105.29	1
C2'-C1'-N9	112.00	118.21	1
O3'-P-OP1	108.00	120.41	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C2'-C1'-N9	112.00	118.20	1
C3'-C2'-O2'	110.70	116.90	1
C3'-C2'-C1'	101.30	105.43	1
O2'-C2'-C1'	108.40	114.59	1
O4'-C4'-C3'	106.10	110.22	1
O4'-C1'-N9	108.50	114.68	2
C4'-O4'-C1'	109.90	105.78	1
O5'-C5'-C4'	111.50	117.68	1
C5'-C4'-C3'	116.00	109.82	1
C3'-C2'-C1'	101.30	105.42	1
O4'-C1'-C2'	107.60	103.48	1
O2-C2-N3	121.90	109.55	1
O4'-C4'-C3'	104.00	108.12	1
C5'-C4'-O4'	109.80	103.63	1
O4'-C1'-C2'	107.60	103.49	1
C5'-C4'-C3'	116.00	109.84	1
O3'-C3'-C2'	113.70	119.85	1
N6-C6-N1	118.60	106.30	1
O2'-C2'-C1'	108.40	114.55	1
C4'-C3'-O3'	113.00	106.85	1
O3'-P-O5'	104.00	110.15	2
O3'-C3'-C2'	113.70	107.55	1
O3'-C3'-C2'	113.70	107.56	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O2'-C2'-C1'	108.40	114.54	1
O5'-C5'-C4'	111.50	117.63	1
C4'-O4'-C1'	109.90	113.98	1
C3'-C2'-C1'	101.30	97.22	1
C4'-O4'-C1'	109.90	105.82	1
C5'-C4'-O4'	109.80	115.91	1
C4'-C3'-O3'	113.00	119.11	1
O4'-C4'-C3'	104.00	99.93	1
C3'-C2'-O2'	110.70	116.81	1
O3'-P-O5'	104.00	110.10	1
C3'-C2'-C1'	101.30	105.37	1
C2'-C1'-N1	112.00	105.90	1
C5'-C4'-O4'	109.10	103.01	1
O4'-C1'-C2'	107.60	103.54	1
C4'-C3'-C2'	102.60	106.66	1
C4'-C3'-C2'	102.60	98.54	1
C5'-C4'-O4'	109.80	115.88	1
O4'-C1'-C2'	107.60	103.55	1
C5'-C4'-C3'	116.00	109.92	1
C3'-C2'-O2'	110.70	116.78	1
C4'-O4'-C1'	109.90	105.85	1
O5'-C5'-C4'	111.50	117.57	1
C2'-C1'-N9	112.00	105.93	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C3'-C2'-O2'	110.70	116.77	2
C4'-C3'-O3'	113.00	106.93	1
C4'-O4'-C1'	109.90	113.95	1
O4'-C1'-N9	108.50	114.57	1
C3'-C2'-C1'	101.30	105.34	1
C5'-C4'-O4'	109.80	115.86	1
C5'-C4'-C3'	116.00	109.94	1
C4'-C3'-O3'	113.00	106.94	1
O5'-C5'-C4'	111.50	105.44	1
C2'-C1'-N9	112.00	105.94	1
O3'-P-OP2	108.00	120.11	1
O4'-C1'-C2'	107.60	111.64	1
O2'-C2'-C1'	111.80	117.85	1
O4'-C4'-C3'	104.00	108.03	1
O2'-C2'-C1'	108.40	114.45	1
C4'-C3'-C2'	102.60	98.57	1
C3'-C2'-C1'	101.30	105.33	1
O4'-C1'-C2'	107.60	103.57	2
C4'-O4'-C1'	109.90	105.87	1
O3'-P-O5'	104.00	110.04	1
O2'-C2'-C1'	108.40	114.43	1
C4'-C3'-C2'	102.60	98.58	1
O4'-C1'-N1	108.50	114.53	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O3'-P-OP2	108.00	120.06	1
C3'-C2'-C1'	101.30	97.28	1
C2'-C1'-N1	112.00	105.97	1
O5'-C5'-C4'	111.50	117.53	1
O2'-C2'-C1'	108.40	114.42	1
C5'-C4'-C3'	115.20	109.18	1
C3'-C2'-C1'	101.30	97.29	1
C2'-C1'-N1	112.00	105.98	1
C4'-C3'-O3'	113.00	119.01	1
C3'-O3'-P	120.20	126.21	1
O3'-C3'-C2'	113.70	119.70	1
O4'-C1'-C2'	107.60	103.60	1
H41-N4-H42	107.91	120.00	1
C2'-O2'-HO2'	96.75	109.00	1
C4'-C5'-H5'	96.69	109.00	1
C4-N4-H41	107.68	120.00	1
H21-N2-H22	107.62	120.00	1
C2'-O2'-HO2'	96.54	109.00	1
C3'-C4'-H4'	96.45	109.00	1
C4'-C3'-H3'	96.44	109.00	1
C4'-C5'-H5"	121.61	109.00	1
O2'-C2'-H2'	121.72	109.00	1
O4'-C4'-H4'	96.23	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C4-N4-H42	107.18	120.00	1
C1'-C2'-H2'	121.92	109.00	1
C4'-C3'-H3'	96.04	109.00	1
O4'-C1'-H1'	122.15	109.00	1
C4'-C5'-H5'	95.84	109.00	1
C2'-O2'-HO2'	95.80	109.00	1
H5'-C5'-H5''	122.22	109.00	1
O4'-C4'-H4'	95.74	109.00	1
C2'-O2'-HO2'	95.54	109.00	1
C2'-O2'-HO2'	122.58	109.00	1
H5'-C5'-H5''	95.40	109.00	1
C3'-C4'-H4'	95.29	109.00	1
O4'-C1'-H1'	95.29	109.00	1
H5'-C5'-H5''	95.06	109.00	1
H5'-C5'-H5''	95.02	109.00	1
O3'-C3'-H3'	123.06	109.00	1
C2'-O2'-HO2'	94.77	109.00	1
C2'-O2'-HO2'	94.27	109.00	1
C3'-C4'-H4'	93.77	109.00	1
O5'-C5'-H5''	93.56	109.00	1
O3'-C3'-H3'	124.45	109.00	1
C2'-O2'-HO2'	93.31	109.00	1
O2'-C2'-H2'	126.37	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C1'-C2'-H2'	126.56	109.00	1
C1'-C2'-H2'	126.57	109.00	1
C1'-C2'-H2'	126.58	109.00	1
C1'-C2'-H2'	126.59	109.00	3
C1'-C2'-H2'	126.60	109.00	5
C1'-C2'-H2'	126.61	109.00	8
C1'-C2'-H2'	126.62	109.00	11
C1'-C2'-H2'	126.63	109.00	18
C1'-C2'-H2'	126.64	109.00	43
C1'-C2'-H2'	126.65	109.00	60
C1'-C2'-H2'	126.66	109.00	94
C1'-C2'-H2'	126.67	109.00	122
C1'-C2'-H2'	126.68	109.00	100
C1'-C2'-H2'	126.69	109.00	117
C1'-C2'-H2'	126.70	109.00	103
C1'-C2'-H2'	126.71	109.00	91
C1'-C2'-H2'	126.72	109.00	73
C1'-C2'-H2'	126.73	109.00	49
C1'-C2'-H2'	126.74	109.00	19
C1'-C2'-H2'	126.75	109.00	25
C1'-C2'-H2'	126.76	109.00	11
C1'-C2'-H2'	126.77	109.00	6
C1'-C2'-H2'	126.78	109.00	4

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C1'-C2'-H2'	126.79	109.00	1
O3'-C3'-H3'	84.39	109.00	1
O3'-C3'-H3'	84.38	109.00	3
O3'-C3'-H3'	84.37	109.00	2
O3'-C3'-H3'	84.36	109.00	10
O3'-C3'-H3'	84.35	109.00	13
O3'-C3'-H3'	84.34	109.00	24
O3'-C3'-H3'	84.33	109.00	28
O3'-C3'-H3'	84.32	109.00	28
O3'-C3'-H3'	84.31	109.00	42
O3'-C3'-H3'	84.30	109.00	75
O3'-C3'-H3'	84.29	109.00	69
O3'-C3'-H3'	84.28	109.00	80
O3'-C3'-H3'	84.27	109.00	78
O3'-C3'-H3'	84.26	109.00	81
O3'-C3'-H3'	84.25	109.00	99
O3'-C3'-H3'	84.24	109.00	69
O3'-C3'-H3'	84.23	109.00	79
O3'-C3'-H3'	84.22	109.00	55
O3'-C3'-H3'	84.21	109.00	41
O3'-C3'-H3'	84.20	109.00	30
O3'-C3'-H3'	84.19	109.00	24
O3'-C3'-H3'	84.18	109.00	10

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O3'-C3'-H3'	84.17	109.00	13
O3'-C3'-H3'	84.16	109.00	5
O3'-C3'-H3'	84.15	109.00	2
O3'-C3'-H3'	84.14	109.00	1
O3'-C3'-H3'	84.13	109.00	1
O3'-C3'-H3'	84.12	109.00	2
O3'-C3'-H3'	84.11	109.00	1
C4'-C3'-H3'	134.61	109.00	1
C4'-C3'-H3'	134.63	109.00	2
C4'-C3'-H3'	134.64	109.00	1
C4'-C3'-H3'	134.65	109.00	1
C4'-C3'-H3'	134.66	109.00	3
C4'-C3'-H3'	134.67	109.00	4
C4'-C3'-H3'	134.68	109.00	11
C4'-C3'-H3'	134.69	109.00	6
C4'-C3'-H3'	134.70	109.00	15
C4'-C3'-H3'	134.71	109.00	17
C4'-C3'-H3'	134.72	109.00	32
C4'-C3'-H3'	134.73	109.00	41
C4'-C3'-H3'	134.74	109.00	32
C4'-C3'-H3'	134.75	109.00	57
C4'-C3'-H3'	134.76	109.00	46
C4'-C3'-H3'	134.77	109.00	42

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C4'-C3'-H3'	134.78	109.00	64
C4'-C3'-H3'	134.79	109.00	49
C4'-C3'-H3'	134.80	109.00	60
C4'-C3'-H3'	134.81	109.00	64
C4'-C3'-H3'	134.82	109.00	57
C4'-C3'-H3'	134.83	109.00	57
C4'-C3'-H3'	134.84	109.00	45
C4'-C3'-H3'	134.85	109.00	43
C4'-C3'-H3'	134.86	109.00	42
C4'-C3'-H3'	134.87	109.00	36
C4'-C3'-H3'	134.88	109.00	33
C4'-C3'-H3'	134.89	109.00	15
C4'-C3'-H3'	134.90	109.00	32
C4'-C3'-H3'	134.91	109.00	20
C4'-C3'-H3'	134.92	109.00	7
C4'-C3'-H3'	134.93	109.00	12
C4'-C3'-H3'	134.94	109.00	4
C4'-C3'-H3'	134.95	109.00	4
C4'-C3'-H3'	134.96	109.00	2
C4'-C3'-H3'	134.97	109.00	2
C4'-C3'-H3'	134.98	109.00	3
C4'-C3'-H3'	134.99	109.00	2
C4'-C3'-H3'	135.00	109.00	2

Too-close contacts

The following all-atom clashscore is based on a MolProbity analysis. All-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The table below contains clashscores for all the models in this entry.

Model ID	Clash score	Number of clashes
1	0.00	0
2	0.00	0
3	0.00	0
4	0.00	0
5	0.00	0
6	0.00	0
7	0.00	0
8	0.00	0
9	0.00	0
10	0.00	0

All 0 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Torsion angles: Protein backbone

In the following table, Ramachandran outliers are listed. The Analysed column shows the number of residues for which the backbone conformation was analysed.

Model ID	Analyzed	Favored	Allowed	Outliers
1	0	0	0	0
2	0	0	0	0
3	0	0	0	0
4	0	0	0	0
5	0	0	0	0
6	0	0	0	0
7	0	0	0	0

Model ID	Analyzed	Favored	Allowed	Outliers
8	0	0	0	0
9	0	0	0	0
10	0	0	0	0

Detailed list of outliers are tabulated below.

Torsion angles: Protein sidechains

In the following table, sidechain outliers are listed. The Analysed column shows the number of residues for which the sidechain conformation was analysed.

Model ID	Analyzed	Favored	Allowed	Outliers
1	0	0	0	0
2	0	0	0	0
3	0	0	0	0
4	0	0	0	0
5	0	0	0	0
6	0	0	0	0
7	0	0	0	0
8	0	0	0	0
9	0	0	0	0
10	0	0	0	0

Detailed list of outliers are tabulated below.

Fit of model to data used for modeling

Single molecule FRET

Validation for this section is under development.

Fit of model to data used for validation

Validation for this section is under development.

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