Integrative Structure Validation Report

July 22, 2024 - 04:10 PM PDT

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	9A0K
PDB-Dev ID	PDBDEV_00000056
Structure Title	A structural model of the endogenoushuman SWI/SNF (BAF) complex bound to the nucleosome informs disease mechanisms
Structure Authors	Mashtalir N; Suzuki H; Farrell DP; Sankar A; Luo J; Filipovski M; D'Avino AR; St.Pierre R; Valencia AM; Onikubo T; Roeder RG; Han Y; He Y; Ranish JA; DiMaio F; Walz T; Kadoch C

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

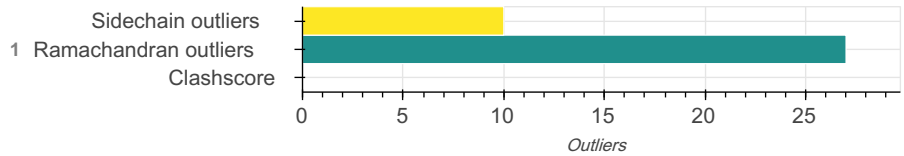
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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



Ensemble information

This entry consists of 0 distinct ensemble(s).

Summary

This entry consists of 1 unique models, with 20 subunits in each model. A total of 49 datasets or restraints were used to build this entry. Each model is represented by 23 rigid bodies and 0 flexible or non-rigid units.

Entry composition

There is 1 unique type of models in this entry. This model is titled Top Model/Best scoring model.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	ACTB	B	B	375
1	2	2	ACTL6A	6	6	429
1	3	3	ARID1A	A	A	2285
1	4	4	DPF2	P	P	391
1	5	5	SMARCA4	4	4	1647
1	6	6	SMARCB1	b	b	385
1	7	7	SMARCC1	1	1	1105
1	8	8	SMARCC2	2	2	1214
1	9	9	SMARCD1	D	D	515
1	10	10	SMARCE1	E	E	411
1	11	11	H2A	V	V	130
1	12	11	H2A	v	v	130
1	13	12	H2B	W	W	126
1	14	12	H2B	w	w	126
1	15	13	H3	X	X	136
1	16	13	H3	x	x	136
1	17	14	H4	Y	Y	103
1	18	14	H4	y	y	103
1	19	15	601 dna fwd	p	p	196
1	20	16	601 dna rev	q	q	196

Datasets used for modeling

There are 49 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	3DEM volume	File	10.5281/zenodo.3998811
2	Crosslinking-MS data	PRIDE	PXD020992
3	Comparative model	File	10.5281/zenodo.3998811
4	Comparative model	File	10.5281/zenodo.3998811
5	Comparative model	File	10.5281/zenodo.3998811
6	Comparative model	File	10.5281/zenodo.3998811
7	Comparative model	File	10.5281/zenodo.3998811
8	Comparative model	File	10.5281/zenodo.3998811
9	Comparative model	File	10.5281/zenodo.3998811
10	Comparative model	File	10.5281/zenodo.3998811
11	Comparative model	File	10.5281/zenodo.3998811
12	Comparative model	File	10.5281/zenodo.3998811
13	Comparative model	File	10.5281/zenodo.3998811
14	Comparative model	File	10.5281/zenodo.3998811
15	Comparative model	File	10.5281/zenodo.3998811
16	Comparative model	File	10.5281/zenodo.3998811
17	Comparative model	File	10.5281/zenodo.3998811
18	Comparative model	File	10.5281/zenodo.3998811
19	Comparative model	File	10.5281/zenodo.3998811
20	Comparative model	File	10.5281/zenodo.3998811
21	Comparative model	File	10.5281/zenodo.3998811
22	Comparative model	File	10.5281/zenodo.3998811
23	Comparative model	File	10.5281/zenodo.3998811
24	De Novo model	File	10.5281/zenodo.3998811
25	De Novo model	File	10.5281/zenodo.3998811
26	Experimental model	PDB	6UXV
27	Experimental model	PDB	6UXV

ID	Dataset type	Database name	Data access code
28	Experimental model	PDB	6UCH
29	Experimental model	PDB	6UXV
30	Experimental model	PDB	5X0Y
31	Experimental model	PDB	5X0Y
32	Experimental model	PDB	5X0Y
33	Experimental model	PDB	6UXV
34	Experimental model	PDB	5X0Y
35	Experimental model	PDB	5X0Y
36	Experimental model	PDB	6UXV
37	Experimental model	PDB	4I6M
38	Experimental model	PDB	5X0Y
39	Experimental model	PDB	6UXV
40	Experimental model	PDB	4I6M
41	Experimental model	PDB	5X0Y
42	Experimental model	PDB	5X0Y
43	Experimental model	PDB	6UXV
44	Experimental model	PDB	5X0Y
45	Experimental model	PDB	5X0Y
46	Experimental model	PDB	4I6M
47	Experimental model	PDB	5X0Y
48	3DEM volume	EMDB	EMD-22476
49	3DEM volume	EMDB	EMD-22478

Representation

This entry has only one representation and includes 23 rigid bodies and 0 flexible units

Chain ID	Rigid bodies	Non-rigid segments
B	1-375	-
6	1-429	-

Chain ID	Rigid bodies	Non-rigid segments
A	1-2285	-
P	1-88	-
4	1-16471-16471-1647	-
b	1-3851-385	-
1	1-1105	-
2	1-1214	-
D	1-515	-
E	220-298	-
V	1-130	-
W	1-126	-
X	1-136	-
Y	1-103	-
v	1-130	-
w	1-126	-
x	1-136	-
y	1-103	-
p	1-196	-
q	1-196	-

Methodology and software

This entry is a result of 1 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	Monte Carlo	Production sampling	None	None	False	False
2	1	trRosetta	trRosetta	None	None	False	False
3	1	Rosetta Hybridize	Rosetta Hybridize	None	None	False	False

There are 3 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	Rosetta	Rosetta version unknown:ff8ee24ee5f65423d5064cba818ede41d012fa87 2020-08-10 10:39:53 -0700 from git@github.com:RosettaCommons/main.git	RosettaCM/hybridize and unpublished 'complex assembly'	https://www.rosettacommons.org/
2	trRosetta	1.0.0	trRosetta	https://github.com/gjoni/trRosetta
3	HHpred	website	protein homology detection	https://toolkit.tuebingen.mpg.de/hhpred

Data quality

3DEM volume

Validation for this section is under development.

Crosslinking-MS

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 35990 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
CG2--2HG2	1.05	0.97	9
CG1--1HG1	1.05	0.97	9
CG1--3HG1	1.05	0.97	5
CD1--1HD1	1.05	0.97	6
CD2--2HD2	1.05	0.97	8
CD2--1HD2	1.05	0.97	5
CB--2HB	1.05	0.97	36
CD1--3HD1	1.05	0.97	12
CB--HB	1.05	0.97	3
CE--2HE	1.05	0.97	4
CB--1HB	1.05	0.97	33

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CG2--1HG2	1.05	0.97	12
CD1--2HD1	1.05	0.97	6
CG--2HG	1.05	0.97	6
CG--HG	1.05	0.97	6
CG1--2HG1	1.05	0.97	6
CA--HA	1.05	0.97	6
CG--1HG	1.05	0.97	4
CD--1HD	1.05	0.97	4
N4--H42	0.94	0.86	1
CB--3HB	1.05	0.97	3
CD2--3HD2	1.05	0.97	4
CG2--3HG2	1.05	0.97	5
CE--1HE	1.05	0.97	3
CD--2HD	1.05	0.97	3
C1'--H1'	1.05	0.97	2
CE--3HE	1.05	0.97	1
CE2--HE2	1.01	0.93	1
CG1--2HG1	1.06	0.97	15
CD1--1HD1	1.06	0.97	25
CE--2HE	1.06	0.97	6
CD1--2HD1	1.06	0.97	32
CG--1HG	1.06	0.97	26
CG2--2HG2	1.06	0.97	31
CG1--1HG1	1.06	0.97	18
CD2--2HD2	1.06	0.97	17
CD2--1HD2	1.06	0.97	13
CB--2HB	1.06	0.97	91
CB--1HB	1.06	0.97	85

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CD2--3HD2	1.06	0.97	17
CG2--1HG2	1.06	0.97	29
N4--H41	0.95	0.86	1
CB--3HB	1.06	0.97	10
CG2--3HG2	1.06	0.97	24
CD--2HD	1.06	0.97	12
CD1--3HD1	1.06	0.97	34
CA--HA	1.06	0.97	31
CB--HB	1.06	0.97	33
CG--HG	1.06	0.97	21
C2'--H2''	1.06	0.97	1
CD--1HD	1.06	0.97	18
CG--2HG	1.06	0.97	23
CG1--3HG1	1.06	0.97	4
CE--3HE	1.06	0.97	3
CE--1HE	1.06	0.97	7
C3'--H3'	1.06	0.97	2
C5'--H5'	1.06	0.97	1
CD1--HD1	1.02	0.93	1
C5'--H5''	1.06	0.97	1
CA--2HA	1.06	0.97	1
C1'--H1'	1.06	0.97	2
CG2--3HG2	1.07	0.97	52
CG1--2HG1	1.07	0.97	37
CD1--3HD1	1.07	0.97	69
CB--1HB	1.07	0.97	184
CG2--2HG2	1.07	0.97	59
CD1--2HD1	1.07	0.97	64

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CD--1HD	1.07	0.97	29
CA--HA	1.07	0.97	126
CG--1HG	1.07	0.97	59
CB--2HB	1.07	0.97	188
CD2--1HD2	1.07	0.97	37
C4'--H4'	1.07	0.97	3
CG--HG	1.07	0.97	46
CG--2HG	1.07	0.97	70
CD1--1HD1	1.07	0.97	48
CG1--3HG1	1.07	0.97	17
CG2--1HG2	1.07	0.97	44
CE--2HE	1.07	0.97	15
CG1--1HG1	1.07	0.97	44
CA--2HA	1.07	0.97	6
CB--HB	1.07	0.97	53
CB--3HB	1.07	0.97	22
CE2--HE2	1.03	0.93	2
CD2--3HD2	1.07	0.97	51
CD--2HD	1.07	0.97	26
CZ--HZ	1.03	0.93	1
CD2--2HD2	1.07	0.97	32
C2'--H2''	1.07	0.97	2
CE--3HE	1.07	0.97	12
CE--1HE	1.07	0.97	9
C3'--H3'	1.07	0.97	2
N2--H22	0.96	0.86	1
N4--H42	0.96	0.86	1
C1'--H1'	1.07	0.97	1

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
N4--H41	0.96	0.86	1
NZ--3HZ	0.99	0.89	1
C2'--H2'	1.07	0.97	1
NZ--2HZ	0.99	0.89	2
CD1--HD1	1.03	0.93	1
C5'--H5'	1.07	0.97	1
N1--H1	0.96	0.86	1
CA--1HA	1.07	0.97	2
CD2--HD2	1.03	0.93	1
CB--1HB	1.08	0.97	403
CG1--3HG1	1.08	0.97	39
CB--2HB	1.08	0.97	381
CG2--2HG2	1.08	0.97	121
CD2--2HD2	1.08	0.97	87
CG1--1HG1	1.08	0.97	74
CA--HA	1.08	0.97	665
CD1--1HD1	1.08	0.97	108
CD--2HD	1.08	0.97	91
CD2--3HD2	1.08	0.97	125
CG2--3HG2	1.08	0.97	137
CD1--2HD1	1.08	0.97	140
CG--2HG	1.08	0.97	216
CD1--3HD1	1.08	0.97	174
NZ--3HZ	1.00	0.89	27
CD--1HD	1.08	0.97	58
CG1--2HG1	1.08	0.97	97
CZ--HZ	1.04	0.93	2

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CB--HB	1.08	0.97	86
CG--1HG	1.08	0.97	170
CG2--1HG2	1.08	0.97	143
CG--HG	1.08	0.97	72
CE--3HE	1.08	0.97	33
CE--2HE	1.08	0.97	47
CA--2HA	1.08	0.97	15
N3--H3	0.97	0.86	1
CB--3HB	1.08	0.97	56
CD1--HD1	1.04	0.93	2
CD2--1HD2	1.08	0.97	63
CE--1HE	1.08	0.97	36
C2'--H2''	1.08	0.97	2
NZ--2HZ	1.00	0.89	26
CA--1HA	1.08	0.97	14
C5'--H5'	1.08	0.97	2
CE2--HE2	1.04	0.93	2
C5'--H5''	1.08	0.97	3
C6--H6	1.04	0.93	1
C1'--H1'	1.08	0.97	7
NZ--1HZ	1.00	0.89	17
N--3H	1.00	0.89	8
N--1H	1.00	0.89	8
N--2H	1.00	0.89	8
OH--HH	0.95	0.84	4
OG--HG	0.95	0.84	8
CD2--HD2	1.04	0.93	1
CE1--HE1	1.04	0.93	2

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
C7--H73	1.08	0.97	1
N6--H61	0.97	0.86	1
C3'--H3'	1.08	0.97	1
C2'--H2'	1.08	0.97	2
N4--H41	0.97	0.86	1
OG1--HG1	0.95	0.84	2
NE2--1HE2	0.97	0.86	1
N6--H62	0.97	0.86	1
C4'--H4'	1.08	0.97	1
CD--1HD	1.09	0.97	510
CB--1HB	1.09	0.97	2220
CE--1HE	1.09	0.97	331
CA--HA	1.09	0.97	2912
CG2--1HG2	1.09	0.97	450
CB--2HB	1.09	0.97	2231
CD--2HD	1.09	0.97	493
CG1--2HG1	1.09	0.97	307
NZ--3HZ	1.01	0.89	202
CB--HB	1.09	0.97	489
CG--1HG	1.09	0.97	960
CD1--1HD1	1.09	0.97	467
CG--2HG	1.09	0.97	912
CG2--2HG2	1.09	0.97	449
CD1--3HD1	1.09	0.97	359
CD1--2HD1	1.09	0.97	405
CD2--1HD2	1.09	0.97	294
CG--HG	1.09	0.97	259
CD2--2HD2	1.09	0.97	278

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CB--3HB	1.09	0.97	209
CG2--3HG2	1.09	0.97	463
CG1--3HG1	1.09	0.97	165
CG1--1HG1	1.09	0.97	305
CA--1HA	1.09	0.97	188
NZ--1HZ	1.01	0.89	226
CD2--3HD2	1.09	0.97	226
NZ--2HZ	1.01	0.89	208
C4'--H4'	1.09	0.97	10
CE--2HE	1.09	0.97	315
CE1--HE1	1.05	0.93	3
N1--H1	0.98	0.86	1
CE--3HE	1.09	0.97	66
CA--2HA	1.09	0.97	182
N2--H21	0.98	0.86	2
C5'--H5''	1.09	0.97	10
CD1--HD1	1.05	0.93	5
OH--HH	0.96	0.84	90
CH2--HH2	1.05	0.93	2
C5'--H5'	1.09	0.97	10
C1'--H1'	1.09	0.97	7
CE3--HE3	1.05	0.93	3
OG--HG	0.96	0.84	152
OG1--HG1	0.96	0.84	128
C2--H2	1.05	0.93	1
N2--H22	0.98	0.86	3
N4--H41	0.98	0.86	1
C2'--H2''	1.09	0.97	13

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
C3'--H3'	1.09	0.97	10
N6--H62	0.98	0.86	2
C2'--H2'	1.09	0.97	11
N--H	0.98	0.86	1
NE2--2HE2	0.98	0.86	1
CE2--HE2	1.05	0.93	5
CD2--HD2	1.05	0.93	6
N--2H	1.01	0.89	6
C8--H8	1.05	0.93	1
N--3H	1.01	0.89	5
N--1H	1.01	0.89	8
NH1--1HH1	0.98	0.86	1
C6--H6	1.05	0.93	2
CZ2--HZ2	1.05	0.93	1
CZ--HZ	1.05	0.93	1
C7--H71	1.09	0.97	1
ND2--1HD2	0.98	0.86	1
C7--H73	1.09	0.97	1
CB--HB	1.10	0.97	15
CD--1HD	1.10	0.97	100
CD1--HD1	1.06	0.93	16
CG--HG	1.10	0.97	14
OG--HG	0.97	0.84	27
CB--1HB	1.10	0.97	191
C2'--H2'	1.10	0.97	261
CD2--1HD2	1.10	0.97	7
NZ--3HZ	1.02	0.89	23
CB--2HB	1.10	0.97	160

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
OH--HH	0.97	0.84	13
C4'--H4'	1.10	0.97	258
C7--H71	1.10	0.97	59
CE--1HE	1.10	0.97	2
CD--2HD	1.10	0.97	87
CG--2HG	1.10	0.97	142
CD1--2HD1	1.10	0.97	6
OG1--HG1	0.97	0.84	42
CB--3HB	1.10	0.97	4
CE2--HE2	1.06	0.93	6
CG--1HG	1.10	0.97	146
CA--HA	1.10	0.97	140
ND2--1HD2	0.99	0.86	8
CG1--2HG1	1.10	0.97	3
CG1--1HG1	1.10	0.97	3
CD2--2HD2	1.10	0.97	4
N4--H42	0.99	0.86	4
C2'--H2''	1.10	0.97	257
CG2--3HG2	1.10	0.97	4
NZ--2HZ	1.02	0.89	13
C5'--H5''	1.10	0.97	261
CD2--HD2	1.06	0.93	8
C5'--H5'	1.10	0.97	259
C1'--H1'	1.10	0.97	246
CE--3HE	1.10	0.97	2
N--3H	1.02	0.89	3
NZ--1HZ	1.02	0.89	12

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CZ--HZ	1.06	0.93	9
SG--HG	1.33	1.20	19
C7--H72	1.10	0.97	58
CG2--1HG2	1.10	0.97	2
ND2--2HD2	0.99	0.86	5
N3--H3	0.99	0.86	2
C7--H73	1.10	0.97	60
C3'--H3'	1.10	0.97	256
CD1--1HD1	1.10	0.97	4
N--H	0.99	0.86	3
CH2--HH2	1.06	0.93	3
CG1--3HG1	1.10	0.97	1
N2--H21	0.99	0.86	3
CE1--HE1	1.06	0.93	11
N1--H1	0.99	0.86	4
N--2H	1.02	0.89	1
NE2--1HE2	0.99	0.86	9
C6--H6	1.06	0.93	1
CE--2HE	1.10	0.97	1
CZ3--HZ3	1.06	0.93	5
CE3--HE3	1.06	0.93	3
N6--H62	0.99	0.86	1
N4--H41	0.99	0.86	2
NE2--2HE2	0.99	0.86	6
NE--HE	0.99	0.86	1
NH2--2HH2	0.99	0.86	1
OG1--HG1	0.98	0.84	35
ND2--1HD2	1.00	0.86	115

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
C2'--H2''	1.11	0.97	11
CG--2HG	1.11	0.97	9
C7--H71	1.11	0.97	2
CE1--HE1	1.07	0.93	16
NZ--2HZ	1.03	0.89	12
C5'--H5''	1.11	0.97	11
ND2--2HD2	1.00	0.86	109
CD--1HD	1.11	0.97	3
CD--2HD	1.11	0.97	16
NZ--1HZ	1.03	0.89	10
N3--H3	1.00	0.86	57
N6--H61	1.00	0.86	56
NE2--1HE2	1.00	0.86	158
N--2H	1.03	0.89	1
NE2--2HE2	1.00	0.86	137
CG--1HG	1.11	0.97	10
ND1--HD1	1.00	0.86	24
CA--HA	1.11	0.97	4
CD1--HD1	1.07	0.93	20
CE3--HE3	1.07	0.93	2
CB--1HB	1.11	0.97	5
C4'--H4'	1.11	0.97	7
CD2--HD2	1.07	0.93	25
C5'--H5'	1.11	0.97	11
CB--2HB	1.11	0.97	10
C1'--H1'	1.11	0.97	10
OG--HG	0.98	0.84	19
C2'--H2'	1.11	0.97	8

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
C3'--H3'	1.11	0.97	10
N2--H21	1.00	0.86	69
SG--HG	1.34	1.20	10
OH--HH	0.98	0.84	7
NH2--2HH2	1.00	0.86	21
CZ--HZ	1.07	0.93	7
CE2--HE2	1.07	0.93	9
C7--H72	1.11	0.97	2
N4--H42	1.00	0.86	71
N2--H22	1.00	0.86	70
N4--H41	1.00	0.86	66
N6--H62	1.00	0.86	55
NH1--1HH1	1.00	0.86	36
N--H	1.00	0.86	70
N1--H1	1.00	0.86	67
C8--H8	1.07	0.93	1
NZ--3HZ	1.03	0.89	8
NE--HE	1.00	0.86	3
CH2--HH2	1.07	0.93	1
NE1--HE1	1.00	0.86	2
CZ2--HZ2	1.07	0.93	2
C6--H6	1.07	0.93	1
NH1--2HH1	1.00	0.86	7
NH2--1HH2	1.00	0.86	8
C2--H2	1.07	0.93	1
C7--H73	1.11	0.97	1
CZ3--HZ3	1.07	0.93	1
NE2--HE2	1.00	0.86	2

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NE1--HE1	1.01	0.86	26
N--H	1.01	0.86	1711
NE2--1HE2	1.01	0.86	15
CG--2HG	1.12	0.97	1
CZ--HZ	1.08	0.93	29
NZ--3HZ	1.04	0.89	11
NH1--2HH1	1.01	0.86	232
CE2--HE2	1.08	0.93	45
C4'--H4'	1.12	0.97	5
CD2--HD2	1.08	0.93	61
OG1--HG1	0.99	0.84	13
CE3--HE3	1.08	0.93	14
NH1--1HH1	1.01	0.86	207
ND2--1HD2	1.01	0.86	8
CD1--HD1	1.08	0.93	55
CE1--HE1	1.08	0.93	46
NH2--2HH2	1.01	0.86	232
N1--H1	1.01	0.86	4
N4--H41	1.01	0.86	7
ND2--2HD2	1.01	0.86	9
NE--HE	1.01	0.86	219
SG--HG	1.35	1.20	12
NE2--2HE2	1.01	0.86	7
C2'--H2''	1.12	0.97	4
NZ--2HZ	1.04	0.89	6
C5'--H5''	1.12	0.97	4
OG--HG	0.99	0.84	17
NH2--1HH2	1.01	0.86	220

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NZ--1HZ	1.04	0.89	5
ND1--HD1	1.01	0.86	10
C7--H72	1.12	0.97	3
C8--H8	1.08	0.93	3
C7--H71	1.12	0.97	1
N2--H21	1.01	0.86	2
CZ2--HZ2	1.08	0.93	6
CH2--HH2	1.08	0.93	9
C5'--H5'	1.12	0.97	5
C5--H5	1.08	0.93	4
CD--2HD	1.12	0.97	1
CZ3--HZ3	1.08	0.93	10
C1'--H1'	1.12	0.97	6
N4--H42	1.01	0.86	3
CB--1HB	1.12	0.97	2
OH--HH	0.99	0.84	7
N3--H3	1.01	0.86	1
NE2--HE2	1.01	0.86	40
N6--H62	1.01	0.86	1
N6--H61	1.01	0.86	2
N2--H22	1.01	0.86	2
CB--2HB	1.12	0.97	1
C6--H6	1.08	0.93	1
CG--1HG	1.12	0.97	1
C3'--H3'	1.12	0.97	1
CA--HA	1.12	0.97	1
C2'--H2'	1.12	0.97	1
N--H	1.02	0.86	1383

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NH2--1HH2	1.02	0.86	21
CZ--HZ	1.09	0.93	83
CD2--HD2	1.09	0.93	248
SG--HG	1.36	1.20	9
NE--HE	1.02	0.86	21
NE2--HE2	1.02	0.86	8
NE2--1HE2	1.02	0.86	13
CE2--HE2	1.09	0.93	185
NH1--1HH1	1.02	0.86	16
ND2--2HD2	1.02	0.86	12
NH2--2HH2	1.02	0.86	14
CD1--HD1	1.09	0.93	187
CH2--HH2	1.09	0.93	26
NH1--2HH1	1.02	0.86	20
N6--H62	1.02	0.86	3
CE1--HE1	1.09	0.93	278
C1'--H1'	1.13	0.97	4
C2--H2	1.09	0.93	2
NE1--HE1	1.02	0.86	8
OG--HG	1.00	0.84	7
NZ--3HZ	1.05	0.89	1
NE2--2HE2	1.02	0.86	18
CZ3--HZ3	1.09	0.93	23
ND2--1HD2	1.02	0.86	6
CE3--HE3	1.09	0.93	19
CZ2--HZ2	1.09	0.93	32
C5'--H5''	1.13	0.97	2
NZ--2HZ	1.05	0.89	6

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
N2--H22	1.02	0.86	4
C5'--H5'	1.13	0.97	1
N6--H61	1.02	0.86	1
C8--H8	1.09	0.93	2
C6--H6	1.09	0.93	6
C3'--H3'	1.13	0.97	3
C2'--H2'	1.13	0.97	5
ND1--HD1	1.02	0.86	4
NZ--1HZ	1.05	0.89	3
OG1--HG1	1.00	0.84	6
N2--H21	1.02	0.86	3
N4--H42	1.02	0.86	1
C4'--H4'	1.13	0.97	3
CD--1HD	1.13	0.97	1
OH--HH	1.00	0.84	3
O3'--HO3'	1.00	0.84	2
C5--H5	1.09	0.93	3
N--H	1.03	0.86	724
CD1--HD1	1.10	0.93	10
NE2--2HE2	1.03	0.86	29
NE2--1HE2	1.03	0.86	5
SG--HG	1.37	1.20	3
CD2--HD2	1.10	0.93	11
CZ3--HZ3	1.10	0.93	2
ND2--2HD2	1.03	0.86	7
NE--HE	1.03	0.86	28
CE1--HE1	1.10	0.93	5
ND2--1HD2	1.03	0.86	1

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NH1--2HH1	1.03	0.86	17
CE2--HE2	1.10	0.93	3
NE2--HE2	1.03	0.86	5
C8--H8	1.10	0.93	129
N1--H1	1.03	0.86	1
NH1--1HH1	1.03	0.86	22
NH2--2HH2	1.03	0.86	11
NH2--1HH2	1.03	0.86	27
C6--H6	1.10	0.93	124
N4--H41	1.03	0.86	1
C2'--H2'	1.14	0.97	1
C4'--H4'	1.14	0.97	3
C2--H2	1.10	0.93	57
C5--H5	1.10	0.93	66
CZ--HZ	1.10	0.93	2
C2'--H2''	1.14	0.97	1
ND1--HD1	1.03	0.86	1
C3'--H3'	1.14	0.97	1
N3--H3	1.03	0.86	1
C5'--H5'	1.14	0.97	1
N2--H21	1.03	0.86	1
OG--HG	1.01	0.84	1
N--H	1.04	0.86	18
C6--H6	1.11	0.93	5
NH1--2HH1	1.04	0.86	17
ND2--2HD2	1.04	0.86	1
C1'--H1'	1.15	0.97	2
NE--HE	1.04	0.86	19

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
ND2--1HD2	1.04	0.86	4
NH2--1HH2	1.04	0.86	15
NH1--1HH1	1.04	0.86	10
C5--H5	1.11	0.93	3
NE2--2HE2	1.04	0.86	5
NH2--2HH2	1.04	0.86	14
C3'--H3'	1.15	0.97	2
C2--H2	1.11	0.93	1
SG--HG	1.38	1.20	1
C8--H8	1.11	0.93	1
NE1--HE1	1.04	0.86	4
OG1--HG1	1.02	0.84	2
CB--2HB	1.15	0.97	1
NE2--HE2	1.04	0.86	4
NE2--1HE2	1.04	0.86	4
C2'--H2'	1.15	0.97	1
N6--H61	1.04	0.86	2
N1--H1	1.04	0.86	1
ND1--HD1	1.04	0.86	1
N2--H22	1.04	0.86	2
C5'--H5'	1.15	0.97	1
C1'--H1'	1.16	0.97	2
C5--H5	1.12	0.93	2
NH2--1HH2	1.05	0.86	2
NE2--2HE2	1.05	0.86	2
NH1--1HH1	1.05	0.86	1
NE--HE	1.05	0.86	2
C8--H8	1.12	0.93	3

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
C7--H72	1.16	0.97	1
NE1--HE1	1.05	0.86	1
C4'--H4'	1.16	0.97	1
ND1--HD1	1.05	0.86	1
NE2--HE2	1.05	0.86	3
N1--H1	1.05	0.86	1
C3'--H3'	1.16	0.97	2
C2--H2	1.12	0.93	2
C2'--H2''	1.16	0.97	1
C6--H6	1.12	0.93	1
C3'--H3'	1.17	0.97	1
N4--H41	1.06	0.86	1
C5--H5	1.13	0.93	3
N2--H21	1.06	0.86	1
C8--H8	1.13	0.93	1
C4'--H4'	1.17	0.97	1
C6--H6	1.13	0.93	1
N6--H62	1.06	0.86	1
C8--H8	1.14	0.93	1
N1--H1	1.07	0.86	1
C3'--H3'	1.18	0.97	1
C6--H6	1.15	0.93	1
N4--H42	1.07	0.86	1
N4--H41	1.07	0.86	1
N1--H1	1.08	0.86	1
C5--H5	1.15	0.93	1
N6--H61	1.08	0.86	1
C7--H73	1.20	0.97	1

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
C8--H8	1.18	0.93	1
C1'--H1'	1.25	0.97	1
C8--H8	1.21	0.93	1
N6--H61	1.14	0.86	1
C8--H8	1.33	0.93	1
N--2H	1.89	0.96	1
N--1H	1.90	0.96	1

Standard geometry: angle outliers

There are 988 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
O2-C2-N3	122.00	0.86	1
N9-C4-C5	105.70	13.06	1
C8-N7-C5	104.20	16.72	1
O2-C2-N3	121.90	37.13	1
N9-C4-C5	105.70	28.32	1
N1-C2-O2	119.20	42.51	1
N9-C4-C5	105.60	29.96	1
N9-C4-C5	105.60	30.16	1
O2-C2-N3	121.90	46.80	1
N9-C4-C5	105.70	30.70	1
N1-C2-O2	119.20	44.26	1
O2-C2-N3	121.90	47.36	1
O2-C2-N3	122.00	48.54	1
N9-C4-C5	105.60	33.63	1
O2-C2-N3	121.90	51.23	1
N1-C2-O2	123.20	52.73	1
N1-C2-O2	119.20	51.76	1
N1-C2-O2	123.20	57.11	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N9-C4-C5	105.70	39.79	1
O2-C2-N3	122.00	56.18	1
N1-C2-N3	114.80	51.60	1
N9-C4-C5	105.60	43.08	1
C8-N7-C5	104.20	44.34	1
C8-N7-C5	103.90	45.28	1
N1-C2-O2	119.20	62.03	1
C8-N9-C4	106.00	49.09	1
C1'-N9-C4	127.00	71.46	1
C8-N9-C4	105.90	51.48	1
N1-C6-C5	122.80	68.43	1
C8-N9-C4	105.90	52.35	1
C8-N9-C4	106.00	53.62	1
C8-N7-C5	104.20	52.87	1
N9-C4-N3	126.00	176.35	1
O2-C2-N3	122.00	72.46	1
C1'-N9-C4	127.05	176.28	1
C1'-N9-C8	127.05	175.82	1
C8-N7-C5	103.90	55.86	1
N1-C6-C5	121.00	73.16	1
C8-N7-C5	103.90	56.49	1
C2-N3-C4	111.80	67.12	1
C8-N9-C4	106.00	61.99	1
C1'-N1-C6	119.35	75.68	1
N1-C6-C5	121.00	77.99	1
N9-C4-N3	126.00	83.78	1
N1-C6-C5	122.80	80.88	1
C8-N7-C5	104.20	62.42	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C8-N9-C4	105.90	64.13	1
C2-N1-C6	121.30	162.99	1
C1'-N1-C2	119.35	78.49	1
N1-C6-C5	121.00	80.28	1
C1'-N9-C8	127.00	86.90	1
N1-C6-C5	121.00	81.11	1
C8-N7-C5	103.90	65.89	1
N1-C2-N3	118.90	81.38	1
C2-N1-C6	120.60	157.89	1
N9-C8-N7	113.80	76.78	1
C2-N3-C4	120.00	85.70	1
C2-N1-C6	121.30	154.17	1
N1-C2-O2	123.20	91.51	1
C2-N3-C4	127.00	95.47	1
C1'-N9-C4	127.00	158.20	1
C2-N3-C4	120.00	88.97	1
C8-N9-C4	105.90	75.53	1
N7-C5-C6	130.10	100.26	1
C1'-N9-C4	127.05	97.44	1
N1-C2-N3	118.90	89.31	1
N9-C8-N7	113.80	84.41	1
C5-C4-N3	126.90	156.21	1
C1'-N9-C8	127.00	156.13	1
C3'-O3'-P	120.20	149.24	1
C2-N3-C4	120.00	91.02	1
C2-N1-C6	121.30	150.25	1
C-N-CA	121.70	154.14	1
N7-C5-C4	110.80	137.45	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C1'-N1-C6	119.70	146.19	1
C8-N9-C4	106.00	79.52	1
C1'-N1-C2	119.70	93.32	1
N9-C4-N3	126.00	99.71	1
N7-C5-C4	110.70	136.98	1
N9-C8-N7	113.50	87.38	1
N9-C8-N7	113.50	138.98	1
C-N-N9-C8-N7	113.80	88.62	1
C6-C5-C4	119.10	93.96	1
C4-C5-C6	119.20	94.42	1
N9-C4-N3	126.00	150.65	1
C-N-CA	121.70	150.97	1
C4'-O4'-C1'	109.70	85.57	1
C1'-N9-C8	127.00	150.97	1
N9-C8-N7	113.50	89.87	1
C2-N3-C4	127.00	103.53	1
O-C-N	123.00	147.55	1
C2-N3-C4	120.00	97.13	1
N1-C6-C5	122.80	100.04	1
C1'-N1-C2	119.35	96.62	1
N1-C2-N3	114.80	92.37	1
CA-C-N	116.20	86.48	1
C1'-N9-C8	127.05	148.92	1
C5-C4-N3	128.40	150.02	1
C5-C6-N1	111.70	132.97	1
N7-C5-C4	110.80	131.94	1
C5-C4-N3	126.90	147.88	1
C-N-CA	121.70	96.81	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N9-C4-N3	126.00	105.85	1
N3-C4-N4	117.90	137.79	1
N1-C2-N2	116.30	135.63	1
C1'-N1-C6	119.35	100.38	1
C2-N1-C6	120.60	139.06	1
N9-C4-N3	127.40	109.10	1
N9-C4-N3	127.40	145.69	1
C1'-N1-C2	119.70	101.53	1
C1'-N9-C8	127.00	109.24	1
C2-N3-C4	110.80	93.13	1
N9-C8-N7	113.50	95.89	1
CA-CB-C4-C5-C6	117.60	100.14	1
C1'-N1-C2	119.70	102.76	1
CA-CB-CG	113.80	102.80	1
C2'-C1'-N9	113.50	129.84	1
C4-C5-C6	117.60	101.54	1
N1-C2-N3	118.90	102.99	1
CA-CB-C8-N9-C4	106.00	121.79	1
N6-C6-N1	119.00	134.77	1
C1'-N1-C2	119.35	103.75	1
C-N-CA	121.70	140.33	1
C1'-N1-C6	119.70	104.24	1
C-N-C1'-N9-C8	127.05	142.29	1
O4-C4-C5	122.60	137.81	1
N7-C5-C4	110.70	125.91	1
C1'-N9-C4	127.05	142.19	1
C2-N1-C6	120.60	135.71	1
C1'-N9-C8	127.05	112.15	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N3-C4-C5	121.80	136.70	1
C1'-N9-C4	127.00	141.81	1
C5-C6-N1	111.70	96.96	1
C2-N3-C4	110.80	96.17	1
C3'-O3'-P	120.20	105.63	1
C2-N3-C4	120.00	134.41	1
C6-C5-C4	116.90	102.56	1
N9-C4-C5	105.60	91.66	1
C5-C6-N6	123.40	137.22	1
C2-N3-C4	110.80	97.12	1
O4'-C1'-N9	108.40	94.77	1
O5'-C5'-C4'	110.80	97.26	1
N1-C2-N3	114.80	101.27	1
C1'-N9-C4	127.00	140.51	1
C1'-N1-C6	119.35	106.00	1
N2-C2-N3	119.70	106.38	1
C-N-C6-N1-C2	118.80	131.76	1
C5-C4-N3	126.90	139.80	1
C1'-N9-C4	127.00	114.16	1
N7-C5-C6	130.10	117.33	1
O-C-N3-C4-O4	122.60	109.95	1
C5-C6-N1	111.70	99.10	1
C2-N3-C4	127.00	114.48	1
C-N-N7-C5-C6	130.10	117.88	1
N9-C8-N7	113.80	101.66	1
N2-C2-N3	119.70	131.78	1
N7-C5-C6	132.30	120.46	1
C1'-N1-C6	119.35	107.57	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O3'-P-O5'	104.00	92.27	1
C-N-CA	121.70	107.66	1
C6-N1-C2	124.90	136.59	1
C4'-C3'-O3'	110.00	98.34	1
O3'-P-O5'	104.00	92.35	1
N3-C4-C5	121.80	110.18	1
CA-CB-CG	113.80	121.50	1
C-N-CA	121.70	135.43	1
N7-C5-C4	110.80	122.14	1
N4-C4-C5	120.30	109.03	1
C5-C6-O6	128.30	117.04	1
C2-N3-C4	111.80	100.61	1
C6-N1-C2	124.90	113.71	1
C-N-CA	121.70	134.96	1
N3-C4-C5	121.80	110.78	1
CA-CB-CG	112.60	119.93	1
N9-C4-N3	127.40	116.43	1
C7-C5-C6	124.00	134.97	1
CA-CB-C1'-N1-C6	119.70	108.78	1
C2'-C1'-N9	113.50	102.73	1
C-N-CA	121.70	134.61	1
C5-C4-N3	128.40	117.67	1
N9-C8-N7	113.50	102.80	1
C-N-CA	121.70	134.40	1
C2-N1-C6	120.60	131.18	1
N-CA-N-CA-C	111.00	130.69	1
C5-C4-N3	126.90	116.40	1
C4-C5-C6	117.60	107.24	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C4'-C3'-O3'	110.00	120.35	1
C-N-CA	121.70	134.08	1
N2-C2-N3	119.70	109.44	1
N7-C5-C4	110.80	121.04	1
C5'-C4'-O4'	109.40	119.58	1
CA-CB-N3-C4-O4	122.60	112.53	1
C-CA-N1-C6-C5	122.80	112.74	1
CA-CB-O6-C6-N1	120.00	109.99	1
O3'-C3'-C2'	111.50	101.49	1
C3'-C2'-C1'	101.60	91.61	1
O4'-C1'-N9	108.40	98.46	1
C-N-CA	121.70	133.61	1
C4-C5-C6	119.20	109.28	1
N2-C2-N3	119.70	129.62	1
O3'-C3'-C2'	111.50	101.65	1
CA-CB-N-CA-C	112.10	95.80	1
C2'-C1'-N9	113.50	123.25	1
C-N-O4'-C1'-N9	108.40	118.11	1
C1'-N9-C8	127.00	117.29	1
C-N-CA	121.70	133.32	1
C6-N1-C2	124.90	134.58	1
CA-CB-CG	113.80	120.25	1
C-N-CA	121.70	133.30	1
CA-C-N1-C2-N3	118.90	109.38	1
N3-C4-O4	122.60	113.10	1
C5-C6-N1	117.60	108.17	1
CA-CB-CG	104.50	116.44	1
CA-CB-CG	113.80	107.53	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-O5'-C5'-C4'	110.80	101.48	1
P-O5'-C5'	120.00	129.32	1
C3'-O3'-P	120.20	129.50	1
N7-C5-C6	132.30	123.09	1
CA-CB-C5'-C4'-O4'	109.40	118.54	1
C-N-CA	121.70	110.78	1
CA-CB-CG	114.10	126.20	1
N4-C4-C5	120.30	111.31	1
N-CA-C4'-O4'-C1'	109.70	118.66	1
N-CA-C	112.10	97.19	1
O6-C6-N1	120.00	128.93	1
C5-C6-O6	128.30	137.20	1
N7-C5-C6	132.30	123.44	1
N1-C2-N2	116.30	125.15	1
CA-CB-C6-N1-C2	118.80	127.63	1
CG-SD-CE	100.90	113.84	1
C1'-N1-C6	119.70	128.50	1
C4-C5-C7	122.40	113.62	1
N1-C2-N3	124.00	115.24	1
O4-C4-C5	122.60	131.34	1
CA-CB-CG	113.80	107.98	1
N4-C4-C5	120.30	111.57	1
C1'-N1-C6	119.35	128.08	1
CA-CB-N-CA-C	112.10	126.61	1
C1'-N1-C2	119.70	111.00	1
C6-C5-C4	119.10	127.80	2
N7-C5-C6	130.10	121.42	1
C-N-O3'-C3'-C2'	111.50	102.85	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C2-N3-C4	127.00	135.61	1
N-CA-C2'-C1'-N1	113.50	104.95	1
N-CA-C	113.30	129.80	1
N3-C4-C5	114.80	123.33	1
CA-CB-O4'-C1'-N9	108.40	116.88	1
C-N-CA	121.70	131.85	1
N3-C4-C5	121.80	130.25	1
N-CA-C	111.00	126.72	1
CA-CB-N-CA-C	112.10	126.09	1
C2-N1-C6	120.60	112.25	1
C-N-CA	121.70	131.71	1
C2-N3-C4	111.80	103.48	1
N-CA-C	111.00	95.49	1
C-N-CA	121.70	131.66	1
C5-C6-N6	123.40	115.10	1
C-N-CA	121.70	131.64	1
N3-C4-N4	117.90	109.62	1
O3'-C3'-C2'	111.50	103.22	1
CA-C-P-O5'-C5'	120.00	111.76	1
C-N-C4-C5-C7	122.40	130.61	1
N-CA-CB	103.00	109.01	1
N7-C5-C4	110.70	118.89	1
CA-CB-CG	112.60	118.06	1
N3-C4-C5	121.80	129.98	1
N-CA-C	111.00	95.75	1
C3'-C2'-C1'	101.60	93.43	1
N-CA-CA-C-N	116.20	127.03	1
CA-CB-CA-CB-N-CA-CB	110.40	118.51	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C6-N1-C2	118.80	110.71	1
C-N-C-N-C-N-CA	121.70	131.38	1
CA-CB-CG	112.60	117.95	1
C2-N3-C4	120.00	128.01	1
O3'-P-O5'	104.00	112.00	1
CA-CB-CG	113.80	108.47	1
C5'-C4'-O4'	109.40	101.45	1
CA-CB-CG	113.80	119.08	1
C-CA-CB	110.10	100.07	1
N-CA-C-N-CA	121.70	131.18	1
O4'-C4'-C3'	105.40	97.51	1
C6-N1-C2	118.80	126.69	1
N-CA-N7-C5-C4	110.70	118.57	1
N-CA-CB	110.50	101.60	1
N3-C4-C5	121.80	129.64	1
N9-C4-N3	127.40	119.56	1
N-CA-N-CA-N9-C4-C5	105.70	97.91	1
C-N-CA	121.70	112.38	1
CA-C-O	120.80	112.00	1
N3-C4-C5	114.80	122.55	1
C4-C5-C6	117.60	109.86	1
CA-C-N	116.90	124.64	1
C4'-C3'-O3'	110.00	102.27	1
N-CA-CB	110.50	101.74	1
N7-C5-C6	132.30	124.58	1
O4'-C1'-C2'	106.40	98.68	1
C-N-O5'-C5'-C4'	110.80	103.11	1
C-CA-CB	110.10	100.38	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA-CB-N-CA-C	111.00	125.16	1
C-N-CA-CB-CG	112.60	117.64	1
C5'-C4'-C3'	114.90	107.34	1
N-CA-CB	111.50	102.93	1
O5'-C5'-C4'	110.80	103.24	1
CA-C-N	116.90	124.46	1
C5-C6-N1	117.60	125.13	1
C5-C6-N1	117.60	110.10	1
CA-C-N	116.20	126.19	1
N-CA-C3'-O3'-P	120.20	127.68	1
CA-CB-C5-C6-N6	123.40	115.93	1
N-CA-C	111.00	124.94	1
N1-C2-N3	118.90	126.37	1
N-CA-C	111.00	124.93	1
N-CA-C	111.00	124.90	1
C-CA-C-CA-CB	110.10	100.69	1
C1'-N1-C2	119.70	112.27	1
CA-CB-CA-CB-CG	112.60	117.54	1
C5-C4-N3	128.40	135.80	1
N-CA-CB	103.00	108.43	1
C6-C5-C4	116.90	109.51	1
N3-C4-O4	122.60	115.22	1
N-CA-C	111.00	124.78	1
C-CA-CB	110.10	100.79	1
CA-CB-N-CA-C4'-O4'-C1'	109.70	102.45	1
C-CA-CA-CB-CA-CB-C-N-N-CA-C	111.00	124.41	1
N-CA-C	112.10	100.15	1
C2'-C1'-N1	113.50	120.67	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C2-N1-C6	120.60	127.75	1
C-N-CA	121.70	113.13	1
CA-CB-CG	112.60	107.84	1
C-CA-CB	110.10	101.05	1
N1-C2-N2	116.30	109.17	1
N9-C4-N3	127.40	120.28	1
CA-C-N-CA-N-CA-CB	110.50	118.55	1
C-N-CA	121.70	113.17	1
CA-C-C-N-CA-CB-CG	113.90	122.41	1
C-N-CA	121.70	113.20	1
CA-C-N	116.90	123.98	1
CA-C-N	116.20	125.64	1
C-N-C-CA-C4'-O4'-C1'	109.70	102.65	1
O2-C2-N3	121.90	128.94	1
CA-C-N	116.90	123.93	1
N-CA-CA-CB-CG	112.60	117.28	1
N-CA-C	111.00	124.10	1
C-N-C-N-CA	121.70	130.11	1
N-CA-CA-CB-CA-CB-CG	113.80	118.46	1
C-N-N-CA-O4'-C4'-C3'	105.40	98.42	1
C4'-O4'-C1'	109.70	102.72	1
CA-CB-CG	113.80	118.45	1
CA-CB-C-N-CA-CB-CG	112.60	117.24	1
C-N-C5-C6-N1	117.60	110.65	1
C5'-C4'-O4'	109.40	102.45	1
C1'-N1-C2	119.35	112.40	1
CA-CB-CG	112.60	117.23	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	113.80	109.18	1
CA-CB-N-CA-CB	110.40	103.50	1
C5-C6-N6	123.40	130.29	1
N-CA-N-CA-C	111.00	123.80	1
P-O5'-C5'	120.00	113.15	1
N3-C4-C5	121.80	128.64	1
O3'-C3'-C2'	111.50	104.67	1
CA-CB-CG	112.60	117.14	1
N-CA-C	111.00	123.68	1
C1'-N9-C4	127.05	120.26	1
N-CA-C	112.10	123.40	1
N-CA-C	111.00	123.64	1
C2-N1-C6	120.60	113.84	1
N1-C2-N3	118.90	112.15	1
O4-C4-C5	122.60	115.87	1
C-CA-CB	110.10	101.59	1
CA-CB-CG	113.80	118.28	1
CA-CB-CG	112.60	117.07	1
N-CA-C	113.30	100.36	1
C2'-C1'-N9	113.50	106.81	1
CA-C-N	116.90	123.57	1
C-N-CA	121.70	129.70	1
N-CA-CA-C-O	120.80	113.30	1
N-CA-CA-C-C-N-CA	121.70	129.62	1
C2'-C1'-N9	113.50	120.09	1
N-CA-CB	110.50	117.94	1
C-N-CA	121.70	129.58	1
C-N-CA	121.70	113.82	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	129.57	1
C-N-CA	121.70	129.56	1
C-CA-CB	110.10	118.37	1
N-CA-C	111.00	123.16	2
O5'-C5'-C4'	110.80	104.30	1
O4'-C1'-C2'	106.40	112.89	1
C-CA-N-CA-CB	110.50	103.19	1
CA-CB-CG	114.10	122.69	1
C5-C4-N3	126.90	133.34	1
N3-C4-C5	114.80	121.24	1
N4-C4-C5	120.30	126.74	1
CA-CB-CG	112.60	116.89	1
CA-CB-CA-C-C-CA-CB	110.10	118.24	1
C-N-CA	121.70	114.00	2
N1-C6-C5	121.00	127.42	1
C-N-CA	121.70	129.40	1
C-N-CA	121.70	129.39	1
CA-C-N	116.90	123.29	1
C5'-C4'-C3'	114.90	121.29	1
N3-C4-O4	122.60	116.22	1
N-CA-N1-C2-N3	129.00	122.63	1
C-N-CA	121.70	114.06	1
CA-CB-CG	112.60	116.84	1
N-CA-CA-CB-CG	113.60	121.63	1
C-N-CA	121.70	129.31	1
C3'-C2'-C1'	101.60	95.26	1
CA-CB-CG	113.80	118.02	1
N7-C5-C6	132.30	125.97	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	116.82	1
C-N-CA	121.70	114.12	2
NE-CZ-NH2	119.20	115.41	1
C-N-N-CA-C	111.00	122.73	1
C3'-C2'-C1'	101.60	107.88	1
N-CA-C	111.00	122.72	1
C-CA-CB	110.10	102.16	1
C-CA-C3'-O3'-P	120.20	126.46	1
C1'-N1-C2	119.35	125.61	1
CA-C-O	120.80	113.71	1
CA-CB-CG	113.80	117.97	1
C-CA-C3'-C2'-C1'	101.60	107.85	1
CA-C-N	116.20	124.53	1
C-N-CA	121.70	129.19	1
O3'-C3'-C2'	111.50	117.74	1
N-CA-CA-CB-CG	113.80	117.96	1
C-N-CA	121.70	129.18	1
C5'-C4'-C3'	114.90	121.11	1
CA-CB-CG	113.80	109.66	1
N-CA-N-CA-C	111.00	122.58	1
CA-CB-CG	113.80	117.93	1
C-N-CA	121.70	114.28	1
N-CA-C	112.10	122.40	1
CA-CB-CG	112.60	116.72	1
C5-C6-O6	128.30	134.47	1
C-N-CA	121.70	114.32	1
NE-CZ-NH2	119.20	115.51	1
CG-SD-C3'-O3'-P	120.20	114.06	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N1-C2-N3	129.00	135.14	1
NE-CZ-CA-CB-C-N-C4-C5-C6	117.60	111.48	1
C3'-C2'-C1'	101.60	107.70	1
C2-N3-C4	111.80	105.71	1
C-N-CG-CD-NE2	116.40	122.49	1
O3'-P-O5'	104.00	97.92	1
N9-C4-N3	126.00	119.92	1
N-CA-C5'-C4'-C3'	114.90	108.85	1
CA-CB-C-CA-CA-CB-CG	113.80	117.83	1
C-N-CA	121.70	114.46	1
N-CA-C	111.00	99.74	1
CA-C-N	116.90	122.93	1
C-N-CA	121.70	114.48	1
O3'-P-O5'	104.00	97.98	1
NE-CZ-C-N-CA	121.70	128.92	1
N1-C2-N3	124.00	117.99	1
NE-CZ-NH2	119.20	115.59	1
CA-C-N	116.90	122.91	1
C3'-C2'-H2''	103.00	109.00	1
C2'-C3'-H3'	115.01	109.00	1
C3'-C2'-H2'	115.02	109.00	1
C3'-C2'-H2''	102.96	109.00	1
O4'-C4'-H4'	115.04	109.00	1
C2'-C3'-H3'	115.04	109.00	1
C3'-C2'-H2''	115.05	109.00	1
C2'-C3'-H3'	115.05	109.00	1
O3'-C3'-H3'	102.95	109.00	1
O4'-C4'-H4'	115.06	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C2'-C3'-H3'	115.06	109.00	1
C3'-C2'-H2''	115.06	109.00	1
C3'-C2'-H2'	115.06	109.00	1
C-N-H	112.16	124.30	1
O4'-C4'-H4'	115.08	109.00	2
CA-N-H	126.17	114.00	1
C3'-C2'-H2''	115.09	109.00	1
C2'-C3'-H3'	115.09	109.00	1
C2'-C3'-H3'	115.12	109.00	1
C3'-C2'-H2'	115.13	109.00	1
C-N-H	112.04	124.30	1
O4'-C4'-H4'	115.13	109.00	1
C2'-C1'-H1'	102.87	109.00	1
C2'-C3'-H3'	115.19	109.00	1
C3'-C2'-H2''	102.81	109.00	1
C4'-C3'-H3'	115.20	109.00	1
C6-N1-H1	111.39	117.60	1
C2'-C3'-H3'	115.20	109.00	1
C2'-C3'-H3'	115.22	109.00	1
O4'-C4'-H4'	115.22	109.00	1
C2'-C3'-H3'	115.23	109.00	3
C-N-H	111.85	124.30	1
H72-C7-H73	102.77	109.00	1
C2'-C3'-H3'	115.25	109.00	3
C3'-C2'-H2''	115.26	109.00	1
C3'-C2'-H2''	102.74	109.00	1
C3'-C2'-H2'	115.28	109.00	1
C2'-C3'-H3'	115.28	109.00	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C4'-C3'-H3'	115.28	109.00	1
C3'-C2'-H2''	115.29	109.00	1
H2'-C2'-H2''	115.30	109.00	1
C2'-C3'-H3'	115.31	109.00	2
C2'-C3'-H3'	115.33	109.00	2
O4'-C4'-H4'	115.35	109.00	1
C2'-C3'-H3'	115.37	109.00	1
C2'-C3'-H3'	115.39	109.00	1
C-N-H	111.52	124.30	1
CB-CA-HA	96.22	109.00	1
C3'-C2'-H2''	102.59	109.00	1
C3'-C2'-H2''	102.55	109.00	1
C2'-C3'-H3'	115.45	109.00	1
CA-N-H	126.90	114.00	1
C-N-H	111.40	124.30	1
C2'-C3'-H3'	115.46	109.00	1
O4'-C4'-H4'	115.47	109.00	1
C3'-C2'-H2'	115.47	109.00	1
O4'-C4'-H4'	115.48	109.00	1
C3'-C2'-H2''	115.48	109.00	1
O4'-C1'-H1'	115.49	109.00	2
O4'-C4'-H4'	115.49	109.00	1
C2'-C3'-H3'	115.49	109.00	1
C3'-C2'-H2'	115.50	109.00	1
C2'-C3'-H3'	115.50	109.00	1
O4'-C4'-H4'	115.51	109.00	1
O4'-C1'-H1'	115.51	109.00	1
C2'-C3'-H3'	115.52	109.00	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C3'-C2'-H2'	115.53	109.00	1
O3'-C3'-H3'	115.53	109.00	1
C3'-C2'-H2''	102.46	109.00	1
C2'-C3'-H3'	115.54	109.00	1
C3'-C2'-H2'	102.45	109.00	1
C1'-C2'-H2''	115.56	109.00	1
C2'-C3'-H3'	115.57	109.00	1
C-N-H	111.15	124.30	1
N9-C1'-H1'	102.41	109.00	1
C2'-C3'-H3'	115.59	109.00	1
C2'-C3'-H3'	115.62	109.00	2
C4'-C3'-H3'	115.62	109.00	1
N9-C1'-H1'	102.37	109.00	1
C2'-C3'-H3'	115.63	109.00	1
C-N-H	111.04	124.30	1
C2'-C3'-H3'	115.64	109.00	1
C2'-C1'-H1'	102.36	109.00	1
C3'-C2'-H2'	115.66	109.00	1
C3'-C2'-H2''	115.67	109.00	1
C2'-C3'-H3'	115.67	109.00	1
O4'-C4'-H4'	115.68	109.00	1
O4'-C1'-H1'	115.68	109.00	1
C2'-C3'-H3'	115.68	109.00	1
C3'-C2'-H2''	102.31	109.00	1
C2'-C3'-H3'	115.72	109.00	1
C3'-C2'-H2'	102.28	109.00	1
C2'-C3'-H3'	115.73	109.00	3
C2'-C3'-H3'	115.74	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C2'-C3'-H3'	115.75	109.00	1
O4'-C4'-H4'	115.75	109.00	1
O4'-C4'-H4'	115.76	109.00	1
O5'-C5'-H5''	115.76	109.00	1
C5'-C4'-H4'	102.22	109.00	1
O4'-C4'-H4'	115.78	109.00	1
C3'-C2'-H2''	115.80	109.00	1
C3'-C2'-H2''	102.19	109.00	1
C4'-C3'-H3'	115.82	109.00	1
C3'-C2'-H2''	102.18	109.00	1
C3'-C2'-H2''	102.17	109.00	1
C3'-C2'-H2''	115.84	109.00	1
C3'-C2'-H2'	115.84	109.00	1
C3'-C2'-H2'	102.16	109.00	1
O4'-C4'-H4'	115.87	109.00	1
C2'-C3'-H3'	115.93	109.00	1
C3'-C2'-H2''	115.93	109.00	1
O3'-C3'-H3'	102.07	109.00	1
C2'-C3'-H3'	115.94	109.00	1
O4'-C1'-H1'	115.94	109.00	1
C2'-C3'-H3'	115.96	109.00	1
C2'-C3'-H3'	115.98	109.00	1
C3'-C2'-H2'	115.98	109.00	1
C2'-C3'-H3'	115.99	109.00	1
N1-C6-H6	112.50	119.50	1
C3'-C2'-H2''	101.99	109.00	1
C2'-C3'-H3'	116.01	109.00	1
O4'-C1'-H1'	116.03	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C3'-C2'-H2'	116.04	109.00	1
C5'-C4'-H4'	101.96	109.00	1
C2'-C3'-H3'	116.04	109.00	1
C3'-C2'-H2'	101.94	109.00	1
C5'-C4'-H4'	101.91	109.00	1
C2'-C3'-H3'	116.09	109.00	1
C3'-C2'-H2''	101.89	109.00	1
H5'-C5'-H5''	101.89	109.00	1
C3'-C2'-H2'	101.87	109.00	1
C3'-C2'-H2''	116.16	109.00	1
C3'-C2'-H2'	101.83	109.00	1
C-N-H	138.71	124.30	1
C2'-C3'-H3'	116.22	109.00	1
C2-N3-H3	109.28	116.50	1
C4'-C3'-H3'	116.23	109.00	1
C3'-C2'-H2''	101.73	109.00	1
C3'-C2'-H2''	116.31	109.00	1
C6-C5-H5	128.53	121.20	1
H61-N6-H62	127.34	120.00	1
C3'-C2'-H2''	116.38	109.00	1
O4'-C4'-H4'	116.39	109.00	1
C4'-C3'-H3'	116.42	109.00	1
C2'-C1'-H1'	116.45	109.00	1
C3'-C2'-H2'	116.45	109.00	1
O4'-C1'-H1'	116.46	109.00	1
C2'-C3'-H3'	116.47	109.00	1
C2'-C3'-H3'	116.52	109.00	1
C3'-C2'-H2''	116.52	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C3'-C2'-H2''	101.45	109.00	1
C1'-C2'-H2''	116.60	109.00	1
C3'-C2'-H2'	116.61	109.00	1
C3'-C2'-H2'	116.63	109.00	1
C2-N2-H21	127.63	120.00	1
C-N-H	108.97	124.30	1
C2'-C3'-H3'	116.68	109.00	1
O4'-C1'-H1'	116.70	109.00	1
N1-C1'-H1'	101.29	109.00	1
C3'-C2'-H2'	116.78	109.00	1
C3'-C2'-H2''	101.21	109.00	1
H5'-C5'-H5''	101.19	109.00	1
C3'-C2'-H2''	116.84	109.00	1
C5'-C4'-H4'	101.13	109.00	1
C3'-C2'-H2''	101.13	109.00	1
O4'-C4'-H4'	116.89	109.00	1
C2'-C3'-H3'	116.90	109.00	1
C3'-C2'-H2'	116.91	109.00	1
O4'-C4'-H4'	116.93	109.00	1
C3'-C2'-H2'	101.06	109.00	1
C3'-C2'-H2''	116.95	109.00	1
C3'-C2'-H2'	116.97	109.00	1
C4-N4-H42	128.01	120.00	1
C3'-C2'-H2''	100.98	109.00	2
O4'-C1'-H1'	117.04	109.00	1
C3'-C2'-H2'	117.05	109.00	1
C3'-C2'-H2'	100.89	109.00	1
H71-C7-H72	117.15	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N1-C1'-H1'	100.84	109.00	1
C3'-C2'-H2'	100.77	109.00	1
C3'-C2'-H2'	100.73	109.00	1
N1-C1'-H1'	100.72	109.00	1
C3'-C2'-H2''	117.28	109.00	1
C2'-C3'-H3'	117.29	109.00	1
N1-C6-H6	127.80	119.50	1
C5'-C4'-H4'	100.69	109.00	1
C2'-C3'-H3'	117.34	109.00	1
C2'-C3'-H3'	117.36	109.00	1
C3'-C2'-H2'	117.37	109.00	1
H2'-C2'-H2''	117.38	109.00	1
C6-N1-H1	109.19	117.60	1
C3'-C2'-H2'	117.41	109.00	1
C3'-C2'-H2''	100.59	109.00	1
C3'-C2'-H2'	100.58	109.00	1
C3'-C2'-H2''	100.58	109.00	2
C3'-C2'-H2''	117.45	109.00	1
O5'-C5'-H5''	117.48	109.00	1
C3'-C2'-H2'	117.50	109.00	1
O4'-C4'-H4'	117.50	109.00	1
C3'-C2'-H2''	100.46	109.00	1
C3'-C2'-H2'	117.60	109.00	1
C3'-C2'-H2'	100.40	109.00	1
C2'-C3'-H3'	117.67	109.00	2
C4'-C5'-H5''	117.68	109.00	1
O4'-C1'-H1'	117.70	109.00	1
C3'-C2'-H2'	117.71	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C5-C6-H6	110.79	119.50	1
O5'-C5'-H5'	117.71	109.00	1
C4-C5-H5	129.93	121.20	1
C3'-C2'-H2'	100.26	109.00	1
C3'-C2'-H2'	117.76	109.00	1
C3'-C2'-H2'	100.21	109.00	1
C3'-C2'-H2'	117.80	109.00	1
C3'-C2'-H2'	117.81	109.00	1
C1'-C2'-H2'	117.84	109.00	1
C2'-C3'-H3'	117.88	109.00	1
O4'-C4'-H4'	117.94	109.00	1
C3'-C2'-H2''	100.05	109.00	1
C3'-C2'-H2'	117.96	109.00	2
C3'-C2'-H2'	100.01	109.00	1
C3'-C2'-H2''	99.99	109.00	1
C-N-H	106.27	124.30	1
O3'-C3'-H3'	99.95	109.00	1
C3'-C2'-H2''	99.95	109.00	1
C3'-C2'-H2'	118.08	109.00	1
C3'-C2'-H2''	99.89	109.00	1
C1'-C2'-H2'	118.17	109.00	1
C3'-C2'-H2''	99.78	109.00	1
O4'-C1'-H1'	118.22	109.00	1
CA-N-2H	90.96	109.47	1
N9-C1'-H1'	99.62	109.00	1
C3'-C2'-H2'	99.61	109.00	1
C3'-C2'-H2'	118.44	109.00	1
H21-N2-H22	129.52	120.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C3'-C2'-H2''	118.56	109.00	1
H41-N4-H42	110.42	120.00	1
C3'-C2'-H2''	118.72	109.00	1
C3'-C2'-H2''	118.87	109.00	1
C3'-C2'-H2''	99.13	109.00	1
C2-N3-H3	126.44	116.50	1
C3'-C2'-H2''	118.96	109.00	1
C4-N4-H41	110.03	120.00	1
C1'-C2'-H2'	118.99	109.00	1
C1'-C2'-H2'	119.06	109.00	1
C3'-C2'-H2'	98.83	109.00	1
C3'-C2'-H2'	119.20	109.00	1
C3'-C2'-H2''	119.23	109.00	1
C5'-C4'-H4'	98.77	109.00	1
C3'-C2'-H2'	119.23	109.00	1
C2-N2-H22	109.75	120.00	1
N7-C8-H8	112.83	123.10	1
CA-N-1H	88.80	109.47	1
N1-C6-H6	109.06	119.50	1
C3'-C2'-H2'	119.44	109.00	1
C2'-C3'-H3'	119.45	109.00	1
C3'-C2'-H2'	98.52	109.00	1
C3'-C2'-H2''	98.44	109.00	1
C3'-C2'-H2''	119.56	109.00	1
O4'-C1'-H1'	119.59	109.00	1
C3'-C2'-H2'	119.64	109.00	1
C3'-C2'-H2''	98.28	109.00	1
C3'-C2'-H2''	119.77	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C3'-C2'-H2'	119.80	109.00	1
C3'-C2'-H2'	119.87	109.00	1
C3'-C2'-H2'	119.90	109.00	1
C3'-C2'-H2'	119.94	109.00	1
C3'-C2'-H2''	119.96	109.00	1
C3'-C2'-H2'	119.98	109.00	1
C3'-C2'-H2'	120.00	109.00	1
C4-N3-H3	127.53	116.50	1
C3'-C2'-H2'	120.09	109.00	1
C4'-C5'-H5'	120.10	109.00	1
C3'-C2'-H2'	120.11	109.00	1
C3'-C2'-H2'	120.14	109.00	1
C3'-C2'-H2''	120.24	109.00	1
O4'-C4'-H4'	120.27	109.00	1
C4'-C3'-H3'	120.28	109.00	1
C3'-C2'-H2'	120.34	109.00	1
C1'-C2'-H2''	97.65	109.00	1
C3'-C2'-H2'	97.60	109.00	1
C3'-C2'-H2'	120.42	109.00	1
C3'-C2'-H2'	120.46	109.00	1
C2'-C3'-H3'	120.47	109.00	1
C3'-C2'-H2'	120.48	109.00	1
N7-C8-H8	134.80	123.30	1
C3'-C2'-H2'	120.61	109.00	1
N9-C1'-H1'	97.37	109.00	1
C3'-C2'-H2'	120.74	109.00	1
C3'-C2'-H2'	97.24	109.00	1
C3'-C2'-H2'	120.79	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C3'-C2'-H2''	120.80	109.00	1
C3'-C2'-H2'	120.83	109.00	1
C3'-C2'-H2'	120.89	109.00	1
C3'-C2'-H2'	97.08	109.00	1
C3'-C2'-H2''	120.99	109.00	1
H61-N6-H62	132.09	120.00	1
C3'-C2'-H2'	121.11	109.00	1
C3'-C2'-H2'	121.16	109.00	1
C3'-C2'-H2''	121.16	109.00	1
C3'-C2'-H2'	121.20	109.00	1
C3'-C2'-H2'	96.80	109.00	1
C3'-C2'-H2''	121.25	109.00	1
C3'-C2'-H2'	121.27	109.00	1
O4'-C1'-H1'	121.27	109.00	1
C2'-C3'-H3'	121.28	109.00	1
C3'-C2'-H2'	121.33	109.00	1
C5'-C4'-H4'	96.64	109.00	1
C3'-C2'-H2''	121.37	109.00	1
C3'-C2'-H2'	96.62	109.00	1
C2-N3-H3	128.93	116.50	1
C3'-C2'-H2'	121.46	109.00	1
C3'-C2'-H2'	121.59	109.00	1
C3'-C2'-H2'	96.37	109.00	1
C3'-C2'-H2''	121.68	109.00	1
C3'-C2'-H2'	121.70	109.00	1
C3'-C2'-H2'	96.27	109.00	1
C3'-C2'-H2'	121.76	109.00	1
C3'-C2'-H2'	121.80	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C3'-C2'-H2'	121.86	109.00	1
C3'-C4'-H4'	96.14	109.00	1
C3'-C2'-H2'	121.93	109.00	1
C3'-C2'-H2'	121.95	109.00	1
O5'-C5'-H5''	95.99	109.00	1
C3'-C2'-H2'	122.04	109.00	1
C3'-C2'-H2''	122.04	109.00	1
C3'-C2'-H2''	122.06	109.00	1
C3'-C2'-H2'	95.84	109.00	1
O4'-C4'-H4'	122.19	109.00	1
C3'-C2'-H2'	122.22	109.00	1
C3'-C2'-H2'	122.26	109.00	1
C3'-C2'-H2'	95.73	109.00	1
C3'-C2'-H2'	122.29	109.00	1
C3'-C2'-H2''	122.30	109.00	2
C3'-C2'-H2'	122.45	109.00	1
C3'-C2'-H2''	122.48	109.00	1
C4'-C3'-H3'	122.55	109.00	1
C3'-C2'-H2'	122.60	109.00	1
C4-N3-H3	130.14	116.50	1
C3'-C2'-H2''	122.72	109.00	1
C3'-C2'-H2'	95.14	109.00	1
C3'-C2'-H2'	122.92	109.00	1
C1'-C2'-H2''	123.00	109.00	1
C3'-C2'-H2'	123.02	109.00	1
C5-C6-H6	104.53	118.60	1
C3'-C2'-H2''	123.21	109.00	1
C3'-C2'-H2''	123.25	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C3'-C2'-H2'	123.27	109.00	1
C3'-C2'-H2'	123.30	109.00	1
C3'-C2'-H2'	123.33	109.00	2
C3'-C2'-H2'	123.35	109.00	1
C3'-C2'-H2'	94.64	109.00	1
C3'-C2'-H2'	123.37	109.00	1
C3'-C2'-H2'	123.38	109.00	1
C3'-C2'-H2''	123.41	109.00	1
C3'-C2'-H2'	94.58	109.00	1
C3'-C2'-H2'	123.47	109.00	1
C3'-C2'-H2'	94.38	109.00	1
C3'-C2'-H2'	123.63	109.00	1
C3'-C2'-H2'	94.31	109.00	1
C3'-C2'-H2'	123.74	109.00	1
C3'-C2'-H2''	123.84	109.00	1
C3'-C2'-H2'	123.95	109.00	1
C3'-C2'-H2'	124.05	109.00	1
C3'-C2'-H2'	124.09	109.00	1
C6-N1-H1	132.77	117.60	1
C3'-C2'-H2'	124.18	109.00	1
C3'-C2'-H2'	124.21	109.00	2
CD-N-1H	139.93	109.47	1
N7-C8-H8	138.54	123.30	1
N1-C1'-H1'	93.68	109.00	1
C3'-C2'-H2'	124.32	109.00	1
C3'-C2'-H2'	124.33	109.00	1
C3'-C2'-H2'	124.41	109.00	1
C3'-C2'-H2''	124.49	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C3'-C2'-H2'	124.49	109.00	1
C3'-C2'-H2'	93.48	109.00	1
C3'-C2'-H2'	124.63	109.00	1
C3'-C2'-H2''	124.67	109.00	1
C3'-C2'-H2'	124.73	109.00	1
C6-N6-H61	104.22	120.00	1
C3'-C2'-H2''	125.00	109.00	1
C5'-C4'-H4'	92.92	109.00	1
C3'-C2'-H2'	92.84	109.00	2
N9-C1'-H1'	92.73	109.00	1
C3'-C2'-H2'	125.29	109.00	1
C3'-C2'-H2''	125.36	109.00	1
C3'-C2'-H2'	92.58	109.00	1
C3'-C2'-H2'	92.46	109.00	1
C3'-C2'-H2'	92.41	109.00	1
C3'-C2'-H2'	125.66	109.00	1
C3'-C2'-H2'	92.27	109.00	1
C5-C6-H6	135.35	118.60	1
C3'-C2'-H2'	125.75	109.00	1
C3'-C2'-H2''	125.79	109.00	1
C6-N1-H1	100.77	117.60	1
CA-N-H	80.33	114.00	1
C3'-C2'-H2'	92.15	109.00	1
C3'-C2'-H2''	125.98	109.00	1
C3'-C2'-H2''	126.00	109.00	1
C3'-C2'-H2'	126.09	109.00	1
C3'-C2'-H2'	126.13	109.00	1
C3'-C2'-H2'	126.14	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C3'-C2'-H2''	126.15	109.00	1
C3'-C2'-H2'	126.21	109.00	1
C3'-C2'-H2''	126.27	109.00	1
C3'-C2'-H2'	126.30	109.00	1
C3'-C2'-H2''	126.36	109.00	1
C3'-C2'-H2'	91.61	109.00	1
C3'-C2'-H2'	126.48	109.00	1
C3'-C2'-H2'	126.50	109.00	1
C3'-C2'-H2'	126.66	109.00	1
C2-N3-H3	134.16	116.50	1
N1-C6-H6	137.34	119.50	1
C3'-C2'-H2''	127.10	109.00	1
C3'-C2'-H2'	127.11	109.00	1
C3'-C2'-H2'	127.19	109.00	1
C3'-C2'-H2''	127.20	109.00	1
C3'-C2'-H2''	127.24	109.00	1
C3'-C2'-H2'	90.74	109.00	1
C3'-C2'-H2''	127.31	109.00	1
C3'-C2'-H2''	127.34	109.00	1
C3'-C2'-H2'	127.46	109.00	1
C3'-C2'-H2'	90.51	109.00	1
C3'-C2'-H2''	127.53	109.00	1
CA-N-H	76.64	114.00	1
N1-C6-H6	138.19	119.50	1
O4'-C1'-H1'	127.77	109.00	1
CD-N-2H	147.18	109.47	1
CA-N-H	76.23	114.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-H	86.51	124.30	1
C3'-C2'-H2''	128.07	109.00	1
C5-C6-H6	138.59	119.50	1
H21-N2-H22	139.14	120.00	1
C3'-C2'-H2''	128.16	109.00	1
C3'-C2'-H2''	128.22	109.00	1
O4'-C4'-H4'	128.34	109.00	1
C6-C5-H5	140.64	121.20	1
C3'-C2'-H2'	89.44	109.00	1
C3'-C2'-H2'	128.61	109.00	1
C3'-C2'-H2'	128.65	109.00	1
C3'-C2'-H2'	128.75	109.00	1
C3'-C2'-H2''	128.79	109.00	1
N9-C1'-H1'	128.84	109.00	1
C3'-C2'-H2''	128.85	109.00	1
C3'-C2'-H2''	129.09	109.00	1
C3'-C2'-H2'	88.88	109.00	1
C3'-C2'-H2''	129.18	109.00	1
C3'-C2'-H2''	129.28	109.00	1
N1-C6-H6	138.88	118.60	1
C3'-C2'-H2''	129.36	109.00	1
N1-C6-H6	140.29	119.50	1
C3'-C2'-H2''	129.92	109.00	1
C2-N2-H22	98.78	120.00	1
C3'-C2'-H2''	130.59	109.00	1
C5-C6-H6	140.24	118.60	1
N9-C8-H8	145.40	123.10	1
C3'-C2'-H2'	85.64	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C3'-C2'-H2''	132.55	109.00	1
C5-C6-H6	143.82	119.50	1
C-N-H	75.59	124.30	1
C3'-C2'-H2'	84.50	109.00	1
C-N-H	75.11	124.30	1
C-N-H	74.83	124.30	1
C3'-C2'-H2''	134.63	109.00	1
C3'-C2'-H2'	83.36	109.00	1
C3'-C2'-H2''	134.65	109.00	1
C3'-C2'-H2'	82.88	109.00	1
C3'-C2'-H2''	135.45	109.00	1
C3'-C2'-H2''	137.12	109.00	1
1H-N-2H	52.60	109.47	1
C3'-C2'-H2''	137.85	109.00	1
C3'-C2'-H2'	79.58	109.00	1
C5-C6-H6	149.49	119.50	1
C3'-C2'-H2''	140.62	109.00	1
N7-C8-H8	91.34	123.10	1
C3'-C2'-H2''	141.37	109.00	1
C3'-C2'-H2'	76.20	109.00	1
C3'-C2'-H2''	142.21	109.00	1
C3'-C2'-H2''	143.68	109.00	1
C3'-C2'-H2'	72.60	109.00	1
C3'-C2'-H2''	145.59	109.00	1
C3'-C2'-H2''	145.97	109.00	1
C3'-C2'-H2''	146.09	109.00	1
C3'-C2'-H2''	146.22	109.00	1
C3'-C2'-H2'	71.67	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C3'-C2'-H2''	146.34	109.00	1
C3'-C2'-H2''	146.56	109.00	1
N9-C8-H8	161.34	123.10	1
C3'-C2'-H2'	70.57	109.00	1
N7-C8-H8	84.56	123.10	1
N9-C8-H8	163.87	123.10	1
N7-C8-H8	82.17	123.30	1
C3'-C2'-H2'	67.68	109.00	1
N7-C8-H8	80.88	123.30	1
N7-C8-H8	79.46	123.10	1
N9-C8-H8	168.26	123.30	1
N9-C8-H8	171.51	123.30	1
C3'-C2'-H2'	60.55	109.00	1
N9-C8-H8	172.04	123.30	1
N1-C6-H6	168.92	119.50	1
C3'-C2'-H2'	58.84	109.00	1
C3'-C2'-H2'	57.19	109.00	1
N1-C6-H6	172.96	118.60	1
C3'-C2'-H2'	53.88	109.00	1
N9-C8-H8	179.95	123.10	1
C3'-C2'-H2'	49.72	109.00	1
C3'-C2'-H2'	49.40	109.00	1
N7-C8-H8	49.45	123.30	1

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

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	4036	3849	160	27

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	3557	3516	31	10

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	1	537	TYR
1	4	1014	LYS
1	4	1074	ASP
1	4	1362	GLU
1	4	1367	PHE
1	4	1375	LYS
1	4	1376	GLU
1	4	1377	VAL
1	A	1834	VAL
1	A	2124	LYS

Fit of model to data used for modeling

3DEM volume

Validation for this section is under development.

Crosslinking-MS

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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