Integrative Structure Validation Report

July 22, 2024 - 04:46 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	9A1Y
PDB-Dev ID	PDBDEV_00000128
Structure Title	Integrative model of Nucleotide excision repair complex of XPA and RPA on 3' junction substrate
Structure Authors	DSouza, A.; Topolska-Wos, A.M.; Chazin, W.J.

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

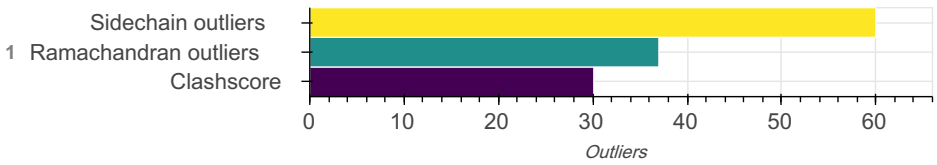
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 8 subunits in each model. A total of 7 datasets or restraints were used to build this entry. Each model is represented by 0 rigid bodies and 14 flexible or non-rigid units.

Entry composition

There is 1 unique type of models in this entry.This model is titled None/None.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	RPA70	A	A	434
1	2	2	RPA32	B	B	226
1	3	3	RPA14	C	C	115
1	4	4	XPA	D	D	239
1	5	5	DNA (40-MER)	E	E	40
1	6	6	DNA (5'-D(P*TP*TP*TP*TP*TP*TP*TP*TP*GP*CP*CP*CP*GP*CP*GP*GP*C)-3')	F	F	17
1	7	7	ZINC ION	G	E	Not available
1	8	8	ZINC ION ON 3-FOLD CRYSTAL AXIS	H	H	Not available

Datasets used for modeling

There are 7 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	SAS data	SASBDB	SASDH44
2	Experimental model	PDB	1JMC
3	Integrative model	PDB-Dev	PDBDEV_00000039
4	Experimental model	PDB	1L1O
5	Experimental model	PDB	1DPU

ID	Dataset type	Database name	Data access code
6	Comparative model	Not available	Not available
7	De Novo model	Not available	Not available

Representation

This entry has only one representation and includes 0 rigid bodies and 14 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	-	1-238, 239-253, 254-434
B	-	1-128, 129-226
C	-	1-115
D	-	1-28, 29-48, 49-97, 98-239
E	-	1-40
F	-	1-17
G	-	None-None
H	-	None-None

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	None	None	None	1	False	False

There are 2 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	Modeller	9v4	model building	https://salilab.org/modeller/
2	FoXSDock	main.c2a7893	model building	https://modbase.compbio.ucsf.edu/foxsdock/

Data quality

SAS:Scattering profile

SAS data used in this integrative model could not be validated as the sascif file is currently unavailable.

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 496 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
C2'--H2''	1.05	0.97	2
C2'--H2'	1.05	0.97	2
C1'--H1'	1.06	0.97	7
C3'--H3'	1.06	0.97	1
C2'--H2''	1.06	0.97	2
C2'--H2'	1.06	0.97	5
C4'--H4'	1.06	0.97	2
C1'--H1'	1.07	0.97	11
C5'--H5''	1.07	0.97	7
C2'--H2'	1.07	0.97	5
C2'--H2''	1.07	0.97	3
N4--H41	0.96	0.86	1
C4'--H4'	1.07	0.97	3
C2'--1H2'	0.87	0.97	1
N4--H42	0.96	0.86	1
C3'--H3'	1.07	0.97	1
C4'--H4'	0.87	0.97	1
C2'--H2'	1.08	0.97	12
C1'--H1'	1.08	0.97	14
C3'--H3'	1.08	0.97	17
C2'--H2''	1.08	0.97	9

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
C4'--H4'	1.08	0.97	13
C5'--H5''	1.08	0.97	6
C5'--H5'	1.08	0.97	7
C2'--H2'	0.86	0.97	1
C6--H6	1.04	0.93	1
N4--H42	0.97	0.86	1
N4--H41	0.97	0.86	1
C3'--H3'	1.09	0.97	11
C5'--H5''	1.09	0.97	24
C2'--H2'	1.09	0.97	10
C2'--H2''	1.09	0.97	18
C4'--H4'	1.09	0.97	13
N4--H41	0.98	0.86	4
C5'--H5'	1.09	0.97	28
C1'--H1'	1.09	0.97	6
N4--H42	0.98	0.86	4
C1'--H1'	0.85	0.97	1
N4--H41	0.99	0.86	3
C5'--H5'	1.10	0.97	5
C6--H6	1.06	0.93	4
C5'--H5''	1.10	0.97	4
C4'--H4'	1.10	0.97	8
C1'--H1'	1.10	0.97	4
C2'--H2''	1.10	0.97	7
O5'--HO5'	0.97	0.84	1
N4--H42	0.99	0.86	5
C5--H5	0.80	0.93	1

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
C3'--H3'	1.10	0.97	9
C2'--H2'	1.10	0.97	3
C5--H5	1.06	0.93	2
N2--H22	0.99	0.86	1
N1--H1	1.00	0.86	3
N4--H42	1.00	0.86	11
N2--H22	1.00	0.86	1
C2'--H2''	1.11	0.97	2
C5--H5	1.07	0.93	3
C5'--H5''	1.11	0.97	1
N4--H41	1.00	0.86	4
C3'--H3'	1.11	0.97	1
C6--H6	1.07	0.93	5
C2'--H2'	1.11	0.97	1
C8--H8	1.07	0.93	1
C4'--H4'	1.11	0.97	1
C3'--H3'	0.83	0.97	1
N4--H42	1.01	0.86	16
N4--H41	1.01	0.86	21
C6--H6	1.08	0.93	7
C5--H5	1.08	0.93	7
C8--H8	1.08	0.93	5
N2--H22	1.01	0.86	6
N2--H21	1.01	0.86	9
N1--H1	1.01	0.86	2
C5--H5	1.09	0.93	8
C6--H6	1.09	0.93	5

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
N2--H22	1.02	0.86	1
N4--H41	1.02	0.86	1
N1--H1	1.02	0.86	4
C8--H8	1.09	0.93	2
N4--H42	1.02	0.86	2
C5'--1H5'	0.81	0.97	1
C5--H5	1.10	0.93	10
C6--H6	1.10	0.93	4
N4--H41	1.03	0.86	1
C4'--H4'	1.14	0.97	1
C2'--H2''	1.14	0.97	1
C8--H8	1.10	0.93	1
C6--H6	1.11	0.93	5
C5'--H5''	1.15	0.97	1
C3'--H3'	1.15	0.97	2
C5--H5	1.11	0.93	3
C2'--H2'	0.79	0.97	1
C6--H6	1.12	0.93	3
C5--H5	1.12	0.93	1
C4'--H4'	0.78	0.97	1
C2'--H2'	1.17	0.97	1
C1'--H1'	1.17	0.97	1
C5--H5	1.13	0.93	1
C6--H6	1.13	0.93	1
N4--H41	1.07	0.86	1
C6--H6	1.15	0.93	1
N4--H41	1.09	0.86	2

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
C5'--H5''	1.22	0.97	1
C2'--H2'	0.70	0.97	1
C6--H6	1.22	0.93	1
C2'--H2''	1.25	0.97	1
C5--H5	1.22	0.93	1
C5'--2H5'	1.31	0.97	1
C5'--H5'	1.38	0.97	1
C2'--2H2'	1.62	0.97	1

Standard geometry: angle outliers

There are 1341 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
C5'-C4'-C3'	114.90	170.70	1
C5'-C4'-C3'	114.90	170.02	1
O-C-OXT	118.00	16.19	1
P-O5'-C5'	120.00	169.25	1
CG-CD1-NE1	110.20	68.59	1
C3'-O3'-P	120.20	168.13	1
CE3-CZ3-CH2	121.10	83.51	1
CD2-CE3-CZ3	118.60	156.15	1
CA-C-O	120.80	168.08	1
CG-CD1-CE1	120.70	165.40	1
C3'-O3'-P	120.20	158.16	1
C-N-CA	121.70	167.18	1
C-N-CA	121.70	165.05	1
C5'-C4'-C3'	114.90	150.88	1
C2-N3-C4	120.00	86.56	1
CB-CG-CD	111.30	160.51	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O5'-C5'-C4'	110.80	79.09	1
CA-CB-CG	112.60	91.74	1
O4'-C1'-N1	108.40	139.53	1
CA-CB-CG1	110.40	145.30	1
CA-C-O	120.80	87.69	1
O3'-P-O5'	104.00	74.91	1
O-C-N	123.00	92.00	1
CD1-CG-CD2	118.60	89.72	1
C-N-CA	121.70	155.77	1
C5'-C4'-O4'	109.40	137.43	1
C-CA-CB	110.10	75.10	1
P-O5'-C5'	120.00	147.62	1
C-CA-CB	110.10	75.54	1
C-N-CA	121.70	153.75	1
C-CA-CB	110.10	76.42	1
C-N-CA	121.70	152.97	1
NE1-CE2-CZ2	130.10	155.96	1
N1-C6-C5	121.00	95.47	1
O5'-C5'-C4'	110.80	136.20	1
C5'-C4'-O4'	109.40	134.18	1
C4'-C3'-O3'	110.00	134.70	1
CB-CG-CD2	131.20	109.90	1
CD2-CE2-NE1	107.40	86.17	1
CA-C-N	116.20	148.76	1
O3'-P-O5'	104.00	79.69	1
CD1-CE1-CZ	120.00	91.31	1
C5'-C4'-O4'	109.40	85.62	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O4'-C1'-C2'	106.40	82.74	1
CA-CB-CG	114.10	145.15	1
O-C-N	123.00	147.77	1
CB-CG-CD1	120.70	146.38	1
C1'-N1-C6	119.70	97.18	1
CA-C-O	120.80	95.31	1
O-C-N	123.00	146.77	1
P-O5'-C5'	120.00	142.07	1
C-CA-CB	110.10	82.15	1
C3'-O3'-P	120.20	142.25	1
N1-C6-C5	121.00	99.10	1
O4'-C1'-C2'	106.40	84.50	1
N-CA-CB	110.50	135.15	1
O-C-N	123.00	100.40	1
CD1-NE1-CE2	108.90	134.25	1
P-O5'-C5'	120.00	141.06	1
CA-C-N	116.90	137.91	1
C-N-CA	121.70	146.84	1
N-CA-CB	110.40	131.26	1
OP1-P-OP2	120.00	161.58	1
O4'-C4'-C3'	105.40	84.67	1
CA-CB-CG	114.10	141.66	1
C-CA-CB	110.50	131.10	1
C-N-CA	121.70	146.11	1
O4'-C4'-C3'	105.40	85.14	1
CA-C-N	116.20	143.20	1
C1'-N1-C6	119.70	99.46	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD	112.60	135.50	1
CB-CG-ND1	122.70	142.30	1
O3'-P-O5'	104.00	123.53	1
C1'-N1-C6	119.70	139.08	1
C-CA-CB	110.50	91.27	1
C1'-N1-C2	119.70	138.88	1
C-N-CA	121.70	144.69	1
O4'-C1'-N1	108.40	127.49	1
P-O5'-C5'	120.00	138.91	1
C3'-O3'-P	120.20	138.92	1
C3'-O3'-P	120.20	138.84	1
C-N-CA	121.70	99.35	1
O4'-C4'-C3'	105.40	86.86	1
C4'-C3'-O3'	110.00	128.49	1
CA-C-N	116.20	140.83	1
C2'-C1'-N1	113.50	95.06	1
N-CA-C	112.10	142.72	1
CA-C-N	116.90	135.25	1
N3-C4-N4	117.90	136.12	1
C3'-C2'-C1'	101.60	119.81	1
C3'-O3'-P	120.20	138.34	1
N-CA-CB	110.50	130.89	1
O3'-P-OP2	108.00	143.88	1
C4'-C3'-O3'	110.00	127.85	1
O-C-N	123.00	141.92	1
C-CA-CB	110.50	92.81	1
N-CA-C	112.10	141.44	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O4'-C1'-N1	108.40	125.89	1
NE-CZ-NH1	121.50	109.99	1
C4'-C3'-O3'	110.00	126.90	1
C-N-CA	121.70	141.93	1
CD2-NE2-CE1	109.00	97.85	1
C-N-CA	121.70	101.65	1
CA-CB-OG1	109.60	126.30	1
C-N-CA	121.70	141.67	1
CA-C-N	116.90	133.51	1
N-CA-CB	110.50	129.20	1
OP1-P-OP2	120.00	152.87	1
P-O5'-C5'	120.00	136.42	1
OP1-P-OP2	120.00	87.32	1
P-O5'-C5'	120.00	136.24	1
N1-C2-N3	118.90	135.13	1
CA-C-N	116.20	137.80	1
C-N-CA	121.70	141.11	1
C5'-C4'-C3'	114.90	131.02	1
OP1-P-O5'	109.00	141.20	1
C3'-O3'-P	120.20	136.24	1
C2'-C1'-N1	113.50	129.52	1
O5'-C5'-C4'	110.80	126.72	1
C-CA-CB	111.40	91.24	1
CA-C-O	120.80	102.84	1
P-O5'-C5'	120.00	135.85	1
CA-C-N	116.20	137.25	1
N4-C4-C5	120.30	104.53	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O3'-P-OP2	108.00	76.73	1
N-CA-CB	103.00	91.70	1
N-CA-C	111.00	139.64	1
C2-N3-C4	120.00	104.68	1
N-CA-C	111.00	139.56	1
C-N-CA	121.70	103.36	1
CA-C-O	120.80	103.49	1
C3'-O3'-P	120.20	135.47	1
CB-CG-CD2	131.20	118.01	1
CD2-CE2-CZ	120.00	138.23	1
C4'-O4'-C1'	109.70	124.84	1
C4'-O4'-C1'	109.70	94.71	1
O5'-C5'-C4'	110.80	125.75	1
C-N-CA	121.70	139.56	1
C-N-CA	121.70	103.93	1
O5'-C5'-C4'	110.80	125.55	1
O4'-C1'-C2'	106.40	91.78	1
CA-CB-OG	111.10	91.93	1
CE2-CZ2-CH2	117.50	105.11	1
CA-CB-CG	113.60	131.62	1
C5'-C4'-C3'	114.90	100.69	1
O3'-C3'-C2'	111.50	125.66	1
NE-CZ-NH1	121.50	112.07	1
N-CA-C	111.00	137.24	1
CA-CB-CG	112.60	121.87	1
C-N-CA	121.70	138.35	1
CA-CB-CG	113.80	122.97	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C3'-O3'-P	120.20	133.95	1
O-C-N	123.00	108.35	1
O-C-N	123.00	108.37	1
CA-C-N	116.20	134.49	1
C-N-CA	121.70	105.35	1
O4'-C4'-C3'	105.40	91.79	1
O-C-N	123.00	108.49	1
C1'-N1-C2	119.70	106.20	1
OE1-CD-NE2	122.60	113.62	1
O5'-C5'-C4'	110.80	97.39	1
C5'-C4'-O4'	109.40	96.00	1
CG-CD1-CE1	120.70	105.52	1
C5'-C4'-C3'	114.90	128.27	1
CG-CD2-CE3	133.90	124.99	1
C4'-C3'-O3'	110.00	123.34	1
P-O5'-C5'	120.00	133.34	1
C-N-CA	121.70	137.67	1
NE-CZ-NH2	119.20	111.23	1
NE-CZ-NH1	121.50	130.36	1
O2-C2-N3	121.90	108.63	1
CA-CB-CG	114.10	131.77	1
P-O5'-C5'	120.00	106.81	1
C-N-CA	121.70	137.31	1
C2-N1-C6	120.60	107.60	1
O-C-N	123.00	109.13	1
CA-CB-CG	112.60	121.26	1
C4'-C3'-C2'	102.40	89.42	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O4'-C1'-C2'	106.40	93.43	1
C2-N1-C6	120.60	107.70	1
CA-C-N	116.20	133.40	1
OD1-CG-ND2	122.60	114.05	1
N-CA-C	111.00	134.91	1
C4'-O4'-C1'	109.70	122.51	1
N-CA-C	111.00	134.86	1
CA-N-CD	112.00	100.11	1
C4'-C3'-O3'	110.00	122.73	1
CB-CG-CD2	126.80	114.94	1
CB-CG1-CD1	113.80	131.56	1
O4'-C1'-N1	108.40	121.05	1
C4'-O4'-C1'	109.70	97.13	1
N1-C6-C5	121.00	133.55	1
O2-C2-N3	121.90	109.37	1
N-CA-CB	110.50	124.64	1
C-N-CA	121.70	136.67	1
O3'-P-O5'	104.00	116.41	1
CB-CG-CD2	131.20	120.48	1
CA-C-N	116.20	132.65	1
CA-CB-CG	114.10	97.74	1
N-CA-C	112.10	132.50	1
CA-C-N	116.20	99.91	1
CA-CB-OG1	109.60	121.79	1
CA-CB-CG	114.10	97.94	1
CB-CG-ND1	122.70	134.81	1
C4'-O4'-C1'	109.70	97.62	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C2-N3-C4	120.00	107.92	1
C-N-CA	121.70	136.19	1
CB-CG-OD1	118.40	136.88	1
C4'-O4'-C1'	109.70	121.72	1
CA-CB-CG	113.90	128.31	1
CA-CB-CG	112.60	104.60	1
N-CA-C	111.00	133.39	1
O2-C2-N3	121.90	109.93	1
O5'-C5'-C4'	110.80	122.69	1
O-C-N	123.00	135.66	1
O2-C2-N3	121.90	110.06	1
C-N-CA	121.70	135.90	1
O5'-C5'-C4'	110.80	122.60	1
C-N-CA	121.70	135.85	1
OD1-CG-OD2	122.90	104.05	1
C4'-C3'-C2'	102.40	114.17	1
C2'-C1'-N1	113.50	125.23	1
O2-C2-N3	121.90	110.18	1
O5'-C5'-C4'	110.80	122.48	1
C-N-CA	121.70	135.71	1
C-N-CA	121.70	135.58	1
N-CA-CB	111.50	124.58	1
O4'-C4'-C3'	105.40	93.87	1
O2-C2-N3	121.90	110.37	1
CB-CG-CD1	126.90	138.39	1
C4'-O4'-C1'	109.70	98.26	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N1-C2-O2	119.20	130.61	1
C4'-C3'-O3'	110.00	121.38	1
O2-C2-N3	121.90	110.53	1
P-O5'-C5'	120.00	131.31	1
N-CA-C	111.00	132.07	1
CA-CB-CG	112.60	120.11	1
CA-C-N	116.20	131.20	1
C-CA-CB	110.10	124.34	1
O4'-C1'-N1	108.40	119.64	1
O2-C2-N3	121.90	110.67	1
O-C-N	123.00	111.03	1
O3'-P-O5'	104.00	115.21	1
O4'-C1'-N1	108.40	119.59	1
C4'-O4'-C1'	109.70	98.52	1
CA-C-N	116.20	101.36	1
O4'-C1'-C2'	106.40	117.53	1
OD1-CG-ND2	122.60	115.26	1
P-O5'-C5'	120.00	130.99	1
C5'-C4'-O4'	109.40	98.50	1
O4'-C1'-C2'	106.40	95.51	1
N-CA-C	111.00	131.29	1
CB-CG-CD2	131.20	121.81	1
NE-CZ-NH1	121.50	128.71	1
CA-CB-OG	111.10	96.70	1
N-CA-C	113.30	134.17	1
O2-C2-N3	121.90	111.13	1
OE1-CD-NE2	122.60	115.44	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C4'-O4'-C1'	109.70	99.01	1
P-O5'-C5'	120.00	130.69	1
N3-C4-N4	117.90	107.22	1
CE2-CD2-CE3	118.80	111.68	1
OE1-CD-NE2	122.60	115.53	1
O-C-N	123.00	111.70	1
CA-CB-CG	113.80	120.85	1
CA-C-O	120.80	108.82	1
O4'-C1'-C2'	106.40	95.84	1
NE-CZ-NH2	119.20	125.53	1
O2-C2-N3	121.90	111.37	1
N-CA-CB	111.50	123.44	1
CA-C-O	120.80	108.87	1
CA-C-N	116.20	130.21	1
O3'-C3'-C2'	111.50	121.99	1
O4'-C1'-C2'	106.40	95.92	1
C4'-C3'-C2'	102.40	91.96	1
O2-C2-N3	121.90	111.47	1
OD1-CG-ND2	122.60	115.66	1
C-N-CA	121.70	134.19	1
CA-C-O	120.80	109.02	1
OD1-CG-ND2	122.60	115.67	1
N-CA-CB	110.50	98.74	1
C1'-N1-C6	119.70	130.04	1
C-N-CA	121.70	134.11	1
CD-NE-CZ	124.40	134.04	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	134.07	1
CA-C-N	116.20	129.91	1
OE1-CD-NE2	122.60	115.76	1
C4'-C3'-O3'	110.00	120.24	1
C-N-CA	121.70	133.96	1
O-C-N	123.00	112.11	1
O2-C2-N3	121.90	111.74	1
C-N-CA	121.70	133.82	1
CA-CB-CG	112.60	119.32	1
CA-C-O	120.80	109.37	1
C5'-C4'-O4'	109.40	99.32	1
N-CA-CB	110.50	121.93	1
N3-C4-C5	121.80	111.73	1
CA-CB-CG	112.60	119.30	1
CA-C-N	116.20	129.59	1
CD-NE-CZ	124.40	133.77	1
O4'-C1'-C2'	106.40	96.38	1
C-N-CA	121.70	133.72	1
N-CA-CB	110.50	99.19	1
N-CA-CB	110.50	99.21	1
O4'-C1'-C2'	106.40	96.45	1
OE1-CD-NE2	122.60	115.98	1
C-CA-CB	110.10	122.67	1
C5'-C4'-O4'	109.40	99.50	1
C1'-N1-C6	119.70	129.57	1
C-N-CA	121.70	133.52	1
OE1-CD-NE2	122.60	116.04	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG2	110.50	121.64	1
O2-C2-N3	121.90	112.09	1
O4'-C1'-N1	108.40	118.20	1
CA-CB-CG2	110.50	121.60	1
C-CA-CB	110.10	97.70	1
C3'-O3'-P	120.20	129.99	1
N3-C4-N4	117.90	108.13	1
CA-CB-CG	112.60	119.11	1
C4'-C3'-C2'	102.40	92.65	1
C-N-CA	121.70	133.40	1
OD1-CG-ND2	122.60	116.11	1
O4'-C1'-N1	108.40	118.09	1
C4'-O4'-C1'	109.70	100.01	1
N-CA-CB	110.40	100.71	1
CZ2-CH2-CZ3	121.50	113.11	1
CB-CG-CD1	120.80	111.12	1
C3'-O3'-P	120.20	129.88	1
CA-CB-CG	113.80	120.25	1
O4'-C1'-N1	108.40	118.07	1
CA-C-N	116.20	129.08	1
C-N-CA	121.70	133.29	1
C-N-CA	121.70	133.23	1
C-N-CA	121.70	133.21	1
C4'-O4'-C1'	109.70	100.12	1
OD1-CG-ND2	122.60	116.21	1
CB-CG-CD2	131.20	122.90	1
O-C-N	123.00	112.79	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C2'-C1'-N1	113.50	123.06	1
C5'-C4'-C3'	114.90	124.46	1
O5'-C5'-C4'	110.80	120.35	1
C-N-CA	121.70	133.14	1
C-N-CA	121.70	133.12	1
O5'-C5'-C4'	110.80	101.32	1
C-N-CA	121.70	133.08	1
CA-CB-CG	114.10	126.71	1
CA-CB-CG	104.50	92.55	1
C-N-CA	121.70	132.98	1
N1-C2-O2	119.20	128.59	1
CA-CB-CG	104.50	92.60	1
CD-NE-CZ	124.40	115.65	1
CG-CD2-CE2	107.20	114.66	1
O4'-C1'-N1	108.40	117.73	1
C4'-O4'-C1'	109.70	100.40	1
O4'-C1'-C2'	106.40	97.10	1
CA-CB-CG	113.80	119.98	1
O4'-C1'-C2'	106.40	97.15	1
CB-CG-CD2	120.80	111.55	1
C-N-CA	121.70	132.78	1
N-CA-CB	110.40	101.17	1
O-C-OXT	118.00	99.55	1
C3'-O3'-P	120.20	129.42	1
O4'-C1'-N1	108.40	117.62	1
CA-C-N	116.90	126.10	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O3'-C3'-C2'	111.50	120.70	1
N1-C2-O2	119.20	128.38	1
CA-CB-CG2	110.40	120.80	1
CE2-CZ2-CH2	117.50	125.42	1
CA-CB-CG1	110.40	120.75	1
CA-CB-CG	112.60	118.68	1
O-C-N	123.00	113.27	1
CB-CG-CD	112.60	102.27	1
C4'-C3'-O3'	110.00	119.11	1
CE2-CD2-CE3	118.80	112.73	1
P-O5'-C5'	120.00	129.08	1
O4'-C4'-C3'	105.40	96.33	1
O2-C2-N3	121.90	112.83	1
CA-CB-CG1	110.40	120.66	1
N1-C2-O2	119.20	110.17	1
CG-CD2-CE3	133.90	139.92	1
CA-CB-CG2	110.40	120.62	1
CG-CD-NE2	116.40	125.40	1
O-C-N	123.00	113.41	1
NE-CZ-NH2	119.20	124.59	1
CD2-CE3-CZ3	118.60	126.37	1
NE-CZ-NH2	119.20	124.56	1
C-N-CA	121.70	132.43	1
CA-C-N	116.20	104.31	1
C-CA-CB	110.10	121.40	1
CA-CB-CG2	110.50	120.60	1
CA-N-CD	112.00	103.69	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.50	119.40	1
CA-CB-CG2	110.50	120.58	1
CA-N-CD	112.00	103.71	1
CB-CG1-CD1	113.80	126.24	1
OD1-CG-ND2	122.60	116.69	1
CA-C-O	120.80	130.82	1
C3'-O3'-P	120.20	129.04	1
CA-CB-CG	113.80	107.91	1
C4-C5-C6	117.60	126.43	1
C1'-N1-C2	119.70	128.52	1
CB-CG-CD	112.60	102.61	1
O4'-C1'-C2'	106.40	97.58	1
C-CA-CB	110.10	121.27	1
CA-C-O	120.80	110.81	1
O3'-P-O5'	104.00	95.23	1
CB-CG-CD	112.60	122.54	1
CA-CB-CG	112.60	106.78	1
CD1-CE1-CZ	120.00	130.47	1
NH1-CZ-NH2	119.30	126.85	1
N-CA-C	111.00	127.23	1
N-CA-CB	110.50	120.34	1
O-C-N	123.00	113.76	1
O2-C2-N3	121.90	113.25	1
CB-CG-CD2	120.80	129.41	1
C1'-N1-C2	119.70	111.09	1
O-C-N	123.00	113.83	1
CB-CG-CD	112.60	122.34	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OG1-CB-CG2	109.30	97.84	1
N-CA-CB	103.00	96.71	1
O5'-C5'-C4'	110.80	119.38	1
NE-CZ-NH2	119.20	114.06	1
C4'-O4'-C1'	109.70	101.13	1
P-O5'-C5'	120.00	111.43	1
C3'-O3'-P	120.20	111.66	1
CB-CG-CD	112.60	122.26	1
C-CA-CB	110.10	99.32	1
CG1-CB-CG2	110.80	98.32	1
O-C-N	123.00	113.93	1
O-C-N	123.00	113.95	1
CA-CB-CG	112.60	118.24	1
CG-CD2-NE2	107.20	101.57	1
C1'-N1-C6	119.70	111.25	1
CA-N-CD	112.00	104.12	1
C2-N3-C4	120.00	111.57	1
CA-CB-CG	114.10	102.86	1
CA-CB-CG	112.60	118.22	1
C4'-C3'-O3'	110.00	118.42	1
CB-CG-CD	111.30	124.21	1
N-CD-CG	103.20	111.61	1
CA-CB-CG	112.60	118.21	1
CA-CB-CG1	110.40	119.92	1
OE1-CD-NE2	122.60	117.01	1
C5'-C4'-C3'	114.90	123.26	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-N	116.90	108.55	1
CA-CB-CG	112.60	107.04	1
C-N-CA	121.70	131.70	1
N1-C2-N3	118.90	127.23	1
CA-CB-CG	112.60	118.15	1
C1'-N1-C6	119.70	128.03	1
OD1-CG-ND2	122.60	117.05	1
ND1-CG-CD2	106.10	111.64	1
C-N-CA	121.70	111.74	1
CB-CG-CD1	120.80	112.50	1
N-CA-CB	110.50	101.10	1
O3'-C3'-C2'	111.50	119.79	1
CA-C-O	120.80	130.20	1
C3'-C2'-C1'	101.60	93.31	1
O3'-P-O5'	104.00	112.26	1
C-N-CA	121.70	131.60	1
C-CA-CB	110.10	120.54	1
N1-C2-O2	119.20	127.44	1
C-N-CA	121.70	131.58	1
CD-NE-CZ	124.40	132.08	1
CA-C-N	116.90	125.12	1
N3-C4-C5	121.80	130.02	1
N-CA-CB	110.50	101.19	1
N-CA-C	112.10	125.79	1
CD1-CG-CD2	110.80	122.83	1
O5'-C5'-C4'	110.80	118.99	1
CA-CB-CG	112.60	107.14	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
P-O5'-C5'	120.00	128.18	1
C2'-C1'-N1	113.50	121.68	1
OE1-CD-NE2	122.60	117.16	1
O4'-C1'-N1	108.40	116.56	1
C5'-C4'-C3'	114.90	123.05	1
C-CA-CB	110.10	120.42	1
C-N-CA	121.70	111.94	1
C-N-CA	121.70	131.45	1
O2-C2-N3	121.90	113.78	1
OD1-CG-ND2	122.60	117.19	1
O5'-C5'-C4'	110.80	118.90	1
O-C-N	123.00	114.37	1
CA-CB-CG2	110.40	119.57	1
CD1-CG-CD2	118.10	110.02	1
C-N-CA	121.70	131.39	1
N1-C2-O2	119.20	127.27	1
O-C-N	123.00	114.40	1
CA-CB-CG	113.80	119.17	2
N3-C4-N4	117.90	109.85	1
N4-C4-C5	120.30	128.35	1
C2'-C1'-N1	113.50	121.55	1
C3'-O3'-P	120.20	128.24	1
C-N-CA	121.70	131.34	1
CA-C-N	116.90	124.93	1
CG-CD-NE	112.00	100.23	1
O-C-N	123.00	114.45	1
CB-CG-CD	111.30	123.56	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG1	110.40	119.46	2
C-N-CA	121.70	131.29	1
CA-CB-CG	113.80	119.12	1
CD2-CE2-CZ2	122.40	127.72	1
CB-CG-CD2	120.80	128.78	1
CA-CB-CG	113.80	108.48	1
C5'-C4'-O4'	109.40	101.43	1
C-CA-CB	110.10	120.19	1
P-O5'-C5'	120.00	112.04	2
C-CA-CB	110.50	102.54	1
O-C-N	123.00	114.51	1
CA-CB-CG	112.60	107.30	1
N1-C2-O2	119.20	127.12	1
CA-C-N	116.20	126.75	1
C3'-O3'-P	120.20	128.10	1
C-CA-CB	110.10	120.10	1
C4'-C3'-O3'	110.00	117.89	1
CB-CG-ND1	122.70	130.58	1
OD1-CG-ND2	122.60	117.35	1
CA-C-O	120.80	129.71	1
C2-N1-C6	120.60	128.45	1
C-N-CA	121.70	131.12	1
O4'-C1'-C2'	106.40	98.55	1
CA-C-N	116.20	126.66	1
N-CA-CB	110.50	119.38	1
O5'-C5'-C4'	110.80	118.64	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C3'-C2'-C1'	101.60	93.76	1
C3'-C2'-C1'	101.60	93.77	1
C-N-CA	121.70	131.10	1
C-N-CA	121.70	131.09	1
C3'-O3'-P	120.20	128.02	1
C2-N1-C6	120.60	112.78	1
CD1-CG-CD2	118.10	125.91	1
C-N-CA	121.70	131.05	1
N1-C2-O2	119.20	126.99	1
CA-CB-CG	113.80	118.99	1
CA-C-N	116.90	124.69	1
CA-CB-CG	104.50	94.65	1
N-CA-CB	110.50	119.32	1
C-CA-CB	110.10	119.94	1
O-C-N	123.00	114.72	1
C4'-C3'-O3'	110.00	117.76	1
CA-C-O	120.80	129.59	1
C5'-C4'-C3'	114.90	107.15	1
CA-C-O	120.80	112.02	1
NE-CZ-NH2	119.20	114.55	1
O3'-P-O5'	104.00	111.74	1
C-CA-CB	110.10	119.89	1
O3'-C3'-C2'	111.50	119.23	1
C-N-CA	121.70	130.97	1
O-C-N	123.00	114.76	1
O4'-C4'-C3'	105.40	97.67	1
C4'-C3'-O3'	110.00	117.72	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	111.40	101.63	1
CA-CB-CG	104.50	94.73	1
C1'-N1-C2	119.70	127.41	1
C-N-CA	121.70	130.95	1
C3'-O3'-P	120.20	112.49	1
N1-C2-O2	119.20	126.90	1
C-CA-CB	110.10	119.85	1
OP1-P-OP2	120.00	135.39	1
C1'-N1-C6	119.70	127.39	1
N3-C4-N4	117.90	110.22	1
C-N-CA	121.70	130.91	1
C-CA-CB	110.50	118.17	1
CA-CB-CG1	110.40	119.09	1
CD-NE-CZ	124.40	131.55	1
C4'-C3'-O3'	110.00	102.35	1
C-N-CA	121.70	130.88	1
CA-C-N	116.20	126.39	1
CA-C-O	120.80	112.15	1
O3'-P-O5'	104.00	96.37	1
O4'-C1'-C2'	106.40	98.77	1
C-CA-CB	110.10	100.46	1
O4'-C4'-C3'	105.40	97.80	1
CA-C-O	120.80	112.19	1
O4'-C1'-C2'	106.40	98.81	1
CE1-CZ-CE2	120.00	110.90	1
C-N-CA	121.70	130.79	1
C4-C5-C6	117.60	125.16	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
P-O5'-C5'	120.00	112.44	1
NH1-CZ-NH2	119.30	112.75	1
N4-C4-C5	120.30	112.75	1
CA-CB-CG	112.60	117.63	1
N1-C2-O2	119.20	126.75	1
O2-C2-N3	121.90	114.35	1
NE-CZ-NH2	119.20	123.72	1
C1'-N1-C6	119.70	127.23	1
C5'-C4'-C3'	114.90	107.38	1
C-N-CA	121.70	130.72	1
C3'-O3'-P	120.20	127.71	1
C5'-C4'-C3'	114.90	122.40	1
CA-CB-CG	114.10	124.09	1
CA-C-N	116.20	126.16	1
O-C-N	123.00	130.97	1
C-N-CA	121.70	130.66	1
N-CA-CB	110.50	118.96	1
CA-C-O	120.80	129.26	1
CA-CB-CG1	110.40	118.86	2
C-N-CA	121.70	130.65	1
CA-CB-CG	113.80	118.77	1
NE-CZ-NH1	121.50	116.53	1
N-CA-CB	110.40	102.95	1
N-CA-CB	110.50	102.06	1
CB-CG-CD	112.60	104.17	1
CA-C-N	116.90	124.34	1
O-C-N	123.00	115.07	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C3'-O3'-P	120.20	127.63	1
CA-CB-CG	112.60	107.65	1
C-N-CA	121.70	130.60	1
CG-CD-NE	112.00	101.14	1
CG-CD-NE2	116.40	109.00	1
N4-C4-C5	120.30	127.70	1
CA-CB-CG	112.60	107.67	1
N1-C6-C5	121.00	113.60	1
O4'-C1'-C2'	106.40	99.01	1
O3'-C3'-C2'	111.50	118.88	1
OD1-CG-ND2	122.60	117.69	1
CD2-CE2-CZ2	122.40	117.50	1
OG1-CB-CG2	109.30	99.51	1
CA-C-N	116.90	124.24	1
O2-C2-N3	121.90	114.57	1
OD1-CG-ND2	122.60	117.72	1
CA-CB-CG	104.50	95.22	1
C3'-O3'-P	120.20	127.51	1
C-N-CA	121.70	130.47	1
O2-C2-N3	121.90	114.60	1
C-CA-CB	109.10	119.81	1
N-CA-CB	110.50	118.77	1
C-N-CA	121.70	130.45	1
N-CA-CB	110.50	102.26	1
C-CA-CB	110.10	119.31	1
ND1-CG-CD2	106.10	110.95	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O2-C2-N3	121.90	114.64	1
C3'-C2'-C1'	101.60	94.34	1
C-N-CA	121.70	130.41	1
CA-CB-CG1	110.40	118.61	1
CA-CB-CG	114.10	123.75	1
CA-C-O	120.80	112.61	1
CA-CB-CG1	110.40	118.59	1
C-N-CA	121.70	113.03	1
N-CA-CB	110.40	117.61	1
CD1-CG-CD2	118.60	125.81	1
CA-CB-SG	114.40	103.35	1
NH1-CZ-NH2	119.30	113.06	1
OD1-CG-ND2	122.60	117.81	1
N-CA-C	111.00	124.41	1
CA-CB-CG2	110.50	102.36	1
CA-C-O	120.80	128.93	1
N1-C2-O2	119.20	112.03	1
C5'-C4'-C3'	114.90	122.07	1
CA-N-CD	112.00	105.33	1
N-CA-CB	110.50	102.41	1
OP2-P-O5'	108.00	122.27	1
C-N-CA	121.70	130.26	1
CB-CG-CD2	120.70	112.62	1
C-N-CA	121.70	130.25	1
CA-C-O	120.80	128.87	1
N-CA-CB	110.50	102.43	1
C-N-CA	121.70	130.23	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CD-NE-CZ	124.40	131.02	1
N-CA-CB	110.50	102.47	1
O3'-C3'-C2'	111.50	118.58	1
O4'-C4'-C3'	105.40	98.32	1
CA-CB-CG	112.60	117.32	1
O3'-P-O5'	104.00	111.08	1
C4'-C3'-O3'	110.00	117.07	2
CA-C-O	120.80	112.79	1
O2-C2-N3	121.90	114.84	1
N-CA-CB	110.40	103.35	1
O-C-N	123.00	115.49	1
CG-CD-CE	111.30	122.10	1
O5'-C5'-C4'	110.80	103.76	1
O-C-N	123.00	115.50	1
CE1-CZ-CE2	120.00	111.56	1
CB-CG-CD2	131.20	125.12	1
CA-C-O	120.80	112.86	1
N-CA-CB	110.50	102.57	1
C2-N1-C6	120.60	127.60	1
CA-CB-CG2	110.40	118.32	1
O-C-N	123.00	115.55	1
CA-C-O	120.80	112.89	1
N-CA-C	111.00	124.02	1
CA-CB-CG2	110.50	118.40	1
C-CA-CB	109.10	119.32	1
C-N-CA	121.70	130.06	1
N-CA-CB	110.50	102.60	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-OD1	118.40	129.08	1
C-CA-CB	110.10	118.92	1
O4'-C1'-N1	108.40	115.36	1
C5'-C4'-C3'	114.90	121.86	1
O4'-C1'-C2'	106.40	99.45	1
C2'-C1'-N1	113.50	120.45	1
O4'-C4'-C3'	105.40	98.45	1
CD-NE-CZ	124.40	130.88	1
CA-CB-CG	114.10	123.35	1
CA-CB-CG	104.50	95.73	1
CA-CB-OG1	109.60	116.52	1
CD-NE-CZ	124.40	117.95	1
O-C-N	123.00	115.63	2
NH1-CZ-NH2	119.30	125.29	1
C-N-CA	121.70	129.99	1
O4'-C1'-C2'	106.40	99.49	1
C-CA-CB	110.10	118.85	1
CA-CB-CG2	110.50	118.32	1
C3'-C2'-C1'	101.60	94.70	1
CA-C-O	120.80	128.61	1
CA-CB-SG	114.40	103.83	1
CB-CG-ND1	122.70	129.59	1
CA-C-N	116.20	125.39	1
C5'-C4'-C3'	114.90	121.79	1
C-N-CA	121.70	129.96	1
NH1-CZ-NH2	119.30	125.25	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.10	101.40	1
C-CA-CB	110.10	101.42	1
CA-C-O	120.80	128.56	1
P-O5'-C5'	120.00	113.15	1
C-N-CA	121.70	129.91	1
C-CA-CB	110.10	101.44	1
P-O5'-C5'	120.00	126.82	1
C3'-O3'-P	120.20	127.02	1
C1'-N1-C6	119.70	112.90	1
C-CA-CB	110.10	118.71	1
NE-CZ-NH1	121.50	116.97	1
C1'-N1-C2	119.70	126.49	1
CA-CB-CG2	110.40	118.10	1
N-CA-CB	111.50	103.80	1
CA-C-N	116.20	125.25	1
C4'-C3'-C2'	102.40	95.62	1
CA-C-O	120.80	128.48	1
CG-ND1-CE1	109.30	101.62	1
CA-C-O	120.80	113.12	1
CA-CB-CG1	110.40	118.07	1
N-CA-CB	110.50	118.17	1
CB-CG-CD	111.30	121.67	1
C3'-O3'-P	120.20	126.96	1
C3'-O3'-P	120.20	113.44	1
C2'-C1'-N1	113.50	120.25	1
C-N-CA	121.70	129.80	1
C-CA-CB	110.10	118.64	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N4-C4-C5	120.30	127.04	1
C2'-C1'-N1	113.50	120.24	1
C5'-C4'-O4'	109.40	102.66	1
C4'-O4'-C1'	109.70	102.97	1
C-N-CA	121.70	129.78	1
C-N-CA	121.70	129.77	1
CD2-NE2-CE1	109.00	104.53	1
N3-C4-N4	117.90	124.61	1
O-C-N	123.00	115.84	1
C4'-C3'-C2'	102.40	109.11	1
CA-CB-OG	111.10	120.04	1
C-N-CA	121.70	129.75	1
C-CA-CB	110.10	118.59	1
C3'-O3'-P	120.20	126.89	1
CB-CG-ND1	122.70	129.39	1
CD2-NE2-CE1	109.00	104.54	1
CB-CG-CD1	120.80	114.12	1
C-N-CA	121.70	129.71	1
CD2-NE2-CE1	109.00	104.55	1
N-CA-C	111.00	123.46	1
OE1-CD-NE2	122.60	118.16	1
C-N-CA	121.70	129.69	1
C5'-C4'-C3'	114.90	121.56	1
CA-CB-CG	104.50	96.07	1
N-CA-CB	110.50	102.96	1
CA-C-N	116.20	125.07	1
CA-N-CD	112.00	105.80	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	129.67	1
O5'-C5'-C4'	110.80	117.44	1
NE-CZ-NH2	119.20	115.22	1
OG1-CB-CG2	109.30	100.45	1
CG1-CB-CG2	110.80	101.07	1
C-CA-CB	110.10	101.70	1
CB-CG-CD	112.60	120.11	1
O-C-N	123.00	115.94	1
C-N-CA	121.70	129.63	1
CA-CB-CG	104.50	96.14	1
CA-CB-CG	112.60	108.20	1
O3'-C3'-C2'	111.50	104.91	1
C-CA-CB	110.10	118.45	1
CB-CG-ND2	116.40	122.99	1
CA-C-N	116.90	123.49	1
N1-C2-O2	119.20	125.78	1
CA-C-N	116.20	124.97	1
CA-C-O	120.80	128.25	1
C3'-O3'-P	120.20	126.77	1
CA-CB-CG	114.10	122.86	1
CA-CB-CG	114.10	122.85	1
C3'-O3'-P	120.20	126.76	1
C-N-CA	121.70	129.57	1
CA-CB-CG	112.60	116.97	1
O5'-C5'-C4'	110.80	117.35	1
CA-CB-CG1	110.40	117.81	1
CD2-NE2-CE1	109.00	104.64	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-C	111.00	123.20	1
C-CA-CB	110.10	118.37	2
CD-NE-CZ	124.40	130.49	1
CA-CB-CG1	110.40	117.80	1
CD2-NE2-CE1	109.00	113.35	1
CA-CB-CG	104.50	96.23	1
O4'-C4'-C3'	105.40	98.88	1
CA-CB-CG	114.10	122.79	1
OD1-CG-ND2	122.60	118.25	1
C5'-C4'-O4'	109.40	115.92	1
N1-C2-O2	119.20	125.72	1
C-CA-CB	110.50	117.02	1
O3'-C3'-C2'	111.50	118.01	1
CA-C-N	116.20	124.88	1
C-N-CA	121.70	129.51	1
CG-CD2-CE3	133.90	138.23	1
CB-CG-CD2	120.80	114.30	1
CB-CG-OD2	118.40	108.44	1
CA-C-O	120.80	113.44	2
C-N-CA	121.70	129.49	1
CA-C-O	120.80	128.15	1
O3'-P-O2P	108.00	120.97	1
CG-CD-OE1	120.80	129.45	1
C-N-CA	122.60	144.20	1
C1'-N1-C2	119.70	126.18	1
C-CA-CB	110.10	118.28	1
CA-C-O	120.80	113.48	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	103.18	1
O4'-C1'-N1	108.40	114.85	1
CA-C-N	116.20	124.79	1
CA-C-N	116.20	124.78	1
O-C-N	123.00	116.14	1
O5'-C5'-C4'	110.80	117.23	1
CA-CB-CG	104.50	96.36	1
C-CA-CB	110.10	118.24	1
C4-C5-C6	117.60	111.18	1
C-N-CA	121.70	129.40	1
N-CA-CB	110.50	103.23	1
N1-C2-N3	118.90	112.48	1
CA-C-O	120.80	113.53	1
C-N-CA	121.70	129.39	2
C-N-CA	121.70	129.38	1
O2-C2-N3	121.90	115.50	1
C1'-N1-C2	119.70	126.09	1
C1'-N1-C2	119.70	113.31	1
CA-N-CD	112.00	106.04	1
N3-C4-C5	121.80	128.19	1
CA-C-O	120.80	113.56	1
C-N-CA	121.70	129.35	1
O-C-N	123.00	116.20	1
CD-NE-CZ	124.40	118.46	1
C1'-N1-C2	119.70	126.07	1
O5'-C5'-C4'	110.80	117.16	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C4'-C3'-O3'	110.00	116.35	1
N1-C2-O2	119.20	125.55	1
C4'-O4'-C1'	109.70	116.05	1
CD2-CE2-CZ	120.00	127.61	1
CA-C-O	120.80	113.61	1
N1-C2-N3	118.90	125.24	1
C1'-N1-C2	119.70	126.03	1
CA-CB-OG1	109.60	115.93	1
N-CA-CB	110.50	117.68	1
CA-CB-CG2	110.50	117.67	1
NE-CZ-NH2	119.20	115.40	1
N-CA-CB	110.50	103.33	1
NH1-CZ-NH2	119.30	113.82	1
N-CA-CB	110.50	117.67	1
O-C-N	123.00	116.25	1
C2-N1-C6	120.60	114.28	1
CB-CG-CD	112.60	119.76	1
N-CA-CB	111.50	104.34	1
CA-CB-CG2	110.50	117.66	1
C-N-CA	121.70	129.28	1
CA-CB-OG1	109.60	115.92	1
N-CA-CB	110.50	103.34	1
CB-CG-CD	112.60	105.45	1
O-C-N	123.00	116.27	1
C4'-C3'-C2'	102.40	96.10	1
CA-N-CD	112.00	106.13	1
O3'-C3'-C2'	111.50	117.79	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CG-CD2-CE3	133.90	138.09	1
CA-C-N	116.20	124.58	1
CA-CB-CG1	110.40	117.52	1
C-CA-CB	110.10	118.05	1
O-C-N	123.00	129.69	1
O-C-N	123.00	116.32	1
P-O5'-C5'	120.00	126.26	1
C2'-C1'-N1	113.50	107.24	1
C4'-C3'-O3'	110.00	116.25	1
O-C-N	123.00	116.33	1
CA-CB-CG1	110.40	117.48	1
C3'-O3'-P	120.20	113.95	1
C1'-N1-C2	119.70	113.46	1
N-CA-CB	103.00	107.58	1
C4'-C3'-C2'	102.40	96.16	1
CD-NE-CZ	124.40	118.58	1
C4'-C3'-C2'	102.40	96.19	1
CA-CB-CG	114.10	122.38	1
CB-CG-CD2	120.80	114.59	1
OD1-CG-ND2	122.60	118.46	1
CA-C-O	120.80	113.76	1
CD2-NE2-CE1	109.00	104.86	1
C5'-C4'-C3'	114.90	121.11	1
CA-CB-CG	104.50	96.64	1
C2'-C1'-N9	113.50	119.70	1
NE-CZ-NH2	119.20	122.92	1
CA-CB-CG2	110.50	117.52	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CG-CD-CE	111.30	120.79	1
CA-CB-CG1	110.40	117.41	1
C-N-CA	121.70	129.12	1
C-N-CA	121.70	114.29	1
N-CA-CB	110.50	103.51	1
N1-C2-N3	118.90	125.07	1
CA-C-O	120.80	127.79	1
N-CA-CB	110.40	104.23	1
CA-CB-CG1	110.40	117.39	1
CA-CB-CG	114.10	105.88	1
CA-CB-CG	104.50	96.70	1
O4'-C1'-C2'	106.40	100.24	1
CB-CG-CD	112.60	105.62	1
C3'-C2'-C1'	101.60	95.45	1
O-C-N	123.00	129.56	1
O5'-C5'-C4'	110.80	104.65	1
C-N-CA	121.70	129.07	2
OP2-P-O5'	108.00	95.71	1
C5'-C4'-C3'	114.90	121.04	1
CA-N-CD	112.00	106.28	1
N-CA-CB	110.50	103.55	1
CA-CB-CG	104.50	96.74	1
O-C-N	123.00	116.47	2
C2-N3-C4	120.00	113.88	1
C-N-CA	121.70	129.04	1
O-C-N	123.00	116.48	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	114.36	1
CA-C-O	120.80	113.88	1
CB-CG-CD1	120.80	126.90	1
CA-C-O	120.80	113.89	1
C4-C5-C7	122.40	116.30	1
O-C-N	123.00	116.50	2
O3'-C3'-C2'	111.50	105.41	1
CB-CG1-CD1	113.80	122.32	1
O3'-P-OP1	108.00	120.18	1
C2-N1-C6	120.60	114.51	1
O3'-C3'-C2'	111.50	105.42	1
C-CA-CB	110.10	117.80	1
CA-C-N	116.20	108.10	1
CA-CB-CG	112.60	108.55	1
N-CA-C	112.10	122.21	1
CA-C-O	120.80	113.92	1
CB-CG-ND2	116.40	122.46	1
CA-CB-CG	114.10	122.18	1
CA-CB-CG	104.50	96.82	1
C-N-CA	121.70	128.97	1
CA-CB-CG	112.60	108.56	1
C-N-CA	121.70	114.44	1
C5'-C4'-O4'	109.40	115.45	1
CA-CB-CG	104.50	96.85	2
C4'-C3'-O3'	110.00	116.04	1
O-C-N	123.00	116.56	1
CA-C-O	120.80	113.96	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OD1-CG-ND2	122.60	118.58	1
O3'-P-O5'	104.00	110.02	1
C5'-C4'-C3'	114.90	120.91	1
O-C-N	123.00	116.59	1
C-N-CA	121.70	128.91	1
CA-C-N	116.20	108.19	1
CA-CB-CG	114.10	122.11	1
NE-CZ-NH1	121.50	125.50	1
H2'-C2'-H2"	103.00	109.00	1
C2'-C1'-H1'	115.00	109.00	1
O4'-C4'-H4'	102.99	109.00	1
C4'-C5'-H5"	115.04	109.00	1
C1'-C2'-H2"	115.04	109.00	1
C4-N4-H41	113.94	120.00	1
O4'-C4'-H4'	115.09	109.00	1
N1-C1'-H1'	115.09	109.00	1
C1'-C2'-H2"	115.10	109.00	1
C5'-C4'-H4'	102.84	109.00	1
H2'-C2'-H2"	102.84	109.00	1
H2'-C2'-H2"	102.83	109.00	1
C4-N4-H42	126.17	120.00	1
C4-N4-H42	126.19	120.00	1
O3'-C3'-H3'	102.81	109.00	1
C3'-C4'-H4'	102.79	109.00	1
O4'-C1'-H1'	102.79	109.00	1
H2'-C2'-H2"	102.78	109.00	1
C4'-C5'-H5"	102.77	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C1'-C2'-H2"	115.24	109.00	1
O4'-C1'-H1'	102.72	109.00	1
C3'-C2'-H2"	115.28	109.00	1
C3'-C2'-H2'	115.28	109.00	1
C3'-C4'-H4'	102.72	109.00	1
H2'-C2'-H2"	102.71	109.00	2
N1-C6-H6	125.81	119.50	1
C2'-C3'-H3'	115.32	109.00	1
C1'-C2'-H2'	115.32	109.00	1
O4'-C4'-H4'	115.33	109.00	1
C1'-C2'-H2'	115.33	109.00	1
H41-N4-H42	126.38	120.00	1
C6-C5-H5	114.81	121.20	1
H2'-C2'-H2"	102.61	109.00	1
C1'-C2'-H2"	115.40	109.00	1
C4'-C5'-H5"	115.41	109.00	1
C5'-C4'-H4'	102.59	109.00	1
H5'-C5'-H5"	102.53	109.00	1
N1-C6-H6	125.98	119.50	1
C1'-C2'-H2"	115.48	109.00	1
N1-C6-H6	126.01	119.50	1
O3'-C3'-H3'	115.53	109.00	1
O3'-C3'-H3'	102.47	109.00	1
H2'-C2'-H2"	102.45	109.00	1
C3'-C4'-H4'	102.44	109.00	1
C3'-C2'-H2'	102.44	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C3'-C2'-H2"	115.57	109.00	1
O4'-C1'-H1'	115.57	109.00	1
H5'-C5'-H5"	115.60	109.00	1
O3'-C3'-H3'	102.38	109.00	1
C3'-C2'-H2'	102.38	109.00	1
C4-N4-H41	126.63	120.00	1
C5'-C4'-H4'	102.34	109.00	1
C4'-C3'-H3'	115.73	109.00	1
C1'-C2'-H2"	115.76	109.00	1
C4'-C3'-H3'	115.78	109.00	1
C3'-C2'-H2"	115.78	109.00	1
H5'-C5'-H5"	115.80	109.00	1
O3'-C3'-H3'	102.19	109.00	1
C3'-C4'-H4'	102.19	109.00	1
C2'-C3'-H3'	115.85	109.00	1
C5'-C4'-H4'	102.15	109.00	1
C3'-C2'-H2'	102.14	109.00	1
C2'-C3'-H3'	115.92	109.00	1
C2'-C1'-H1'	115.92	109.00	1
C4-N4-H41	113.07	120.00	1
C3'-C2'-H2'	115.94	109.00	1
H5'-C5'-H5"	115.94	109.00	1
N1-C6-H6	126.49	119.50	1
C4'-C3'-H3'	116.02	109.00	1
O3'-C3'-H3'	101.96	109.00	1
C1'-C2'-H2"	116.08	109.00	1
C2'-C3'-H3'	101.91	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C4'-C3'-H3'	116.13	109.00	1
C3'-C2'-H2''	116.14	109.00	1
H41-N4-H42	112.85	120.00	1
N9-C1'-H1'	101.82	109.00	1
H2'-C2'-H2''	101.80	109.00	1
H5'-C5'-H5''	101.75	109.00	1
H2'-C2'-H2''	101.74	109.00	1
O3'-C3'-H3'	101.73	109.00	1
C5'-C4'-H4'	101.73	109.00	1
C3'-C4'-H4'	101.72	109.00	1
C5'-C4'-H4'	101.71	109.00	1
C4-N4-H41	112.70	120.00	1
C2'-C3'-H3'	116.30	109.00	1
C2'-C3'-H3'	116.31	109.00	1
C3'-C2'-H2''	116.38	109.00	1
C4'-C5'-H5''	116.38	109.00	1
C5'-C4'-H4'	101.61	109.00	1
C4-N4-H42	112.61	120.00	1
C3'-C4'-H4'	101.61	109.00	1
C1'-C2'-H2'	116.41	109.00	2
N1-C6-H6	112.08	119.50	1
C1'-C2'-H2'	116.44	109.00	1
C1'-C2'-H2''	101.56	109.00	1
C4'-C5'-H5''	116.46	109.00	1
C4'-C5'-H5'	116.46	109.00	1
C2'-C3'-H3'	116.47	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O4'-C4'-H4'	116.48	109.00	1
N1-C1'-H1'	101.51	109.00	1
C1'-C2'-H2''	101.48	109.00	1
C1'-C2'-H2''	116.54	109.00	1
C4'-C5'-H5'	101.45	109.00	1
O4'-C1'-H1'	116.56	109.00	1
O5'-C5'-H5'	116.61	109.00	1
C4'-C3'-H3'	101.39	109.00	1
C1'-C2'-H2''	116.64	109.00	1
O4'-C4'-H4'	116.64	109.00	1
O4'-C4'-H4'	116.65	109.00	1
N1-C1'-H1'	101.34	109.00	1
C1'-C2'-H2''	101.34	109.00	1
O5'-C5'-H5'	101.33	109.00	1
C5-C6-H6	127.21	119.50	1
O5'-C5'-H5'	101.28	109.00	1
C3'-C4'-H4'	101.27	109.00	1
C3'-C4'-H4'	101.25	109.00	1
C3'-C4'-H4'	116.77	109.00	1
C2'-C1'-H1'	116.82	109.00	1
O4'-C1'-H1'	101.17	109.00	1
O4'-C4'-H4'	116.83	109.00	1
C6-C5-H5	129.06	121.20	1
C4'-C3'-H3'	101.13	109.00	1
C2'-C1'-H1'	116.88	109.00	1
C6-C5-H5	113.28	121.20	1
O5'-C5'-H5'	101.08	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C4'-C5'-H5'	116.92	109.00	1
C3'-C2'-H2''	116.94	109.00	1
C5-C6-H6	111.55	119.50	1
C5'-C4'-H4'	101.04	109.00	1
C1'-C2'-H2''	117.03	109.00	1
C4'-C5'-H5''	117.04	109.00	1
C3'-C4'-H4'	100.95	109.00	1
O3'-C3'-H3'	117.07	109.00	1
C5-C6-H6	111.43	119.50	1
C1'-C2'-H2''	117.08	109.00	1
C2'-C3'-H3'	100.91	109.00	1
N1-C6-H6	127.59	119.50	1
C4-N4-H41	111.89	120.00	1
C5'-C4'-H4'	100.88	109.00	1
C1'-C2'-H2''	117.14	109.00	1
C1'-C2'-H2'	117.17	109.00	2
C1'-C2'-H2''	117.18	109.00	1
O4'-C4'-H4'	117.19	109.00	1
C1'-C2'-H2'	117.20	109.00	1
C4-C5-H5	129.43	121.20	1
H41-N4-H42	128.23	120.00	1
C4-N4-H42	111.76	120.00	1
C4'-C5'-H5''	100.76	109.00	1
C4-C5-H5	112.94	121.20	1
C3'-C2'-H2'	117.32	109.00	1
C1'-C2'-H2'	117.33	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C5'-C4'-H4'	100.66	109.00	1
H2'-C2'-H2''	100.64	109.00	1
O4'-C4'-H4'	117.38	109.00	1
C2'-C3'-H3'	117.39	109.00	2
C1'-C2'-H2''	100.58	109.00	1
C4-C5-H5	129.63	121.20	1
C4'-C5'-H5'	100.57	109.00	1
N1-C1'-H1'	100.56	109.00	1
C4-N4-H42	111.54	120.00	1
O3'-C3'-H3'	100.53	109.00	1
C3'-C2'-H2''	117.48	109.00	1
C2'-C3'-H3'	117.49	109.00	1
C4-N4-H41	111.47	120.00	1
C3'-C2'-H2''	117.60	109.00	1
C6-C5-H5	112.58	121.20	1
H2'-C2'-H2''	100.36	109.00	1
C4-N4-H42	128.67	120.00	1
C1'-C2'-H2'	117.68	109.00	1
C4'-C3'-H3'	117.68	109.00	1
O5'-C5'-H5'	117.73	109.00	1
O4'-C4'-H4'	117.75	109.00	1
C3'-C2'-H2''	117.75	109.00	1
O4'-C1'-H1'	100.19	109.00	1
O3'-C3'-H3'	100.19	109.00	1
C2'-C3'-H3'	117.81	109.00	1
C3'-C2'-H2'	117.88	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C4'-C5'-H5'	100.12	109.00	1
O5'-C5'-H5'	117.92	109.00	1
H2'-C2'-H2''	100.06	109.00	1
O5'-C5'-H5'	100.06	109.00	1
H2'-C2'-H2''	100.03	109.00	1
C1'-C2'-H2''	117.98	109.00	1
C1'-C2'-H2'	118.04	109.00	1
C6-C5-H5	130.25	121.20	1
C2'-C1'-H1'	118.07	109.00	1
O4'-C1'-H1'	99.91	109.00	1
C3'-C2'-H2''	118.10	109.00	1
O4'-C4'-H4'	118.11	109.00	1
O4'-C4'-H4'	118.16	109.00	1
C4-N4-H42	110.84	120.00	1
H5'-C5'-H5''	99.81	109.00	1
C3'-C4'-H4'	99.79	109.00	1
C5-C6-H6	110.28	119.50	1
O4'-C1'-H1'	118.22	109.00	1
O3'-C3'-H3'	99.72	109.00	1
C4'-C3'-H3'	118.28	109.00	1
N1-C1'-H1'	99.68	109.00	1
C4'-C5'-H5''	99.68	109.00	1
O4'-C4'-H4'	118.33	109.00	1
H2'-C2'-H2''	99.63	109.00	1
C1'-C2'-H2''	118.37	109.00	1
O4'-C4'-H4'	118.38	109.00	1
C1'-C2'-H2''	118.38	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O4'-C4'-H4'	118.42	109.00	1
C5-C6-H6	110.07	119.50	1
H41-N4-H42	110.50	120.00	1
C4'-C5'-H5"	118.52	109.00	1
C2'-C3'-H3'	118.53	109.00	1
C1'-C2'-H2"	118.61	109.00	1
C3'-C4'-H4'	99.32	109.00	1
O4'-C4'-H4'	118.73	109.00	1
C2'-C3'-H3'	118.76	109.00	1
C5-C6-H6	109.63	119.50	1
O4'-C4'-H4'	118.88	109.00	1
C4'-C5'-H5"	118.91	109.00	1
C4-N4-H41	110.05	120.00	1
O4'-C4'-H4'	119.03	109.00	2
C4-C5-H5	111.15	121.20	1
O5'-C5'-H5'	119.10	109.00	1
N1-C6-H6	129.62	119.50	1
C4-N4-H41	109.88	120.00	1
C2'-C3'-H3'	119.14	109.00	1
C1'-C2'-H2'	98.84	109.00	1
O4'-C4'-H4'	119.16	109.00	1
C1'-C2'-H2"	119.19	109.00	1
O4'-C4'-H4'	119.26	109.00	1
H41-N4-H42	130.30	120.00	1
H41-N4-H42	130.39	120.00	1
H5'-C5'-H5"	98.58	109.00	1
C4-N4-H42	109.53	120.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C6-C5-H5	131.69	121.20	1
O4'-C4'-H4'	119.54	109.00	1
C6-C5-H5	110.65	121.20	1
C4-N4-H41	109.44	120.00	1
C5-C6-H6	108.92	119.50	1
H2'-C2'-H2''	98.36	109.00	1
O4'-C4'-H4'	98.35	109.00	1
C2'-C3'-H3'	119.67	109.00	1
O4'-C4'-H4'	119.72	109.00	1
C3'-C2'-H2'	119.76	109.00	1
C3'-C4'-H4'	119.77	109.00	1
C4'-C3'-H3'	98.16	109.00	1
C1'-C2'-H2''	98.09	109.00	1
H5'-C5'-H5''	119.99	109.00	1
O4'-C4'-H4'	120.04	109.00	1
C4'-C5'-H5''	120.05	109.00	1
N1-C1'-H1'	97.91	109.00	1
O4'-C4'-H4'	120.11	109.00	1
C4'-C5'-H5'	120.19	109.00	1
C3'-C2'-H2''	120.22	109.00	1
C3'-C2'-H2''	120.29	109.00	1
O4'-C4'-H4'	120.29	109.00	1
C2'-C3'-H3'	120.44	109.00	1
C1'-C2'-H2'	120.47	109.00	1
H41-N4-H42	131.48	120.00	1
H41-N4-H42	131.49	120.00	1
C2'-C1'-H1'	97.51	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C4'-C3'-H3'	120.50	109.00	1
O4'-C4'-H4'	120.54	109.00	1
C3'-C2'-H2'	120.57	109.00	1
C4'-C3'-H3'	120.64	109.00	1
C4'-C3'-H3'	120.67	109.00	1
H5'-C5'-H5"	120.69	109.00	1
C1'-C2'-H2'	120.82	109.00	1
C3'-C2'-H2'	120.93	109.00	1
C3'-C2'-H2"	120.93	109.00	1
O4'-C4'-H4'	121.04	109.00	1
H41-N4-H42	132.06	120.00	1
C2'-C1'-H1'	121.06	109.00	1
C3'-C2'-H2'	121.25	109.00	1
C1'-C2'-1H2'	96.62	109.00	1
C1'-C2'-H2'	121.46	109.00	1
H5'-C5'-H5"	96.53	109.00	1
C2'-C3'-H3'	121.50	109.00	1
C2'-C3'-H3'	121.51	109.00	1
H2'-C2'-H2"	96.45	109.00	1
C6-C5-H5	108.47	121.20	1
O4'-C4'-H4'	121.80	109.00	1
C4-N4-H41	107.15	120.00	1
C1'-C2'-H2"	121.96	109.00	1
C4'-C5'-H5"	121.97	109.00	1
C3'-C4'-H4'	96.01	109.00	1
C4-C5-H5	108.20	121.20	1
C2'-C3'-H3'	122.06	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O4'-C4'-H4'	122.07	109.00	1
O5'-C5'-H5''	122.11	109.00	1
C3'-C2'-H2''	122.12	109.00	1
C3'-C2'-H2''	122.23	109.00	1
C6-C5-H5	107.94	121.20	1
C1'-C2'-2H2'	95.65	109.00	1
C3'-C4'-H4'	95.62	109.00	1
O4'-C1'-H1'	95.61	109.00	1
H41-N4-H42	133.46	120.00	1
O4'-C1'-H1'	122.76	109.00	1
C1'-C2'-H2''	95.23	109.00	1
C1'-C2'-H2'	122.82	109.00	1
O5'-C5'-H5'	122.90	109.00	1
C1'-C2'-H2'	122.94	109.00	1
N1-C6-H6	133.52	119.50	1
C1'-C2'-H2'	123.03	109.00	1
1H5'-C5'-2H5'	123.06	109.00	1
C3'-C2'-H2''	123.18	109.00	1
C4-C5-H5	106.98	121.20	1
C4'-C3'-H3'	123.23	109.00	1
C1'-C2'-H2'	123.29	109.00	1
H41-N4-H42	134.41	120.00	1
C3'-C2'-H2''	123.49	109.00	1
C2'-C3'-H3'	123.52	109.00	1
C2'-C1'-H1'	123.57	109.00	1
H5'-C5'-H5''	94.21	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O4'-C1'-H1'	123.85	109.00	1
C5-C6-H6	104.59	119.50	1
C4-N4-H42	135.31	120.00	1
C4-C5-H5	105.79	121.20	1
C1'-C2'-H2'	93.50	109.00	1
C4-N4-H42	104.33	120.00	1
C5-C6-H6	135.41	119.50	1
C2'-C1'-H1'	93.06	109.00	1
H41-N4-H42	136.00	120.00	1
C5-C6-H6	135.72	119.50	1
C3'-C2'-H2''	125.52	109.00	1
H2'-C2'-H2''	92.41	109.00	1
C5'-C4'-H4'	92.24	109.00	1
O4'-C1'-H1'	92.22	109.00	1
C3'-C2'-H2''	92.19	109.00	1
N1-C1'-H1'	126.48	109.00	1
O4'-C4'-H4'	126.53	109.00	1
O3'-C3'-H3'	91.02	109.00	1
C3'-C4'-H4'	90.58	109.00	1
N1-C6-H6	101.07	119.50	1
C5'-C4'-H4'	90.50	109.00	1
C3'-C4'-H4'	127.55	109.00	1
C3'-C2'-1H2'	127.59	109.00	1
O5'-C5'-1H5'	127.64	109.00	1
C3'-C2'-H2'	89.20	109.00	1
C5-C6-H6	99.61	119.50	1
C4'-C5'-H5'	129.07	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C6-C5-H5	141.42	121.20	1
O4'-C4'-H4'	129.47	109.00	1
C6-C5-H5	141.68	121.20	1
C4'-C5'-H5'	88.11	109.00	1
C2'-C3'-H3'	131.26	109.00	1
C3'-C4'-H4'	133.17	109.00	1
N1-C1'-H1'	83.57	109.00	1
C3'-C2'-H2''	83.11	109.00	1
C2'-C3'-H3'	81.47	109.00	1
C3'-C4'-H4'	80.21	109.00	1
C1'-C2'-H2''	138.88	109.00	1
O5'-C5'-H5'	140.05	109.00	1
H41-N4-H42	88.89	120.00	1
C4'-C5'-2H5'	76.84	109.00	1
C4-N4-H41	152.77	120.00	1
O5'-C5'-H5''	74.61	109.00	1
C1'-C2'-H2'	144.21	109.00	1
C3'-C2'-2H2'	144.54	109.00	1
C3'-C2'-H2''	144.56	109.00	1
O5'-C5'-2H5'	72.85	109.00	1
C4'-C3'-H3'	70.39	109.00	1
O4'-C4'-H4'	148.27	109.00	1
C3'-C2'-H2'	157.00	109.00	1
O4'-C4'-H4'	175.66	109.00	1
1H2'-C2'-2H2'	38.48	109.00	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	30.10	195

All 195 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:20:LEU:CD1	D:20:LEU:CG	1.628
1	D:180:LEU:HD21	E:11:DC:C5'	1.595
1	B:134:ALA:C	B:134:ALA:CA	1.584
1	D:180:LEU:CD2	E:11:DC:H5'	1.569
1	B:134:ALA:CA	B:134:ALA:N	1.558
1	B:129:ASN:CA	B:129:ASN:N	1.543
1	D:20:LEU:CA	D:20:LEU:CB	1.541
1	B:129:ASN:C	B:129:ASN:CA	1.539
1	B:130:SER:C	B:130:SER:CA	1.539
1	E:12:DC:C1'	E:12:DC:N1	1.527
1	B:133:SER:C	B:133:SER:CA	1.523
1	B:207:ASN:CA	B:207:ASN:CB	1.495
1	B:130:SER:CA	B:130:SER:N	1.480
1	D:20:LEU:C	D:20:LEU:CA	1.460
1	D:20:LEU:CA	D:20:LEU:N	1.454
1	D:98:MET:C	D:99:GLU:N	1.437
1	B:207:ASN:HB2	B:208:GLU:N	1.430
1	B:207:ASN:C	B:208:GLU:N	1.346
1	B:130:SER:C	B:130:SER:CB	1.294
1	B:207:ASN:CB	B:208:GLU:N	1.224
1	B:207:ASN:C	B:207:ASN:CB	1.218
1	F:1:DT:C2'	F:2:DT:H71	1.208
1	B:133:SER:C	B:133:SER:HA	1.130
1	B:130:SER:HB3	B:130:SER:O	1.128

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:180:LEU:HD21	E:11:DC:H5"	1.126
1	D:180:LEU:CD2	E:11:DC:C5'	1.122
1	B:130:SER:HA	B:130:SER:N	1.119
1	B:134:ALA:HA	B:134:ALA:N	1.104
1	D:131:ASP:OD1	E:13:DC:N4	1.095
1	F:1:DT:H2"	F:2:DT:C7	1.077
1	F:1:DT:H2"	F:2:DT:H71	1.076
1	D:180:LEU:HD23	E:11:DC:H5'	1.050
1	E:22:DC:C2	E:22:DC:C4	1.039
1	B:130:SER:C	B:130:SER:HB3	1.009
1	D:138:LEU:O	E:12:DC:OP1	0.986
1	D:131:ASP:CG	E:13:DC:N4	0.984
1	D:20:LEU:CD1	D:20:LEU:HG	0.965
1	B:129:ASN:HA	B:129:ASN:N	0.958
1	F:1:DT:C2'	F:2:DT:C7	0.922
1	D:150:LEU:HD11	D:186:ILE:HG23	0.884
1	B:172:ILE:HD13	B:181:LEU:HD23	0.878
1	E:12:DC:H1'	E:12:DC:N1	0.866
1	B:205:LEU:HA	B:208:GLU:HG2	0.854
1	D:98:MET:C	D:99:GLU:CA	0.853
1	F:1:DT:O3'	F:2:DT:H5"	0.853
1	D:131:ASP:OD2	E:13:DC:N4	0.844
1	D:131:ASP:OD1	E:13:DC:C4	0.826
1	F:1:DT:H2'	F:2:DT:H71	0.815
1	D:137:LYS:HD3	D:183:LYS:HD2	0.811
1	D:104:ILE:HA	D:112:PHE:HA	0.806
1	F:1:DT:H2"	F:2:DT:C5	0.800

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:207:ASN:C	B:207:ASN:HB2	0.790
1	B:165:GLN:HA	B:168:VAL:HG22	0.777
1	B:207:ASN:HB2	B:208:GLU:CA	0.759
1	F:1:DT:O3'	F:2:DT:C5'	0.750
1	B:134:ALA:C	B:134:ALA:CB	0.746
1	E:12:DC:C1'	E:12:DC:C2	0.743
1	F:4:DT:O3'	F:5:DT:O5'	0.735
1	D:178:MET:HE3	D:180:LEU:HD11	0.733
1	D:140:THR:H	D:143:GLU:HB2	0.731
1	B:130:SER:CB	B:130:SER:O	0.730
1	B:207:ASN:C	B:208:GLU:CA	0.722
1	F:1:DT:H2''	F:2:DT:C6	0.721
1	B:169:LEU:HD21	B:225:ALA:HB3	0.715
1	B:134:ALA:C	B:134:ALA:HA	0.695
1	D:20:LEU:CA	D:20:LEU:H	0.686
1	B:207:ASN:CA	B:207:ASN:CG	0.683
1	B:177:ARG:HH21	B:181:LEU:HA	0.666
1	B:130:SER:C	B:130:SER:OG	0.641
1	B:169:LEU:HD13	B:205:LEU:HD13	0.636
1	B:156:MET:HG2	B:158:ALA:HB2	0.625
1	D:154:ASP:HA	D:161:PRO:HG2	0.625
1	F:7:DT:H1'	F:8:DT:H5'	0.625
1	D:137:LYS:HB3	D:183:LYS:HG3	0.621
1	D:180:LEU:CD2	E:11:DC:C4'	0.608
1	D:227:ARG:HG2	D:239:THR:HA	0.605
1	B:207:ASN:CB	B:207:ASN:N	0.604
1	B:156:MET:CG	B:158:ALA:HB2	0.598

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:133:ASP:OD1	E:14:DC:N4	0.591
1	B:134:ALA:H	B:134:ALA:HA	0.589
1	D:178:MET:HE3	D:180:LEU:HD21	0.588
1	D:150:LEU:HD21	D:190:SER:HB3	0.587
1	B:131:GLN:HB3	B:132:PRO:HD3	0.585
1	F:2:DT:H2''	F:3:DT:H71	0.572
1	D:161:PRO:HB2	D:162:LEU:HD23	0.563
1	D:217:LYS:HD3	E:2:DC:H4'	0.563
1	D:160:PRO:HB2	D:161:PRO:HD3	0.558
1	F:1:DT:C2'	F:2:DT:C5	0.556
1	B:170:ASN:ND2	B:173:LYS:HE3	0.545
1	D:102:TYR:HD2	D:104:ILE:HG13	0.545
1	B:161:LEU:HB2	B:166:ASN:HD21	0.544
1	B:212:TYR:CD2	D:38:LEU:HD22	0.543
1	D:48:TYR:CE2	D:50:ALA:HB2	0.541
1	D:180:LEU:HD21	E:11:DC:H5'	0.535
1	D:113:MET:SD	D:124:PRO:HA	0.532
1	B:207:ASN:CA	B:208:GLU:N	0.528
1	D:103:VAL:HG12	D:113:MET:HB3	0.526
1	B:193:MET:CB	B:198:ILE:HD11	0.519
1	B:136:ARG:CG	B:137:ALA:H	0.518
1	B:168:VAL:HG12	B:190:LEU:HD12	0.512
1	B:169:LEU:HD11	B:210:HIS:HB3	0.511
1	D:102:TYR:CD2	D:104:ILE:HG13	0.510
1	D:20:LEU:C	D:20:LEU:CB	0.506
1	D:180:LEU:CD2	E:11:DC:H5''	0.503
1	B:133:SER:C	B:133:SER:CB	0.502

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:186:LEU:CD1	B:198:ILE:HD12	0.502
1	B:164:ALA:HB1	B:193:MET:HE1	0.497
1	B:208:GLU:HG3	B:210:HIS:ND1	0.486
1	D:98:MET:C	D:99:GLU:CB	0.485
1	B:129:ASN:C	B:129:ASN:HA	0.484
1	D:141:LYS:CG	D:155:LEU:HD13	0.484
1	B:139:ILE:HD13	B:140:SER:H	0.477
1	F:1:DT:H2'	F:2:DT:C7	0.477
1	B:173:LYS:HE2	B:226:GLU:HA	0.465
1	D:20:LEU:CB	D:20:LEU:CD1	0.463
1	B:212:TYR:HB3	D:38:LEU:HB3	0.458
1	D:180:LEU:HD23	E:11:DC:C5'	0.458
1	B:156:MET:HG3	B:157:PRO:HD2	0.457
1	D:20:LEU:CB	D:20:LEU:N	0.457
1	D:217:LYS:HB2	E:3:DC:OP2	0.456
1	D:141:LYS:HG3	D:155:LEU:HD13	0.455
1	D:121:PHE:CZ	D:182:LEU:HG	0.454
1	D:178:MET:CE	D:180:LEU:HD11	0.454
1	B:161:LEU:HB2	B:166:ASN:ND2	0.452
1	D:150:LEU:CD1	D:186:ILE:HG23	0.452
1	B:136:ARG:HD2	B:137:ALA:O	0.449
1	D:137:LYS:HB3	D:183:LYS:CG	0.449
1	F:6:DT:H1'	F:7:DT:H5'	0.449
1	B:169:LEU:CD1	B:210:HIS:HB3	0.448
1	B:169:LEU:HD22	B:210:HIS:HD2	0.448
1	D:139:ILE:HD11	D:183:LYS:HG2	0.446
1	B:177:ARG:HA	B:178:PRO:HD3	0.445

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:179:GLU:HA	B:219:HIS:NE2	0.445
1	D:143:GLU:O	D:147:GLU:HG2	0.445
1	B:219:HIS:CE1	B:221:LYS:HD2	0.444
1	D:65:ALA:HA	D:66:PRO:HD3	0.442
1	B:170:ASN:HA	B:173:LYS:HG2	0.440
1	B:183:PHE:CZ	B:195:VAL:HG23	0.440
1	F:1:DT:C6	F:2:DT:H73	0.440
1	D:139:ILE:HA	E:11:DC:O3'	0.438
1	D:183:LYS:HA	D:186:ILE:HD12	0.438
1	B:168:VAL:O	B:172:ILE:HG12	0.436
1	D:220:ASP:O	D:224:LYS:HG3	0.436
1	D:202:GLU:O	D:206:VAL:HG23	0.435
1	D:164:PHE:CD2	D:179:LYS:HB3	0.434
1	D:168:LYS:O	D:170:PRO:HD3	0.434
1	B:181:LEU:HD23	B:186:LEU:HD23	0.431
1	D:219:PHE:O	D:223:VAL:HG23	0.431
1	B:219:HIS:HE1	B:221:LYS:HD2	0.429
1	D:189:ARG:O	D:193:VAL:HG23	0.428
1	B:181:LEU:CD2	B:186:LEU:HD23	0.427
1	D:126:CYS:SG	D:128:ASN:HB3	0.427
1	B:170:ASN:HD22	B:173:LYS:HE3	0.426
1	D:137:LYS:HD3	D:183:LYS:CD	0.426
1	B:171:LEU:O	B:181:LEU:HD22	0.425
1	D:120:HIS:CB	D:165:ILE:HG12	0.425
1	D:226:LEU:O	D:230:VAL:HG23	0.425
1	F:1:DT:O3'	F:2:DT:H5'	0.425

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:129:CYS:HB3	D:136:HIS:CD2	0.423
1	D:141:LYS:HG3	D:155:LEU:HB3	0.422
1	D:20:LEU:C	D:20:LEU:HA	0.421
1	B:131:GLN:HB3	B:132:PRO:CD	0.419
1	D:166:VAL:HG13	D:177:ASP:OD1	0.419
1	D:180:LEU:CD2	E:11:DC:H4'	0.418
1	B:183:PHE:HZ	B:195:VAL:HG23	0.417
1	D:204:LYS:O	D:208:GLN:HG3	0.417
1	D:20:LEU:HB3	D:20:LEU:O	0.416
1	E:12:DC:C5	E:13:DC:H5	0.415
1	D:167:LYS:HB3	D:167:LYS:HE2	0.414
1	D:183:LYS:O	D:187:VAL:HG23	0.414
1	B:190:LEU:HD22	B:192:HIS:HE1	0.413
1	B:207:ASN:CG	B:207:ASN:N	0.412
1	D:99:GLU:HB3	D:102:TYR:HE1	0.412
1	D:137:LYS:HB3	D:183:LYS:CD	0.412
1	B:197:SER:O	B:200:GLN:HB3	0.411
1	B:193:MET:HB3	B:198:ILE:HD11	0.409
1	D:121:PHE:CE2	D:182:LEU:HG	0.409
1	D:159:GLU:CG	D:160:PRO:HD3	0.409
1	D:220:ASP:OD2	D:224:LYS:HE3	0.408
1	B:208:GLU:HG3	B:210:HIS:CG	0.407
1	D:63:LYS:HD3	D:64:ALA:N	0.407
1	D:210:ASN:O	D:214:MET:HG2	0.407
1	F:4:DT:O3'	F:5:DT:C5'	0.406
1	B:129:ASN:C	B:129:ASN:CB	0.405
1	B:168:VAL:HG12	B:190:LEU:CD1	0.405

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:130:ARG:CZ	D:130:ARG:HB3	0.405
1	D:178:MET:HE3	D:180:LEU:CD1	0.405
1	D:187:VAL:O	D:191:LEU:HG	0.405
1	D:167:LYS:O	D:177:ASP:HB2	0.404
1	D:150:LEU:CD2	D:190:SER:HB3	0.403
1	D:167:LYS:C	D:178:MET:H	0.403
1	D:208:GLN:O	D:212:GLU:HG2	0.403
1	B:139:ILE:HG23	B:140:SER:O	0.401
1	D:114:ASP:OD2	D:117:LEU:HD13	0.401
1	D:200:LEU:O	D:204:LYS:HG3	0.400

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	1006	872	97	37

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	882	790	32	60

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	3	VAL
1	A	4	PRO
1	A	10	PRO
1	A	65	PRO
1	A	82	ILE
1	A	85	LYS

Model ID	Chain	Residue ID	Residue type
1	A	106	PRO
1	A	114	PRO
1	A	153	ARG
1	A	161	LYS
1	A	192	PRO
1	A	221	PRO
1	A	224	PRO
1	A	273	GLN
1	A	277	PRO
1	A	292	GLU
1	A	300	PRO
1	A	306	LYS
1	A	324	GLU
1	A	326	PRO
1	A	414	PRO
1	A	422	ARG
1	B	5	PRO
1	B	44	PRO
1	B	58	PRO
1	B	78	PRO
1	B	79	PRO
1	B	88	HIS
1	B	105	PRO
1	B	121	ASN
1	B	130	SER
1	B	132	PRO

Model ID	Chain	Residue ID	Residue type
1	B	138	PRO
1	B	139	ILE
1	B	142	PRO
1	B	176	PRO
1	B	178	PRO
1	B	197	SER
1	B	211	ILE
1	C	6	PRO
1	C	22	PRO
1	C	56	PRO
1	C	61	ILE
1	C	64	ILE
1	C	91	PRO
1	C	108	PRO
1	C	112	PRO
1	D	9	PRO
1	D	17	PRO
1	D	20	LEU
1	D	21	PRO
1	D	47	PRO
1	D	63	LYS
1	D	66	PRO
1	D	94	PRO
1	D	96	PRO
1	D	124	PRO
1	D	170	PRO
1	D	172	HIS

Model ID	Chain	Residue ID	Residue type
1	D	178	MET

Fit of model to data used for modeling

SAS data used in this integrative model could not be validated as the sascif file is currently unavailable.

Fit of model to data used for validation

Validation for this section is under development.

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