

Integrative Structure Validation Report

July 22, 2024 - 05:23 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	9A3O
PDB-Dev ID	PDBDEV_00000209
Structure Title	CLOCK-BMAL1 bound to a nucleosome at SHL -6.2
Structure Authors	Michael, A.K.; Kempf, G.; Cavadini, S.; Thoma, N.

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

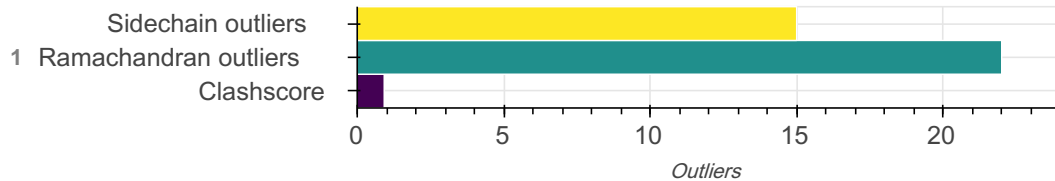
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the  symbol.

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 16 subunits in each model. A total of 5 datasets or restraints were used to build this entry. Each model is represented by 0 rigid bodies and 16 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	Histone H3.1	A	A	139
1	2	1	Histone H3.1	E	E	139
1	3	2	Histone H4	B	B	106
1	4	2	Histone H4	F	F	106
1	5	3	Histone H2A	C	C	133
1	6	3	Histone H2A	G	G	133
1	7	4	Histone H2B	D	D	128
1	8	4	Histone H2B	H	H	128
1	9	5	DNA (128-MER)	I	I	153
1	10	6	DNA (128-MER)	J	J	153
1	11	7	Circadian locomoter output cycles protein kaput	K	M	84

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	12	7	Circadian locomoter output cycles protein kaput	K	M	280
1	13	7	Circadian locomoter output cycles protein kaput	K	M	11
1	14	8	Basic helix-loop-helix ARNT-like protein 1	L	N	71
1	15	8	Basic helix-loop-helix ARNT-like protein 1	L	N	305
1	16	8	Basic helix-loop-helix ARNT-like protein 1	L	N	8

Datasets used for modeling

There are 5 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
2	Crosslinking-MS data	PRIDE	PXD033181
1	3DEM volume	EMDB	EMD-17155
3	Experimental model	PDB	6T93
4	Experimental model	PDB	4F3L
5	Experimental model	PDB	8OSJ

Representation

This entry has only one representation and includes 0 rigid bodies and 16 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	-	1-139
E	-	1-139

Chain ID	Rigid bodies	Non-rigid segments
B	-	1-106
F	-	1-106
C	-	1-133
G	-	1-133
D	-	1-128
H	-	1-128
I	-	1-153
J	-	1-153
K	-	1-84, 85-364, 365-375
L	-	1-71, 72-376, 377-384

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	Manual fitting	Manual fitting	None	None	False	False
2	1	Rosetta Dock	Rosetta Dock with crosslink filter and density scoring	None	None	False	False

There are 2 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
2	Coot	0.9.6	model building	https://www2.mrc-lmb.cam.ac.uk/personal/pemsley/coot/

ID	Software name	Software version	Software classification	Software location
1	Rosetta	Not available	protein docking and model building	https://www.rosettacommons.org/

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

Standard geometry: bond outliers ?

Bond length outliers can not be evaluated for this model

Standard geometry: angle outliers ?

There are 993 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
CA-N-CD	112.00	24.76	1
N-CD-CG	103.20	17.34	1
CA-N-CD	112.00	36.33	1
CA-N-CD	112.00	36.82	1
N-CD-CG	103.20	26.13	1
N-CD-CG	103.20	28.09	1
N-CD-CG	103.20	28.39	1
C1'-N1-C2	119.70	47.64	1
C1'-N1-C2	119.70	47.67	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C1'-N1-C2	119.70	47.72	1
C1'-N1-C2	119.70	47.73	2
C1'-N1-C2	119.70	47.74	1
C1'-N1-C2	119.70	47.77	1
C1'-N1-C2	119.70	47.83	1
C1'-N1-C2	119.70	47.84	1
C1'-N1-C2	119.35	47.52	1
C1'-N1-C2	119.70	47.89	1
C1'-N1-C2	119.70	47.90	2
C1'-N1-C2	119.70	47.93	1
C1'-N1-C2	119.70	47.94	1
C1'-N1-C2	119.70	47.96	1
C1'-N1-C2	119.70	47.97	1
C1'-N1-C2	119.70	47.98	1
C1'-N1-C2	119.35	47.64	1
C1'-N1-C2	119.35	47.66	1
C1'-N1-C2	119.35	47.69	1
C1'-N1-C2	119.70	48.05	1
C1'-N1-C2	119.35	47.74	1
C1'-N1-C2	119.35	47.90	1
C1'-N1-C2	119.35	47.92	1
C1'-N1-C2	119.35	47.94	1
C1'-N1-C2	119.35	47.96	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C1'-N1-C2	119.35	48.04	2
CA-N-CD	112.00	46.58	1
CA-N-CD	112.00	46.83	1
C1'-N1-C2	119.70	50.02	1
C1'-N1-C2	119.70	50.12	1
C1'-N1-C2	119.70	50.24	1
C1'-N1-C2	119.70	50.29	1
C1'-N1-C2	119.70	50.32	1
C1'-N1-C2	119.70	50.36	1
C1'-N1-C2	119.70	50.37	1
C1'-N1-C2	119.35	50.03	1
C1'-N1-C2	119.70	50.39	1
C1'-N1-C2	119.70	50.44	1
C1'-N1-C2	119.35	50.14	1
C1'-N1-C2	119.70	50.50	1
C1'-N1-C2	119.35	50.16	2
C1'-N1-C2	119.35	50.19	1
C1'-N1-C2	119.35	50.24	1
C1'-N1-C2	119.70	50.62	1
C1'-N1-C2	119.35	50.28	1
C1'-N1-C2	119.70	50.65	1
C1'-N1-C2	119.70	50.66	1
C1'-N1-C2	119.35	50.34	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C1'-N1-C2	119.70	50.70	1
C1'-N1-C2	119.35	50.42	1
C1'-N1-C2	119.35	50.46	1
C1'-N1-C2	119.70	50.83	1
C1'-N1-C2	119.35	50.53	1
C1'-N1-C2	119.35	50.54	1
CA-N-CD	112.00	47.84	1
C1'-N1-C2	119.35	50.63	1
C1'-N1-C2	119.70	51.03	1
C1'-N1-C2	119.70	51.08	1
C1'-N1-C2	119.35	50.74	1
C1'-N1-C2	119.70	51.11	1
C1'-N1-C2	119.35	50.80	1
C1'-N1-C2	119.35	50.85	1
C1'-N1-C2	119.35	50.86	1
C1'-N1-C2	119.35	50.95	1
N-CD-CG	103.20	34.87	1
C1'-N1-C2	119.35	51.08	1
N-CD-CG	103.20	35.06	1
CA-N-CD	112.00	56.12	1
N-CD-CG	103.20	43.89	1
N-CD-CG	103.20	44.77	1
CA-N-CD	112.00	60.79	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-N-CD	112.00	62.42	1
C1'-N1-C6	119.70	69.74	1
C1'-N1-C6	119.70	69.94	1
C1'-N1-C6	119.70	70.09	1
C1'-N1-C6	119.70	70.31	1
C1'-N1-C6	119.70	70.42	1
C1'-N1-C6	119.35	70.14	1
C1'-N1-C6	119.70	70.58	1
C1'-N1-C6	119.70	70.65	2
C1'-N1-C6	119.70	70.66	2
C1'-N1-C6	119.70	70.68	1
C1'-N1-C6	119.70	70.69	1
C1'-N1-C6	119.35	70.34	1
C1'-N1-C6	119.35	70.36	1
C1'-N1-C6	119.70	70.72	1
C1'-N1-C6	119.70	70.74	1
C1'-N1-C6	119.35	70.40	1
C1'-N1-C6	119.70	70.77	1
C1'-N1-C6	119.70	70.78	1
C1'-N1-C6	119.70	70.79	1
C1'-N1-C6	119.35	70.51	1
C1'-N1-C6	119.35	70.55	1
C1'-N1-C6	119.70	71.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C1'-N1-C6	119.35	70.73	1
C1'-N1-C6	119.35	70.79	1
C1'-N1-C6	119.35	70.81	1
C1'-N1-C6	119.35	70.88	1
C1'-N1-C6	119.35	70.98	1
C1'-N1-C6	119.70	73.76	1
C1'-N1-C6	119.70	73.83	1
C1'-N1-C6	119.70	73.93	1
C1'-N1-C6	119.70	73.95	1
C1'-N1-C6	119.35	73.66	1
C1'-N1-C6	119.70	74.08	2
C1'-N1-C6	119.35	73.77	1
C1'-N1-C6	119.70	74.13	1
C1'-N1-C6	119.70	74.14	1
C1'-N1-C6	119.70	74.20	2
C1'-N1-C6	119.35	73.85	1
C1'-N1-C6	119.70	74.22	1
C1'-N1-C6	119.70	74.26	1
C1'-N1-C6	119.70	74.27	1
C1'-N1-C6	119.70	74.28	1
C1'-N1-C6	119.35	73.97	1
C1'-N1-C6	119.70	74.35	1
C1'-N1-C6	119.35	74.03	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C1'-N1-C6	119.70	74.41	1
C1'-N1-C6	119.70	74.54	1
C1'-N1-C6	119.35	74.22	1
C1'-N1-C6	119.35	74.24	3
C1'-N1-C6	119.35	74.25	1
C1'-N1-C6	119.35	74.26	1
C1'-N1-C6	119.35	74.28	1
C1'-N1-C6	119.35	74.31	1
C1'-N1-C6	119.70	74.68	1
C1'-N1-C6	119.35	74.41	1
C1'-N1-C6	119.35	74.45	1
C1'-N1-C6	119.35	74.46	1
C1'-N1-C6	119.35	74.50	1
C1'-N1-C6	119.35	74.54	1
C1'-N1-C6	119.35	74.64	1
N-CD-CG	103.20	58.93	1
C2'-C1'-N1	113.50	138.99	1
C2'-C1'-N1	113.50	138.72	1
C2'-C1'-N1	113.50	138.39	1
CB-CG-CD2	131.20	109.98	1
C2'-C1'-N1	113.50	137.22	1
C2'-C1'-N1	113.50	136.44	1
C2'-C1'-N1	113.50	135.26	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C2'-C1'-N1	113.50	134.82	1
C2'-C1'-N1	113.50	134.20	1
C2'-C1'-N1	113.50	134.03	1
C2'-C1'-N1	113.50	133.93	1
C2'-C1'-N1	113.50	133.78	1
C2'-C1'-N1	113.50	133.75	1
C2'-C1'-N1	113.50	133.35	1
CB-CG-CD2	126.80	108.74	1
C2'-C1'-N1	113.50	132.73	1
C2'-C1'-N1	113.50	132.34	1
C2'-C1'-N1	113.50	132.27	1
C2'-C1'-N1	113.50	132.21	1
C2'-C1'-N1	113.50	132.17	1
C2'-C1'-N1	113.50	132.11	1
C2'-C1'-N1	113.50	131.92	1
C2'-C1'-N1	113.50	131.85	1
C2'-C1'-N1	113.50	131.84	1
C2'-C1'-N1	113.50	131.79	1
C2'-C1'-N1	113.50	131.66	1
C2'-C1'-N1	113.50	131.64	1
C2'-C1'-N1	113.50	131.60	1
C2'-C1'-N1	113.50	131.58	1
C2'-C1'-N1	113.50	131.55	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C2'-C1'-N1	113.50	131.52	1
C2'-C1'-N1	113.50	131.46	1
C2'-C1'-N1	113.50	131.37	1
C2'-C1'-N1	113.50	131.30	1
C2'-C1'-N1	113.50	131.29	1
C2'-C1'-N1	113.50	131.21	1
C2'-C1'-N1	113.50	131.04	1
C2'-C1'-N1	113.50	131.02	1
C2'-C1'-N1	113.50	130.93	1
C2'-C1'-N1	113.50	130.50	1
C2'-C1'-N1	113.50	130.42	1
C2'-C1'-N1	113.50	130.38	1
C2'-C1'-N1	113.50	130.30	1
C2'-C1'-N1	113.50	130.20	1
C2'-C1'-N1	113.50	130.07	1
C2-N3-C4	127.00	110.46	1
CB-CG-CD1	126.90	110.36	1
C2'-C1'-N1	113.50	130.02	1
C2-N3-C4	110.80	127.28	1
C2-N3-C4	127.00	110.54	1
C2'-C1'-N1	113.50	129.95	1
C2-N3-C4	110.80	127.24	1
C2-N3-C4	127.00	110.57	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C2-N3-C4	127.00	110.58	1
C2-N3-C4	127.00	110.59	1
C2-N3-C4	110.80	127.21	1
C2-N3-C4	127.00	110.60	1
C2-N3-C4	110.80	127.20	1
C2-N3-C4	127.00	110.63	1
C2-N3-C4	110.80	127.16	1
C2-N3-C4	127.00	110.64	1
C2-N3-C4	127.00	110.65	1
C2-N3-C4	127.00	110.67	1
C2-N3-C4	110.80	127.09	1
C2-N3-C4	110.80	127.08	1
C2'-C1'-N1	113.50	129.73	1
C2-N3-C4	127.00	110.78	1
C2-N3-C4	110.80	127.01	1
C2-N3-C4	110.80	126.94	1
CG-CD2-CE2	107.20	120.08	1
C2-N3-C4	110.80	126.89	1
C2-N3-C4	110.80	126.88	1
C2-N3-C4	110.80	126.84	1
C2'-C1'-N1	113.50	129.52	1
C2'-C1'-N1	113.50	129.46	1
C2'-C1'-N1	113.50	129.43	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C2'-C1'-N1	113.50	129.41	1
C2'-C1'-N1	113.50	129.27	1
C2'-C1'-N1	113.50	129.24	1
C2-N3-C4	111.80	127.47	1
C2'-C1'-N1	113.50	129.11	1
C2'-C1'-N1	113.50	129.05	1
C2-N3-C4	111.80	127.33	1
C2-N3-C4	111.80	127.29	2
C2'-C1'-N1	113.50	128.93	1
C2-N3-C4	111.80	127.22	1
C2-N3-C4	111.80	127.21	1
C2-N3-C4	111.80	127.19	1
C2-N3-C4	111.80	127.17	1
C2'-C1'-N1	113.50	128.84	1
C2-N3-C4	111.80	127.12	1
C2-N3-C4	111.80	127.03	2
C2-N3-C4	127.00	111.79	1
C2-N3-C4	127.00	111.80	1
C2-N3-C4	111.80	126.99	1
C2-N3-C4	127.00	111.83	1
C2-N3-C4	127.00	111.85	1
C2'-C1'-N1	113.50	128.63	1
C2-N3-C4	127.00	111.87	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C2-N3-C4	127.00	111.89	2
C2-N3-C4	127.00	111.90	1
C2-N3-C4	111.80	126.89	2
C2-N3-C4	127.00	111.91	1
C2-N3-C4	127.00	111.93	1
C2-N3-C4	127.00	111.94	2
C2-N3-C4	127.00	111.95	1
C2-N3-C4	111.80	126.85	1
C2'-C1'-N1	113.50	128.54	1
C2-N3-C4	127.00	111.97	1
C2'-C1'-N1	113.50	128.53	1
C2-N3-C4	127.00	111.98	1
C2-N3-C4	127.00	111.99	1
C2-N3-C4	127.00	112.00	2
C2-N3-C4	127.00	112.09	1
C2'-C1'-N1	113.50	128.34	1
C2'-C1'-N1	113.50	128.33	1
N1-C2-N3	114.80	129.62	1
N1-C2-N3	114.80	129.48	1
N1-C2-N3	129.00	114.38	1
N1-C2-N3	114.80	129.41	1
N1-C2-N3	114.80	129.39	1
N1-C2-N3	129.00	114.41	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N1-C2-N3	114.80	129.36	1
N1-C2-N3	129.00	114.46	1
C2'-C1'-N1	113.50	128.03	1
N1-C2-N3	114.80	129.32	1
N1-C2-N3	129.00	114.48	1
N1-C2-N3	129.00	114.52	1
N1-C2-N3	114.80	129.28	1
N1-C2-N3	129.00	114.55	1
N1-C2-N3	114.80	129.24	1
N1-C2-N3	129.00	114.57	1
N1-C2-N3	114.80	129.21	1
N1-C2-N3	129.00	114.60	2
C2'-C1'-N1	113.50	127.87	1
N1-C2-N3	114.80	129.17	2
N1-C2-N3	129.00	114.64	1
N1-C2-N3	129.00	114.65	1
C2'-C1'-N1	113.50	127.78	1
N1-C2-N3	129.00	114.75	1
C2'-C1'-N1	113.50	127.67	1
C5-C4-N3	114.80	128.88	1
C5-C4-N3	114.80	128.85	1
C5-C4-N3	114.80	128.78	1
CB-CG-CD2	131.20	119.09	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C5-C4-N3	114.80	128.77	1
C5-C4-N3	114.80	128.76	1
C5-C4-N3	114.80	128.74	1
C5-C4-N3	114.80	128.73	1
C5-C4-N3	114.80	128.72	2
C5-C4-N3	114.80	128.68	2
C5-C4-N3	114.80	128.66	1
CA-CB-CG	113.80	104.59	1
C5-C4-N3	114.80	128.60	1
O4'-C1'-N1	108.40	122.18	1
C5-C4-N3	114.80	128.54	1
C5-C4-N3	114.80	128.42	3
C5-C4-N3	114.80	128.35	1
C5-C4-N3	114.80	128.30	1
C2'-C1'-N1	113.50	126.97	1
N3-C4-C5	128.40	115.03	1
CA-CB-CG	113.80	104.92	1
O4'-C1'-N1	108.40	121.72	1
N3-C4-C5	128.40	115.11	1
O4'-C1'-N1	108.40	121.69	1
N3-C4-C5	128.40	115.17	1
CB-CG-CD2	131.20	119.73	1
N3-C4-C5	128.40	115.19	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N3-C4-C5	128.40	115.20	2
N3-C4-C5	128.40	115.21	1
N3-C4-C5	128.40	115.23	1
O4'-C1'-N1	108.40	121.54	1
N3-C4-C5	128.40	115.28	1
N3-C4-C5	128.40	115.30	1
N3-C4-C5	128.40	115.31	1
CB-CG-CD2	131.20	119.86	2
N3-C4-C5	128.40	115.36	1
O4'-C1'-N1	108.40	121.43	1
N3-C4-C5	128.40	115.40	1
N3-C4-C5	128.40	115.43	1
N3-C4-C5	128.40	115.47	1
CA-CB-CG	112.60	104.02	1
CD1-CG-CD2	106.30	119.94	1
O4'-C1'-N1	108.40	121.15	1
O4'-C1'-N1	108.40	121.12	1
O4'-C1'-N1	108.40	121.08	2
CB-CG-CD2	131.20	120.30	1
O4'-C1'-N1	108.40	120.82	1
N-CA-CB	103.00	112.07	1
O4'-C1'-N1	108.40	120.72	1
N-CA-CB	103.00	111.95	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C5-C4-N3	114.80	126.95	1
N1-C6-C5	111.70	123.83	3
N-CA-CB	103.00	111.89	1
N1-C6-C5	111.70	123.82	1
O4'-C1'-N1	108.40	120.51	1
N1-C6-C5	111.70	123.81	2
CB-CG-CD2	131.20	120.72	1
N1-C6-C5	111.70	123.79	2
N1-C6-C5	111.70	123.78	1
N1-C6-C5	111.70	123.77	1
C5-C4-N3	114.80	126.86	2
N1-C6-C5	111.70	123.75	2
O4'-C1'-N1	108.40	120.45	1
C5-C4-N3	114.80	126.85	1
C5-C4-N3	114.80	126.84	1
N1-C6-C5	111.70	123.74	1
C5-C4-N3	114.80	126.78	1
C5-C4-N3	114.80	126.77	1
C5-C4-N3	114.80	126.76	1
N1-C6-C5	111.70	123.62	1
C5-C4-N3	114.80	126.71	1
O4'-C1'-N1	108.40	120.31	1
C-N-CD	125.00	157.54	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	103.00	111.73	1
O4'-C1'-N1	108.40	120.27	1
N1-C6-C5	111.70	123.57	1
N-CA-CB	103.00	111.68	1
C-N-CD	125.00	157.35	1
O4'-C1'-N1	108.40	120.23	1
C5-C4-N3	114.80	126.62	1
N3-C4-C5	126.90	115.08	1
CB-CG-CD2	120.80	109.07	1
N3-C4-C5	126.90	115.18	1
N3-C4-C5	126.90	115.19	1
N3-C4-C5	126.90	115.22	1
C5-C4-N3	114.80	126.45	1
N3-C4-C5	126.90	115.25	2
CB-CG-CD2	120.80	109.15	1
N-CA-CB	103.00	111.54	1
N3-C4-C5	126.90	115.29	1
N-CA-CB	103.00	111.48	1
N3-C4-C5	126.90	115.35	1
N3-C4-C5	126.90	115.36	1
N3-C4-C5	126.90	115.37	1
O4'-C1'-N1	108.40	119.93	1
N3-C4-C5	126.90	115.38	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD2	120.80	109.29	1
N3-C4-C5	126.90	115.44	1
N-CA-CB	103.00	111.38	1
N-CA-CB	103.00	111.34	1
O4'-C1'-N1	108.40	119.77	1
C5-C6-N1	122.80	111.46	1
C-N-CD	125.00	155.96	1
C5-C6-N1	122.80	111.49	1
N-CA-CB	103.00	111.28	1
O4'-C1'-N1	108.40	119.67	1
N-CA-CB	103.00	111.24	1
C5-C6-N1	122.80	111.57	3
C5-C6-N1	122.80	111.59	1
C5-C6-N1	122.80	111.60	2
C5-C6-N1	122.80	111.64	1
C5-C6-N1	122.80	111.65	1
C-N-CD	125.00	155.48	1
N-CA-CB	103.00	111.18	1
C5-C6-N1	122.80	111.69	1
C5-C6-N1	122.80	111.72	1
C5-C6-N1	122.80	111.74	3
C5-C6-N1	122.80	111.76	1
O4'-C1'-N1	108.40	119.43	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C5-C6-N1	122.80	111.77	1
N-CA-CB	103.00	111.08	1
N-CA-CB	103.00	111.07	1
N-CA-CB	103.00	111.06	1
C5-C6-N1	122.80	111.82	1
C5-C6-N1	122.80	111.84	1
N-CA-CB	103.00	111.03	1
CB-CG-CD1	120.80	109.87	1
CB-CG-CD1	120.80	109.90	1
N-CA-CB	103.00	110.97	1
N-CA-CB	103.00	110.94	1
O4'-C1'-N1	108.40	119.19	1
O4'-C1'-N1	108.40	119.11	1
N-CA-CB	103.00	110.85	1
O4'-C1'-N1	108.40	119.09	1
O4'-C1'-N1	108.40	119.08	1
N1-C2-N3	118.90	129.53	1
N-CA-CB	103.00	110.79	1
N1-C2-N3	118.90	129.47	2
CB-CG-CD2	120.70	108.73	1
CB-CG-CD1	120.80	110.24	1
O4'-C1'-N1	108.40	118.96	1
N-CA-CB	103.00	110.74	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N1-C2-N3	118.90	129.46	1
N-CA-CB	103.00	110.72	2
N1-C2-N3	118.90	129.43	1
N1-C2-N3	118.90	129.42	1
N-CA-CB	103.00	110.70	1
N1-C2-N3	118.90	129.38	1
N1-C2-N3	118.90	129.35	1
N-CA-CB	103.00	110.66	1
N1-C2-N3	118.90	129.33	2
O4'-C1'-N1	108.40	118.83	1
N-CA-CB	103.00	110.64	1
N1-C2-N3	118.90	129.29	1
N1-C2-N3	118.90	129.28	2
N1-C2-N3	118.90	129.27	1
N-CA-CB	103.00	110.58	1
CB-CG-CD2	110.70	131.34	1
CB-CG-CD2	110.70	131.33	1
N1-C2-N3	118.90	129.20	1
N1-C2-N3	118.90	129.19	1
O4'-C1'-N1	108.40	118.68	1
N1-C2-N3	118.90	129.18	1
N-CA-CB	103.00	110.53	1
N1-C2-N3	118.90	129.16	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD2	110.70	131.12	2
CB-CG-CD2	120.70	109.13	1
O4'-C1'-N1	108.40	118.57	1
CB-CG-CD2	120.70	109.19	1
N-CA-CB	103.00	110.45	1
CB-CG-CD2	110.70	131.00	1
CB-CG-CD2	110.70	130.94	1
N-CA-CB	103.00	110.42	1
N-CA-CB	103.00	110.41	1
N-CA-CB	103.00	110.40	1
N-CA-CB	103.00	110.39	2
N-CA-CB	103.00	110.38	2
CB-CG-CD2	120.70	109.37	1
CB-CG-CD2	120.80	130.72	1
N1-C2-N3	129.00	119.09	1
N-CA-CB	103.00	110.24	1
N-CA-CB	103.00	110.22	1
N-CA-CB	103.00	110.21	1
N1-C2-N3	129.00	119.18	1
N1-C2-N3	129.00	119.19	1
N1-C2-N3	129.00	119.20	1
N-CA-CB	103.00	110.18	1
N1-C6-C5	111.70	121.49	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	104.50	116.88	1
N-CA-CB	103.00	110.15	2
N-CA-CB	103.00	110.14	1
N1-C2-N3	129.00	119.27	1
CB-CG-CD2	120.70	109.68	1
N1-C2-N3	129.00	119.29	1
N-CA-CB	103.00	110.12	1
CB-CG-CD1	120.70	109.70	1
N1-C2-N3	129.00	119.31	1
N-CA-CB	103.00	110.09	1
N1-C2-N3	129.00	119.34	1
N1-C2-N3	129.00	119.36	1
N1-C6-C5	111.70	121.34	1
N1-C6-C5	111.70	121.33	1
N1-C2-N3	129.00	119.37	1
N-CA-CB	103.00	110.05	1
N1-C6-C5	111.70	121.32	1
N1-C2-N3	124.00	114.39	1
N1-C2-N3	129.00	119.39	1
CB-CG-CD2	120.70	109.81	1
O4'-C1'-N1	108.40	118.00	1
N1-C6-C5	111.70	121.30	1
N1-C6-C5	111.70	121.29	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	103.00	110.04	1
N1-C2-N3	124.00	114.41	1
N1-C6-C5	111.70	121.28	2
N1-C2-N3	124.00	114.42	1
C2-N3-C4	110.80	120.38	1
N1-C6-C5	111.70	121.25	1
N1-C2-N3	124.00	114.47	1
N1-C6-C5	111.70	121.23	1
N1-C2-N3	129.00	119.48	1
N1-C2-N3	124.00	114.48	1
N1-C6-C5	111.70	121.22	1
N-CA-CB	103.00	109.98	1
CB-CG-CD1	120.70	109.93	1
C2-N3-C4	120.00	110.49	1
N1-C6-C5	111.70	121.21	1
N1-C6-C5	111.70	121.20	1
N1-C2-N3	124.00	114.51	2
C5-C6-N1	121.00	111.51	1
C2-N3-C4	120.00	110.52	2
N1-C2-N3	124.00	114.52	2
C5-C6-N1	121.00	111.53	1
N1-C6-C5	111.70	121.17	2
N-CA-CB	103.00	109.94	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C5-C6-N1	121.00	111.54	1
C2-N3-C4	120.00	110.54	1
N1-C2-N3	114.80	124.25	1
N1-C2-N3	124.00	114.55	1
C2-N3-C4	120.00	110.55	1
N1-C2-N3	124.00	114.56	1
C2-N3-C4	120.00	110.56	1
C5-C6-N1	121.00	111.56	1
N1-C6-C5	111.70	121.13	4
C2-N3-C4	120.00	110.57	1
N1-C2-N3	129.00	119.58	1
C2-N3-C4	120.00	110.59	3
N1-C2-N3	114.80	124.21	1
N1-C6-C5	111.70	121.10	1
C-N-CD	125.00	150.70	1
CB-CG-CD1	120.70	110.05	1
N1-C2-N3	114.80	124.19	1
N1-C2-N3	124.00	114.62	1
N1-C6-C5	111.70	121.08	1
C5-C6-N1	121.00	111.63	1
C2-N3-C4	120.00	110.63	1
CA-CB-CG	104.50	116.37	1
N1-C2-N3	114.80	124.17	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N1-C2-N3	124.00	114.63	1
N1-C6-C5	111.70	121.07	1
N1-C2-N3	114.80	124.16	3
C5-C6-N1	121.00	111.64	1
C2-N3-C4	120.00	110.64	1
C5-C6-N1	121.00	111.65	1
N1-C6-C5	111.70	121.05	1
N1-C6-C5	111.70	121.04	2
C2-N3-C4	120.00	110.66	1
C5-C6-N1	121.00	111.66	1
O4'-C1'-N1	108.40	117.73	1
C5-C6-N1	121.00	111.67	1
N1-C6-C5	111.70	121.02	1
CB-CG-CD1	120.70	110.14	1
CA-CB-CG	104.50	116.30	1
C5-C6-N1	121.00	111.68	1
C2-N3-C4	110.80	120.12	1
N1-C2-N3	114.80	124.11	1
C2-N3-C4	110.80	120.11	1
N1-C6-C5	111.70	121.01	1
C2-N3-C4	120.00	110.69	1
N1-C2-N3	114.80	124.10	1
CB-CG-CD2	120.70	131.24	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C2-N3-C4	120.00	110.70	1
N1-C2-N3	114.80	124.09	2
C5-C6-N1	121.00	111.71	1
N1-C2-N3	114.80	124.08	1
C5-C6-N1	121.00	111.73	1
N1-C2-N3	124.00	114.73	1
N1-C2-N3	114.80	124.06	1
O4'-C1'-N1	108.40	117.66	1
CB-CG-CD1	120.70	110.22	1
N1-C2-N3	124.00	114.75	1
C5-C6-N1	121.00	111.77	2
N1-C2-N3	114.80	124.03	2
C5-C6-N1	121.00	111.78	1
CB-CG-CD1	120.70	110.26	1
C5-C6-N1	121.00	111.79	1
N1-C2-N3	114.80	124.00	1
C2-N3-C4	110.80	119.99	1
N-CA-CB	103.00	109.74	1
CB-CG-CD2	120.70	131.10	1
C2-N3-C4	120.00	110.83	1
N1-C2-N3	114.80	123.96	1
C5-C6-N1	121.00	111.85	1
N-CA-CB	103.00	109.71	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C2-N3-C4	110.80	119.93	1
C2-N3-C4	120.00	110.88	1
C5-C6-N1	121.00	111.88	1
C2-N3-C4	120.00	110.92	1
O4'-C1'-N1	108.40	117.47	2
O4'-C1'-N1	108.40	117.46	1
C-N-CD	125.00	149.74	1
C2-N3-C4	110.80	119.85	1
C2-N3-C4	110.80	119.84	2
N1-C2-N3	114.80	123.83	1
C2-N3-C4	110.80	119.81	1
CB-CG-CD2	120.70	130.81	1
N-CA-CB	103.00	109.51	1
CA-CB-CG	104.50	115.74	1
N-CA-CB	103.00	109.50	1
O4'-C1'-N1	108.40	117.27	1
C2-N3-C4	110.80	119.65	1
O4'-C1'-N1	108.40	117.19	1
O4'-C1'-N1	108.40	117.17	1
C2-N3-C4	110.80	119.55	1
N-CA-CB	103.00	109.41	1
O4'-C1'-N1	108.40	117.10	1
O4'-C1'-N1	108.40	117.09	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C2-N3-C4	110.80	119.44	1
C2-N3-C4	111.80	120.39	1
CA-CB-CG	104.50	115.37	1
O4'-C1'-N1	108.40	116.97	1
N-CA-CB	111.50	101.79	1
CA-CB-CG	104.50	115.36	1
C2-N3-C4	110.80	119.31	1
N-CA-CB	111.50	101.86	1
O4'-C1'-N1	108.40	116.87	1
O4'-C1'-N1	108.40	116.86	1
N-CA-CB	111.50	101.92	1
CA-CB-CG	104.50	115.19	1
O4'-C1'-N1	108.40	116.80	1
O4'-C1'-N1	108.40	116.79	1
CA-CB-CG	104.50	115.12	1
C2-N3-C4	111.80	120.18	1
C2-N3-C4	111.80	120.17	1
N-CA-CB	111.50	102.01	1
CA-CB-CG	104.50	115.09	1
C2-N3-C4	111.80	120.16	1
CD1-CG-CD2	118.60	110.28	1
N-CA-CB	111.50	102.09	1
C2-N3-C4	111.80	120.08	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	111.50	102.12	1
C2-N3-C4	111.80	120.03	1
N-CA-CB	111.50	102.18	1
N-CA-CB	111.50	102.19	1
C2-N3-C4	111.80	119.98	1
C2-N3-C4	120.00	111.84	1
N-CA-CB	111.50	102.25	1
CA-CB-CG	104.50	114.83	1
C2-N3-C4	111.80	119.94	1
O4'-C1'-N1	108.40	116.54	1
C2-N3-C4	120.00	111.87	1
C2-N3-C4	111.80	119.93	1
C2-N3-C4	120.00	111.88	1
C2-N3-C4	120.00	111.89	1
O4'-C1'-N1	108.40	116.50	1
C2-N3-C4	120.00	111.91	2
N-CA-CB	111.50	102.34	1
C2-N3-C4	120.00	111.92	2
C2-N3-C4	120.00	111.93	1
C2-N3-C4	120.00	111.94	1
C2-N3-C4	120.00	111.95	2
CA-CB-CG	104.50	114.68	1
C2-N3-C4	120.00	111.97	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C2-N3-C4	111.80	119.82	1
C2-N3-C4	111.80	119.81	1
C2-N3-C4	111.80	119.78	1
CA-CB-CG	104.50	114.60	1
C2-N3-C4	111.80	119.77	1
C2-N3-C4	120.00	112.03	1
C2-N3-C4	120.00	112.04	1
C2-N3-C4	120.00	112.05	2
C2-N3-C4	120.00	112.06	1
CD1-CG-CD2	118.60	110.70	1
C2-N3-C4	111.80	119.66	1
CA-CB-CG	104.50	114.45	1
CA-CB-CG	104.50	114.42	1
C2-N3-C4	111.80	119.62	1
CD1-CG-CD2	118.60	110.78	1
C2-N3-C4	111.80	119.61	1
C2-N3-C4	111.80	119.58	2
C2-N3-C4	111.80	119.57	1
CA-CB-CG	104.50	114.34	1
C2-N3-C4	111.80	119.56	1
C2-N3-C4	127.00	119.24	1
N-CA-CB	110.50	101.71	1
C2-N3-C4	127.00	119.25	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	104.50	114.32	1
C2-N3-C4	111.80	119.55	1
CA-CB-CG	104.50	114.31	1
CA-CB-CG	104.50	114.29	1
C2-N3-C4	127.00	119.28	1
CD1-CG-CD2	118.10	110.39	1
N-CA-CB	110.50	101.77	1
C2-N3-C4	111.80	119.50	1
C2-N3-C4	111.80	119.48	1
CA-CB-CG	113.90	104.69	1
N-CA-CB	110.50	101.81	1
N-CA-CB	110.50	101.82	1
N-CA-CB	110.50	101.89	1
C2-N3-C4	111.80	119.40	1
C2-N3-C4	127.00	119.40	1
N-CA-CB	110.50	101.90	1
O4'-C1'-N1	108.40	115.95	1
N-CA-CB	110.50	101.95	2
C2-N3-C4	127.00	119.45	1
C2-N3-C4	127.00	119.46	1
C2-N3-C4	111.80	119.33	1
N-CA-CB	110.50	101.97	1
N-CA-CB	110.50	101.98	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	114.10	104.08	1
C2-N3-C4	127.00	119.50	1
N3-C4-C5	114.80	122.30	1
CD1-CG-CD2	118.10	110.61	1
N3-C4-C5	114.80	122.29	1
C2-N3-C4	111.80	119.29	1
CA-CB-CG	114.10	104.12	1
CA-CB-CG	114.10	104.13	1
C2-N3-C4	111.80	119.27	1
C2-N3-C4	127.00	119.53	1
CA-CB-CG	114.10	104.14	1
CD1-CG-CD2	118.60	111.14	1
N-CA-CB	111.50	103.05	1
N-CA-CB	110.50	102.06	1
CA-CB-CG	114.10	104.17	1
N3-C4-C5	114.80	122.24	1
C2-N3-C4	120.00	127.44	1
C2-N3-C4	127.00	119.57	1
C2-N3-C4	111.80	119.23	1
C2-N3-C4	127.00	119.58	1
N3-C4-C5	114.80	122.22	1
CD1-CG-CD2	118.60	111.18	1
CA-CB-CG	114.10	104.24	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	114.10	104.27	1
C2-N3-C4	120.00	127.36	1
N-CA-CB	110.50	102.16	2
CA-CB-CG	114.10	104.29	1
N-CA-CB	110.50	102.17	1
C2-N3-C4	120.00	127.35	1
N3-C4-C5	114.80	122.15	1
N3-C4-C5	114.80	122.14	1
CB-CG-CD2	126.80	119.97	1
N3-C4-C5	114.80	122.12	1
CD1-CG-CD2	118.10	110.78	1
O4'-C1'-N1	108.40	115.71	1
N3-C4-C5	114.80	122.10	2
CA-CB-CG	104.50	113.73	1
N-CA-CB	110.50	102.25	1
CA-CB-CG	104.50	113.71	1
O4'-C1'-N1	108.40	115.66	1
CA-CB-CG	114.10	104.42	1
N3-C4-C5	114.80	122.06	1
CA-CB-CG	114.10	104.43	1
N-CA-CB	110.50	102.31	1
C2-N3-C4	120.00	127.22	1
C2-N3-C4	120.00	127.21	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	114.10	104.49	1
C2-N3-C4	127.00	119.80	1
N-CA-CB	110.50	102.35	1
N3-C4-C5	114.80	121.98	1
C2-N3-C4	127.00	119.82	1
CA-CB-CG	104.50	113.59	1
C2-N3-C4	120.00	127.17	1
N3-C4-C5	114.80	121.97	1
C2-N3-C4	120.00	127.16	2
N3-C4-C5	114.80	121.96	1
CA-CB-CG	104.50	113.57	1
C2-N3-C4	120.00	127.15	2
N3-C4-C5	114.80	121.95	1
N3-C4-C5	114.80	121.94	1
C2-N3-C4	127.00	119.87	1
C2-N3-C4	120.00	127.10	2
O4'-C1'-N1	108.40	115.49	1
N3-C4-C5	114.80	121.88	1
C2-N3-C4	120.00	127.07	1
O4'-C1'-N1	108.40	115.45	1
C5-C4-N3	121.80	128.84	1
C2-N3-C4	127.00	119.96	1
C5-C4-N3	121.80	128.83	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	102.54	2
CA-CB-CG	114.10	104.75	1
CB-CG-CD	112.60	104.66	1
CA-CB-CG	114.10	104.76	1
O4'-C1'-N1	108.40	115.41	1
C5-C4-N3	121.80	128.80	1
C2-N3-C4	127.00	120.01	1
CD1-CG-CD2	118.60	111.63	1
C2-N3-C4	127.00	120.03	1
CA-CB-CG	114.10	104.82	1
C5-C4-N3	121.80	128.75	2
C2-N3-C4	120.00	126.94	1
CA-CB-CG	104.50	113.26	1
C5-C4-N3	121.80	128.68	1
N-CA-CB	110.50	102.71	1
CB-CG-CD1	126.90	120.03	1
C5-C4-N3	121.80	128.67	1
C2-N3-C4	120.00	126.86	1
C5-C4-N3	121.80	128.66	1
C5-C4-N3	121.80	128.63	1
C6-N1-C2	124.90	118.09	1
C6-N1-C2	124.90	118.10	1
N-CA-CB	110.50	102.80	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O4'-C1'-N1	108.40	115.18	1
C5-C4-N3	121.80	128.57	1
N3-C4-C5	121.80	115.04	1
C6-N1-C2	124.90	118.14	1
CB-CG-CD	112.60	104.94	1
C5-C4-N3	121.80	128.56	1
C5-C4-N3	121.80	128.53	1
C5-C4-N3	121.80	128.52	1
CA-CB-CG	114.10	105.15	1
N3-C4-C5	128.40	121.69	1
N3-C4-C5	121.80	115.10	1
C5-C4-N3	121.80	128.48	1
C5-C4-N3	121.80	128.46	1
N-CA-CB	110.50	102.95	1
N3-C4-C5	121.80	115.14	1
CB-CG-CD	112.60	105.07	1
C6-N1-C2	124.90	118.26	2
N-CA-CB	110.50	102.98	1
C5-C4-N3	121.80	128.43	1
C6-N1-C2	124.90	118.27	1
N3-C4-C5	121.80	115.18	2
C6-N1-C2	124.90	118.29	1
N3-C4-C5	128.40	121.80	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N3-C4-C5	121.80	115.21	1
N3-C4-C5	121.80	115.22	1
N3-C4-C5	128.40	121.82	1
O4'-C1'-N1	108.40	114.97	1
N3-C4-C5	128.40	121.84	1
N3-C4-C5	121.80	115.24	1
N3-C4-C5	121.80	115.25	2
C2-N3-C4	120.00	126.55	1
N3-C4-C5	128.40	121.85	1
N3-C4-C5	121.80	115.26	1
C5-C4-N3	121.80	128.34	1
N3-C4-C5	121.80	115.27	2
N3-C4-C5	128.40	121.88	1
CB-CG-CD	112.60	105.25	1
N3-C4-C5	128.40	121.92	1
N3-C4-C5	121.80	115.32	1
N3-C4-C5	128.40	121.93	1
C6-N1-C2	118.80	125.27	1
N3-C4-C5	128.40	121.94	1
C5-C4-N3	121.80	128.25	1
N3-C4-C5	128.40	121.95	2
C6-N1-C2	124.90	118.46	1
N3-C4-C5	128.40	121.96	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N3-C4-C5	128.40	121.98	1
CA-CB-CG	104.50	112.63	1
C6-N1-C2	124.90	118.48	1
N3-C4-C5	128.40	122.00	1
CA-CB-CG	112.60	116.86	1
N1-C6-C5	117.60	123.97	1
C6-N1-C2	124.90	118.54	1
C6-N1-C2	118.80	125.16	1
CA-CB-CG	112.60	116.84	1
O4'-C1'-N1	108.40	114.75	1
N3-C4-C5	128.40	122.06	1
N3-C4-C5	128.40	122.07	1
C6-N1-C2	124.90	118.58	1
N3-C4-C5	128.40	122.09	2
C6-N1-C2	118.80	125.11	1
N1-C6-C5	117.60	123.91	1
N3-C4-C5	128.40	122.10	1
O4'-C1'-N1	108.40	114.70	1
C5-C6-N1	111.70	117.99	1
N3-C4-C5	128.40	122.11	1
CA-CB-CG	104.50	112.46	1
C5-C6-N1	111.70	117.98	1
N3-C4-C5	128.40	122.12	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C6-N1-C2	118.80	125.07	1
N3-C4-C5	128.40	122.14	2
N3-C4-C5	121.80	115.54	1
C5-C6-N1	111.70	117.95	1
N1-C6-C5	117.60	123.83	1
N1-C6-C5	117.60	123.82	2
C5-C6-N1	111.70	117.92	1
C6-N1-C2	118.80	125.00	1
N1-C6-C5	117.60	123.80	1
C5-C6-N1	111.70	117.90	1
N3-C4-C5	121.80	115.61	1
CD1-CG-CD2	110.80	119.88	1
N1-C6-C5	117.60	123.79	1
C6-N1-C2	118.80	124.99	1
N1-C6-C5	117.60	123.78	2
C6-N1-C2	118.80	124.98	1
C5-C6-N1	117.60	111.42	1
N3-C4-C5	128.40	122.22	2
CA-CB-CG	104.50	112.30	1
C5-C6-N1	111.70	117.86	1
N3-C4-C5	128.40	122.26	1
O4'-C1'-N1	108.40	114.54	1
N3-C4-C5	128.40	122.27	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C6-N1-C2	118.80	124.92	1
N1-C6-C5	117.60	123.71	1
C5-C6-N1	111.70	117.80	3
C5-C6-N1	117.60	111.51	1
CD1-CG-CD2	110.80	119.73	1
N1-C6-C5	117.60	123.68	1
C5-C6-N1	117.60	111.53	2
C6-N1-C2	118.80	124.87	1
N1-C6-C5	117.60	123.67	1
CD1-CG-CD2	110.80	119.68	2
C5-C6-N1	111.70	117.76	1
C5-C6-N1	117.60	111.55	1
CA-CB-CG	112.60	116.63	1
C5-C6-N1	111.70	117.74	1
C6-N1-C2	118.80	124.82	1
C5-C6-N1	117.60	111.58	1
CD1-CG-CD2	110.80	119.61	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	0.92	21

All 21 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Model ID	Atom-1	Atom-2	Clash overlap (Å)
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Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	I:118:DT:H3	J:11:DG:H1	0.944
1	I:117:DG:H1	J:12:DT:H3	0.901
1	I:47:DG:H1	J:82:DT:H3	0.893
1	K:56:LYS:O	K:60:PHE:CG	0.614
1	J:103:DA:H2"	J:104:DG:C5'	0.529
1	K:226:GLU:N	K:227:ASP:CD	0.520
1	K:56:LYS:HG2	K:60:PHE:NE2	0.498
1	K:227:ASP:N	K:228:ARG:CD	0.491
1	G:30:PRO:N	G:31:VAL:CD	0.484
1	I:115:DT:H2"	I:116:DA:C8	0.462
1	D:82:SER:NZ	K:216:THR:OE2	0.459
1	K:278:GLY:O	L:130:ASP:NH1	0.424
1	C:30:PRO:N	C:31:VAL:CD	0.421
1	F:9:LYS:N	F:10:GLY:CD	0.412
1	J:103:DA:H2"	J:104:DG:H5"	0.412
1	I:126:DC:C2	J:4:DA:C2	0.409
1	I:85:DC:C2	J:45:DT:C2	0.407
1	K:101:PHE:NE2	K:155:LEU:O	0.407
1	B:9:LYS:N	B:10:GLY:CD	0.406
1	F:30:ILE:N	F:30:ILE:OE1	0.403
1	J:103:DA:H2"	J:104:DG:H5'	0.401

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	1290	1228	40	22

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	130	106	9	15

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	20	PRO
1	B	66	LEU
1	D	12	PRO
1	D	49	LEU
1	E	20	PRO
1	F	66	LEU
1	H	12	PRO
1	H	49	LEU
1	K	5	PRO
1	K	150	LEU
1	K	162	PRO
1	K	252	PRO
1	K	301	LEU
1	L	180	PRO
1	L	235	PRO

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.

Acknowledgements

Development of integrative model validation metrics, implementation of a model validation pipeline, and creation of a validation report for integrative structures, are funded by NSF ABI awards (DBI-1756248, DBI-2112966, DBI-2112967, DBI-2112968, and DBI-1756250). The [PDB-Dev team](#) and members of [Sali lab](#) contributed model validation metrics and software packages.

Implementation of validation methods for SAS data and SAS-based models are funded by [RCSB PDB](#) (grant number DBI-1832184). Dr. Stephen Burley, Dr. John Westbrook, and Dr. Jasmine Young from [RCSB PDB](#), Dr. Jill Trehwella, Dr. Dina Schneidman, and members of the [SASBDB](#) repository are acknowledged for their advice and support in implementing SAS validation methods.

Members of the [wwPDB Integrative/Hybrid Methods Task Force](#) provided recommendations and community support for the project.