

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	9A3P
PDB-Dev ID	PDBDEV_00000210
Structure Title	CLOCK-BMAL1 bound to the native Por nucleosome
Structure Authors	Michael, A.K.; Stoos, L.; Kempf, G.; Cavadini, S.; Thoma, N.H.

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

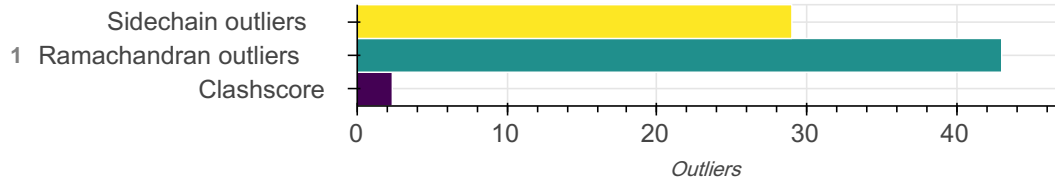
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the  symbol.

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 22 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 22 flexible or non-rigid units.

Entry composition ?

There is 1 unique type of models in this entry. This model is titled Fitted model/Fitted 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 (147-MER)	I	I	147
1	10	6	DNA (147-MER)	J	J	147
1	11	7	Circadian locomoter output cycles protein kaput	K	K	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	K	280
1	13	7	Circadian locomoter output cycles protein kaput	K	K	11
1	14	7	Circadian locomoter output cycles protein kaput	M	M	84
1	15	7	Circadian locomoter output cycles protein kaput	M	M	280
1	16	7	Circadian locomoter output cycles protein kaput	M	M	11
1	17	8	Basic helix-loop-helix ARNT-like protein 1	L	L	71
1	18	8	Basic helix-loop-helix ARNT-like protein 1	L	L	305
1	19	8	Basic helix-loop-helix ARNT-like protein 1	L	L	8
1	20	8	Basic helix-loop-helix ARNT-like protein 1	N	N	71
1	21	8	Basic helix-loop-helix ARNT-like protein 1	N	N	305
1	22	8	Basic helix-loop-helix ARNT-like protein 1	N	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-17160

ID	Dataset type	Database name	Data access code
3	Experimental model	PDB	6T93
4	Experimental model	PDB	4F3L
5	Experimental model	PDB	8OSL

Representation ?

This entry has only one representation and includes 0 rigid bodies and 22 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	-	1-139
L	-	1-71, 72-376, 377-384
N	-	1-71, 72-376, 377-384
M	-	1-84, 85-364, 365-375
K	-	1-84, 85-364, 365-375
E	-	1-139
B	-	1-106
F	-	1-106
C	-	1-133
G	-	1-133
D	-	1-128
H	-	1-128
I	-	1-147
J	-	1-147

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	MDFF	MDFF with distance and map restraints	None	None	False	False

There are 2 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	ChimeraX/Isolde	Not available	model building	Not available
2	Coot	0.9.6	model building	https://www2.mrc-lmb.cam.ac.uk/personal/pemsley/coot/

Data quality

Crosslinking-MS

Validation for this section is under development.

3DEM volume

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 8 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
N--H1	0.86	0.96	6
CD1--HD2	3.22	0.97	2

Standard geometry: angle outliers

There are 345 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	21.75	1
N-CD-CG	103.20	16.09	1
N-CD-CG	103.20	17.18	1
N-CD-CG	103.20	19.00	1
N-CD-CG	103.20	20.76	1
N-CD-CG	103.20	20.94	1
CA-N-CD	112.00	35.25	1
N-CD-CG	103.20	21.01	1
CA-N-CD	112.00	35.69	1
CA-N-CD	112.00	36.54	1
CA-N-CD	112.00	37.56	1
N-CD-CG	103.20	23.70	1
CA-N-CD	112.00	37.82	1
N-CD-CG	103.20	23.76	1
N-CD-CG	103.20	23.82	1
CA-N-CD	112.00	38.36	1
CA-N-CD	112.00	39.12	1
N-CD-CG	103.20	26.04	1
CA-N-CD	112.00	43.51	1
N-CD-CG	103.20	33.01	1
N-CD-CG	103.20	34.30	1
N-CD-CG	103.20	35.07	1
N-CD-CG	103.20	35.21	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CD-CG	103.20	35.24	1
N-CD-CG	103.20	35.41	1
N-CD-CG	103.20	35.64	1
N-CD-CG	103.20	36.10	1
CA-N-CD	112.00	50.51	1
CA-N-CD	112.00	54.94	1
CA-N-CD	112.00	55.14	1
CA-N-CD	112.00	57.63	1
CA-N-CD	112.00	58.85	1
N-CD-CG	103.20	46.88	1
CA-N-CD	112.00	59.71	1
CA-N-CD	112.00	59.85	1
N-CD-CG	103.20	47.63	1
CA-N-CD	112.00	60.19	1
CA-N-CD	112.00	60.89	1
CA-N-CD	112.00	61.75	1
CA-N-CD	112.00	62.38	1
CA-N-CD	112.00	62.60	1
CA-N-CD	112.00	67.72	1
N-CD-CG	103.20	56.10	1
N-CD-CG	103.20	57.47	1
CA-N-CD	112.00	70.63	1
N-CD-CG	103.20	67.76	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CD-CG	103.20	73.61	1
CA-N-CD	112.00	85.93	1
CB-CG-CD2	131.20	109.93	1
CB-CG-CD2	131.20	110.70	1
CB-CG-CD2	131.20	110.90	1
CB-CG-CD2	131.20	111.31	1
CB-CG-CD2	131.20	111.44	1
CB-CG-CD2	131.20	111.48	1
CB-CG-CD2	131.20	111.59	1
CB-CG-CD2	126.80	110.60	1
CB-CG-CD1	126.90	111.17	1
C-N-CD	125.00	163.51	1
CA-CB-CG	113.80	104.43	1
C-N-CD	125.00	163.40	1
CA-CB-CG	113.80	104.45	1
CG-CD2-CE2	121.20	107.17	1
CG-CD2-CE2	121.20	107.27	1
CA-CB-CG	113.80	104.62	1
C-N-CD	125.00	162.38	1
CB-CG-CD2	131.20	119.45	1
CA-CB-CG	112.60	103.60	1
CA-CB-CG	113.80	104.83	1
C-N-CD	125.00	160.77	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	103.95	1
CA-CB-CG	112.60	104.00	1
N-CA-CB	103.00	112.32	1
C-N-CD	125.00	159.41	1
CA-CB-CG	112.60	104.23	1
N-CA-CB	103.00	112.19	1
CB-CG-CD2	131.20	120.42	1
CA-CB-CG	112.60	104.37	1
CD1-CG-CD2	118.60	106.27	1
CB-CG-CD2	131.20	120.54	1
CB-CG-CD2	131.20	120.58	1
CD1-CG-CD2	118.10	105.93	1
CB-CG-CD2	131.20	120.67	1
CA-CB-CG	112.60	104.51	1
CB-CG-CD2	131.20	120.69	1
CA-CB-CG	112.60	104.53	1
N-CA-CB	103.00	111.82	1
CB-CG-CD2	131.20	120.84	1
N-CA-CB	103.00	111.76	1
CD1-CG-CD2	118.10	106.18	1
CA-CB-CG	112.60	104.66	1
CB-CG-CD2	131.20	120.88	1
CB-CG-CD2	131.20	120.90	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	103.00	111.72	1
CB-CG-CD2	131.20	120.96	1
CB-CG-CD2	131.20	120.99	1
N-CA-CB	103.00	111.64	1
CG-CD2-CE2	120.70	107.41	1
CB-CG-CD2	131.20	121.05	1
N-CA-CB	103.00	111.57	1
C-N-CD	125.00	156.86	1
CA-CB-CG	112.60	104.83	1
N-CA-CB	103.00	111.53	1
CA-CB-CG	104.50	119.20	1
N-CA-CB	103.00	111.42	1
N-CA-CB	103.00	111.39	1
C-N-CD	125.00	155.83	1
N-CA-CB	103.00	111.24	1
N-CA-CB	103.00	111.20	1
N-CA-CB	103.00	111.08	2
C-N-CD	125.00	155.10	1
N-CA-CB	103.00	111.01	1
CB-CG-CD2	120.80	109.97	1
CB-CG-CD2	110.70	131.88	1
CB-CG-CD2	120.80	110.27	1
CB-CG-CD2	120.80	110.28	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	103.00	110.69	1
CB-CG-CD2	120.80	131.15	1
N-CA-CB	103.00	110.58	1
CB-CG-CD2	110.70	131.35	1
N-CA-CB	103.00	110.57	1
CB-CG-CD2	110.70	131.22	1
CB-CG-CD2	110.70	131.19	1
CB-CG-CD2	110.70	131.18	1
CB-CG-CD2	110.70	131.16	1
CB-CG-CD2	110.70	131.11	1
CB-CG-CD2	110.70	131.07	1
CB-CG-CD2	110.70	131.04	1
N-CA-CB	103.00	110.45	1
CB-CG-CD1	120.80	110.66	1
CB-CG-CD2	120.80	110.66	1
CB-CG-CD1	120.80	110.70	1
N-CA-CB	103.00	110.40	1
N-CA-CB	103.00	110.38	2
CA-CB-CG	112.60	119.30	1
N-CA-CB	103.00	110.34	1
N-CA-CB	103.00	110.33	1
N-CA-CB	103.00	110.32	1
N-CA-CB	103.00	110.31	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	103.00	110.29	1
CB-CG-CD2	120.80	130.74	1
N-CA-CB	103.00	110.28	1
N-CA-CB	103.00	110.25	2
N-CA-CB	103.00	110.24	2
CB-CG-CD2	120.70	109.52	1
CB-CG-CD2	120.80	110.95	1
N-CA-CB	103.00	110.17	1
N-CA-CB	103.00	110.14	1
CB-CG-CD1	120.80	111.11	2
N-CA-CB	103.00	110.09	2
N-CA-CB	103.00	110.07	2
N-CA-CB	103.00	110.04	2
N-CA-CB	103.00	110.03	1
CA-CB-CG	112.60	118.96	1
CA-CB-CG	104.50	116.59	1
N-CA-CB	103.00	109.99	1
N-CA-CB	103.00	109.98	1
CA-CB-CG	104.50	116.54	1
CA-CB-CG	104.50	116.53	1
N-CA-CB	103.00	109.96	1
N-CA-CB	103.00	109.94	1
N-CA-CB	103.00	109.93	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	103.00	109.92	2
CB-CG-CD1	120.80	111.38	1
CA-CB-CG	104.50	116.42	2
N-CA-CB	103.00	109.90	2
N-CA-CB	103.00	109.89	1
N-CA-CB	103.00	109.87	1
N-CA-CB	103.00	109.86	2
N-CA-CB	103.00	109.81	1
CB-CG-CD2	120.70	131.21	1
N-CA-CB	103.00	109.80	2
CB-CG-CD2	120.70	131.16	1
N-CA-CB	103.00	109.72	1
N-CA-CB	103.00	109.71	2
N-CA-CB	103.00	109.70	1
N-CA-CB	103.00	109.63	1
N-CA-CB	103.00	109.62	1
CB-CG-CD2	120.70	110.55	1
CA-CB-CG	104.50	115.81	1
N-CA-CB	103.00	109.51	1
CA-CB-CG	104.50	115.70	1
CA-CB-CG	112.60	118.41	1
N-CA-CB	103.00	109.37	1
CA-CB-CG	104.50	115.43	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CD1-CG-CD2	118.60	109.99	1
CA-CB-CG	104.50	115.39	1
CB-CG-CD2	120.70	110.96	1
CB-CG-CD1	120.70	111.14	1
CA-CB-CG	104.50	115.14	1
N-CA-CB	103.00	109.15	1
CB-CG-CD1	120.70	111.21	1
CD1-CG-CD2	118.60	110.32	1
N-CA-CB	103.00	109.06	1
N-CA-CB	103.00	109.03	1
CA-CB-CG	112.60	118.06	1
C-N-CD	125.00	147.35	1
N-CA-CB	103.00	108.98	1
CB-CG-CD2	110.70	126.98	1
CA-CB-CG	104.50	114.76	1
CB-CG-CD1	120.70	111.53	1
CA-CB-CG	104.50	114.73	1
CA-CB-CG	104.50	114.72	1
CB-CG-CD1	110.70	126.83	1
CA-CB-CG	104.50	114.70	1
C-N-CD	125.00	146.99	1
CA-CB-CG	104.50	114.64	2
CD1-CG-CD2	118.60	110.60	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	103.00	108.86	1
CD1-CG-CD2	118.10	110.15	1
CA-CB-CG	113.90	104.42	1
CA-CB-CG	104.50	114.50	1
CA-CB-CG	104.50	114.47	1
CA-CB-CG	112.60	117.84	1
CA-CB-CG	113.90	104.57	1
N-CA-CB	103.00	108.70	1
C-N-CD	125.00	103.76	1
CD1-CG-CD2	118.10	110.35	1
CA-CB-CG	114.10	103.79	1
CA-CB-CG	104.50	114.22	1
CA-CB-CG	113.90	104.71	1
CA-CB-CG	114.10	103.91	1
CA-CB-CG	114.10	103.92	1
CA-CB-CG	104.50	114.17	2
CD1-CG-CD2	118.10	110.52	1
CA-CB-CG	114.10	104.02	1
CA-CB-CG	114.10	104.06	1
CA-CB-CG	114.10	104.13	1
N-CA-CB	110.40	102.93	1
CA-CB-CG	104.50	113.95	1
CA-CB-CG	104.50	113.93	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	114.10	104.19	1
CD1-CG-CD2	118.10	110.70	1
CA-CB-CG	104.50	113.85	1
N-CA-CB	110.50	102.16	1
CD1-CG-CD2	118.10	110.75	1
CA-CB-CG	114.10	104.30	1
CA-CB-CG	104.50	113.79	1
CA-CB-CG	114.10	104.34	1
CA-CB-CG	114.10	104.35	1
CA-CB-CG	104.50	113.75	2
CA-CB-CG	104.50	113.74	2
N-CA-CB	111.50	103.24	1
CA-CB-CG	112.60	117.46	1
N-CA-CB	111.50	103.25	1
CA-CB-CG	104.50	113.69	1
CA-CB-CG	114.10	104.43	1
N-CA-CB	111.50	103.28	1
CA-CB-CG	114.10	104.44	1
CA-CB-CG	104.50	113.67	1
CA-CB-CG	112.60	117.42	1
N-CA-CB	111.50	103.32	1
CA-CB-CG	104.50	113.64	1
CA-CB-CG	104.50	113.50	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	111.50	103.45	1
N-CA-CB	111.50	103.46	2
CB-CG-CD2	120.80	127.88	1
CA-CB-CG	104.50	113.46	1
CA-CB-CG	112.60	117.29	1
CA-CB-CG	114.10	104.74	1
CA-CB-CG	104.50	113.36	1
CA-CB-CG	104.50	113.35	1
N-CA-CB	110.50	102.74	1
N-CA-CB	110.50	102.78	1
N-CA-CB	110.50	102.81	2
N-CA-CB	110.50	102.84	1
N-CA-CB	110.50	102.90	1
CA-CB-CG	114.10	105.17	1
C-N-CD	125.00	143.31	1
N-CA-CB	110.50	102.94	1
CA-CB-CG	112.60	117.04	1
N-CA-CB	110.50	102.99	1
CB-CG-CD	112.60	105.09	1
N-CA-CB	110.50	103.01	1
N-CA-CB	110.50	103.02	2
N-CA-CB	110.50	103.05	1
CA-CB-CG	112.60	116.97	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	103.07	2
CB-CG-CD	112.60	105.18	1
N-CA-CB	110.50	103.08	1
N-CA-CB	110.50	103.09	1
N-CA-CB	110.50	103.12	2
CA-CB-CG	104.50	112.72	1
N-CA-CB	110.50	103.15	1
CA-CB-CG	104.50	112.70	1
N-CA-CB	110.50	103.18	1
N-CA-CB	110.50	103.19	1
CA-CB-CG	104.50	112.62	1
N-CA-CB	110.50	103.25	2
CA-CB-CG	104.50	112.60	1
CA-CB-CG	104.50	112.59	1
N-CA-CB	110.50	103.27	1
CA-CB-CG	104.50	112.57	1
N-CA-CB	110.50	103.28	1
C-N-CD	125.00	142.36	1
CA-CB-CG	104.50	112.54	1
N-CA-CB	110.50	103.31	2
N-CA-CB	110.50	103.32	2
N-CA-CB	110.50	103.33	1
N-CA-CB	110.50	103.34	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	103.35	1
CB-CG-CD	112.60	105.45	1
N-CA-CB	110.50	103.38	1
N-CA-CB	110.50	103.39	1
CB-CG-CD1	120.80	127.03	1
N-CA-CB	110.50	103.45	2
N-CA-CB	110.50	103.50	1
CA-CB-CG	112.60	116.67	1
N-CA-CB	110.50	103.61	1
CA-CB-CG	112.60	116.61	1
CA-CB-CG	104.50	112.12	1
CB-CG-CD1	120.70	127.51	1
N-CD-HD2	123.24	109.00	1
N-CD-HD3	123.54	109.00	1
N-CD-HD2	89.92	109.00	1
HD1-CD1-HD2	142.09	110.00	1
HD1-CD1-HD2	142.24	110.00	1
N-CD-HD3	61.89	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	2.34	73

All 73 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	A:61:SER:O	A:65:LEU:HD22	0.727
1	E:61:SER:O	E:65:LEU:HD22	0.699
1	L:103:LEU:NE2	M:81:LYS:OD1	0.657
1	J:44:DG:H2'	J:45:DT:H72	0.625
1	I:130:DC:H2'	I:131:DG:C8	0.578
1	A:79:ALA:N	I:69:DC:OP1	0.578
1	I:97:DA:H4'	I:98:DA:OP1	0.573
1	I:110:DT:H2"	I:111:DC:C5	0.562
1	K:24:LYS:CD2	K:41:LEU:HD23	0.560
1	E:78:ILE:N	J:73:DG:OP1	0.547
1	I:145:DT:H2"	I:146:DG:C8	0.546
1	I:134:DT:H2"	I:135:DG:C8	0.543
1	I:135:DG:C2	J:14:DA:C2	0.531
1	I:52:DC:H2'	I:53:DT:H72	0.526
1	M:149:ILE:CE1	M:165:LEU:HD13	0.526
1	I:132:DT:H2'	I:133:DT:H72	0.516
1	A:78:ILE:H	I:69:DC:P	0.513
1	E:20:PRO:N	E:20:PRO:OE1	0.513
1	I:144:DG:H2'	I:145:DT:C6	0.509
1	C:2:SER:NH1	I:29:DG:OP2	0.506
1	J:51:DT:H2"	J:52:DC:C6	0.503
1	J:115:DA:H2'	J:116:DT:H71	0.500
1	E:34:PRO:HD3	F:2:SER:HA	0.497

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	E:14:SER:HA	I:8:DC:OP1	0.485
1	B:15:GLY:NH1	I:59:DT:OP2	0.484
1	B:27:ARG:N	J:83:DC:OP1	0.484
1	L:236:PRO:OE1	L:239:MET:NH2	0.482
1	M:267:LEU:HD23	M:310:GLN:HA	0.481
1	I:134:DT:C2'	I:135:DG:C8	0.479
1	J:91:DA:H4'	J:92:DC:H5'	0.478
1	I:134:DT:H2"	I:135:DG:H8	0.477
1	I:92:DC:H2'	I:93:DT:H71	0.474
1	I:104:DC:O2	J:44:DG:N2	0.474
1	J:92:DC:H2"	J:93:DC:OP2	0.473
1	I:129:DA:C2	J:20:DG:C2	0.471
1	I:130:DC:C2'	I:131:DG:C8	0.471
1	N:84:THR:HA	N:107:GLY:HA2	0.468
1	F:14:LEU:NH2	I:80:DA:OP2	0.466
1	J:61:DT:H72	J:61:DT:OP2	0.465
1	K:292:TYR:CE3	K:292:TYR:H	0.465
1	B:27:ARG:H	J:83:DC:P	0.464
1	I:135:DG:N2	J:14:DA:N3	0.459
1	L:81:TYR:HA	L:104:PHE:HA	0.458
1	J:91:DA:H4'	J:92:DC:OP1	0.453
1	J:17:DC:H2'	J:18:DG:C8	0.446
1	K:109:GLY:CE1	K:121:LEU:HD22	0.442

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	I:107:DC:H4'	I:108:DT:OP1	0.441
1	I:138:DG:H2'	I:139:DT:H72	0.437
1	L:15:LYS:HA	L:18:ARG:NE	0.437
1	A:24:LEU:HA	A:24:LEU:NE	0.433
1	I:144:DG:C2	J:5:DG:C2	0.433
1	N:270:GLN:OG	N:290:ASP:OD1	0.432
1	I:58:DT:C2'	I:59:DT:H71	0.429
1	D:61:LYS:O	D:65:ILE:HG23	0.428
1	J:80:DA:H4'	J:81:DC:OP1	0.427
1	A:1:GLY:HA2	J:86:DT:H5'	0.425
1	J:92:DC:H1'	J:93:DC:C6	0.423
1	J:113:DG:H2"	J:114:DC:C6	0.423
1	D:57:GLY:OG1	D:60:SER:OE1	0.423
1	I:87:DA:H2"	I:88:DG:C8	0.421
1	L:78:GLU:O	M:105:ILE:CD	0.421
1	I:115:DC:H2"	I:116:DA:C8	0.417
1	J:44:DG:H2'	J:45:DT:C7	0.412
1	J:27:DG:C6	J:28:DA:C6	0.411
1	I:133:DT:H1'	I:134:DT:O4'	0.411
1	J:62:DC:H2"	J:63:DT:H71	0.410
1	J:95:DA:C6	J:96:DG:C6	0.410
1	I:34:DG:H2"	I:35:DC:C6	0.409
1	L:79:ALA:O	M:106:MET:N	0.409

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	J:62:DC:C2'	J:63:DT:H71	0.407
1	J:2:DC:H2"	J:3:DA:C8	0.403
1	J:91:DA:H2"	J:92:DC:C6	0.401
1	F:15:GLY:NH2	J:63:DT:OP1	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	1845	1729	73	43

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	171	134	8	29

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	20	PRO
1	A	34	PRO
1	C	84	PRO
1	D	14	PRO
1	E	20	PRO
1	E	34	PRO
1	G	84	PRO
1	H	12	PRO
1	K	42	PRO

Model ID	Chain	Residue ID	Residue type
1	K	269	LEU
1	K	274	PRO
1	K	285	LEU
1	K	308	LEU
1	L	44	PRO
1	L	142	PRO
1	L	236	PRO
1	M	5	PRO
1	M	42	PRO
1	M	139	PRO
1	M	252	PRO
1	M	275	PRO
1	M	281	PRO
1	M	285	LEU
1	N	44	PRO
1	N	53	LEU
1	N	142	PRO
1	N	171	PRO
1	N	269	PRO
1	N	271	PRO

Fit of model to data used for modeling ?

Crosslinking-MS

Validation for this section is under development.

3DEM volume

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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