

Integrative Structure Validation Report ?

February 18, 2025 - 08:37 AM PST

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

Integrative Modeling Validation Version 2.0

Python-IHM Version 1.8

MolProbity Version 4.5.2

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.
Deposited on	2023-04-26

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

We welcome your comments at helpdesk@pdb-ihm.org

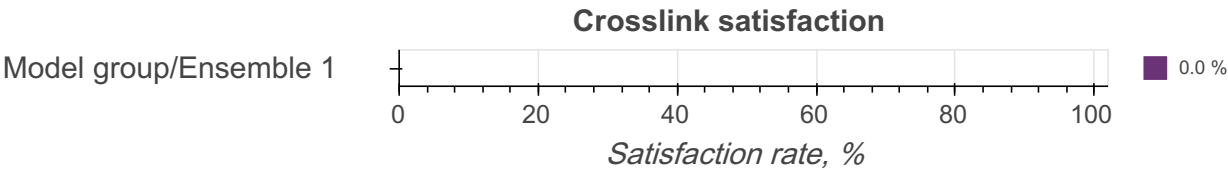
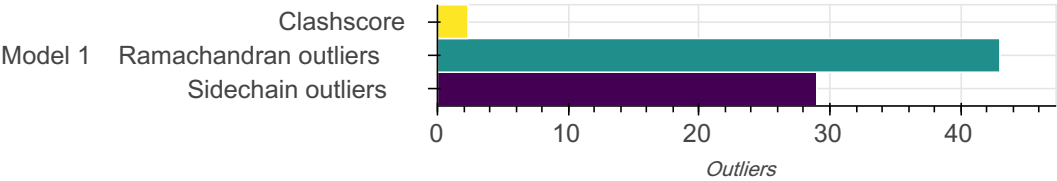
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 and fit to model assessments for SAS and crosslinking-MS 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 model(s). A total of 5 datasets were used to build this entry.

Representation ?

This entry has 1 representation(s).

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
1	1	1	Histone H3.1	A	139	-	1-139	100.00 / 100.00	Atomic
				E					
		2	Histone H4	B	106	-	1-106	100.00 / 100.00	Atomic
				F					
		3	Histone H2A	C	133	-	1-133	100.00 / 100.00	Atomic
				G					
		4	Histone H2B	D	128	-	1-128	100.00 / 100.00	Atomic
				H					
		5	DNA (147-MER)	I	147	-	1-147	100.00 / 100.00	Atomic

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		6	DNA (147-MER)	J	147	-	1-147	100.00 / 100.00	Atomic
		7	Circadian locomotor output cycles protein kaput	K	375	-	1-84, 85-364, 365-375	100.00 / 100.00	Atomic
				M					
		8	Basic helix-loop-helix ARNT-like protein 1	L	384	-	1-71, 72-376, 377-384	100.00 / 100.00	Atomic
				N					

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
3	Experimental model	PDB	6T93
4	Experimental model	PDB	4F3L
5	Experimental model	PDB	8OSL

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 with distance and map restraints	MDFF	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	https://tristanic.github.io/isolde/
2	Coot	0.9.6	model building	https://www2.mrc-lmb.cam.ac.uk/personal/pemsley/coot/

Data quality ?

Crosslinking-MS

At the moment, data validation is only available for crosslinking-MS data deposited as a fully [compliant](#) dataset in the [PRIDE Crosslinking](#) database. Correspondence between crosslinking-MS and entry entities is established using [pyHMMER](#). Only residue pairs that passed the reported threshold are used for the analysis. The values in the report have to be interpreted in the context of the experiment (i.e. only a minor fraction of in-situ or in-vivo dataset can be used for modeling).

Crosslinking-MS dataset is not available in the [PRIDE Crosslinking](#) database.

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 70 bond length outliers in this entry (0.40% of 17316 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
N	269	PRO	N-CD	252.98	5.01	1.47	1	1
M	281	PRO	N-CD	252.61	5.01	1.47	1	1
L	142	PRO	N-CD	250.48	4.98	1.47	1	1
K	274	PRO	N-CD	250.22	4.98	1.47	1	1
K	42	PRO	N-CD	249.25	4.96	1.47	1	1
A	34	PRO	N-CD	248.88	4.96	1.47	1	1
E	34	PRO	N-CD	247.81	4.94	1.47	1	1
M	5	PRO	N-CD	226.22	4.64	1.47	1	1
N	171	PRO	N-CD	219.41	4.54	1.47	1	1
N	142	PRO	N-CD	213.17	4.46	1.47	1	1
M	139	PRO	N-CD	212.33	4.45	1.47	1	1
N	44	PRO	N-CD	211.91	4.44	1.47	1	1
L	236	PRO	N-CD	211.03	4.43	1.47	1	1
D	14	PRO	N-CD	210.99	4.43	1.47	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
N	271	PRO	N-CD	210.91	4.43	1.47	1	1
A	20	PRO	N-CD	206.67	4.37	1.47	1	1
C	84	PRO	N-CD	205.54	4.35	1.47	1	1
M	252	PRO	N-CD	205.41	4.35	1.47	1	1
L	44	PRO	N-CD	189.68	4.13	1.47	1	1
M	42	PRO	N-CD	174.12	3.91	1.47	1	1
G	84	PRO	N-CD	166.58	3.81	1.47	1	1
M	275	PRO	N-CD	149.76	3.57	1.47	1	1
H	12	PRO	N-CD	120.05	3.15	1.47	1	1
E	20	PRO	N-CD	115.22	3.09	1.47	1	1
M	271	HIS	CG-CD2	15.53	1.52	1.35	1	1
K	124	HIS	CG-CD2	15.52	1.52	1.35	1	1
L	93	HIS	CG-CD2	15.43	1.52	1.35	1	1
L	65	HIS	CG-CD2	15.41	1.52	1.35	1	1
K	176	HIS	CG-CD2	15.31	1.52	1.35	1	1
E	43	HIS	CG-CD2	15.22	1.52	1.35	1	1
A	43	HIS	CG-CD2	15.11	1.52	1.35	1	1
L	121	PHE	CG-CD1	6.67	1.52	1.38	1	1
D	69	PHE	CG-CD1	6.61	1.52	1.38	1	1
L	121	PHE	CG-CD2	6.61	1.52	1.38	1	1
M	102	PHE	CG-CD2	6.49	1.52	1.38	1	1
M	102	PHE	CG-CD1	6.47	1.52	1.38	1	1
L	126	TYR	CG-CD1	6.42	1.52	1.39	1	1
F	76	TYR	CG-CD2	6.42	1.52	1.39	1	1
D	69	PHE	CG-CD2	6.39	1.52	1.38	1	1
L	126	TYR	CG-CD2	6.37	1.52	1.39	1	1
B	76	TYR	CG-CD2	6.36	1.52	1.39	1	1
C	43	TYR	CG-CD1	6.32	1.52	1.39	1	1
G	43	TYR	CG-CD1	6.32	1.52	1.39	1	1
C	43	TYR	CG-CD2	6.31	1.52	1.39	1	1
F	76	TYR	CG-CD1	6.25	1.52	1.39	1	1
G	43	TYR	CG-CD2	6.20	1.52	1.39	1	1
B	76	TYR	CG-CD1	6.20	1.52	1.39	1	1
L	234	TRP	CG-CD1	6.17	1.52	1.36	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
C	67	LEU	CG-CD2	5.09	1.35	1.52	1	1
G	67	LEU	CG-CD2	5.08	1.35	1.52	1	1
D	49	LEU	CG-CD2	5.07	1.35	1.52	1	1
K	98	LEU	CG-CD2	5.07	1.35	1.52	1	1
L	170	LEU	CG-CD2	5.06	1.35	1.52	1	1
E	74	LEU	CG-CD2	5.06	1.35	1.52	1	1
N	241	LEU	CG-CD2	5.04	1.35	1.52	1	1
A	74	LEU	CG-CD2	5.04	1.35	1.52	1	1
K	150	LEU	CG-CD2	5.04	1.35	1.52	1	1
L	234	TRP	CG-CD2	4.94	1.52	1.43	1	1
K	280	LEU	CG-CD2	4.69	1.37	1.52	1	1
A	65	LEU	CG-CD1	4.18	1.38	1.52	1	1
E	65	LEU	CG-CD1	4.14	1.38	1.52	1	1
E	65	LEU	CG-CD2	4.13	1.38	1.52	1	1
K	298	LEU	CG-CD1	4.12	1.39	1.52	1	1
A	65	LEU	CG-CD2	4.11	1.39	1.52	1	1
K	269	LEU	CG-CD2	4.03	1.39	1.52	1	1
K	298	LEU	CG-CD2	4.03	1.39	1.52	1	1
N	53	LEU	CG-CD1	4.02	1.39	1.52	1	1
K	285	LEU	CG-CD2	4.01	1.39	1.52	1	1
N	53	LEU	CG-CD2	4.00	1.39	1.52	1	1
K	269	LEU	CG-CD1	4.00	1.39	1.52	1	1

Standard geometry: angle outliers ?

There are 339 bond angle outliers in this entry (1.37% of 24698 assessed bonds). A summary is provided below. The output is limited to 100 rows.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
L	236	PRO	CA-N-CD	64.46	21.75	112.00	1	1
N	171	PRO	N-CD-CG	58.08	16.09	103.20	1	1
M	5	PRO	N-CD-CG	57.35	17.18	103.20	1	1
N	271	PRO	N-CD-CG	56.13	19.00	103.20	1	1
C	84	PRO	N-CD-CG	54.96	20.76	103.20	1	1
N	142	PRO	N-CD-CG	54.84	20.94	103.20	1	1
M	281	PRO	CA-N-CD	54.82	35.25	112.00	1	1
M	139	PRO	N-CD-CG	54.79	21.01	103.20	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
N	269	PRO	CA-N-CD	54.51	35.69	112.00	1	1
L	142	PRO	CA-N-CD	53.90	36.54	112.00	1	1
K	42	PRO	CA-N-CD	53.17	37.56	112.00	1	1
N	44	PRO	N-CD-CG	53.00	23.70	103.20	1	1
K	274	PRO	CA-N-CD	52.98	37.82	112.00	1	1
D	14	PRO	N-CD-CG	52.96	23.76	103.20	1	1
A	20	PRO	N-CD-CG	52.92	23.82	103.20	1	1
A	34	PRO	CA-N-CD	52.60	38.36	112.00	1	1
E	34	PRO	CA-N-CD	52.05	39.12	112.00	1	1
M	252	PRO	N-CD-CG	51.44	26.04	103.20	1	1
M	5	PRO	CA-N-CD	48.92	43.51	112.00	1	1
N	269	PRO	N-CD-CG	46.80	33.01	103.20	1	1
M	281	PRO	N-CD-CG	45.93	34.30	103.20	1	1
L	142	PRO	N-CD-CG	45.42	35.07	103.20	1	1
A	34	PRO	N-CD-CG	45.33	35.21	103.20	1	1
K	42	PRO	N-CD-CG	45.31	35.24	103.20	1	1
L	44	PRO	N-CD-CG	45.19	35.41	103.20	1	1
E	34	PRO	N-CD-CG	45.04	35.64	103.20	1	1
K	274	PRO	N-CD-CG	44.73	36.10	103.20	1	1
M	42	PRO	CA-N-CD	43.92	50.51	112.00	1	1
G	84	PRO	CA-N-CD	40.76	54.94	112.00	1	1
N	171	PRO	CA-N-CD	40.61	55.14	112.00	1	1
M	275	PRO	CA-N-CD	38.84	57.63	112.00	1	1
N	142	PRO	CA-N-CD	37.97	58.85	112.00	1	1
M	42	PRO	N-CD-CG	37.55	46.88	103.20	1	1
D	14	PRO	CA-N-CD	37.35	59.71	112.00	1	1
M	139	PRO	CA-N-CD	37.25	59.85	112.00	1	1
G	84	PRO	N-CD-CG	37.05	47.63	103.20	1	1
N	44	PRO	CA-N-CD	37.01	60.19	112.00	1	1
N	271	PRO	CA-N-CD	36.51	60.89	112.00	1	1
A	20	PRO	CA-N-CD	35.89	61.75	112.00	1	1
M	252	PRO	CA-N-CD	35.44	62.38	112.00	1	1
C	84	PRO	CA-N-CD	35.29	62.60	112.00	1	1
H	12	PRO	CA-N-CD	31.63	67.72	112.00	1	1
M	275	PRO	N-CD-CG	31.40	56.10	103.20	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
L	236	PRO	N-CD-CG	30.49	57.47	103.20	1	1
L	44	PRO	CA-N-CD	29.55	70.63	112.00	1	1
H	12	PRO	N-CD-CG	23.63	67.76	103.20	1	1
E	20	PRO	N-CD-CG	19.72	73.61	103.20	1	1
E	20	PRO	CA-N-CD	18.62	85.93	112.00	1	1
A	43	HIS	CB-CG-CD2	16.36	109.93	131.20	1	1
E	43	HIS	CB-CG-CD2	15.77	110.70	131.20	1	1
K	176	HIS	CB-CG-CD2	15.61	110.90	131.20	1	1
K	124	HIS	CB-CG-CD2	15.30	111.31	131.20	1	1
L	65	HIS	CB-CG-CD2	15.20	111.44	131.20	1	1
L	93	HIS	CB-CG-CD2	15.17	111.48	131.20	1	1
M	271	HIS	CB-CG-CD2	15.09	111.59	131.20	1	1
L	234	TRP	CB-CG-CD2	11.57	110.60	126.80	1	1
L	234	TRP	CB-CG-CD1	10.49	111.17	126.90	1	1
L	43	VAL	C-N-CD	9.39	163.51	125.00	1	1
M	135	PHE	CA-CB-CG	9.37	104.43	113.80	1	1
N	43	VAL	C-N-CD	9.37	163.40	125.00	1	1
K	231	PHE	CA-CB-CG	9.35	104.45	113.80	1	1
K	292	TYR	CG-CD2-CE2	9.35	107.17	121.20	1	1
M	279	TYR	CG-CD2-CE2	9.29	107.27	121.20	1	1
A	82	PHE	CA-CB-CG	9.18	104.62	113.80	1	1
M	251	GLU	C-N-CD	9.12	162.38	125.00	1	1
L	226	HIS	CB-CG-CD2	9.04	119.45	131.20	1	1
C	94	ASP	CA-CB-CG	9.00	103.60	112.60	1	1
E	82	PHE	CA-CB-CG	8.97	104.83	113.80	1	1
E	33	ALA	C-N-CD	8.72	160.77	125.00	1	1
G	94	ASP	CA-CB-CG	8.65	103.95	112.60	1	1
M	28	ASP	CA-CB-CG	8.60	104.00	112.60	1	1
L	200	PRO	N-CA-CB	8.47	112.32	103.00	1	1
A	33	ALA	C-N-CD	8.39	159.41	125.00	1	1
L	175	ASP	CA-CB-CG	8.37	104.23	112.60	1	1
M	281	PRO	N-CA-CB	8.36	112.19	103.00	1	1
K	271	HIS	CB-CG-CD2	8.30	120.42	131.20	1	1
M	99	ASP	CA-CB-CG	8.23	104.37	112.60	1	1
M	213	PHE	CD1-CG-CD2	8.22	106.27	118.60	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
F	79	HIS	CB-CG-CD2	8.20	120.54	131.20	1	1
B	79	HIS	CB-CG-CD2	8.17	120.58	131.20	1	1
K	292	TYR	CD1-CG-CD2	8.12	105.93	118.10	1	1
N	93	HIS	CB-CG-CD2	8.10	120.67	131.20	1	1
K	296	ASP	CA-CB-CG	8.09	104.51	112.60	1	1
K	64	HIS	CB-CG-CD2	8.08	120.69	131.20	1	1
K	136	ASN	CA-CB-CG	8.07	104.53	112.60	1	1
M	275	PRO	N-CA-CB	8.02	111.82	103.00	1	1
G	35	HIS	CB-CG-CD2	7.97	120.84	131.20	1	1
L	75	PRO	N-CA-CB	7.96	111.76	103.00	1	1
M	279	TYR	CD1-CG-CD2	7.95	106.18	118.10	1	1
L	33	ASN	CA-CB-CG	7.94	104.66	112.60	1	1
C	35	HIS	CB-CG-CD2	7.94	120.88	131.20	1	1
H	86	HIS	CB-CG-CD2	7.92	120.90	131.20	1	1
E	42	PRO	N-CA-CB	7.92	111.72	103.00	1	1
M	260	HIS	CB-CG-CD2	7.88	120.96	131.20	1	1
M	307	HIS	CB-CG-CD2	7.85	120.99	131.20	1	1
N	269	PRO	N-CA-CB	7.85	111.64	103.00	1	1
M	213	PHE	CG-CD2-CE2	7.82	107.41	120.70	1	1
N	226	HIS	CB-CG-CD2	7.81	121.05	131.20	1	1
A	42	PRO	N-CA-CB	7.79	111.57	103.00	1	1
K	41	LEU	C-N-CD	7.77	156.86	125.00	1	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 atomic models in this entry.

Model ID	Clash score	Number of clashes
1	2.34	73

There are 73 clashes. The table below contains the detailed list of all clashes based on a MolProbity analysis. Bad clashes are ≥ 0.4 Angstrom.

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:61:SER:O	A:65:LEU:HD12	0.73	1	1
E:61:SER:O	E:65:LEU:HD12	0.70	1	1
L:103:LEU:NE2	M:81:LYS:OD1	0.66	1	1
J:44:DG:H2'	J:45:DT:H72	0.62	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
I:130:DC:H2'	I:131:DG:C8	0.58	1	1
A:79:ALA:N	I:69:DC:OP1	0.58	1	1
I:97:DA:H4'	I:98:DA:OP1	0.57	1	1
I:110:DT:H2"	I:111:DC:C5	0.56	1	1
K:24:LYS:CD2	K:41:LEU:HD23	0.56	1	1
E:78:ILE:N	J:73:DG:OP1	0.55	1	1
I:145:DT:H2"	I:146:DG:C8	0.55	1	1
I:134:DT:H2"	I:135:DG:C8	0.54	1	1
I:135:DG:C2	J:14:DA:C2	0.53	1	1
I:52:DC:H2'	I:53:DT:H72	0.53	1	1
M:149:ILE:CE1	M:165:LEU:HD23	0.53	1	1
I:132:DT:H2'	I:133:DT:H72	0.52	1	1
A:78:ILE:H	I:69:DC:P	0.51	1	1
E:20:PRO:N	E:20:PRO:OE1	0.51	1	1
I:144:DG:H2'	I:145:DT:C6	0.51	1	1
C:2:SER:NH1	I:29:DG:OP2	0.51	1	1
J:51:DT:H2"	J:52:DC:C6	0.50	1	1
J:115:DA:H2'	J:116:DT:H71	0.50	1	1
E:34:PRO:HD3	F:2:SER:HA	0.50	1	1
E:14:SER:HA	I:8:DC:OP1	0.48	1	1
B:15:GLY:NH1	I:59:DT:OP2	0.48	1	1
B:27:ARG:N	J:83:DC:OP1	0.48	1	1
L:236:PRO:OE1	L:239:MET:NH2	0.48	1	1
M:267:LEU:HD13	M:310:GLN:HA	0.48	1	1
I:134:DT:C2'	I:135:DG:C8	0.48	1	1
J:91:DA:H4'	J:92:DC:H5'	0.48	1	1
I:134:DT:H2"	I:135:DG:H8	0.48	1	1
I:92:DC:H2'	I:93:DT:H71	0.47	1	1
I:104:DC:O2	J:44:DG:N2	0.47	1	1
J:92:DC:H2"	J:93:DC:OP2	0.47	1	1
I:129:DA:C2	J:20:DG:C2	0.47	1	1
I:130:DC:C2'	I:131:DG:C8	0.47	1	1
N:84:THR:HA	N:107:GLY:HA2	0.47	1	1
F:14:LEU:NH2	I:80:DA:OP2	0.47	1	1
J:61:DT:H72	J:61:DT:OP2	0.47	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
K:292:TYR:CE3	K:292:TYR:H	0.47	1	1
B:27:ARG:H	J:83:DC:P	0.46	1	1
I:135:DG:N2	J:14:DA:N3	0.46	1	1
L:81:TYR:HA	L:104:PHE:HA	0.46	1	1
J:91:DA:H4'	J:92:DC:OP1	0.45	1	1
J:17:DC:H2'	J:18:DG:C8	0.45	1	1
K:109:GLY:CE1	K:121:LEU:HD12	0.44	1	1
I:107:DC:H4'	I:108:DT:OP1	0.44	1	1
I:138:DG:H2'	I:139:DT:H72	0.44	1	1
L:15:LYS:HA	L:18:ARG:NE	0.44	1	1
A:24:LEU:HA	A:24:LEU:NE	0.43	1	1
I:144:DG:C2	J:5:DG:C2	0.43	1	1
N:270:GLN:OG	N:290:ASP:OD1	0.43	1	1
I:58:DT:C2'	I:59:DT:H71	0.43	1	1
D:61:LYS:O	D:65:ILE:HG23	0.43	1	1
J:80:DA:H4'	J:81:DC:OP1	0.43	1	1
A:1:GLY:HA2	J:86:DT:H5'	0.42	1	1
J:92:DC:H1'	J:93:DC:C6	0.42	1	1
J:113:DG:H2"	J:114:DC:C6	0.42	1	1
D:57:GLY:OG1	D:60:SER:OE1	0.42	1	1
I:87:DA:H2"	I:88:DG:C8	0.42	1	1
L:78:GLU:O	M:105:ILE:CD	0.42	1	1
I:115:DC:H2"	I:116:DA:C8	0.42	1	1
J:44:DG:H2'	J:45:DT:C7	0.41	1	1
J:27:DG:C6	J:28:DA:C6	0.41	1	1
I:133:DT:H1'	I:134:DT:O4'	0.41	1	1
J:62:DC:H2"	J:63:DT:H71	0.41	1	1
J:95:DA:C6	J:96:DG:C6	0.41	1	1
I:34:DG:H2"	I:35:DC:C6	0.41	1	1
L:79:ALA:O	M:106:MET:N	0.41	1	1
J:62:DC:C2'	J:63:DT:H71	0.41	1	1
J:2:DC:H2"	J:3:DA:C8	0.40	1	1
J:91:DA:H2"	J:92:DC:C6	0.40	1	1
F:15:GLY:NH2	J:63:DT:OP1	0.40	1	1

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	Analysed	Favored	Allowed	Outliers
1	1845	1729	73	43

There are 43 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	5	ALA	1
A	19	ALA	1
A	42	PRO	1
B	78	GLU	1
C	91	ILE	1
D	4	MET	1
E	5	ALA	1
E	19	ALA	1
E	42	PRO	1
F	78	GLU	1
G	91	ILE	1
H	14	PRO	1
K	34	ILE	1
K	105	ILE	1
K	264	TRP	1
K	276	ILE	1
K	281	PRO	1
L	75	PRO	1
L	142	PRO	1
L	145	ILE	1
L	176	ILE	1
L	197	CYS	1
L	200	PRO	1
M	81	LYS	1
M	82	PRO	1
M	162	PRO	1
M	235	VAL	1
M	263	GLU	1
M	275	PRO	1

Chain	Res	Type	Models (Total)
M	281	PRO	1
N	73	THR	1
N	82	LYS	1
N	83	PRO	1
N	105	VAL	1
N	148	VAL	1
N	171	PRO	1
N	179	GLY	1
N	199	ARG	1
N	200	PRO	1
N	247	PRO	1
N	263	LEU	1
N	269	PRO	1
N	271	PRO	1

Torsion angles : Protein sidechains ?

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

Model ID	Analysed	Favored	Allowed	Outliers
1	171	134	8	29

There are 29 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	20	PRO	1
A	34	PRO	1
A	65	LEU	1
C	84	PRO	1
D	14	PRO	1
E	20	PRO	1
E	34	PRO	1
E	65	LEU	1
G	84	PRO	1
H	12	PRO	1
K	42	PRO	1
K	121	LEU	1
K	274	PRO	1

Chain	Res	Type	Models (Total)
K	298	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	165	LEU	1
M	252	PRO	1
M	275	PRO	1
M	281	PRO	1
N	44	PRO	1
N	142	PRO	1
N	171	PRO	1
N	269	PRO	1
N	271	PRO	1

Fit of model to data used for modeling ?

Fit of model(s) to crosslinking-MS data

Restraint types

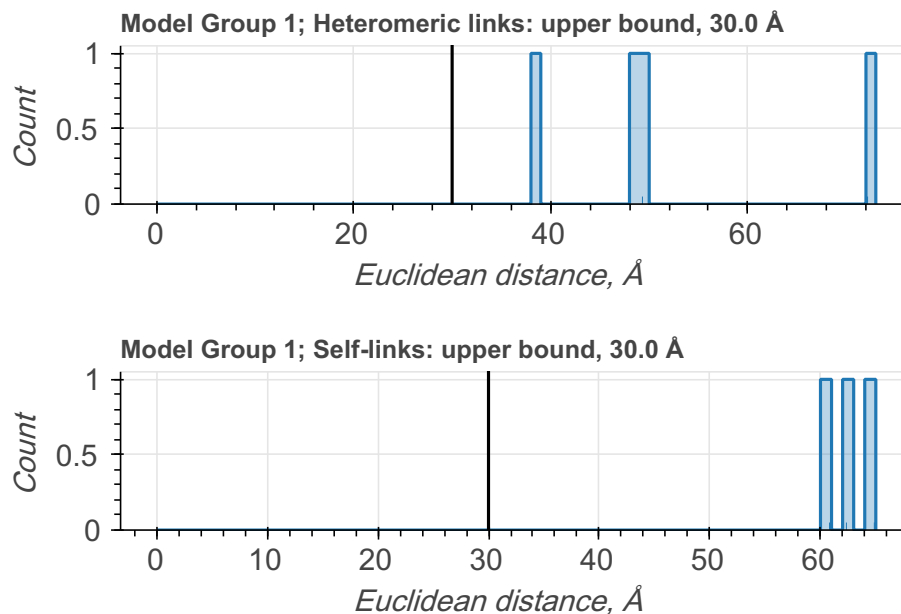
Restraint types are summarized in the table below. Restraints assigned "*by-residue*" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "*coarse-grained*". *Restraint group* represents a set of crosslinking restraints applied collectively in the modeling.

There are 9 crosslinking restraints combined in 9 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
DSSO	LYS	CA	LYS	CA	upper bound	30.0	9

Distograms of individual restraints

Restraints with identical thresholds are grouped into one plot. Only the best distance per restraint per model group/ensemble is plotted. Inter- and intramolecular (including self-links) restraints are also grouped into one plot. Distance for a restraint between coarse-grained beads is calculated as a minimal distance between shells; if beads intersect, the distance will be reported as 0.0. A bead with the highest available resolution for a given residue is used for the assessment.



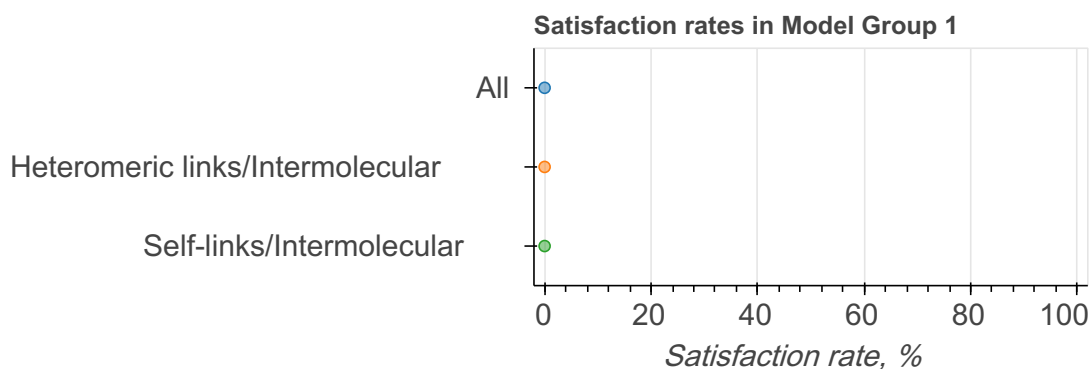
Satisfaction of restraints

Satisfaction of restraints is calculated on a [restraint group](#) (a set of crosslinking restraints applied collectively in the modeling) level. Satisfaction of a restraint group depends on satisfaction of individual restraints in the group and the conditionality (all/any). A restraint group is considered satisfied, if the condition was met in at least one model of the model group/ensemble. The number of measured restraints can be smaller than the total number of restraint groups if crosslinks involve non-modeled residues. Only deposited models are used for validation right now.

State group	State	Model group	# of Deposited models/Total	Restraint group type	Satisfied (%)	Violated (%)	Count (Total=9)
1	1	1	1/1	All	0.00	100.00	7
				Heteromeric links/ Intermolecular	0.00	100.00	4
				Self-links/ Intermolecular	0.00	100.00	3

Per-model satisfaction rates in ensembles

Every point represents one model in a model group/ensemble. Where possible, boxplots with quartile marks are also plotted.



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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