

# 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	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.
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](mailto:helpdesk@pdb-ihm.org)*

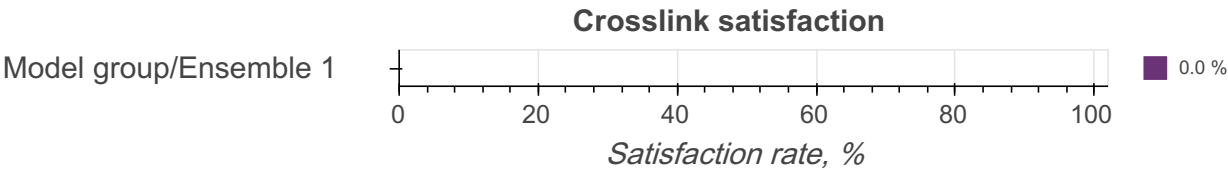
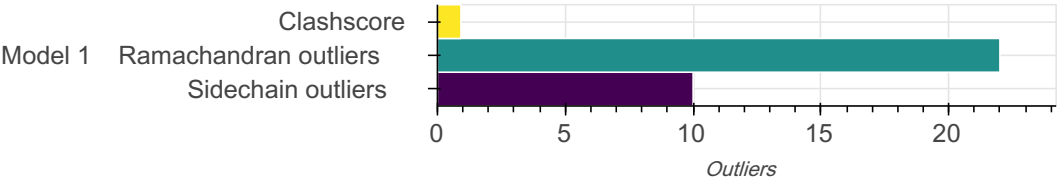
*A user guide is available at [https://pdb-ihm.org/validation\\_help.html](https://pdb-ihm.org/validation_help.html) with specific help available everywhere you see the ? symbol.*

*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 (128-MER)	I	153	-	1-153	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 (128-MER)	J	153	-	1-153	100.00 / 100.00	Atomic
		7	Circadian locomotor output cycles protein kaput	K [M]	375	-	1-84, 85-364, 365-375	100.00 / 100.00	Atomic
		8	Basic helix-loop-helix ARNT-like protein 1	L [N]	384	-	1-71, 72-376, 377-384	100.00 / 100.00	Atomic

### 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	<a href="#">PXD033181</a>
1	3DEM volume	EMDB	<a href="#">EMD-17155</a>
3	Experimental model	PDB	<a href="#">6T93</a>
4	Experimental model	PDB	<a href="#">4F3L</a>
5	Experimental model	PDB	<a href="#">8OSJ</a>

### 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 with crosslink filter and density scoring	Rosetta Dock	None	None	False	False

There are 2 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
2	<a href="#">Coot</a>	0.9.6	model building	<a href="https://www2.mrc-lmb.cam.ac.uk/personal/pemsley/cool/">https://www2.mrc-lmb.cam.ac.uk/personal/pemsley/cool/</a>
1	<a href="#">Rosetta</a>	Not available	protein docking and model building	<a href="https://www.rosettacommons.org/">https://www.rosettacommons.org/</a>

## 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 131 bond length outliers in this entry (1.04% of 12558 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	235	PRO	N-CD	249.41	4.96	1.47	1	1
K	252	PRO	N-CD	248.67	4.95	1.47	1	1
K	162	PRO	N-CD	232.44	4.73	1.47	1	1
K	5	PRO	N-CD	217.92	4.52	1.47	1	1
A	20	PRO	N-CD	208.64	4.39	1.47	1	1
L	180	PRO	N-CD	208.49	4.39	1.47	1	1
E	20	PRO	N-CD	205.21	4.35	1.47	1	1
D	12	PRO	N-CD	183.51	4.04	1.47	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
H	12	PRO	N-CD	182.20	4.02	1.47	1	1
J	107	DC	C1'-N1	122.83	5.17	1.49	1	1
I	119	DC	C1'-N1	122.51	5.17	1.49	1	1
J	57	DC	C1'-N1	122.43	5.16	1.49	1	1
J	5	DC	C1'-N1	122.22	5.16	1.49	1	1
I	115	DT	C1'-N1	122.19	5.16	1.49	1	1
I	108	DT	C1'-N1	121.94	5.15	1.49	1	1
J	99	DT	C1'-N1	121.87	5.15	1.49	1	1
I	60	DT	C1'-N1	121.81	5.14	1.49	1	1
J	88	DC	C1'-N1	121.80	5.14	1.49	1	1
J	66	DC	C1'-N1	121.72	5.14	1.49	1	1
I	15	DC	C1'-N1	121.70	5.14	1.49	1	1
I	128	DC	C1'-N1	121.68	5.14	1.49	1	1
I	56	DC	C1'-N1	121.65	5.14	1.49	1	1
J	117	DC	C1'-N1	121.62	5.14	1.49	1	1
I	92	DT	C1'-N1	121.58	5.14	1.49	1	1
I	54	DC	C1'-N1	121.57	5.14	1.49	1	1
I	85	DC	C1'-N1	121.55	5.14	1.49	1	1
I	126	DC	C1'-N1	121.54	5.14	1.49	1	1
I	38	DT	C1'-N1	121.52	5.14	1.49	1	1
J	19	DC	C1'-N1	121.51	5.14	1.49	1	1
I	34	DT	C1'-N1	121.48	5.13	1.49	1	1
J	29	DC	C1'-N1	121.41	5.13	1.49	1	1
J	45	DT	C1'-N1	121.40	5.13	1.49	1	1
J	30	DC	C1'-N1	121.35	5.13	1.49	1	1
J	86	DT	C1'-N1	121.34	5.13	1.49	1	1
J	102	DT	C1'-N1	121.31	5.13	1.49	1	1
I	98	DC	C1'-N1	121.26	5.13	1.49	1	1
J	96	DC	C1'-N1	121.23	5.13	1.49	1	1
J	48	DT	C1'-N1	121.14	5.12	1.49	1	1
I	96	DC	C1'-N1	120.54	5.11	1.49	1	1
J	16	DT	C1'-N1	120.49	5.10	1.49	1	1
J	108	DT	C1'-N1	120.33	5.10	1.49	1	1
I	78	DT	C1'-N1	120.31	5.10	1.49	1	1
I	45	DC	C1'-N1	120.23	5.10	1.49	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
I	35	DT	C1'-N1	120.20	5.10	1.49	1	1
I	95	DC	C1'-N1	120.14	5.09	1.49	1	1
J	78	DC	C1'-N1	120.02	5.09	1.49	1	1
J	53	DT	C1'-N1	119.96	5.09	1.49	1	1
I	3	DC	C1'-N1	119.89	5.09	1.49	1	1
J	118	DC	C1'-N1	119.83	5.09	1.49	1	1
J	68	DC	C1'-N1	119.83	5.08	1.49	1	1
J	25	DC	C1'-N1	119.80	5.08	1.49	1	1
I	17	DT	C1'-N1	119.69	5.08	1.49	1	1
I	13	DC	C1'-N1	119.66	5.08	1.49	1	1
J	54	DT	C1'-N1	119.63	5.08	1.49	1	1
J	27	DT	C1'-N1	119.63	5.08	1.49	1	1
J	23	DC	C1'-N1	119.54	5.08	1.49	1	1
I	20	DT	C1'-N1	119.54	5.08	1.49	1	1
I	2	DT	C1'-N1	119.52	5.08	1.49	1	1
J	111	DC	C1'-N1	119.49	5.07	1.49	1	1
J	122	DT	C1'-N1	119.49	5.07	1.49	1	1
J	80	DC	C1'-N1	119.42	5.07	1.49	1	1
J	60	DT	C1'-N1	119.39	5.07	1.49	1	1
I	39	DC	C1'-N1	119.38	5.07	1.49	1	1
I	71	DT	C1'-N1	119.34	5.07	1.49	1	1
J	50	DC	C1'-N1	119.30	5.07	1.49	1	1
J	110	DT	C1'-N1	119.28	5.07	1.49	1	1
J	38	DT	C1'-N1	119.26	5.07	1.49	1	1
I	50	DC	C1'-N1	119.25	5.07	1.49	1	1
J	18	DT	C1'-N1	119.19	5.07	1.49	1	1
J	52	DC	C1'-N1	119.18	5.07	1.49	1	1
I	29	DC	C1'-N1	119.17	5.07	1.49	1	1
I	89	DT	C1'-N1	119.12	5.06	1.49	1	1
I	121	DC	C1'-N1	119.10	5.06	1.49	1	1
J	92	DT	C1'-N1	118.99	5.06	1.49	1	1
I	80	DT	C1'-N1	118.99	5.06	1.49	1	1
L	264	HIS	CG-CD2	15.08	1.52	1.35	1	1
E	82	PHE	CG-CD1	7.06	1.53	1.38	1	1
A	82	PHE	CG-CD1	7.01	1.53	1.38	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
K	102	PHE	CG-CD1	6.91	1.53	1.38	1	1
L	104	PHE	CG-CD1	6.86	1.53	1.38	1	1
L	104	PHE	CG-CD2	6.81	1.53	1.38	1	1
K	137	PHE	CG-CD1	6.81	1.53	1.38	1	1
K	190	TYR	CG-CD1	6.76	1.53	1.39	1	1
D	46	TYR	CG-CD1	6.61	1.53	1.39	1	1
K	80	TRP	CG-CD1	6.59	1.53	1.36	1	1
K	102	PHE	CG-CD2	6.59	1.52	1.38	1	1
K	137	PHE	CG-CD2	6.56	1.52	1.38	1	1
L	209	PHE	CG-CD2	6.47	1.52	1.38	1	1
H	46	TYR	CG-CD1	6.45	1.52	1.39	1	1
K	190	TYR	CG-CD2	6.42	1.52	1.39	1	1
D	46	TYR	CG-CD2	6.27	1.52	1.39	1	1
E	82	PHE	CG-CD2	6.20	1.51	1.38	1	1
L	209	PHE	CG-CD1	6.18	1.51	1.38	1	1
A	82	PHE	CG-CD2	6.17	1.51	1.38	1	1
H	46	TYR	CG-CD2	6.15	1.52	1.39	1	1
B	53	LEU	CG-CD2	5.20	1.35	1.52	1	1
F	53	LEU	CG-CD2	5.16	1.35	1.52	1	1
L	53	LEU	CG-CD2	5.15	1.35	1.52	1	1
K	54	LEU	CG-CD2	5.09	1.35	1.52	1	1
E	69	LEU	CG-CD2	5.02	1.36	1.52	1	1

### Standard geometry: angle outliers ?

There are 993 bond angle outliers in this entry (5.65% of 17562 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	180	PRO	CA-N-CD	62.31	24.76	112.00	1	1
K	5	PRO	N-CD-CG	57.24	17.34	103.20	1	1
L	235	PRO	CA-N-CD	54.05	36.33	112.00	1	1
K	252	PRO	CA-N-CD	53.70	36.82	112.00	1	1
A	20	PRO	N-CD-CG	51.38	26.13	103.20	1	1
K	162	PRO	N-CD-CG	50.08	28.09	103.20	1	1
E	20	PRO	N-CD-CG	49.88	28.39	103.20	1	1
J	66	DC	C1'-N1-C2	48.04	47.64	119.70	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
J	96	DC	C1'-N1-C2	48.02	47.67	119.70	1	1
I	54	DC	C1'-N1-C2	47.99	47.72	119.70	1	1
J	117	DC	C1'-N1-C2	47.98	47.73	119.70	1	1
I	85	DC	C1'-N1-C2	47.98	47.73	119.70	1	1
I	126	DC	C1'-N1-C2	47.98	47.74	119.70	1	1
I	15	DC	C1'-N1-C2	47.96	47.77	119.70	1	1
J	19	DC	C1'-N1-C2	47.91	47.83	119.70	1	1
J	5	DC	C1'-N1-C2	47.91	47.84	119.70	1	1
J	86	DT	C1'-N1-C2	47.89	47.52	119.35	1	1
I	119	DC	C1'-N1-C2	47.88	47.89	119.70	1	1
I	128	DC	C1'-N1-C2	47.87	47.90	119.70	1	1
J	88	DC	C1'-N1-C2	47.86	47.90	119.70	1	1
J	29	DC	C1'-N1-C2	47.85	47.93	119.70	1	1
J	30	DC	C1'-N1-C2	47.84	47.94	119.70	1	1
J	107	DC	C1'-N1-C2	47.83	47.96	119.70	1	1
I	56	DC	C1'-N1-C2	47.82	47.97	119.70	1	1
I	98	DC	C1'-N1-C2	47.81	47.98	119.70	1	1
I	115	DT	C1'-N1-C2	47.80	47.64	119.35	1	1
J	45	DT	C1'-N1-C2	47.79	47.66	119.35	1	1
I	34	DT	C1'-N1-C2	47.78	47.69	119.35	1	1
J	57	DC	C1'-N1-C2	47.76	48.05	119.70	1	1
J	102	DT	C1'-N1-C2	47.74	47.74	119.35	1	1
I	108	DT	C1'-N1-C2	47.63	47.90	119.35	1	1
J	48	DT	C1'-N1-C2	47.62	47.92	119.35	1	1
I	38	DT	C1'-N1-C2	47.61	47.94	119.35	1	1
I	92	DT	C1'-N1-C2	47.59	47.96	119.35	1	1
I	60	DT	C1'-N1-C2	47.54	48.04	119.35	1	1
J	99	DT	C1'-N1-C2	47.54	48.04	119.35	1	1
D	12	PRO	CA-N-CD	46.73	46.58	112.00	1	1
H	12	PRO	CA-N-CD	46.55	46.83	112.00	1	1
I	29	DC	C1'-N1-C2	46.45	50.02	119.70	1	1
I	121	DC	C1'-N1-C2	46.39	50.12	119.70	1	1
J	52	DC	C1'-N1-C2	46.31	50.24	119.70	1	1
I	39	DC	C1'-N1-C2	46.28	50.29	119.70	1	1
I	50	DC	C1'-N1-C2	46.26	50.32	119.70	1	1



Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
J	50	DC	C1'-N1-C2	46.22	50.36	119.70	1	1
J	80	DC	C1'-N1-C2	46.22	50.37	119.70	1	1
J	38	DT	C1'-N1-C2	46.22	50.03	119.35	1	1
J	118	DC	C1'-N1-C2	46.21	50.39	119.70	1	1
I	13	DC	C1'-N1-C2	46.17	50.44	119.70	1	1
J	122	DT	C1'-N1-C2	46.14	50.14	119.35	1	1
I	3	DC	C1'-N1-C2	46.14	50.50	119.70	1	1
J	92	DT	C1'-N1-C2	46.13	50.16	119.35	1	1
I	89	DT	C1'-N1-C2	46.13	50.16	119.35	1	1
I	2	DT	C1'-N1-C2	46.10	50.19	119.35	1	1
I	71	DT	C1'-N1-C2	46.08	50.24	119.35	1	1
J	111	DC	C1'-N1-C2	46.05	50.62	119.70	1	1
J	60	DT	C1'-N1-C2	46.04	50.28	119.35	1	1
J	78	DC	C1'-N1-C2	46.03	50.65	119.70	1	1
I	45	DC	C1'-N1-C2	46.03	50.66	119.70	1	1
I	80	DT	C1'-N1-C2	46.01	50.34	119.35	1	1
J	68	DC	C1'-N1-C2	46.00	50.70	119.70	1	1
J	18	DT	C1'-N1-C2	45.96	50.42	119.35	1	1
J	27	DT	C1'-N1-C2	45.93	50.46	119.35	1	1
J	23	DC	C1'-N1-C2	45.92	50.83	119.70	1	1
J	110	DT	C1'-N1-C2	45.88	50.53	119.35	1	1
I	17	DT	C1'-N1-C2	45.87	50.54	119.35	1	1
K	162	PRO	CA-N-CD	45.83	47.84	112.00	1	1
I	20	DT	C1'-N1-C2	45.81	50.63	119.35	1	1
J	25	DC	C1'-N1-C2	45.78	51.03	119.70	1	1
I	95	DC	C1'-N1-C2	45.74	51.08	119.70	1	1
I	78	DT	C1'-N1-C2	45.74	50.74	119.35	1	1
I	96	DC	C1'-N1-C2	45.73	51.11	119.70	1	1
J	108	DT	C1'-N1-C2	45.70	50.80	119.35	1	1
J	16	DT	C1'-N1-C2	45.66	50.85	119.35	1	1
I	35	DT	C1'-N1-C2	45.66	50.86	119.35	1	1
J	53	DT	C1'-N1-C2	45.60	50.95	119.35	1	1
L	235	PRO	N-CD-CG	45.55	34.87	103.20	1	1
J	54	DT	C1'-N1-C2	45.52	51.08	119.35	1	1
K	252	PRO	N-CD-CG	45.43	35.06	103.20	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
K	5	PRO	CA-N-CD	39.92	56.12	112.00	1	1
D	12	PRO	N-CD-CG	39.54	43.89	103.20	1	1
H	12	PRO	N-CD-CG	38.95	44.77	103.20	1	1
A	20	PRO	CA-N-CD	36.58	60.79	112.00	1	1
E	20	PRO	CA-N-CD	35.41	62.42	112.00	1	1
J	107	DC	C1'-N1-C6	33.31	69.74	119.70	1	1
J	57	DC	C1'-N1-C6	33.18	69.94	119.70	1	1
I	119	DC	C1'-N1-C6	33.07	70.09	119.70	1	1
J	5	DC	C1'-N1-C6	32.92	70.31	119.70	1	1
J	88	DC	C1'-N1-C6	32.86	70.42	119.70	1	1
I	60	DT	C1'-N1-C6	32.81	70.14	119.35	1	1
I	56	DC	C1'-N1-C6	32.75	70.58	119.70	1	1
J	19	DC	C1'-N1-C6	32.70	70.65	119.70	1	1
J	66	DC	C1'-N1-C6	32.70	70.65	119.70	1	1
I	15	DC	C1'-N1-C6	32.70	70.66	119.70	1	1
I	54	DC	C1'-N1-C6	32.69	70.66	119.70	1	1
I	126	DC	C1'-N1-C6	32.68	70.68	119.70	1	1
I	98	DC	C1'-N1-C6	32.67	70.69	119.70	1	1
I	108	DT	C1'-N1-C6	32.67	70.34	119.35	1	1
I	115	DT	C1'-N1-C6	32.66	70.36	119.35	1	1
J	117	DC	C1'-N1-C6	32.65	70.72	119.70	1	1
I	128	DC	C1'-N1-C6	32.64	70.74	119.70	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	0.92	21

There are 21 clashes. The table below contains the detailed list of all clashes based on a MolProbity analysis. Bad clashes are  $\geq 0.4$  Angstrom.

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
I:118:DT:H3	J:11:DG:H1	0.94	1	1
I:117:DG:H1	J:12:DT:H3	0.90	1	1
I:47:DG:H1	J:82:DT:H3	0.89	1	1
K:56:LYS:O	K:60:PHE:CG	0.61	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
J:103:DA:H2"	J:104:DG:C5'	0.53	1	1
K:226:GLU:N	K:227:ASP:CD	0.52	1	1
K:56:LYS:HG2	K:60:PHE:NE2	0.50	1	1
K:227:ASP:N	K:228:ARG:CD	0.49	1	1
G:30:PRO:N	G:31:VAL:CD	0.48	1	1
I:115:DT:H2"	I:116:DA:C8	0.46	1	1
D:82:SER:NZ	K:216:THR:OE2	0.46	1	1
K:278:GLY:O	L:130:ASP:NH1	0.42	1	1
C:30:PRO:N	C:31:VAL:CD	0.42	1	1
F:9:LYS:N	F:10:GLY:CD	0.41	1	1
J:103:DA:H2"	J:104:DG:H5"	0.41	1	1
I:126:DC:C2	J:4:DA:C2	0.41	1	1
I:85:DC:C2	J:45:DT:C2	0.41	1	1
K:101:PHE:NE2	K:155:LEU:O	0.41	1	1
B:9:LYS:N	B:10:GLY:CD	0.41	1	1
F:30:ILE:N	F:30:ILE:OE1	0.40	1	1
J:103:DA:H2"	J:104:DG:H5'	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	1290	1228	40	22

There are 22 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	34	PRO	1
B	72	ASP	1
B	77	THR	1
D	14	PRO	1
D	54	PRO	1
E	34	PRO	1
F	77	THR	1
H	14	PRO	1
H	53	HIS	1
H	54	PRO	1

Chain	Res	Type	Models (Total)
K	82	PRO	1
K	239	THR	1
K	240	PRO	1
K	274	PRO	1
L	69	LEU	1
L	83	PRO	1
L	159	PRO	1
L	175	ASP	1
L	199	ARG	1
L	200	PRO	1
L	247	PRO	1
L	269	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	130	113	7	10

There are 10 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	20	PRO	1
D	12	PRO	1
E	20	PRO	1
H	12	PRO	1
K	5	PRO	1
K	162	PRO	1
K	252	PRO	1
L	180	PRO	1
L	235	PRO	1
L	254	LEU	1

### Fit of model to data used for modeling ?

Fit of model(s) to crosslinking-MS data

## Restraint types

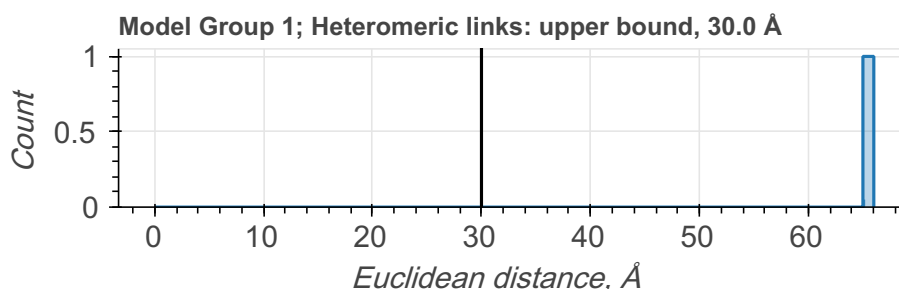
Restraint types are summarized in the table below. Restraints assigned "*by-residue*" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "*coarse-grained*". *Restraint group* represents a set of crosslinking restraints applied collectively in the modeling.

There are 1 crosslinking restraints combined in 1 restraint groups.

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

## 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.



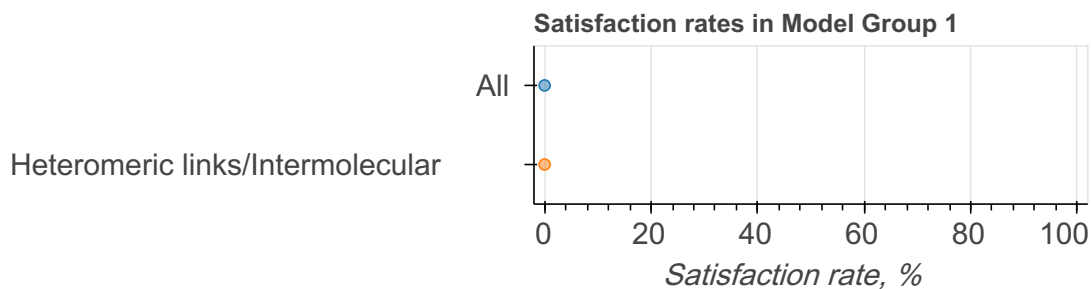
## Satisfaction of restraints

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=1)
1	1	1	1/1	All	0.00	100.00	1
				Heteromeric links/ Intermolecular	0.00	100.00	1

## 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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