

Integrative Structure Validation Report ?

February 18, 2025 - 08:28 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	8ZZS
PDB-Dev ID	PDBDEV_00000028
Structure Title	Complex of RNF168-RING domain and the nucleosome
Structure Authors	Horn V; Uckelmann M; Zhang H; Eerland J; Aarsman I; le Paige UB; Davidovich C; Sixma TK; van Ingen H
Deposited on	2019-01-16

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

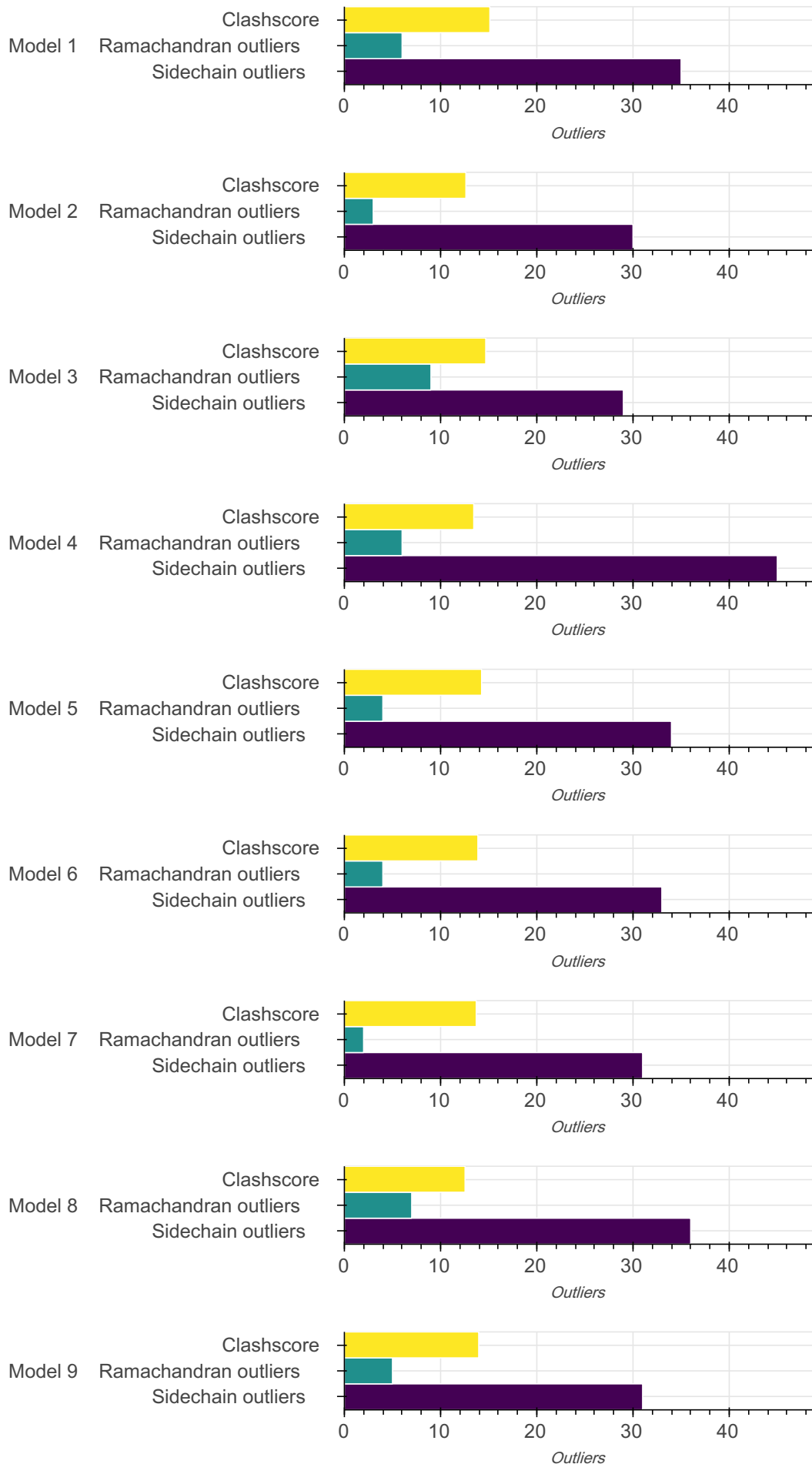
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

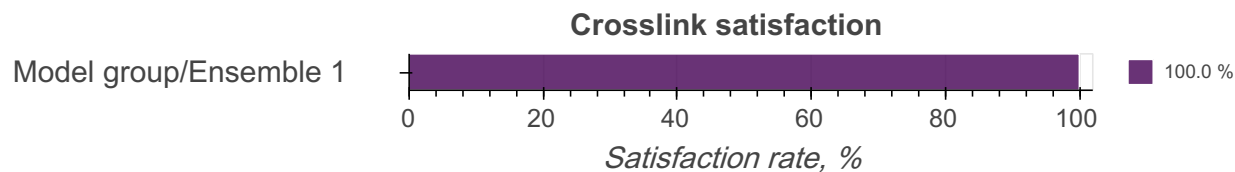
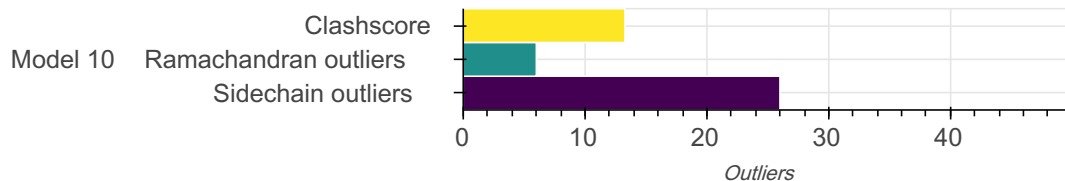
List of references used to build this report is available [here](#).

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 10 model(s). A total of 7 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	1-10	1	H3	A	99	-	1-99	100.00 / 100.00	Atomic
				E					
		2	H4	B	80	-	1-80	100.00 / 100.00	Atomic
				F					
		3	H2A	C	107	-	1-107	100.00 / 100.00	Atomic
				G					
		4	H2B	D	95	-	1-95	100.00 / 100.00	Atomic
				H					
		5	DNA strand 1	I	147	-	1-147	100.00 / 100.00	Atomic
		6	DNA strand 2	J	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
		7	RNF168 RING domain	K	91	-	1-91	100.00 / 100.00	Atomic

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	Experimental model	PDB	2PYO
2	Experimental model	PDB	4GB0
3	Mutagenesis data	Not available	10.1038/s41467-019-09756-z
4	NMR data	BMRB	27786
5	NMR data	BMRB	27791
6	NMR data	BMRB	27792
7	Crosslinking-MS data	PRIDE	PXD012723

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	None	False	False

There are 2 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	HADDOCK	2.20	molecular docking	http://haddock.science.uu.nl/services/HADDOCK/
2	JWALK	1.10	XL-MS validation	http://jwalk.ismb.lon.ac.uk/jwalk/download/

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.

Mutagenesis

Validation for this section is under development.

NMR

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 no bond length outliers.

Standard geometry: angle outliers ?

There are no bond angle outliers.

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	15.12	352
2	12.63	294
3	14.69	342
4	13.45	313
5	14.26	332
6	13.88	323
7	13.71	319
8	12.55	292
9	13.96	325
10	13.28	309

There are 3201 clashes. The table below contains the detailed list of all clashes based on a MolProbity analysis. Bad clashes are ≥ 0.4 Angstrom. The output is limited to 100 rows.

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
I:146:DA:H2"	I:147:DT:H5"	1.02	7	7
J:91:DT:H2'	J:92:DT:H71	0.98	6	4
J:145:DG:H2"	J:146:DA:H5'	0.96	7	4
J:116:DA:H2"	J:117:DC:H5"	0.96	3	4
H:5:GLU:HA	I:123:DG:H5'	0.92	3	2
I:124:DT:H2"	I:125:DA:H5"	0.92	5	3
J:146:DA:H2"	J:147:DT:H5"	0.92	1	8
C:29:ARG:HG2	J:113:DT:H5'	0.91	1	4
J:13:DC:H2"	J:14:DT:H5'	0.91	4	4
I:47:DC:H2"	I:48:DT:H72	0.89	4	1
I:47:DC:H2"	I:48:DT:H71	0.87	9	2
J:69:DC:H2"	J:70:DT:H71	0.87	7	6
I:121:DT:H2"	I:122:DG:C8	0.87	3	4
J:126:DG:H2"	J:127:DT:H5"	0.86	5	3
I:44:DC:H2"	I:45:DT:H5'	0.86	3	4
J:22:DC:H2"	J:23:DT:H5'	0.83	1	2
I:114:DA:H2"	I:115:DC:H5"	0.83	3	2
H:3:ARG:HG3	I:123:DG:H4'	0.83	8	2
I:69:DC:H2"	I:70:DT:H71	0.83	10	4
I:33:DG:H2"	I:34:DT:H5"	0.83	7	4
J:97:DT:H2"	J:98:DG:H5"	0.82	1	1
J:10:DC:H2'	J:11:DA:C8	0.82	5	3
J:47:DC:H2'	J:48:DT:H72	0.82	8	2
J:137:DT:H2"	J:138:DG:H5'	0.81	1	2
A:29:LEU:HD23	J:91:DT:H5"	0.81	6	6
A:4:ARG:HG2	J:84:DA:H4'	0.81	10	1
I:135:DG:H2"	I:136:DG:H5"	0.81	9	1
J:1:DA:H2'	J:2:DT:C6	0.80	5	1
J:55:DA:H2'	J:56:DA:C8	0.80	8	3
D:5:GLU:HA	J:123:DG:H5'	0.80	2	2
H:56:ARG:HD2	J:40:DG:H5"	0.80	5	3
J:57:DA:H2"	J:58:DG:C8	0.79	8	7
H:9:ILE:HD11	I:122:DG:H5"	0.79	9	1
J:72:DG:H2"	J:73:DA:H5'	0.79	4	1
I:45:DT:H2"	I:46:DG:C8	0.79	1	7

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
D:86:LYS:HE2	K:46:SER:HA	0.79	8	1
J:72:DG:H2'	J:73:DA:C8	0.78	4	4
J:121:DT:H2"	J:122:DG:C8	0.78	4	4
J:38:DT:H2"	J:39:DG:N7	0.78	5	10
I:47:DC:H2"	I:48:DT:C7	0.78	10	5
J:6:DT:H2"	J:7:DA:H5"	0.78	9	1
K:16:ILE:HD11	K:33:LEU:HB2	0.78	1	1
I:125:DA:H2"	I:126:DG:H5"	0.78	3	4
J:79:DG:H2"	J:80:DC:C5	0.77	6	6
I:88:DG:H4'	I:89:DC:H5'	0.77	5	3
I:38:DT:H2"	I:39:DG:N7	0.77	7	10
J:133:DC:H2"	J:134:DA:C8	0.77	9	7
I:143:DT:H2"	I:144:DT:H5'	0.77	1	1
I:38:DT:H2"	I:39:DG:C8	0.77	10	8
I:36:DT:H2'	I:37:DT:C6	0.77	7	5
J:88:DG:H4'	J:89:DC:H5'	0.77	1	4
I:32:DT:H2"	I:33:DG:H5'	0.77	2	1
J:131:DT:H2"	J:132:DG:C8	0.76	9	7
J:20:DT:H2"	J:21:DA:H5'	0.76	4	2
J:119:DT:H2'	J:120:DT:C6	0.76	6	2
J:38:DT:H2"	J:39:DG:C8	0.76	2	10
J:99:DG:H1'	J:100:DA:N7	0.76	5	7
I:97:DT:H2'	I:98:DG:C8	0.76	9	6
E:6:ARG:HG3	J:145:DG:H5'	0.76	9	2
J:53:DC:H2"	J:54:DA:H5'	0.75	5	2
I:58:DG:H2"	I:59:DG:N7	0.75	8	4
H:73:PRO:HD2	H:76:LEU:HB2	0.75	9	5
J:64:DT:H2'	J:65:DT:C6	0.75	9	4
I:73:DA:H2'	I:74:DA:C8	0.75	4	5
I:128:DA:H2'	I:129:DT:C6	0.75	7	4
F:54:ALA:HA	H:54:ASN:HD21	0.75	2	1
C:51:GLU:HG2	K:58:SER:HB2	0.75	5	1
I:81:DT:H2"	I:82:DG:C8	0.74	5	10
I:67:DA:H2"	I:68:DG:C8	0.74	9	7
J:26:DC:H2"	J:27:DA:C8	0.74	1	7

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
H:5:GLU:HA	I:123:DG:H5"	0.74	9	4
I:35:DA:H2'	I:36:DT:C6	0.74	3	1
I:130:DC:H2'	I:131:DT:H71	0.74	8	3
E:29:LEU:HB3	E:30:PRO:HD3	0.73	4	10
E:10:VAL:HG21	I:83:DA:H3'	0.73	4	3
I:109:DC:H2"	I:110:DA:C8	0.73	4	9
J:20:DT:H2'	J:21:DA:C8	0.73	9	3
I:88:DG:H2"	I:89:DC:C5	0.73	8	5
J:16:DC:H2"	J:17:DA:N7	0.73	9	8
I:58:DG:H4'	I:59:DG:H5'	0.73	5	1
J:102:DC:H2"	J:103:DA:C8	0.73	7	2
J:10:DC:H2"	J:11:DA:C8	0.72	7	2
B:2:ASP:HB3	B:5:GLN:HB2	0.72	3	1
J:69:DC:H2"	J:70:DT:C7	0.72	8	5
J:119:DT:H2"	J:120:DT:H5'	0.72	4	2
I:67:DA:H2"	I:68:DG:N7	0.72	4	8
J:134:DA:H2"	J:135:DG:C8	0.72	10	8
J:90:DC:H2"	J:91:DT:C7	0.72	2	1
I:139:DG:H2'	I:140:DA:C8	0.72	6	4
J:136:DG:H2'	J:137:DT:H71	0.72	5	1
I:125:DA:C2'	I:126:DG:H5"	0.72	3	3
E:6:ARG:HG3	J:145:DG:H5"	0.72	7	4
H:68:VAL:HG13	H:72:LEU:HD12	0.72	7	5
J:18:DG:H2'	J:19:DA:C8	0.72	9	1
J:67:DA:H1'	J:68:DG:N7	0.72	3	2
J:58:DG:H1'	J:59:DG:N7	0.72	5	2
J:82:DG:H2"	J:83:DA:H5"	0.72	8	1
J:8:DT:H2'	J:9:DC:C6	0.72	10	4
D:5:GLU:HA	J:123:DG:H5"	0.72	7	6
I:6:DT:H2'	I:7:DA:C8	0.72	10	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	835	802	27	6

Model ID	Analysed	Favored	Allowed	Outliers
2	835	798	34	3
3	835	798	28	9
4	835	803	26	6
5	835	800	31	4
6	835	802	29	4
7	835	804	29	2
8	835	793	35	7
9	835	797	33	5
10	835	801	28	6

There are 15 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
C	105	LYS	10
D	73	PRO	6
G	106	LYS	6
C	106	LYS	5
H	73	PRO	5
H	74	GLY	5
K	45	ALA	4
A	45	ASP	2
C	104	PRO	2
D	2	LYS	2
A	7	PRO	1
A	98	ARG	1
E	7	PRO	1
F	74	THR	1
K	56	VAL	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	719	641	43	35
2	719	648	41	30
3	719	636	54	29
4	719	625	49	45

Model ID	Analysed	Favored	Allowed	Outliers
5	719	648	37	34
6	719	640	46	33
7	719	641	47	31
8	719	630	53	36
9	719	646	42	31
10	719	643	50	26

There are 122 unique sidechain outliers. Detailed list of outliers are tabulated below. The output is limited to 100 rows.

Chain	Res	Type	Models (Total)
G	85	SER	10
K	1	LEU	10
D	61	SER	9
E	44	THR	9
H	61	SER	9
A	44	THR	8
B	51	THR	8
E	51	SER	8
K	10	SER	8
C	63	THR	7
C	88	THR	7
E	22	THR	7
F	74	THR	7
G	63	THR	7
K	57	SER	7
K	68	SER	7
A	40	GLN	6
A	51	SER	6
B	74	THR	6
C	85	SER	6
E	50	SER	5
G	5	SER	5
K	29	CYS	5
A	22	THR	4
A	50	SER	4

Chain	Res	Type	Models (Total)
C	3	SER	4
D	22	THR	4
F	51	THR	4
G	3	SER	4
H	93	SER	4
K	41	THR	4
D	57	SER	3
D	86	LYS	3
D	92	THR	3
E	23	GLU	3
G	76	ASN	3
H	57	SER	3
K	4	ASP	3
K	30	ASN	3
K	46	SER	3
K	47	LEU	3
A	4	ARG	2
A	32	GLN	2
A	41	ASP	2
B	52	GLU	2
C	5	SER	2
C	51	GLU	2
C	59	ASP	2
D	37	ASN	2
E	21	SER	2
E	27	ARG	2
E	41	ASP	2
E	45	ASP	2
G	6	ASN	2
G	59	ASP	2
H	21	ASP	2
K	34	CYS	2
K	52	CYS	2
K	55	ARG	2
K	75	TRP	2

Chain	Res	Type	Models (Total)
K	89	ARG	2
A	23	GLU	1
A	28	LYS	1
A	37	GLU	1
A	79	LYS	1
B	12	ILE	1
B	46	ASP	1
B	48	VAL	1
B	49	THR	1
C	7	ARG	1
C	25	ASN	1
C	29	ARG	1
C	42	MET	1
C	45	LEU	1
C	58	ARG	1
C	76	ASN	1
C	82	LYS	1
C	87	VAL	1
C	94	VAL	1
D	5	GLU	1
D	6	SER	1
D	14	VAL	1
D	21	ASP	1
D	26	SER	1
D	48	SER	1
D	56	ARG	1
D	58	THR	1
D	83	GLU	1
D	93	SER	1
E	4	ARG	1
E	48	PHE	1
E	49	GLN	1
E	69	GLU	1
E	79	LYS	1
F	8	THR	1

Chain	Res	Type	Models (Total)
F	24	ILE	1
F	36	LEU	1
F	52	GLU	1
F	75	LEU	1
G	12	PHE	1

Fit of model to data used for modeling ?

Fit of model(s) to crosslinking-MS data

Restraint types

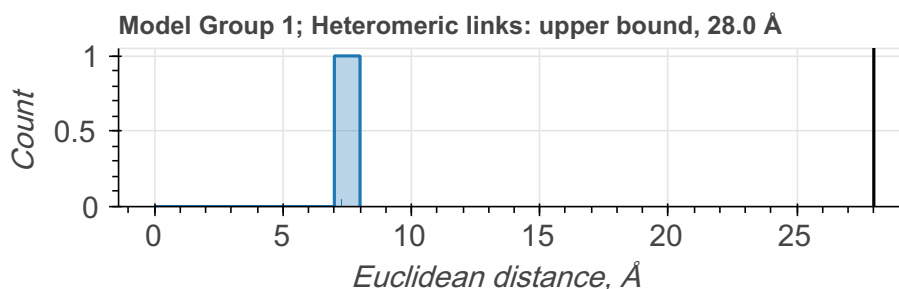
Restraint types are summarized in the table below. Restraints assigned "by-residue" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "coarse-grained". *Restraint group* represents a set of crosslinking restraints applied collectively in the modeling.

There are 1 crosslinking restraints combined in 1 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
BS3	LYS	CA	LYS	CA	upper bound	28.0	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.



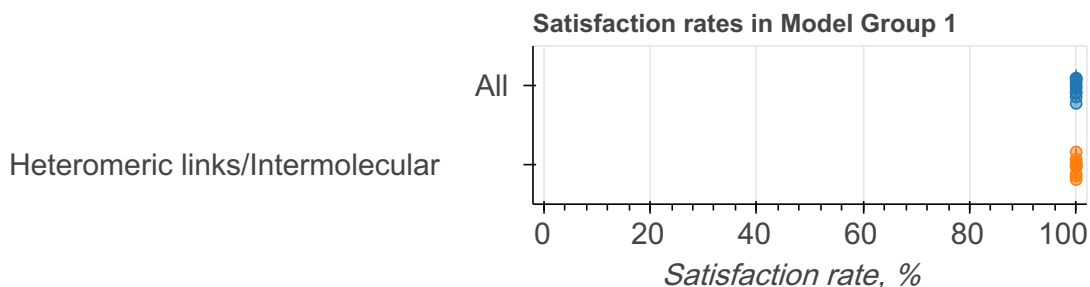
Satisfaction of restraints

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	10/10	All	100.00	0.00	1
				Heteromeric links/ Intermolecular	100.00	0.00	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.



Mutagenesis

Validation for this section is under development.

NMR

Validation for this section is under development.

Fit of model to data used for validation ?

Validation for this section is under development.

Acknowledgments

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