

# Integrative Structure Validation Report ?

March 27, 2025 - 09:57 AM PDT

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

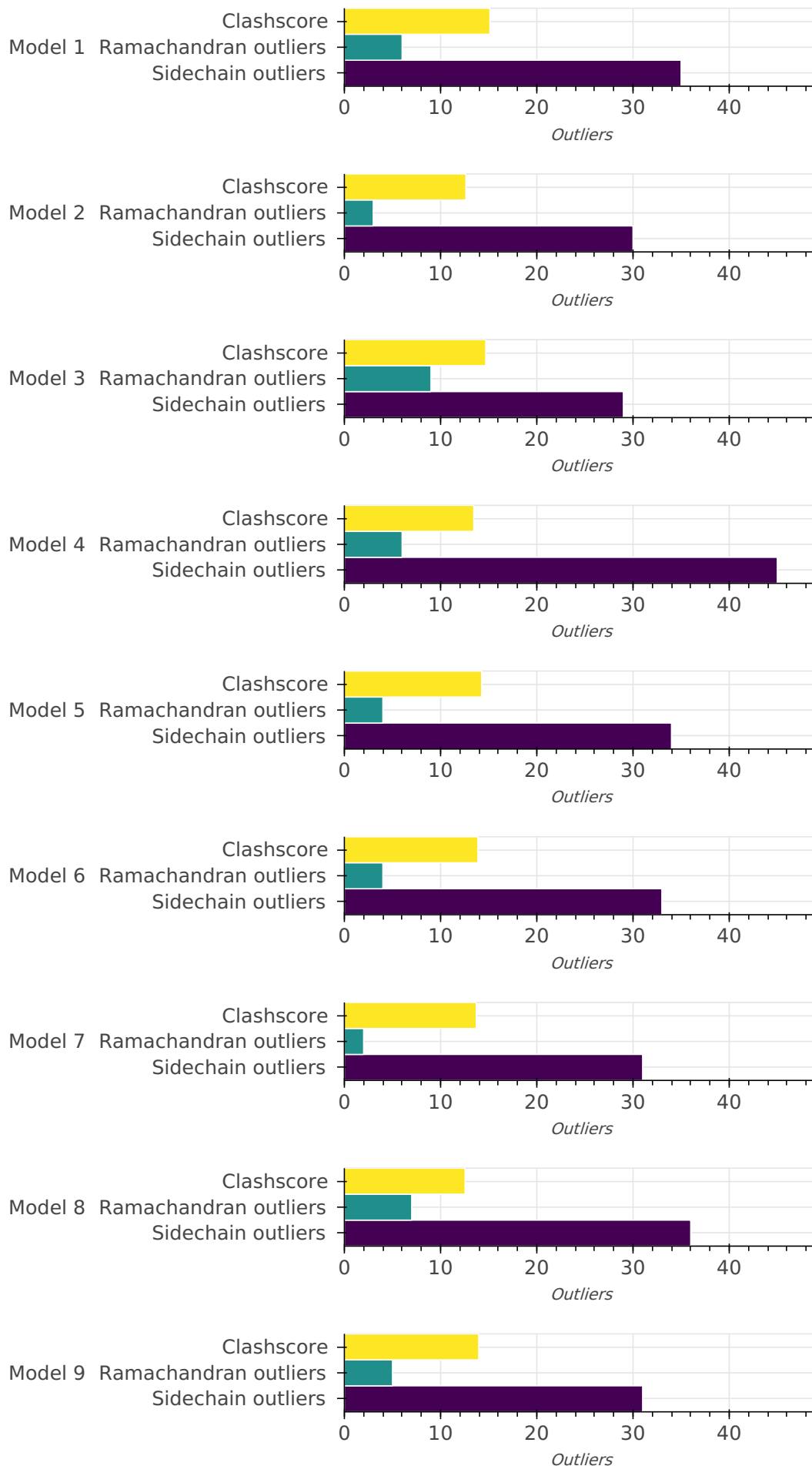
*A user guide is available at [https://pdb-ihm.org/validation\\_help.html](https://pdb-ihm.org/validation_help.html) with specific help available everywhere you see the ? symbol.*

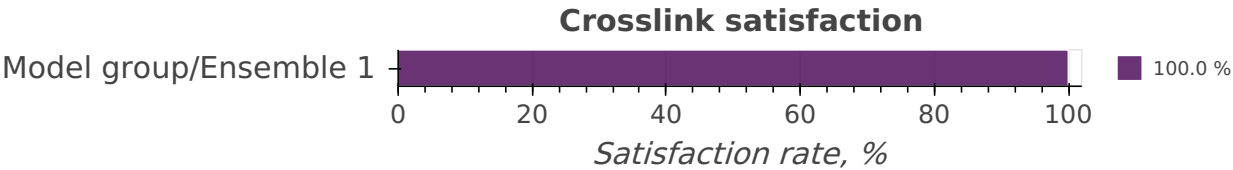
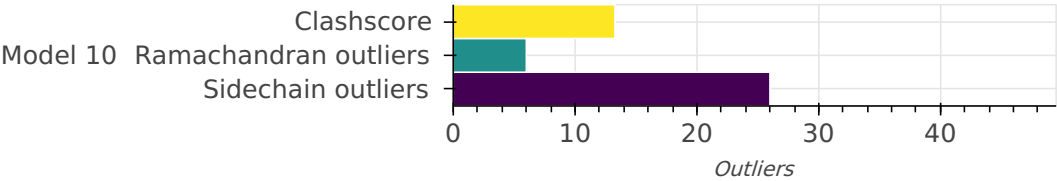
*List of references used to build this report is available [here](#).*

## 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 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

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		6	DNA strand 2	J	147	-	1-147	100.00 / 100.00	Atomic
		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	<a href="#">2PYO</a>
2	Experimental model	PDB	<a href="#">4GB0</a>
3	Mutagenesis data	Not available	<a href="#">10.1038/s41467-019-09756-z</a>
4	NMR data	BMRB	<a href="#">27786</a>
5	NMR data	BMRB	<a href="#">27791</a>
6	NMR data	BMRB	<a href="#">27792</a>
7	Crosslinking-MS data	PRIDE	<a href="#">PXD012723</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	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	<a href="#">HADDOCK</a>	2.20	molecular docking	<a href="http://haddock.science.uu.nl/services/HADDOCK/">http://haddock.science.uu.nl/services/HADDOCK/</a>
2	<a href="#">JWALK</a>	1.10	XL-MS validation	<a href="http://jwalk.ismb.lon.ac.uk/jwalk/download/">http://jwalk.ismb.lon.ac.uk/jwalk/download/</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.

### 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

Model ID	Clash score	Number of clashes
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  $\geq 0.4$  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

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
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
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

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
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
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
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
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

Chain	Res	Type	Models (Total)
G	5	SER	5
K	29	CYS	5
A	22	THR	4
A	50	SER	4
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

Chain	Res	Type	Models (Total)
K	34	CYS	2
K	52	CYS	2
K	55	ARG	2
K	75	TRP	2
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

Chain	Res	Type	Models (Total)
E	49	GLN	1
E	69	GLU	1
E	79	LYS	1
F	8	THR	1
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*".

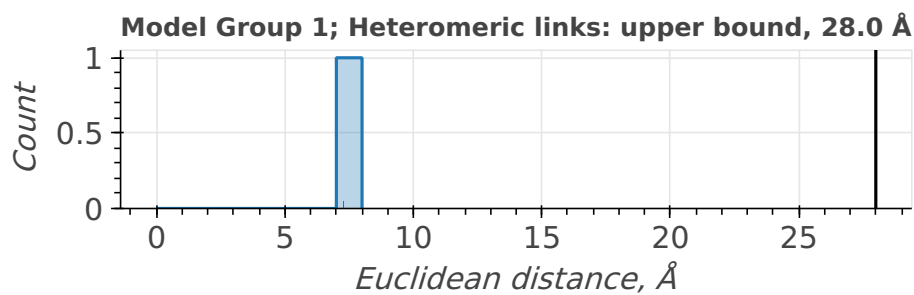
*Restraint group* represents a set of crosslinking restraints applied collectively in the modeling.

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

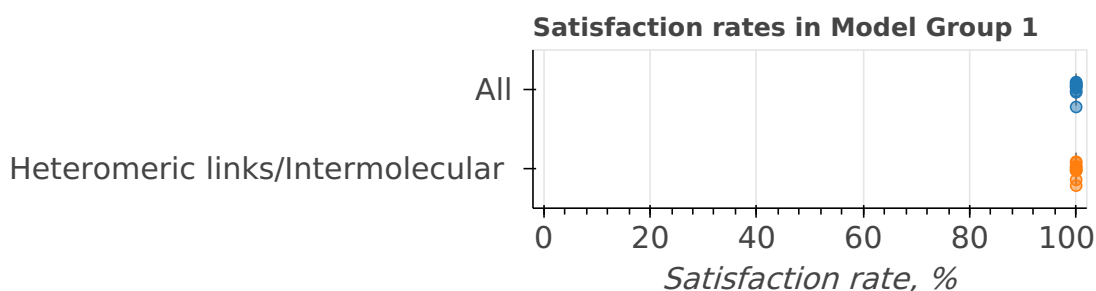
Satisfaction of restraints is calculated on a *restraint group* (a set of crosslinking restraints applied

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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