

Integrative Structure Validation Report ?

February 27, 2025 - 12:16 PM 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	9A18
PDB-Dev ID	PDBDEV_00000080
Structure Title	Integrative model of full-length RAGE in complex with S100B
Structure Authors	Moysa A; Steczkiewicz K; Niedzialek D; Hammerschmid D; Zhukova L; Sobott F; Dadlez M
Deposited on	2021-01-26

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

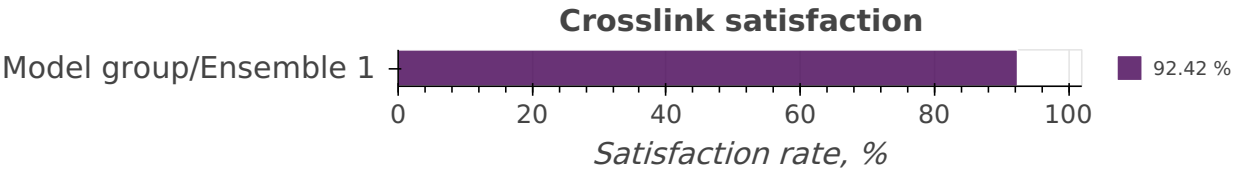
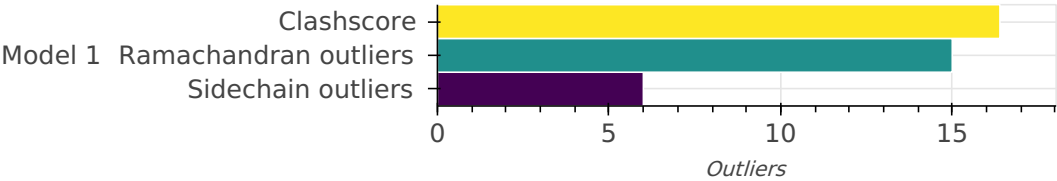
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 6 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	RAGE	A	383	-	1-301, 302-383	100.00 / 78.59	Atomic
				B					
				C					
				D					
		2	S100B	E	91	-	1-91	100.00 / 100.00	Atomic
				F					
				G					
				H					

Datasets used for modeling ?

There are 6 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Experimental model	PDB	4ybh
2	Experimental model	PDB	4xyn
3	Experimental model	PDB	5d7f
4	Crosslinking-MS data	MASSIVE	MSV000086438
5	Crosslinking-MS data	MASSIVE	MSV000086437
6	H/D exchange data	MASSIVE	MSV000086718

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	modeling	–	–	–	False	False

There is 1 software package reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	ROSETTA	Not available	model building	https://github.com/RosettaCommons

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.

H/D exchange

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 17 bond length outliers in this entry (0.12% of 14765 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	341	LEU	C-N	81.97	0.18	1.33	1	1
C	341	LEU	C-N	81.95	0.18	1.33	1	1
A	341	LEU	C-N	81.92	0.18	1.33	1	1
D	341	LEU	C-N	81.91	0.18	1.33	1	1
B	323	ALA	C-N	74.31	0.29	1.33	1	1
A	45	PRO	N-CD	23.88	1.81	1.47	1	1
C	45	PRO	N-CD	18.74	1.74	1.47	1	1
B	50	PRO	N-CD	12.19	1.64	1.47	1	1
B	95	ARG	C-N	9.96	1.19	1.33	1	1
B	213	PRO	N-CD	9.71	1.61	1.47	1	1
B	307	PRO	N-CD	7.88	1.36	1.47	1	1
B	302	PRO	N-CD	7.76	1.58	1.47	1	1
B	203	PRO	N-CD	5.35	1.55	1.47	1	1
A	50	PRO	N-CD	5.25	1.55	1.47	1	1
C	59	PRO	N-CD	4.75	1.54	1.47	1	1
A	307	PRO	N-CD	4.39	1.53	1.47	1	1
B	244	PRO	N-CD	4.21	1.41	1.47	1	1

Standard geometry: angle outliers ?

There are 55 bond angle outliers in this entry (0.27% of 20058 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	323	ALA	C-N-CA	33.86	60.74	121.70	1	1
B	323	ALA	CA-C-N	32.04	52.11	116.20	1	1
A	341	LEU	O-C-N	31.28	72.95	123.00	1	1
D	341	LEU	O-C-N	31.22	73.04	123.00	1	1
C	341	LEU	O-C-N	31.18	73.11	123.00	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	341	LEU	O-C-N	31.12	73.21	123.00	1	1
C	44	SER	C-N-CD	22.90	31.12	125.00	1	1
A	341	LEU	CA-C-N	22.38	160.97	116.20	1	1
C	341	LEU	CA-C-N	22.23	160.65	116.20	1	1
B	341	LEU	CA-C-N	22.22	160.63	116.20	1	1
D	341	LEU	CA-C-N	22.20	160.60	116.20	1	1
A	44	SER	C-N-CD	20.50	40.96	125.00	1	1
B	323	ALA	O-C-N	19.87	154.79	123.00	1	1
A	341	LEU	C-N-CA	17.87	153.87	121.70	1	1
B	341	LEU	C-N-CA	17.66	153.48	121.70	1	1
C	341	LEU	C-N-CA	17.62	153.42	121.70	1	1
D	341	LEU	C-N-CA	17.58	153.34	121.70	1	1
A	45	PRO	CA-N-CD	17.12	88.03	112.00	1	1
C	45	PRO	CA-N-CD	12.83	94.04	112.00	1	1
B	213	PRO	CA-N-CD	12.21	94.90	112.00	1	1
B	302	PRO	CA-N-CD	11.64	95.71	112.00	1	1
B	312	VAL	C-N-CA	10.64	140.84	121.70	1	1
B	312	VAL	CA-C-N	10.31	136.83	116.20	1	1
B	50	PRO	CA-N-CD	8.23	100.47	112.00	1	1
B	312	VAL	O-C-N	8.19	109.90	123.00	1	1
B	309	ALA	O-C-N	7.27	111.37	123.00	1	1
B	309	ALA	CA-C-N	6.66	129.53	116.20	1	1
B	95	ARG	C-N-CA	6.06	132.61	121.70	1	1
B	309	ALA	C-N-CA	5.69	131.95	121.70	1	1
B	307	PRO	CA-N-CD	5.60	104.16	112.00	1	1
B	147	GLU	N-CA-C	5.00	96.99	111.00	1	1
A	150	VAL	N-CA-C	4.92	97.21	111.00	1	1
C	153	LYS	N-CA-C	4.91	97.26	111.00	1	1
B	283	THR	N-CA-C	4.88	97.33	111.00	1	1
B	310	GLY	C-N-CA	4.86	130.46	121.70	1	1
A	382	GLY	N-CA-C	4.69	99.70	113.30	1	1
A	22	LYS	N-CA-C	4.67	97.93	111.00	1	1
B	288	GLY	N-CA-C	4.58	100.00	113.30	1	1
D	226	GLY	N-CA-C	4.55	100.09	113.30	1	1
B	312	VAL	CA-C-O	4.54	113.09	120.80	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	307	PRO	N-CD-CG	4.48	96.48	103.20	1	1
A	195	ARG	N-CA-C	4.47	98.48	111.00	1	1
A	316	GLY	N-CA-C	4.47	100.34	113.30	1	1
A	376	GLY	N-CA-C	4.46	100.35	113.30	1	1
A	349	GLY	N-CA-C	4.44	100.43	113.30	1	1
B	313	GLY	CA-C-N	4.25	124.69	116.20	1	1
B	149	GLY	N-CA-C	4.19	101.14	113.30	1	1
C	347	ARG	N-CA-C	4.15	99.38	111.00	1	1
A	217	VAL	N-CA-C	4.14	99.42	111.00	1	1
C	17	CYS	N-CA-C	4.12	99.48	111.00	1	1
B	146	ASN	N-CA-C	4.09	99.54	111.00	1	1
B	314	GLY	CA-C-N	4.09	124.37	116.20	1	1
B	307	PRO	O-C-N	4.08	116.48	123.00	1	1
A	288	GLY	N-CA-C	4.06	101.53	113.30	1	1
B	247	GLN	N-CA-C	4.03	99.72	111.00	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	16.39	470

There are 470 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)
C:44:SER:O	C:45:PRO:CG	1.42	1	1
B:319:THR:OG1	C:317:LEU:CB	1.39	1	1
A:154:GLU:OE1	B:22:LYS:CE	1.34	1	1
B:321:ALA:CB	C:317:LEU:HB2	1.28	1	1
B:52:ASP:OD1	C:104:GLU:HA	1.27	1	1
A:195:ARG:NH2	B:11:GLU:OE1	1.25	1	1
B:51:TRP:CZ3	C:104:GLU:HB3	1.24	1	1
B:321:ALA:HB3	C:317:LEU:CB	1.21	1	1
B:322:LEU:HD11	D:319:THR:CG2	1.20	1	1
B:321:ALA:CB	C:317:LEU:CB	1.19	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:16:LYS:HD2	A:16:LYS:O	1.14	1	1
B:322:LEU:CD1	D:319:THR:HG23	1.13	1	1
B:319:THR:CB	C:317:LEU:HB3	1.13	1	1
A:11:GLU:HG3	B:195:ARG:HH21	1.13	1	1
B:238:CYS:SG	B:280:CYS:SG	1.11	1	1
C:45:PRO:CD	C:45:PRO:N	1.11	1	1
B:319:THR:OG1	C:317:LEU:HB3	1.10	1	1
B:52:ASP:OD1	C:104:GLU:CA	1.09	1	1
A:16:LYS:C	A:16:LYS:HD2	1.08	1	1
A:154:GLU:OE1	B:22:LYS:CD	1.07	1	1
A:11:GLU:CG	B:195:ARG:HH21	1.07	1	1
C:44:SER:CA	C:45:PRO:CD	1.06	1	1
A:154:GLU:OE1	B:22:LYS:NZ	1.06	1	1
B:49:GLY:HA3	C:102:LYS:HB3	1.04	1	1
B:51:TRP:CZ3	C:104:GLU:CB	1.01	1	1
A:154:GLU:OE1	B:22:LYS:HD3	0.98	1	1
A:154:GLU:CG	B:22:LYS:HE2	0.98	1	1
A:154:GLU:HG3	B:22:LYS:HE2	0.98	1	1
A:144:VAL:CG1	B:59:PRO:HG2	0.96	1	1
B:217:VAL:HG13	B:219:LEU:O	0.96	1	1
B:148:LYS:NZ	D:170:GLU:OE1	0.96	1	1
A:154:GLU:OE1	B:22:LYS:HE2	0.95	1	1
B:319:THR:C	C:317:LEU:HD13	0.94	1	1
C:155:GLN:NE2	C:168:GLN:OE1	0.92	1	1
A:11:GLU:HG3	B:195:ARG:NH2	0.91	1	1
A:154:GLU:CD	B:22:LYS:HE2	0.90	1	1
C:44:SER:CA	C:45:PRO:HD3	0.90	1	1
A:16:LYS:HB3	B:133:THR:OG1	0.88	1	1
B:323:ALA:HB2	C:319:THR:OG1	0.87	1	1
E:57:VAL:O	E:57:VAL:HG13	0.87	1	1
B:321:ALA:HB2	C:317:LEU:O	0.86	1	1
C:44:SER:C	C:45:PRO:CD	0.86	1	1
A:146:ASN:HA	A:150:VAL:O	0.85	1	1
A:11:GLU:CD	B:195:ARG:HH21	0.84	1	1
B:319:THR:CG2	C:317:LEU:HB3	0.84	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:203:PRO:HD3	A:244:PRO:HD3	0.83	1	1
B:326:ILE:HD11	D:326:ILE:HG22	0.82	1	1
A:154:GLU:CD	B:22:LYS:CE	0.82	1	1
A:5:ILE:HB	A:94:VAL:HA	0.82	1	1
B:319:THR:OG1	C:317:LEU:CD2	0.82	1	1
B:319:THR:HG1	C:317:LEU:HD22	0.81	1	1
A:16:LYS:C	A:16:LYS:CD	0.80	1	1
A:147:GLU:HB3	C:153:LYS:CB	0.80	1	1
B:321:ALA:HB2	C:317:LEU:C	0.79	1	1
B:319:THR:OG1	C:317:LEU:HD22	0.79	1	1
A:40:TRP:CD1	A:40:TRP:H	0.79	1	1
B:319:THR:OG1	C:317:LEU:CG	0.79	1	1
B:56:ARG:NH1	C:105:ILE:O	0.77	1	1
B:217:VAL:HG22	B:219:LEU:H	0.77	1	1
A:147:GLU:HB3	C:153:LYS:HB3	0.76	1	1
B:322:LEU:HD11	D:319:THR:HG23	0.76	1	1
B:321:ALA:HB2	C:317:LEU:CB	0.76	1	1
C:317:LEU:HG	C:317:LEU:O	0.76	1	1
A:148:LYS:HD2	C:153:LYS:HG2	0.76	1	1
B:112:LEU:N	B:207:ARG:O	0.76	1	1
B:217:VAL:CG1	B:219:LEU:O	0.76	1	1
A:123:CYS:SG	A:187:CYS:SG	0.75	1	1
A:147:GLU:CB	C:153:LYS:HB3	0.75	1	1
B:51:TRP:HZ3	C:104:GLU:CB	0.74	1	1
A:41:LYS:NZ	A:72:ASP:OD1	0.74	1	1
B:147:GLU:OE2	D:168:GLN:NE2	0.73	1	1
G:90:GLU:HG2	G:90:GLU:O	0.73	1	1
A:203:PRO:CD	A:244:PRO:HD3	0.73	1	1
A:16:LYS:CB	B:133:THR:OG1	0.72	1	1
B:216:GLU:C	B:217:VAL:HG12	0.72	1	1
E:90:GLU:HG3	E:90:GLU:O	0.72	1	1
A:190:SER:O	B:16:LYS:NZ	0.72	1	1
A:144:VAL:HG13	B:59:PRO:HG2	0.72	1	1
G:58:MET:O	G:62:ASP:N	0.71	1	1
A:203:PRO:HG3	A:242:ALA:O	0.71	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:203:PRO:CG	A:242:ALA:O	0.71	1	1
A:40:TRP:H	A:40:TRP:HD1	0.71	1	1
C:44:SER:O	C:45:PRO:HD3	0.71	1	1
B:51:TRP:CH2	C:104:GLU:HB3	0.70	1	1
A:11:GLU:CD	B:195:ARG:NH2	0.70	1	1
A:154:GLU:CD	B:20:ALA:O	0.70	1	1
B:218:GLN:CB	B:292:SER:HA	0.70	1	1
B:319:THR:HG1	C:317:LEU:CD2	0.69	1	1
E:72:GLN:N	E:72:GLN:OE1	0.69	1	1
C:156:THR:O	C:156:THR:HG23	0.69	1	1
A:45:PRO:C	A:45:PRO:CD	0.68	1	1
B:27:ARG:HG2	C:160:PRO:HD2	0.68	1	1
A:22:LYS:HD2	B:152:VAL:HB	0.68	1	1
A:120:VAL:CG1	A:204:ILE:HD11	0.68	1	1
B:232:GLY:O	B:269:GLU:N	0.68	1	1
C:44:SER:C	C:45:PRO:HD3	0.67	1	1
H:88:PHE:C	H:88:PHE:CD1	0.67	1	1
B:326:ILE:HD11	D:326:ILE:CG2	0.67	1	1
A:6:THR:O	B:195:ARG:CA	0.67	1	1
A:120:VAL:CG1	A:204:ILE:CD1	0.66	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	1878	1778	85	15

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

Chain	Res	Type	Models (Total)
A	45	PRO	1
A	146	ASN	1
A	213	PRO	1
B	43	LEU	1
B	195	ARG	1
B	213	PRO	1
B	217	VAL	1

Chain	Res	Type	Models (Total)
B	302	PRO	1
C	45	PRO	1
C	156	THR	1
C	212	VAL	1
D	50	PRO	1
D	312	VAL	1
D	347	ARG	1
E	57	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	1574	1553	15	6

There are 6 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	16	LYS	1
A	40	TRP	1
A	45	PRO	1
B	50	PRO	1
B	213	PRO	1
C	45	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.

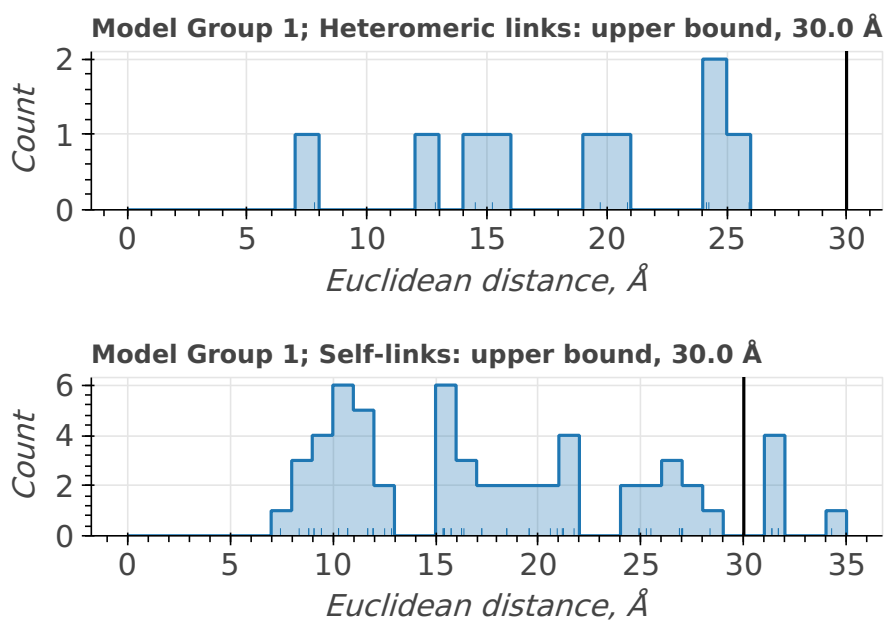
There are 66 crosslinking restraints combined in 66 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
BS3	LYS	CA	MET	CA	upper bound	30.0	7
BS3	MET	CA	THR	CA	upper bound	30.0	2

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
BS3	MET	CA	SER	CA	upper bound	30.0	1
BS3	LYS	CA	LYS	CA	upper bound	30.0	35
BS3	LYS	CA	THR	CA	upper bound	30.0	12
BS3	LYS	CA	SER	CA	upper bound	30.0	7
BS3	LYS	CA	TYR	CA	upper bound	30.0	2

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.



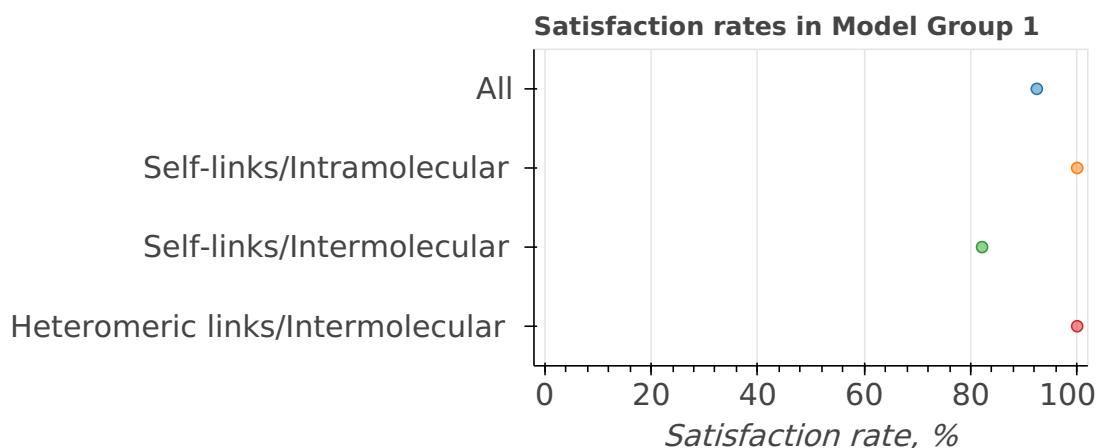
Satisfaction of restraints

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=66)
1	1	1	1/1	All	92.42	7.58	66
				Self-links/ Intramolecular	100.00	0.00	29
				Self-links/ Intermolecular	82.14	17.86	28
				Heteromeric links/ Intermolecular	100.00	0.00	9

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.



H/D exchange

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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