

Integrative Structure Validation Report ?

February 18, 2025 - 08:30 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	9A0U
PDB-Dev ID	PDBDEV_00000066
Structure Title	Docking model of HLA class I with HLA class II
Structure Authors	Armony G; Heck AJR; Wu W
Deposited on	2020-11-24

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

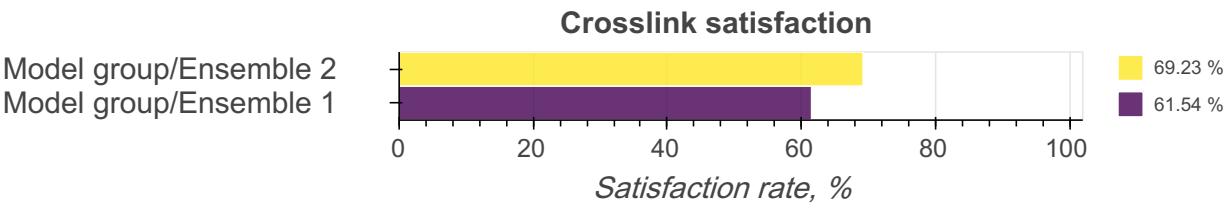
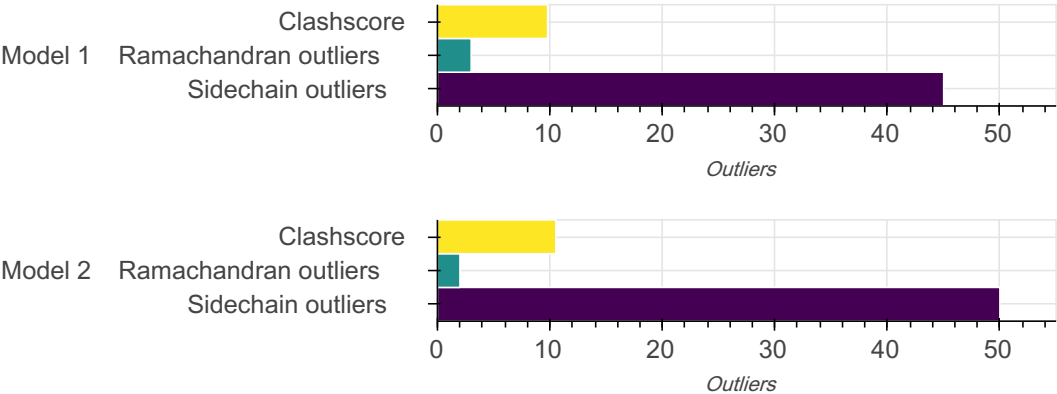
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 2 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	1-2	1	CLASS I HISTOCOMPATIBILITY ANTIGEN (HLA-A*0201) (ALPHA CHAIN)	A	275	1-275	-	100.00 / 100.00	Atomic
		2	BETA 2-MICROGLOBULIN	B	100	1-100	-	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
		3	INFLUENZA A MATRIX PROTEIN M1 (RESIDUES 58-66)	C	9	1-9	-	100.00 / 100.00	Atomic
		4	GLY residue	D	1	1	-	100.00 / 0.00	Atomic
				H					
		5	HLA class II histocompatibility antigen, DR alpha chain	E	179	1-179	-	100.00 / 100.00	Atomic
		6	HLA class II histocompatibility antigen, DRB1-4 beta chain	F	193	1-193	-	100.00 / 100.00	Atomic
		7	Alpha-enolase	G	14	1-14	-	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
1	Experimental model	PDB	1HHI
2	Experimental model	PDB	5NI9
3	Crosslinking-MS data	PRIDE	PXD022675
4	Other	Not available	Not available
5	Other	Not available	Not available

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	Rigid-body minimization	Rigid-body minimization in HADDOCK (it0)	None	1000	True	False

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
2	1	Simulated annealing	Semi-flexible SA in HADDOCK (it1)	None	200	True	False
3	1	Refinement	Water refinement in HADDOCK (itw)	None	200	True	False

There is 1 software package reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	Haddock	2.20	docking	https://alcazar.science.uu.nl/services/HADDOCK2.2/

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.

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	9.80	121

Model ID	Clash score	Number of clashes
2	10.53	130

There are 251 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)
F:96:PRO:HB3	F:121:PHE:HB3	0.88	2	2
A:224:GLN:HG3	A:227:ASP:HB2	0.85	2	1
F:28:ARG:HG2	F:38:ARG:HG3	0.79	2	2
E:20:GLU:HA	E:35:MET:HE1	0.78	2	1
F:66:LEU:HD11	G:9:GLU:HG3	0.77	2	2
A:5:MET:HB2	A:168:LEU:HD13	0.77	1	2
A:23:ILE:HG21	B:55:LEU:HB3	0.76	2	2
A:261:VAL:HB	A:270:LEU:HB2	0.75	2	2
A:207:SER:HA	A:240:THR:HB	0.74	1	2
A:128:GLU:HB2	E:66:LYS:HE2	0.74	2	1
B:37:GLU:HB3	B:84:ASN:HB3	0.72	2	2
E:69:LEU:HB2	F:8:GLU:HB2	0.71	2	2
A:214:THR:HB	A:262:GLN:HB2	0.71	2	2
A:102:ASP:HB2	A:111:ARG:HB2	0.69	2	2
A:13:SER:HA	A:20:PRO:HB3	0.68	2	2
E:72:MET:HE1	F:52:LEU:HB3	0.65	2	2
F:86:GLU:HG2	F:90:VAL:HB	0.64	2	2
B:30:GLY:HA2	B:62:SER:HB2	0.64	2	2
A:249:VAL:HG11	A:254:GLU:HA	0.64	2	2
B:14:HIS:HB3	B:15:PRO:HD2	0.63	1	2
B:97:ASP:HB3	B:100:MET:HB2	0.62	2	2
F:126:ILE:HB	F:176:HIS:HD2	0.62	2	2
E:6:ILE:HG12	E:25:PHE:HD1	0.61	1	2
A:207:SER:HA	A:240:THR:CB	0.61	1	1
A:106:ASP:OD2	A:108:ARG:HD3	0.60	1	2
E:29:GLU:HB2	E:137:LEU:HD22	0.59	2	2
E:25:PHE:HB2	E:30:ILE:HD11	0.59	2	2
A:185:PRO:HB3	A:208:PHE:HB3	0.58	1	1
E:104:LEU:HG	E:152:PHE:CE1	0.58	1	2
A:235:PRO:HG2	B:66:LEU:HD22	0.57	1	2

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:255:GLN:O	A:273:ARG:HD3	0.57	2	1
B:6:PRO:HB3	B:31:PHE:HB3	0.57	1	2
F:115:VAL:HG22	F:159:MET:HG3	0.56	1	2
B:74:THR:HG22	B:76:LYS:H	0.55	2	1
F:114:LEU:O	F:159:MET:HA	0.55	2	2
A:50:PRO:HA	A:53:GLU:OE1	0.55	2	2
A:23:ILE:HG13	B:55:LEU:HD23	0.55	1	2
A:8:PHE:HB2	A:25:VAL:HG23	0.54	2	2
E:118:VAL:HA	E:163:ARG:O	0.54	2	2
F:17:PHE:HB2	F:22:ARG:HB3	0.54	2	2
E:159:VAL:HB	E:176:HIS:HE1	0.53	1	2
F:75:ASP:OD1	F:79:ARG:HD2	0.53	1	2
E:159:VAL:HB	E:176:HIS:CE1	0.53	1	1
F:75:ASP:HA	F:79:ARG:HB2	0.53	2	2
A:44:ARG:HA	A:64:THR:HG23	0.53	2	2
F:127:GLU:HB2	F:175:GLU:HB2	0.53	2	2
E:25:PHE:CE2	F:89:THR:HB	0.52	2	2
F:54:ARG:HB3	F:55:PRO:HD3	0.52	2	2
E:21:PHE:HZ	G:5:LYS:HG3	0.52	2	2
A:203:CYS:HB2	A:217:TRP:CZ2	0.52	1	2
F:27:ASP:HB3	F:39:PHE:HB3	0.52	1	2
A:168:LEU:O	A:172:LEU:HG	0.51	2	2
F:36:TYR:HA	F:50:THR:OG1	0.51	2	2
A:37:ASP:HB3	A:40:ALA:HB2	0.51	1	1
F:6:PHE:HA	F:32:HIS:HE1	0.51	1	2
A:238:ASP:HB3	B:13:ARG:HD3	0.51	2	1
F:126:ILE:HB	F:176:HIS:CD2	0.51	2	2
B:25:ASN:HB3	B:66:LEU:HD11	0.50	2	2
A:44:ARG:HH22	A:61:ASP:CG	0.50	2	1
A:24:ALA:HB3	A:36:PHE:HB3	0.50	1	2
A:13:SER:O	A:15:PRO:HD3	0.50	2	2
A:44:ARG:HG2	A:64:THR:HG21	0.49	2	2
A:117:ALA:HB2	B:61:TRP:CE2	0.49	2	2
B:24:LEU:O	B:68:TYR:HA	0.49	1	2
F:66:LEU:O	F:70:LYS:HG2	0.49	1	2

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
F:80:HIS:O	F:84:VAL:HG23	0.49	2	2
E:10:GLU:HB2	F:10:VAL:CG1	0.49	1	2
F:64:LYS:O	F:68:GLU:HG2	0.49	2	2
E:165:GLU:HG2	E:172:PRO:HB3	0.48	1	1
E:72:MET:HE2	F:31:TYR:HB2	0.48	2	2
A:11:SER:HA	A:21:ARG:O	0.48	2	2
E:86:PRO:HB3	E:111:PHE:HB3	0.48	1	2
E:109:ASP:OD1	E:139:ARG:HD2	0.48	1	2
A:47:PRO:HB2	A:53:GLU:HG2	0.48	2	2
F:13:GLU:HB2	F:26:LEU:HB2	0.48	2	1
B:7:LYS:O	B:28:VAL:HA	0.48	2	2
A:115:GLN:HG3	B:61:TRP:CH2	0.48	2	2
A:219:ARG:HA	A:256:ARG:O	0.48	2	2
A:187:THR:HG21	A:261:VAL:HG21	0.47	1	1
F:98:VAL:HG21	F:174:VAL:HG21	0.47	2	2
F:148:GLN:HG3	F:154:PHE:CE2	0.47	1	2
A:229:GLU:O	A:245:ALA:HA	0.47	1	2
A:96:GLN:HB2	A:117:ALA:HB3	0.47	2	2
E:88:VAL:HG21	E:164:VAL:HG21	0.47	2	2
B:24:LEU:HB3	B:69:THR:HG22	0.47	2	2
B:30:GLY:HA2	B:62:SER:CB	0.47	1	2
A:206:LEU:HD23	A:242:GLN:HB3	0.46	1	1
E:71:ILE:HA	E:74:LYS:HE2	0.46	2	2
F:126:ILE:HD11	F:174:VAL:HG13	0.46	2	2
G:9:GLU:HA	G:9:GLU:OE1	0.46	2	2
A:19:GLU:OE2	A:20:PRO:HD2	0.46	2	2
A:259:CYS:O	A:271:THR:HA	0.46	2	1
E:115:VAL:O	E:166:HIS:HD2	0.46	2	1
A:49:ALA:O	A:52:ILE:HG22	0.46	1	2
A:147:TRP:CZ2	C:9:LEU:HD23	0.46	2	2
E:34:ASP:O	E:38:LYS:HA	0.45	1	1
B:26:CYS:HB2	B:40:LEU:HD21	0.45	1	2
A:236:ALA:HB1	B:13:ARG:HG3	0.45	2	1
A:127:LYS:HD2	A:132:SER:OG	0.45	1	2
E:10:GLU:HG2	E:21:PHE:CD2	0.45	1	2

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	758	712	43	3
2	758	711	45	2

There are 4 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
F	32	HIS	2
A	220	ASP	1
A	221	GLY	1
E	135	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	683	575	63	45
2	683	571	62	50

There are 59 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	42	SER	2
A	68	LYS	2
A	129	ASP	2
A	163	THR	2
A	177	GLU	2
A	216	THR	2
A	224	GLN	2
A	251	SER	2
A	258	THR	2
B	5	THR	2
B	34	SER	2
B	58	SER	2
B	78	GLU	2
B	89	SER	2

Chain	Res	Type	Models (Total)
E	2	GLU	2
E	28	ASP	2
E	82	THR	2
E	91	LEU	2
E	92	THR	2
E	94	SER	2
E	156	THR	2
F	2	THR	2
F	20	THR	2
F	33	GLN	2
F	87	SER	2
F	99	THR	2
F	105	THR	2
F	111	HIS	2
F	125	SER	2
F	139	THR	2
F	166	SER	2
F	175	GLU	2
F	180	THR	2
F	181	SER	2
F	184	THR	2
F	186	GLU	2
A	35	ARG	1
A	212	GLU	1
A	214	THR	1
A	222	GLU	1
B	10	VAL	1
B	12	SER	1
B	74	THR	1
C	8	THR	1
E	70	GLU	1
E	112	THR	1
E	128	THR	1
E	129	THR	1
E	131	VAL	1

Chain	Res	Type	Models (Total)
E	132	SER	1
E	133	GLU	1
E	148	HIS	1
E	155	SER	1
E	174	LEU	1
F	9	GLN	1
F	30	PHE	1
F	191	SER	1
G	9	GLU	1
G	10	LYS	1

Fit of model to data used for modeling ?

Fit of model(s) to crosslinking-MS data

Restraint types

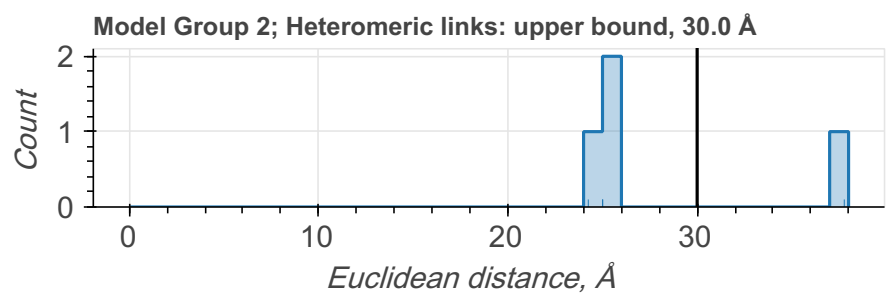
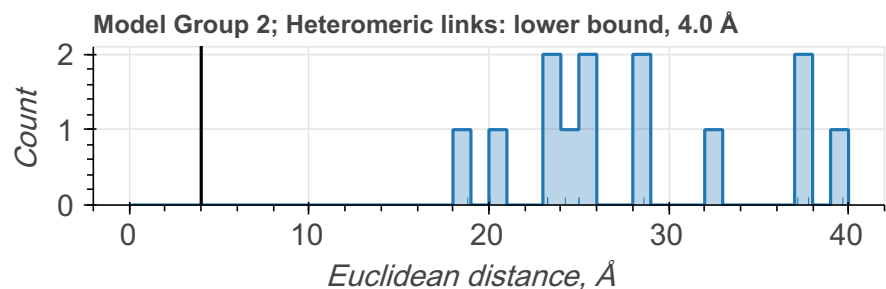
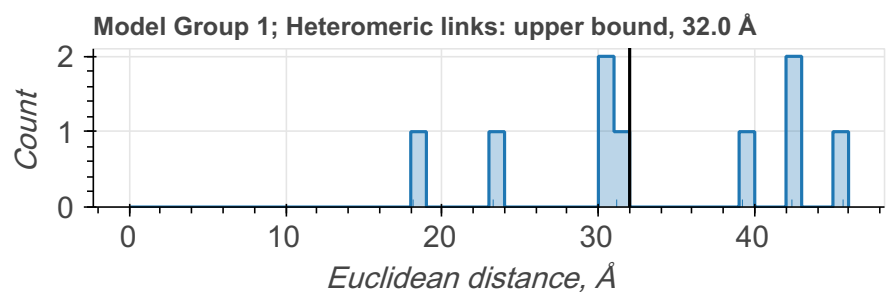
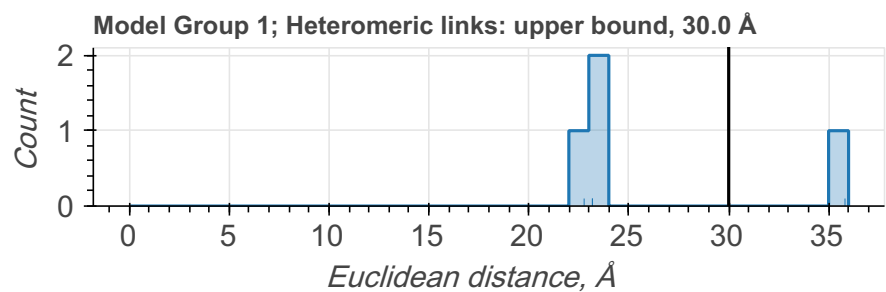
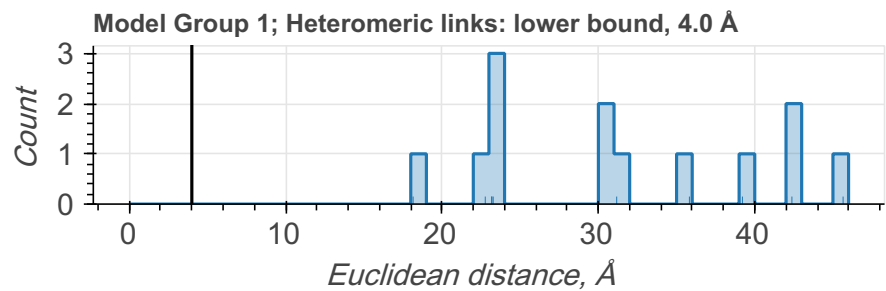
Restraint types are summarized in the table below. Restraints assigned "by-residue" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "coarse-grained". *Restraint group* represents a set of crosslinking restraints applied collectively in the modeling.

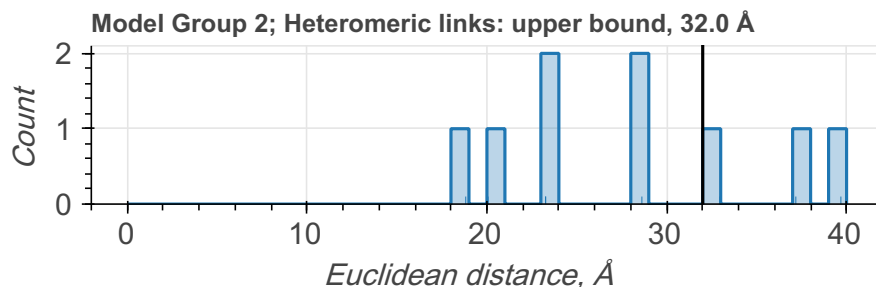
There are 26 crosslinking restraints combined in 13 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
DSSO	ASP	CA	LYS	CA	upper bound	32.0	7
DSSO	ASP	CA	LYS	CA	lower bound	4.0	7
DSSO	LYS	CA	LYS	CA	upper bound	30.0	2
DSSO	LYS	CA	LYS	CA	lower bound	4.0	2
DSSO	GLY	CA	LYS	CA	upper bound	30.0	2
DSSO	GLY	CA	LYS	CA	lower bound	4.0	2
DSSO	ASP	CA	GLY	CA	upper bound	32.0	2
DSSO	ASP	CA	GLY	CA	lower bound	4.0	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.





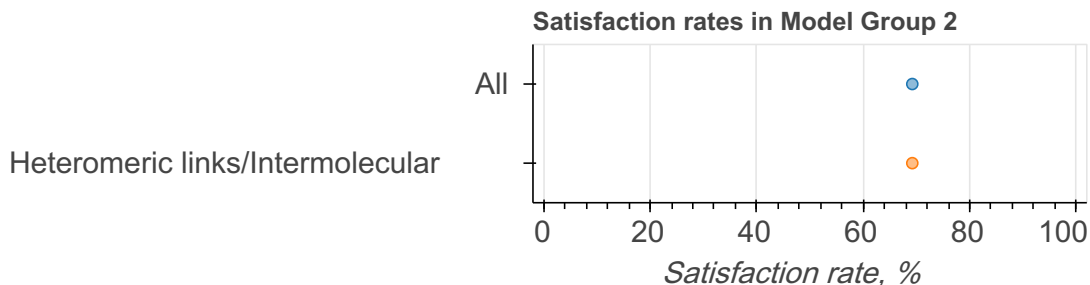
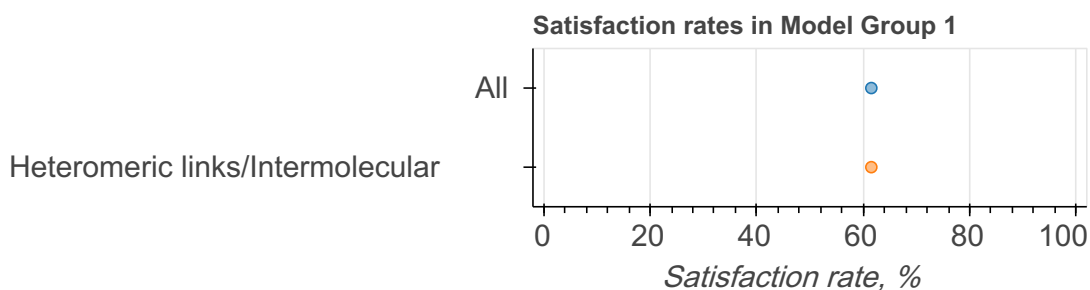
Satisfaction of restraints

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=13)
1	1	1	1/1	All	61.54	38.46	13
				Heteromeric links/Intermolecular	61.54	38.46	13
2	2	2	1/1	All	69.23	30.77	13
				Heteromeric links/Intermolecular	69.23	30.77	13

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.



Fit of model to data used for validation ?

Validation for this section is under development.

Acknowledgments

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