

Integrative Structure Validation Report ?

April 09, 2025 - 08:36 PM 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	9A4O
PDB-Dev ID	PDBDEV_00000245
Structure Title	Integrative model of IF2-TAGH by crosslinking MS and deep learning
Structure Authors	Kolja Stahl; Oliver Brock; Juri Rappsilber
Deposited on	2024-01-23

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

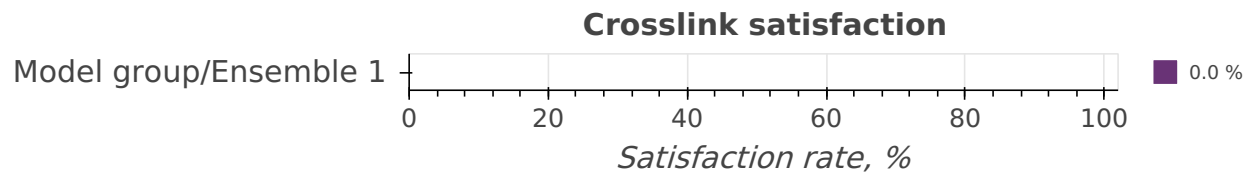
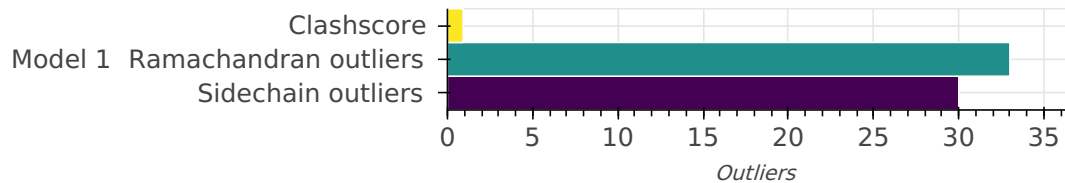
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 1 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	IF2_BACSU	A	716	-	1-716	100.00 / 0.00	Atomic
		2	TAGH_BACSU	B	527	-	1-527	100.00 / 0.00	Atomic

Datasets used for modeling ?

There is 1 unique dataset used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Crosslinking-MS data	PRIDE	PXD035508

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	AlphaLink2	AlphaLink2	None	1	False	False

There is 1 software package reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	AlphaLink2	1.00	model building	https://github.com/Rappsilber-Laboratory/AlphaLink2

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 71 bond length outliers in this entry (0.72% of 9830 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	313	GLY	N-CA	8.52	1.59	1.45	1	1
B	313	GLY	CA-C	7.73	1.66	1.52	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	316	PRO	N-CA	7.57	1.58	1.47	1	1
B	309	ILE	N-CA	7.35	1.60	1.46	1	1
B	308	THR	N-CA	7.27	1.60	1.46	1	1
B	315	ILE	N-CA	7.17	1.59	1.46	1	1
B	307	ARG	N-CA	7.08	1.59	1.46	1	1
B	305	PRO	N-CA	7.05	1.57	1.47	1	1
B	319	GLU	N-CA	6.98	1.59	1.46	1	1
B	317	GLN	N-CA	6.93	1.59	1.46	1	1
B	312	PHE	CA-C	6.88	1.67	1.52	1	1
B	318	ASN	CA-C	6.86	1.67	1.52	1	1
B	315	ILE	CA-C	6.84	1.67	1.52	1	1
B	306	LEU	CA-C	6.76	1.67	1.52	1	1
B	310	ALA	C-N	6.76	1.42	1.33	1	1
B	304	ALA	CA-C	6.70	1.67	1.52	1	1
B	307	ARG	CA-C	6.69	1.67	1.52	1	1
B	317	GLN	CA-C	6.69	1.67	1.52	1	1
B	314	ALA	N-CA	6.68	1.58	1.46	1	1
B	309	ILE	C-N	6.68	1.42	1.33	1	1
B	314	ALA	C-N	6.65	1.42	1.33	1	1
B	308	THR	CA-C	6.64	1.66	1.52	1	1
B	314	ALA	CA-C	6.63	1.66	1.52	1	1
B	311	SER	C-N	6.61	1.42	1.33	1	1
B	316	PRO	C-N	6.61	1.42	1.33	1	1
B	311	SER	N-CA	6.60	1.58	1.46	1	1
B	302	PHE	N-CA	6.59	1.58	1.46	1	1
B	317	GLN	C-N	6.59	1.42	1.33	1	1
B	316	PRO	CA-C	6.58	1.66	1.52	1	1
B	305	PRO	C-N	6.48	1.42	1.33	1	1
B	312	PHE	C-N	6.47	1.42	1.33	1	1
B	313	GLY	C-N	6.44	1.42	1.33	1	1
B	310	ALA	N-CA	6.44	1.58	1.46	1	1
B	318	ASN	N-CA	6.42	1.58	1.46	1	1
B	306	LEU	N-CA	6.42	1.58	1.46	1	1
B	303	ASN	CA-C	6.41	1.66	1.52	1	1
B	302	PHE	C-N	6.39	1.42	1.33	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	308	THR	C-N	6.35	1.42	1.33	1	1
B	300	MET	N-CA	6.33	1.58	1.46	1	1
B	310	ALA	CA-C	6.30	1.66	1.52	1	1
B	306	LEU	C-N	6.27	1.42	1.33	1	1
B	319	GLU	CA-C	6.26	1.66	1.52	1	1
B	305	PRO	CA-C	6.19	1.66	1.52	1	1
B	311	SER	CA-C	6.17	1.65	1.52	1	1
B	304	ALA	N-CA	6.14	1.57	1.46	1	1
B	312	PHE	N-CA	6.11	1.57	1.46	1	1
B	319	GLU	C-N	6.05	1.41	1.33	1	1
B	318	ASN	C-N	6.03	1.41	1.33	1	1
B	303	ASN	C-N	5.95	1.41	1.33	1	1
B	320	VAL	N-CA	5.93	1.57	1.46	1	1
B	298	GLY	N-CA	5.92	1.55	1.45	1	1
B	301	PHE	C-N	5.88	1.41	1.33	1	1
B	301	PHE	N-CA	5.84	1.57	1.46	1	1
B	299	THR	CA-C	5.83	1.65	1.52	1	1
B	300	MET	C-N	5.73	1.41	1.33	1	1
B	303	ASN	N-CA	5.73	1.57	1.46	1	1
B	309	ILE	CA-C	5.66	1.64	1.52	1	1
B	315	ILE	C-N	5.65	1.43	1.34	1	1
B	307	ARG	C-N	5.64	1.41	1.33	1	1
B	301	PHE	CA-C	5.60	1.64	1.52	1	1
B	298	GLY	CA-C	5.57	1.62	1.52	1	1
B	302	PHE	CA-C	5.45	1.64	1.52	1	1
B	299	THR	N-CA	5.40	1.56	1.46	1	1
B	298	GLY	C-N	5.38	1.40	1.33	1	1
B	304	ALA	C-N	5.32	1.43	1.34	1	1
B	300	MET	CA-C	5.23	1.63	1.52	1	1
B	320	VAL	C-N	4.61	1.39	1.33	1	1
B	321	LYS	N-CA	4.53	1.54	1.46	1	1
B	299	THR	C-N	4.48	1.39	1.33	1	1
B	320	VAL	CA-C	4.47	1.62	1.52	1	1
B	297	ALA	CA-C	4.09	1.61	1.52	1	1

Standard geometry: angle outliers ?

There are 251 bond angle outliers in this entry (1.90% of 13231 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)
B	310	ALA	C-N-CA	16.83	151.99	121.70	1	1
B	309	ILE	C-N-CA	15.99	150.49	121.70	1	1
B	311	SER	C-N-CA	15.28	149.20	121.70	1	1
B	302	PHE	C-N-CA	14.47	147.74	121.70	1	1
B	310	ALA	CA-C-N	11.56	139.31	116.20	1	1
B	311	SER	CA-C-N	11.50	139.21	116.20	1	1
B	309	ILE	CA-C-N	10.39	136.98	116.20	1	1
B	302	PHE	CA-C-N	10.16	136.53	116.20	1	1
A	76	GLN	C-N-CA	9.78	139.30	121.70	1	1
A	26	ASN	C-N-CA	9.76	139.27	121.70	1	1
A	38	LEU	C-N-CA	9.39	138.61	121.70	1	1
A	58	LYS	C-N-CA	9.36	138.54	121.70	1	1
B	299	THR	N-CA-C	8.67	135.27	111.00	1	1
A	77	GLN	C-N-CA	8.57	137.13	121.70	1	1
A	6	VAL	C-N-CA	8.51	137.01	121.70	1	1
A	85	LYS	C-N-CA	8.45	136.91	121.70	1	1
B	310	ALA	O-C-N	8.38	109.60	123.00	1	1
B	307	ARG	N-CA-C	8.36	134.42	111.00	1	1
A	65	THR	C-N-CA	8.31	136.65	121.70	1	1
A	7	TYR	C-N-CA	8.26	136.57	121.70	1	1
A	86	ILE	C-N-CA	8.09	136.27	121.70	1	1
B	299	THR	CA-C-N	8.07	132.33	116.20	1	1
B	311	SER	O-C-N	8.04	110.13	123.00	1	1
A	92	ASN	CA-CB-CG	8.03	120.63	112.60	1	1
A	101	LYS	C-N-CA	7.96	136.03	121.70	1	1
B	308	THR	N-CA-C	7.81	132.88	111.00	1	1
A	23	ALA	C-N-CA	7.80	135.74	121.70	1	1
A	79	ALA	C-N-CA	7.68	135.52	121.70	1	1
A	114	ASN	C-N-CA	7.37	134.97	121.70	1	1
B	309	ILE	O-C-N	7.30	111.32	123.00	1	1
B	302	PHE	O-C-N	7.22	111.45	123.00	1	1
B	321	LYS	N-CA-C	7.21	131.20	111.00	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	306	LEU	N-CA-C	7.20	131.17	111.00	1	1
A	11	LYS	C-N-CA	7.14	134.55	121.70	1	1
A	37	MET	C-N-CA	7.10	134.48	121.70	1	1
A	112	LYS	C-N-CA	6.99	134.28	121.70	1	1
B	318	ASN	N-CA-C	6.99	130.57	111.00	1	1
A	15	VAL	C-N-CA	6.92	134.15	121.70	1	1
A	38	LEU	CA-C-N	6.90	130.00	116.20	1	1
B	316	PRO	CA-N-CD	6.86	102.40	112.00	1	1
B	308	THR	C-N-CA	6.81	133.96	121.70	1	1
A	77	GLN	CA-C-N	6.78	129.76	116.20	1	1
A	96	ASN	C-N-CA	6.75	133.84	121.70	1	1
A	71	PRO	C-N-CA	6.72	133.80	121.70	1	1
A	4	MET	C-N-CA	6.69	133.74	121.70	1	1
A	31	VAL	CA-CB-CG1	6.68	121.76	110.40	1	1
B	315	ILE	CA-C-N	6.63	126.85	116.90	1	1
A	94	VAL	C-N-CA	6.62	133.62	121.70	1	1
B	297	ALA	C-N-CA	6.46	133.34	121.70	1	1
B	301	PHE	C-N-CA	6.44	133.29	121.70	1	1
A	66	ASN	CA-CB-CG	6.43	119.03	112.60	1	1
B	312	PHE	CA-C-N	6.35	128.91	116.20	1	1
B	298	GLY	N-CA-C	6.34	131.67	113.30	1	1
A	26	ASN	CA-C-N	6.29	128.79	116.20	1	1
A	59	SER	C-N-CA	6.28	133.01	121.70	1	1
B	305	PRO	CA-N-CD	6.22	103.29	112.00	1	1
A	63	ALA	C-N-CA	6.21	132.88	121.70	1	1
B	304	ALA	CA-C-N	6.21	126.22	116.90	1	1
A	1	MET	C-N-CA	6.21	132.88	121.70	1	1
B	318	ASN	C-N-CA	6.20	132.87	121.70	1	1
B	319	GLU	C-N-CA	6.18	132.83	121.70	1	1
A	77	GLN	O-C-N	6.18	113.12	123.00	1	1
B	307	ARG	C-N-CA	6.10	132.68	121.70	1	1
A	7	TYR	CA-C-N	6.07	128.34	116.20	1	1
A	47	ASP	C-N-CA	6.02	132.54	121.70	1	1
A	98	GLN	C-N-CA	5.99	132.48	121.70	1	1
B	311	SER	CA-C-O	5.96	110.66	120.80	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	526	GLN	OE1-CD-NE2	5.96	116.64	122.60	1	1
B	316	PRO	N-CA-C	5.88	126.80	112.10	1	1
A	604	ASP	CA-CB-CG	5.83	118.43	112.60	1	1
B	305	PRO	N-CA-C	5.83	126.67	112.10	1	1
B	314	ALA	C-N-CA	5.81	132.15	121.70	1	1
A	49	LYS	C-N-CA	5.80	132.14	121.70	1	1
B	319	GLU	N-CA-C	5.78	127.19	111.00	1	1
B	306	LEU	CA-C-N	5.78	127.76	116.20	1	1
A	94	VAL	CA-CB-CG2	5.77	120.20	110.40	1	1
A	59	SER	CA-C-N	5.76	127.72	116.20	1	1
B	300	MET	N-CA-C	5.76	127.13	111.00	1	1
B	310	ALA	CA-C-O	5.72	111.08	120.80	1	1
B	303	ASN	CA-C-N	5.72	127.63	116.20	1	1
A	76	GLN	CA-C-N	5.71	127.63	116.20	1	1
A	7	TYR	O-C-N	5.70	113.89	123.00	1	1
B	307	ARG	CA-C-N	5.68	127.57	116.20	1	1
A	109	LYS	C-N-CA	5.60	131.78	121.70	1	1
B	316	PRO	C-N-CA	5.60	131.77	121.70	1	1
A	16	SER	C-N-CA	5.59	131.77	121.70	1	1
A	92	ASN	CA-C-N	5.58	127.37	116.20	1	1
A	27	MET	C-N-CA	5.52	131.63	121.70	1	1
B	304	ALA	N-CA-C	5.50	126.40	111.00	1	1
B	317	GLN	N-CA-C	5.45	126.26	111.00	1	1
A	69	LYS	C-N-CA	5.43	131.47	121.70	1	1
B	317	GLN	CA-C-N	5.42	127.04	116.20	1	1
B	318	ASN	CA-C-N	5.41	127.01	116.20	1	1
A	6	VAL	CA-C-N	5.41	127.01	116.20	1	1
B	299	THR	O-C-N	5.40	114.37	123.00	1	1
A	516	ASP	CA-CB-CG	5.38	117.98	112.60	1	1
B	309	ILE	CA-C-O	5.36	111.69	120.80	1	1
A	96	ASN	CA-C-N	5.35	126.89	116.20	1	1
A	660	ARG	CD-NE-CZ	5.31	131.84	124.40	1	1
A	103	LYS	C-N-CA	5.30	131.24	121.70	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	18

There are 18 clashes. The table below contains the detailed list of all clashes based on a MolProbity analysis. Bad clashes are ≥ 0.4 Angstrom.

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:15:VAL:HG21	A:22:THR:H	0.67	1	1
A:86:ILE:H	A:87:ARG:HB2	0.58	1	1
A:6:VAL:HG13	A:30:GLU:CD	0.53	1	1
A:11:LYS:HZ3	A:30:GLU:CD	0.50	1	1
A:223:THR:HB	A:290:THR:HG21	0.50	1	1
B:71:LYS:HE3	B:82:MET:SD	0.47	1	1
B:240:PHE:O	B:248:LYS:HE3	0.46	1	1
A:86:ILE:H	A:87:ARG:CB	0.45	1	1
B:202:ILE:HG21	B:234:LYS:HE3	0.45	1	1
A:61:LYS:HB3	A:62:PRO:HD3	0.44	1	1
A:65:THR:HB	A:66:ASN:HB3	0.44	1	1
A:7:TYR:H	A:8:GLU:HB2	0.43	1	1
A:93:ASP:HB3	A:94:VAL:HG22	0.43	1	1
A:65:THR:HB	A:66:ASN:CB	0.42	1	1
A:294:ILE:HD11	A:376:ILE:HD11	0.42	1	1
B:62:LYS:HE2	B:198:VAL:CG1	0.42	1	1
B:112:MET:HA	B:112:MET:HE2	0.41	1	1
A:31:VAL:CG1	A:32:ASN:HA	0.41	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	1239	1110	96	33

There are 33 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	5	ARG	1
A	7	TYR	1

Chain	Res	Type	Models (Total)
A	8	GLU	1
A	12	ALA	1
A	15	VAL	1
A	17	SER	1
A	21	LEU	1
A	26	ASN	1
A	28	ASP	1
A	30	GLU	1
A	33	ASN	1
A	48	ALA	1
A	50	TYR	1
A	57	ALA	1
A	60	GLN	1
A	62	PRO	1
A	64	GLU	1
A	66	ASN	1
A	70	GLN	1
A	71	PRO	1
A	74	VAL	1
A	78	SER	1
A	83	PRO	1
A	84	ASN	1
A	92	ASN	1
A	102	ASN	1
A	107	ASN	1
A	113	ARG	1
A	575	ASN	1
A	676	PHE	1
B	298	GLY	1
B	305	PRO	1
B	316	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	1055	963	62	30

There are 30 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	11	LYS	1
A	13	LEU	1
A	15	VAL	1
A	25	LYS	1
A	35	MET	1
A	38	LEU	1
A	39	GLU	1
A	40	GLU	1
A	94	VAL	1
A	99	PHE	1
A	105	ASN	1
A	122	HIS	1
A	143	LEU	1
A	477	THR	1
A	600	TYR	1
A	680	VAL	1
B	176	THR	1
B	267	PHE	1
B	270	PHE	1
B	286	ILE	1
B	292	LEU	1
B	293	THR	1
B	305	PRO	1
B	308	THR	1
B	312	PHE	1
B	316	PRO	1
B	318	ASN	1
B	319	GLU	1
B	336	THR	1
B	479	ASN	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".

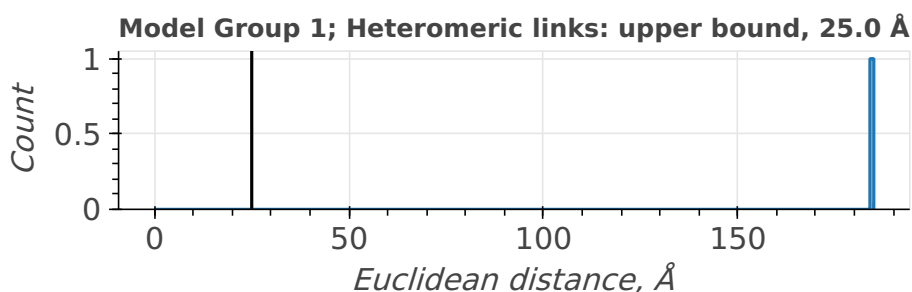
Restraint group represents a set of crosslinking restraints applied collectively in the modeling.

There are 1 crosslinking restraints combined in 1 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
SDA	LYS	CA	LYS	CA	upper bound	25.0	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

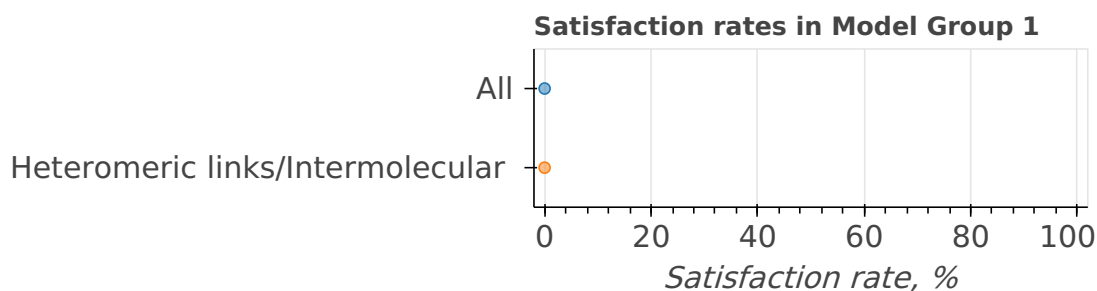
Satisfaction of restraints is calculated on a *restraint group* (a set of crosslinking restraints applied collectively in the modeling) level. Satisfaction of a restraint group depends on satisfaction of individual restraints in the group and the conditionality (all/any). A restraint group is considered 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.



Fit of model to data used for validation ?

Validation for this section is under development.

Acknowledgments

The development of integrative model validation metrics, implementation of a model validation pipeline, and creation of a validation report for integrative structures are funded by NSF awards to the [PDB-IHM team](#) (DBI-1756248, DBI-2112966, DBI-2112967, DBI-2112968, and DBI-1756250) and awards from NSF, NIH, and DOE to the [RCSB PDB](#) (DBI-2321666, R01GM157729, and DE-SC0019749). The PDB-IHM team and members of the [Sali lab](#) contributed model validation metrics and software packages.

Dr. Jill Trewhella, Dr. Dina Schneidman, and members of the [SASBDB](#) repository are acknowledged for their advice and support in implementing SAS validation methods. Team members from the labs of Dr. Juri Rappsilber, Dr. Alexander Leitner, Dr. Andrea Graziadei, and members of [PRIDE](#) database are acknowledged for their advice and support in implementing crosslinking-MS validation methods. We are grateful to Dr. Shruthi Viswanath for discussions about uncertainty assessment of integrative structural models.

Members of the [wwPDB Integrative/Hybrid Methods Task Force](#) provided recommendations and community support for the project.