

Integrative Structure Validation Report ?

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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	9A4E
PDB-Dev ID	PDBDEV_00000235
Structure Title	Integrative model of ATPA-ATPF by crosslinking MS and deep learning
Structure Authors	Kolja Stahl; Oliver Brock; Juri Rappsilber
Deposited on	2024-01-22

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

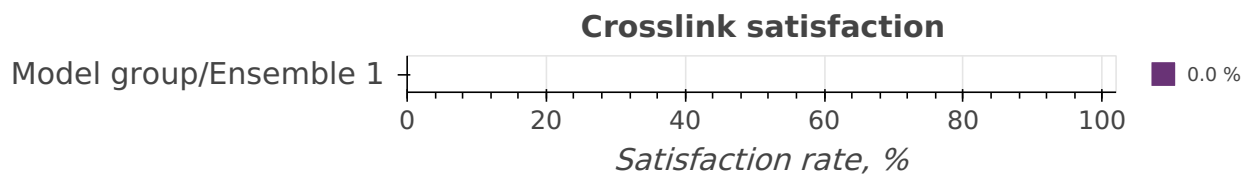
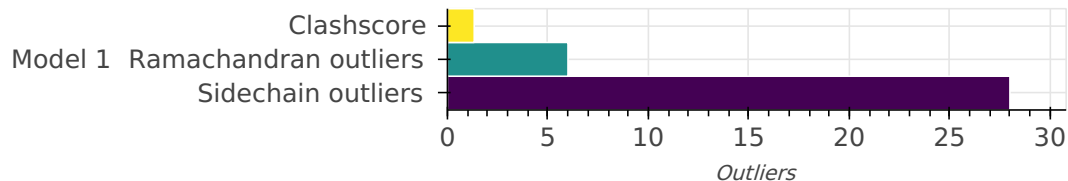
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

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	ATPA_BACSU	A	502	-	1-502	100.00 / 0.00	Atomic
		2	ATPF_BACSU	B	170	-	1-170	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 no bond length outliers.

Standard geometry: angle outliers ?

There are 37 bond angle outliers in this entry (0.52% of 7089 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	1	MET	C-N-CA	6.61	133.61	121.70	1	1
A	147	GLN	OE1-CD-NE2	5.10	117.50	122.60	1	1
B	125	GLN	OE1-CD-NE2	5.02	117.58	122.60	1	1
B	80	GLN	OE1-CD-NE2	4.98	117.62	122.60	1	1
B	66	GLN	OE1-CD-NE2	4.93	117.67	122.60	1	1
A	425	ASN	OD1-CG-ND2	4.88	117.72	122.60	1	1
B	20	GLN	OE1-CD-NE2	4.75	117.85	122.60	1	1
A	172	GLN	OE1-CD-NE2	4.71	117.89	122.60	1	1
A	341	GLN	OE1-CD-NE2	4.70	117.90	122.60	1	1
B	102	GLN	OE1-CD-NE2	4.67	117.93	122.60	1	1
A	466	GLN	OE1-CD-NE2	4.63	117.97	122.60	1	1
B	83	GLN	OE1-CD-NE2	4.62	117.98	122.60	1	1
B	3	GLN	OE1-CD-NE2	4.57	118.03	122.60	1	1
A	20	GLN	OE1-CD-NE2	4.53	118.07	122.60	1	1
B	155	GLN	OE1-CD-NE2	4.49	118.11	122.60	1	1
B	153	GLN	OE1-CD-NE2	4.46	118.14	122.60	1	1
B	160	GLN	OE1-CD-NE2	4.38	118.22	122.60	1	1
B	65	GLN	OE1-CD-NE2	4.36	118.24	122.60	1	1
A	64	GLN	OE1-CD-NE2	4.34	118.26	122.60	1	1
B	71	GLN	OE1-CD-NE2	4.33	118.27	122.60	1	1
A	502	ASN	CA-CB-CG	4.32	116.92	112.60	1	1
A	322	GLN	OE1-CD-NE2	4.31	118.29	122.60	1	1
A	397	GLN	OE1-CD-NE2	4.27	118.33	122.60	1	1
A	163	GLN	OE1-CD-NE2	4.25	118.35	122.60	1	1
A	266	GLN	OE1-CD-NE2	4.25	118.35	122.60	1	1
B	45	GLN	OE1-CD-NE2	4.25	118.35	122.60	1	1
A	14	GLN	OE1-CD-NE2	4.21	118.39	122.60	1	1
B	133	GLN	OE1-CD-NE2	4.17	118.43	122.60	1	1
A	17	GLN	OE1-CD-NE2	4.15	118.45	122.60	1	1
B	49	HIS	CB-CG-CD2	4.12	125.85	131.20	1	1
A	26	GLN	OE1-CD-NE2	4.12	118.48	122.60	1	1
A	70	ASN	OD1-CG-ND2	4.10	118.50	122.60	1	1
A	407	GLN	OE1-CD-NE2	4.09	118.51	122.60	1	1
A	404	GLN	OE1-CD-NE2	4.09	118.51	122.60	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	96	GLN	OE1-CD-NE2	4.07	118.53	122.60	1	1
A	42	HIS	CB-CG-CD2	4.03	125.97	131.20	1	1
A	33	GLN	OE1-CD-NE2	4.00	118.60	122.60	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	1.33	14

There are 14 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:348:LEU:HD11	A:390:ARG:HH22	0.84	1	1
A:95:MET:HE1	A:237:LEU:HD13	0.61	1	1
A:41:VAL:HG21	A:73:ILE:HD12	0.55	1	1
A:348:LEU:HD11	A:390:ARG:NH2	0.53	1	1
A:53:VAL:HG21	A:73:ILE:HD13	0.50	1	1
A:107:ILE:HD11	A:209:VAL:HG11	0.48	1	1
A:389:TYR:CD1	A:413:GLY:HA3	0.46	1	1
A:32:ILE:HD11	A:42:HIS:HB2	0.45	1	1
B:146:ILE:HA	B:150:LEU:HD13	0.45	1	1
A:129:ILE:HG23	A:240:TYR:HB3	0.43	1	1
A:217:ALA:HA	A:220:TYR:CE2	0.43	1	1
A:41:VAL:CG2	A:73:ILE:HD12	0.42	1	1
A:55:PHE:CD2	A:88:VAL:HG22	0.41	1	1
A:74:VAL:CG1	A:233:PRO:CG	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	668	650	12	6

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

Chain	Res	Type	Models (Total)
A	20	GLN	1

Chain	Res	Type	Models (Total)
A	21	SER	1
A	22	ASP	1
A	23	ILE	1
A	24	GLU	1
A	25	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	557	494	35	28

There are 28 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	10	THR	1
A	11	LEU	1
A	19	TYR	1
A	157	ILE	1
A	273	LEU	1
A	386	LEU	1
A	407	GLN	1
A	410	LEU	1
A	487	PHE	1
B	4	LEU	1
B	6	LEU	1
B	8	LEU	1
B	10	LEU	1
B	18	LEU	1
B	22	LEU	1
B	27	LEU	1
B	31	LEU	1
B	36	LEU	1
B	39	LEU	1
B	67	LEU	1
B	75	LEU	1

Chain	Res	Type	Models (Total)
B	84	THR	1
B	85	LEU	1
B	111	LEU	1
B	137	LEU	1
B	156	GLU	1
B	158	LEU	1
B	162	TYR	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".

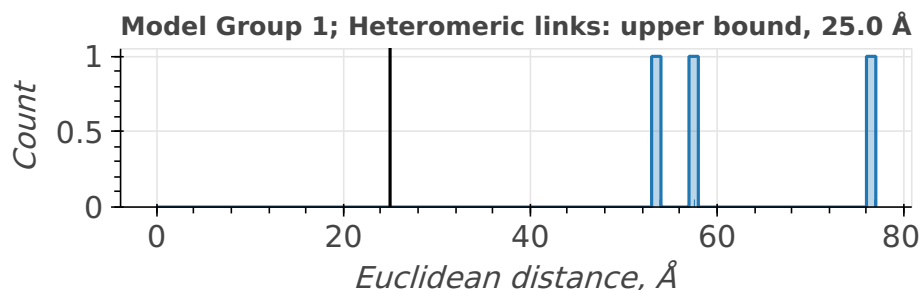
Restraint group represents a set of crosslinking restraints applied collectively in the modeling.

There are 3 crosslinking restraints combined in 3 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	3

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

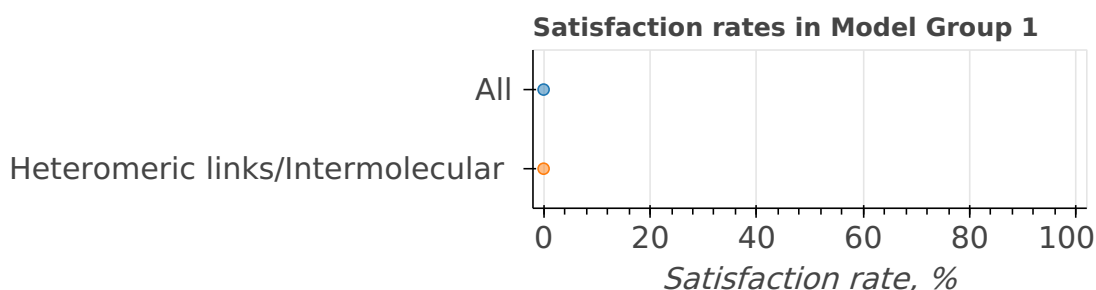
Satisfaction of restraints is calculated on a *restraint group* (a set of crosslinking restraints applied collectively in the modeling) level. Satisfaction of a restraint group depends on satisfaction of individual restraints in the group and the conditionality (all/any). A restraint group is considered 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=3)
1	1	1	1/1	All	0.00	100.00	3
				Heteromeric links/Intermolecular	0.00	100.00	3

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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