

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	9A7C
PDB-Dev ID	PDBDEV_00000341
Structure Title	Integrative model of NUSA-RPOB 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

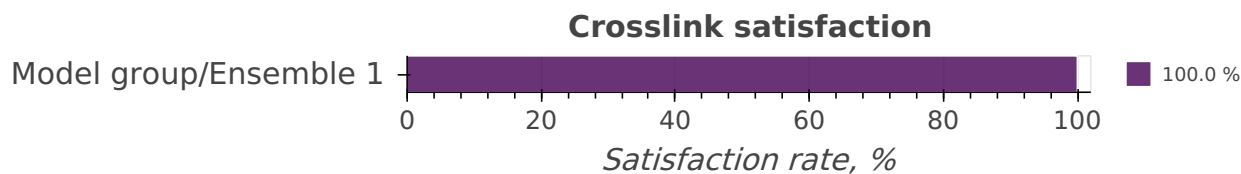
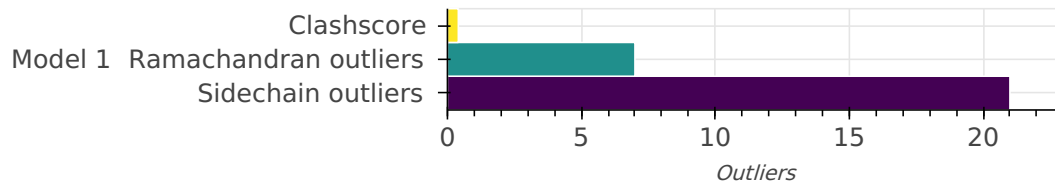
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

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	NUSA_BACSU	A	371	-	1-371	100.00 / 0.00	Atomic
		2	RPOB_BACSU	B	1193	-	1-1193	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 1 bond length outliers in this entry (0.01% of 12540 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	1186	GLU	CA-C	4.07	1.61	1.52	1	1

Standard geometry: angle outliers ?

There are 88 bond angle outliers in this entry (0.52% of 16958 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	1185	VAL	C-N-CA	12.72	144.59	121.70	1	1
B	1182	SER	C-N-CA	10.89	141.31	121.70	1	1
B	1188	ASP	C-N-CA	10.73	141.02	121.70	1	1
B	1183	ALA	C-N-CA	10.60	140.77	121.70	1	1
B	1186	GLU	C-N-CA	9.74	139.24	121.70	1	1
B	1186	GLU	CA-C-N	8.87	133.94	116.20	1	1
B	1185	VAL	CA-C-N	8.53	133.26	116.20	1	1
B	1183	ALA	CA-C-N	7.80	131.80	116.20	1	1
B	1185	VAL	O-C-N	7.66	110.74	123.00	1	1
B	1188	ASP	CA-C-N	7.61	131.41	116.20	1	1
B	1186	GLU	O-C-N	7.35	111.24	123.00	1	1
B	1179	GLU	C-N-CA	6.88	134.08	121.70	1	1
A	362	THR	C-N-CA	6.71	133.78	121.70	1	1
B	1183	ALA	O-C-N	6.58	112.47	123.00	1	1
B	1188	ASP	O-C-N	6.54	112.53	123.00	1	1
B	280	HIS	CB-CG-CD2	6.04	123.35	131.20	1	1
B	1189	VAL	CA-CB-CG2	6.04	120.66	110.40	1	1
A	312	GLN	OE1-CD-NE2	5.39	117.21	122.60	1	1
B	403	HIS	CB-CG-CD2	5.22	124.41	131.20	1	1
B	773	ASP	CA-CB-CG	5.10	117.70	112.60	1	1
B	175	ASP	CA-CB-CG	5.05	117.65	112.60	1	1
B	128	ASN	CA-CB-CG	5.00	117.60	112.60	1	1
B	438	GLN	OE1-CD-NE2	4.94	117.66	122.60	1	1
B	1182	SER	CA-C-N	4.89	125.98	116.20	1	1
B	390	ASN	CA-CB-CG	4.87	117.47	112.60	1	1
B	967	ASN	OD1-CG-ND2	4.84	117.76	122.60	1	1
B	355	GLN	OE1-CD-NE2	4.81	117.79	122.60	1	1
B	1011	ARG	CD-NE-CZ	4.73	131.02	124.40	1	1
B	1190	VAL	N-CA-C	4.72	124.21	111.00	1	1
B	1182	SER	O-C-N	4.69	115.50	123.00	1	1
A	41	GLN	OE1-CD-NE2	4.67	117.93	122.60	1	1
B	701	GLN	OE1-CD-NE2	4.63	117.97	122.60	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	271	ASP	CA-CB-CG	4.62	117.22	112.60	1	1
B	1180	THR	CA-CB-OG1	4.62	116.53	109.60	1	1
B	426	ARG	NH1-CZ-NH2	4.61	113.31	119.30	1	1
B	469	GLN	OE1-CD-NE2	4.60	118.00	122.60	1	1
B	280	HIS	CB-CG-ND1	4.60	129.60	122.70	1	1
B	576	GLN	OE1-CD-NE2	4.60	118.00	122.60	1	1
A	84	HIS	CB-CG-CD2	4.58	125.25	131.20	1	1
A	193	GLN	OE1-CD-NE2	4.54	118.06	122.60	1	1
B	657	PHE	CA-CB-CG	4.53	118.33	113.80	1	1
B	1191	THR	N-CA-C	4.51	123.64	111.00	1	1
B	1101	ASP	CA-CB-CG	4.50	117.10	112.60	1	1
A	359	PRO	C-N-CA	4.47	129.74	121.70	1	1
B	50	GLN	OE1-CD-NE2	4.44	118.16	122.60	1	1
B	1179	GLU	O-C-N	4.43	115.91	123.00	1	1
A	43	GLN	OE1-CD-NE2	4.43	118.17	122.60	1	1
B	308	GLN	OE1-CD-NE2	4.42	118.18	122.60	1	1
B	1165	GLN	OE1-CD-NE2	4.41	118.19	122.60	1	1
B	538	ASN	CA-CB-CG	4.40	117.00	112.60	1	1
B	791	HIS	CB-CG-CD2	4.38	125.50	131.20	1	1
B	359	GLN	OE1-CD-NE2	4.36	118.24	122.60	1	1
B	280	HIS	CA-CB-CG	4.36	118.16	113.80	1	1
B	1042	HIS	CB-CG-CD2	4.35	125.54	131.20	1	1
B	1184	ASP	C-N-CA	4.35	129.54	121.70	1	1
B	507	HIS	CB-CG-CD2	4.34	125.56	131.20	1	1
A	361	PHE	CA-CB-CG	4.33	118.13	113.80	1	1
A	200	HIS	CB-CG-CD2	4.32	125.58	131.20	1	1
A	257	ARG	NH1-CZ-NH2	4.32	113.68	119.30	1	1
B	582	ASP	CA-CB-CG	4.31	116.91	112.60	1	1
B	1187	ARG	CA-CB-CG	4.31	105.49	114.10	1	1
B	419	GLN	OE1-CD-NE2	4.26	118.34	122.60	1	1
B	121	ASP	CA-CB-CG	4.25	116.85	112.60	1	1
B	12	ARG	CD-NE-CZ	4.25	130.35	124.40	1	1
B	51	ASP	CA-CB-CG	4.24	116.84	112.60	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	259	GLN	OE1-CD-NE2	4.23	118.37	122.60	1	1
A	256	GLN	OE1-CD-NE2	4.22	118.38	122.60	1	1
A	175	HIS	CB-CG-CD2	4.21	125.72	131.20	1	1
B	652	GLN	OE1-CD-NE2	4.21	118.39	122.60	1	1
B	375	ASN	OD1-CG-ND2	4.21	118.39	122.60	1	1
A	143	GLN	OE1-CD-NE2	4.20	118.40	122.60	1	1
B	402	ASP	CA-CB-CG	4.20	108.40	112.60	1	1
B	689	ASN	CA-CB-CG	4.20	116.80	112.60	1	1
B	825	ASP	CA-CB-CG	4.19	116.79	112.60	1	1
B	362	ASN	CA-CB-CG	4.18	116.78	112.60	1	1
B	28	ASN	OD1-CG-ND2	4.17	118.43	122.60	1	1
B	13	GLN	OE1-CD-NE2	4.17	118.43	122.60	1	1
B	11	HIS	CB-CG-CD2	4.16	125.79	131.20	1	1
B	446	GLN	OE1-CD-NE2	4.12	118.48	122.60	1	1
B	1049	HIS	CB-CG-CD2	4.11	125.86	131.20	1	1
A	112	GLN	OE1-CD-NE2	4.07	118.53	122.60	1	1
A	116	GLN	OE1-CD-NE2	4.05	118.55	122.60	1	1
A	108	GLN	OE1-CD-NE2	4.04	118.56	122.60	1	1
B	1069	GLN	OE1-CD-NE2	4.04	118.56	122.60	1	1
B	578	ASN	OD1-CG-ND2	4.03	118.57	122.60	1	1
B	606	ASN	CA-CB-CG	4.02	116.62	112.60	1	1
B	720	GLN	OE1-CD-NE2	4.00	118.60	122.60	1	1
B	10	ARG	NE-CZ-NH1	4.00	125.50	121.50	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	0.41	10

There are 10 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)
B:1188:ASP:HB3	B:1189:VAL:HG22	0.55	1	1
B:791:HIS:CE1	B:1043:MET:HE1	0.50	1	1
B:471:MET:HE1	B:483:LYS:HE3	0.48	1	1
B:777:MET:HG3	B:781:LEU:HD12	0.45	1	1
B:781:LEU:HD11	B:954:ASP:HB3	0.44	1	1
B:849:LYS:HE2	B:852:THR:HG21	0.43	1	1
B:928:ARG:HH21	B:973:GLU:CD	0.42	1	1
B:976:MET:HE1	B:987:ILE:HG21	0.42	1	1
A:245:ASP:CG	A:248:GLY:H	0.42	1	1
A:232:ARG:HH21	A:271:ASP: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	1560	1495	58	7

There are 7 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	364	PRO	1
B	268	ALA	1
B	1041	ALA	1
B	1061	GLN	1
B	1187	ARG	1
B	1189	VAL	1
B	1191	THR	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	1352	1289	42	21

There are 21 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	98	THR	1
A	348	ILE	1

Chain	Res	Type	Models (Total)
B	48	MET	1
B	57	ASP	1
B	159	THR	1
B	223	LYS	1
B	311	ASP	1
B	319	LEU	1
B	519	THR	1
B	753	LEU	1
B	802	THR	1
B	976	MET	1
B	1011	ARG	1
B	1044	VAL	1
B	1169	LEU	1
B	1179	GLU	1
B	1180	THR	1
B	1185	VAL	1
B	1188	ASP	1
B	1189	VAL	1
B	1191	THR	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.

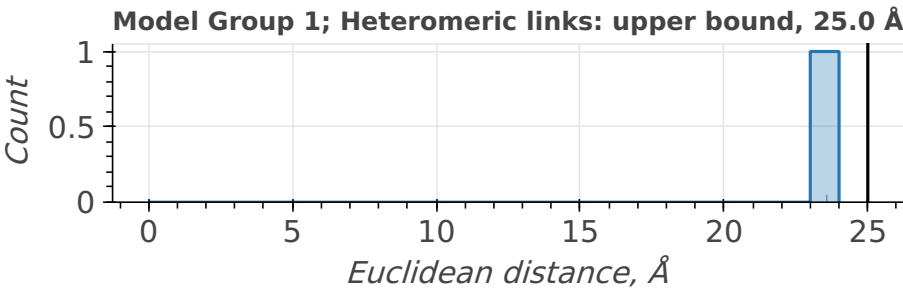
There are 1 crosslinking restraints combined in 1 restraint groups.

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.



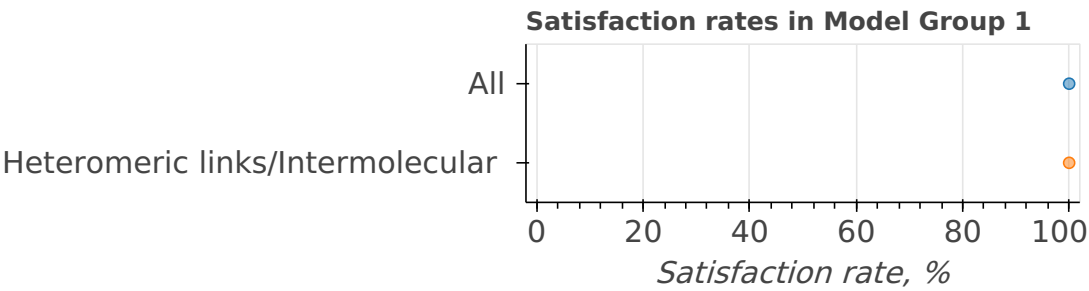
Satisfaction of restraints

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	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.



Fit of model to data used for validation ?

Validation for this section is under development.

Acknowledgments

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