

Integrative Structure Validation Report ?

April 10, 2025 - 05:26 AM 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	9A7U
PDB-Dev ID	PDBDEV_00000359
Structure Title	Integrative model of RPOC-GREA by crosslinking MS and deep learning
Structure Authors	Kolja Stahl; Oliver Brock; Juri Rappsilber
Deposited on	2024-01-24

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

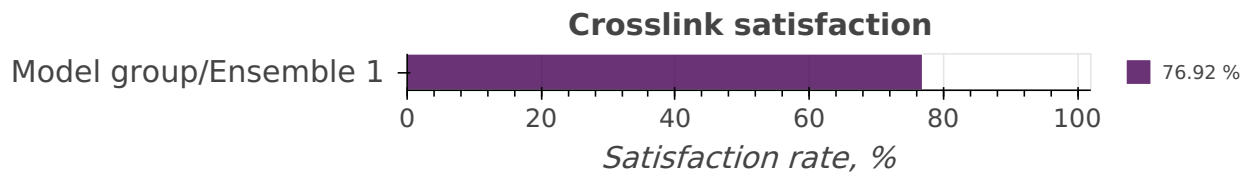
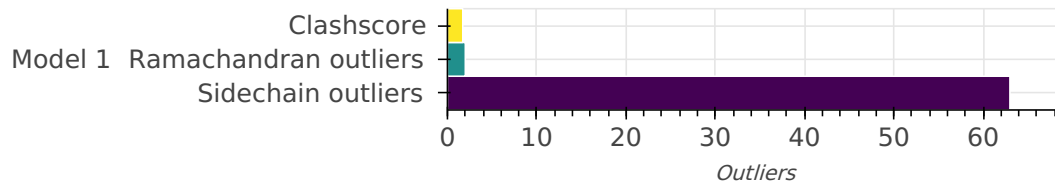
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 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	RPOC_BACSU	A	1199	-	1-1199	100.00 / 0.00	Atomic
		2	GREa_BACSU	B	157	-	1-157	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 49 bond angle outliers in this entry (0.34% of 14571 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	107	PHE	CA-CB-CG	10.86	124.66	113.80	1	1
A	585	ASN	OD1-CG-ND2	5.40	117.20	122.60	1	1
A	668	ASP	CA-CB-CG	5.14	117.74	112.60	1	1
A	382	ASN	CA-CB-CG	5.13	117.73	112.60	1	1
A	948	ASP	CA-CB-CG	5.02	117.62	112.60	1	1
A	527	GLN	OE1-CD-NE2	5.01	117.59	122.60	1	1
A	180	GLN	OE1-CD-NE2	5.00	117.60	122.60	1	1
A	869	ASP	CA-CB-CG	4.98	117.58	112.60	1	1
A	768	ARG	NE-CZ-NH2	4.93	123.64	119.20	1	1
A	968	GLN	OE1-CD-NE2	4.93	117.67	122.60	1	1
A	741	PHE	CA-CB-CG	4.89	108.91	113.80	1	1
A	439	HIS	CB-CG-CD2	4.87	124.87	131.20	1	1
A	1140	GLN	OE1-CD-NE2	4.85	117.75	122.60	1	1
A	933	GLN	OE1-CD-NE2	4.76	117.84	122.60	1	1
A	994	GLN	OE1-CD-NE2	4.68	117.92	122.60	1	1
A	394	GLN	OE1-CD-NE2	4.67	117.93	122.60	1	1
A	1044	GLN	OE1-CD-NE2	4.65	117.95	122.60	1	1
A	821	ASP	CA-CB-CG	4.64	117.24	112.60	1	1
A	925	GLN	OE1-CD-NE2	4.60	118.00	122.60	1	1
A	753	ASN	OD1-CG-ND2	4.56	118.04	122.60	1	1
A	988	GLN	OE1-CD-NE2	4.53	118.07	122.60	1	1
A	329	GLN	OE1-CD-NE2	4.52	118.08	122.60	1	1
A	670	GLN	OE1-CD-NE2	4.50	118.10	122.60	1	1
A	532	HIS	CB-CG-CD2	4.46	125.40	131.20	1	1
A	382	ASN	OD1-CG-ND2	4.43	118.17	122.60	1	1
A	713	GLN	OE1-CD-NE2	4.43	118.17	122.60	1	1
B	15	GLN	OE1-CD-NE2	4.37	118.23	122.60	1	1
A	1190	GLN	OE1-CD-NE2	4.36	118.24	122.60	1	1
B	74	ASN	OD1-CG-ND2	4.33	118.27	122.60	1	1
A	887	ARG	NE-CZ-NH2	4.33	123.09	119.20	1	1
B	19	GLN	OE1-CD-NE2	4.31	118.29	122.60	1	1
A	419	HIS	CB-CG-CD2	4.30	125.61	131.20	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	243	GLN	OE1-CD-NE2	4.27	118.33	122.60	1	1
A	608	GLN	OE1-CD-NE2	4.26	118.34	122.60	1	1
A	957	GLN	OE1-CD-NE2	4.26	118.34	122.60	1	1
A	947	ASP	C-N-CA	4.24	129.32	121.70	1	1
B	43	GLY	C-N-CA	4.21	129.28	121.70	1	1
A	449	ASP	CA-CB-CG	4.21	116.81	112.60	1	1
A	349	HIS	CB-CG-CD2	4.18	125.76	131.20	1	1
A	743	GLN	OE1-CD-NE2	4.17	118.43	122.60	1	1
A	413	ASN	OD1-CG-ND2	4.14	118.46	122.60	1	1
A	448	ALA	C-N-CA	4.14	129.15	121.70	1	1
A	201	GLN	OE1-CD-NE2	4.11	118.49	122.60	1	1
A	181	ASP	CA-CB-CG	4.10	116.70	112.60	1	1
B	73	ARG	NE-CZ-NH2	4.10	122.89	119.20	1	1
A	253	ASP	CA-CB-CG	4.08	116.68	112.60	1	1
A	408	HIS	CB-CG-CD2	4.06	125.92	131.20	1	1
A	854	HIS	CB-CG-CD2	4.06	125.92	131.20	1	1
A	1066	HIS	CB-CG-CD2	4.02	125.97	131.20	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	1.72	37

There are 37 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:808:ALA:CB	A:1070:MET:HE1	0.81	1	1
A:808:ALA:HB2	A:1070:MET:HE1	0.79	1	1
A:234:ILE:HD11	A:316:LEU:HD21	0.71	1	1
A:978:VAL:CG2	A:1018:ILE:HD11	0.70	1	1
A:726:ILE:HG21	A:741:PHE:CE1	0.69	1	1
A:726:ILE:HG21	A:741:PHE:CD1	0.68	1	1
A:317:SER:HB3	A:321:LYS:HE2	0.62	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:234:ILE:HD11	A:316:LEU:CD2	0.62	1	1
A:371:MET:HE3	A:383:ILE:HG23	0.60	1	1
A:978:VAL:HG22	A:1018:ILE:HD11	0.59	1	1
A:503:THR:HG21	A:615:PHE:CD2	0.59	1	1
A:559:ILE:HD11	A:596:LEU:HD11	0.58	1	1
A:747:MET:HE2	A:749:GLY:HA2	0.57	1	1
A:441:LEU:HD21	A:495:MET:HE1	0.57	1	1
A:978:VAL:HG23	A:1018:ILE:HD11	0.54	1	1
A:84:ARG:O	A:87:VAL:HG22	0.53	1	1
A:991:ILE:HD11	A:1010:LEU:CD2	0.53	1	1
A:559:ILE:HD11	A:596:LEU:CD1	0.52	1	1
A:895:PRO:HA	A:1097:HIS:CD2	0.51	1	1
A:808:ALA:HB1	A:1070:MET:HE1	0.50	1	1
A:317:SER:HB3	A:321:LYS:CE	0.50	1	1
A:1086:THR:HG22	A:1106:VAL:HG21	0.50	1	1
A:506:ARG:HH21	A:723:LEU:HD22	0.48	1	1
A:581:PRO:HB2	A:619:ILE:CD1	0.47	1	1
A:820:THR:HG22	A:887:ARG:HH21	0.47	1	1
A:137:THR:O	A:146:LYS:HE3	0.46	1	1
A:720:LEU:HD11	A:741:PHE:CE2	0.45	1	1
A:495:MET:HE3	A:644:LYS:HA	0.45	1	1
A:371:MET:CE	A:383:ILE:HG23	0.44	1	1
A:751:MET:HE1	A:782:GLY:HA3	0.43	1	1
A:506:ARG:HE	A:723:LEU:CD2	0.43	1	1
A:107:PHE:HB2	A:114:MET:CE	0.43	1	1
A:705:TRP:CD2	A:762:PRO:HG3	0.42	1	1
B:95:PHE:CD1	B:151:VAL:HG11	0.42	1	1
A:705:TRP:CH2	A:764:LYS:HE2	0.42	1	1
A:346:VAL:HG22	A:450:PHE:CE2	0.41	1	1
A:1009:ARG:CZ	B:73:ARG:HD2	0.40	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	1352	1307	43	2

There are 2 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	1194	ASP	1
B	44	ASP	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	1162	1023	76	63

There are 63 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	2	LEU	1
A	55	THR	1
A	76	ASP	1
A	107	PHE	1
A	125	LEU	1
A	135	VAL	1
A	159	LEU	1
A	187	GLU	1
A	195	LEU	1
A	260	ARG	1
A	287	MET	1
A	345	VAL	1
A	352	MET	1
A	357	LEU	1
A	363	LEU	1
A	373	GLU	1
A	381	HIS	1
A	382	ASN	1
A	385	SER	1
A	412	LEU	1
A	431	VAL	1

Chain	Res	Type	Models (Total)
A	438	LEU	1
A	444	THR	1
A	453	ASP	1
A	474	LEU	1
A	497	LEU	1
A	504	LEU	1
A	519	THR	1
A	531	VAL	1
A	583	LYS	1
A	634	THR	1
A	641	ASP	1
A	646	LEU	1
A	706	SER	1
A	716	LEU	1
A	751	MET	1
A	753	ASN	1
A	761	LEU	1
A	765	SER	1
A	774	LEU	1
A	781	HIS	1
A	809	GLN	1
A	810	ASP	1
A	816	THR	1
A	869	ASP	1
A	932	THR	1
A	935	THR	1
A	950	THR	1
A	974	ILE	1
A	977	THR	1
A	999	THR	1
A	1003	THR	1
A	1018	ILE	1
A	1041	THR	1
A	1042	THR	1
A	1130	THR	1

Chain	Res	Type	Models (Total)
A	1171	VAL	1
A	1177	MET	1
B	46	SER	1
B	89	LEU	1
B	141	THR	1
B	150	LEU	1
B	151	VAL	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".

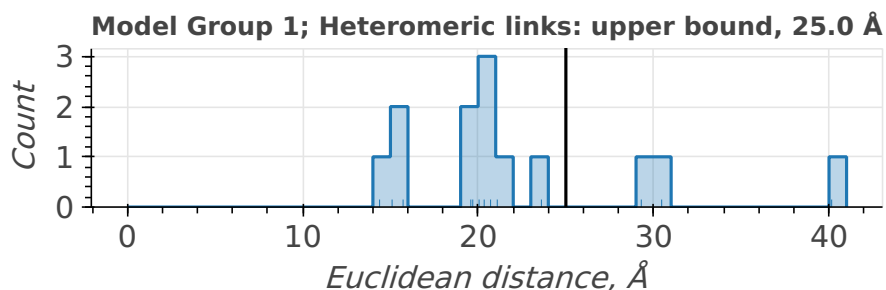
Restraint group represents a set of crosslinking restraints applied collectively in the modeling.

There are 13 crosslinking restraints combined in 13 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	13

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

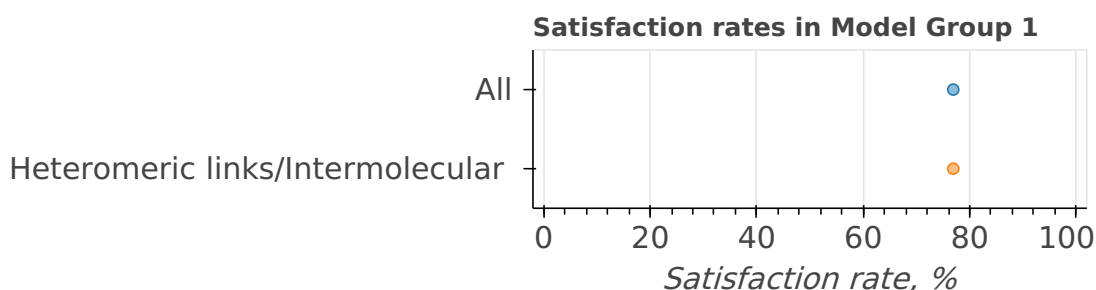
Satisfaction of restraints is calculated on a *restraint group* (a set of crosslinking restraints applied collectively in the modeling) level. Satisfaction of a restraint group depends on satisfaction of individual restraints in the group and the conditionality (all/any). A restraint group is considered 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	76.92	23.08	13
				Heteromeric links/ Intermolecular	76.92	23.08	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

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.