

# 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	9A7J
PDB-Dev ID	PDBDEV_00000348
Structure Title	Integrative model of F16PC-GLPD 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](mailto:helpdesk@pdb-ihm.org)*

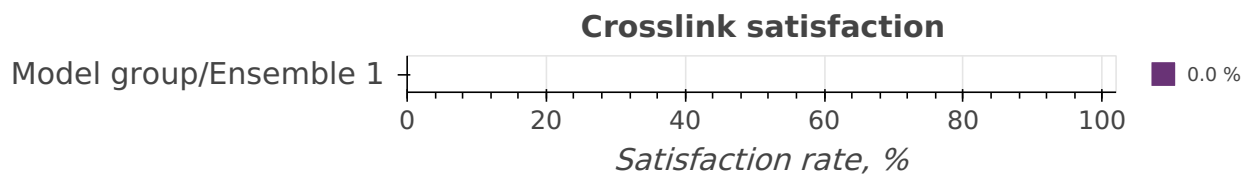
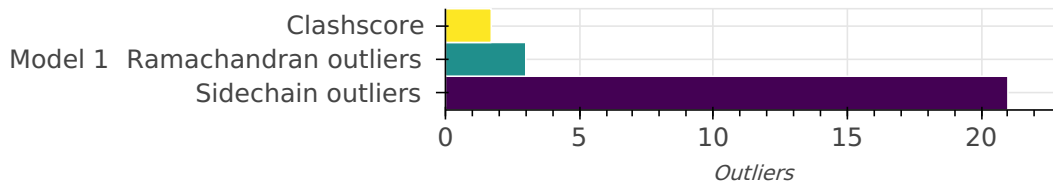
*A user guide is available at [https://pdb-ihm.org/validation\\_help.html](https://pdb-ihm.org/validation_help.html) with specific help available everywhere you see the ? symbol.*

*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	F16PC_BACSU	A	641	-	1-641	100.00 / 0.00	Atomic
		2	GLPD_BACSU	B	555	-	1-555	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	<a href="#">PXD035508</a>

## 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	<a href="#">AlphaLink2</a>	1.00	model building	<a href="https://github.com/Rappsilber-Laboratory/AlphaLink2">https://github.com/Rappsilber-Laboratory/AlphaLink2</a>

## 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 9845 assessed bonds). A summary is provided below.*

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	555	GLN	CA-C	4.85	1.63	1.52	1	1

### Standard geometry: angle outliers ?

*There are 54 bond angle outliers in this entry (0.41% of 13269 assessed bonds). A summary is provided below.*

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	555	GLN	O-C-OXT	16.77	168.30	118.00	1	1
B	555	GLN	CA-C-OXT	13.01	81.98	121.00	1	1
B	555	GLN	CA-C-O	11.55	86.36	121.00	1	1
A	201	ASP	C-N-CA	5.86	132.24	121.70	1	1
A	67	ASP	CA-CB-CG	5.55	118.15	112.60	1	1
B	555	GLN	OE1-CD-NE2	5.54	117.06	122.60	1	1
B	123	ILE	C-CA-CB	5.23	122.06	111.60	1	1
A	186	GLN	OE1-CD-NE2	5.17	117.43	122.60	1	1
B	173	ASP	CA-CB-CG	5.04	117.64	112.60	1	1
A	255	ASP	CA-CB-CG	4.94	117.54	112.60	1	1
B	263	GLN	OE1-CD-NE2	4.92	117.68	122.60	1	1
B	527	ARG	NH1-CZ-NH2	4.92	112.91	119.30	1	1
A	205	GLN	OE1-CD-NE2	4.91	117.69	122.60	1	1
A	322	ASN	CA-CB-CG	4.84	117.44	112.60	1	1
A	48	GLN	OE1-CD-NE2	4.79	117.81	122.60	1	1
B	447	GLN	OE1-CD-NE2	4.77	117.83	122.60	1	1
A	192	HIS	CB-CG-CD2	4.76	125.02	131.20	1	1
B	306	HIS	CB-CG-CD2	4.75	125.03	131.20	1	1
A	5	TYR	CA-CB-CG	4.74	105.38	113.90	1	1
B	527	ARG	NE-CZ-NH2	4.70	123.43	119.20	1	1
A	638	ARG	NE-CZ-NH2	4.67	123.40	119.20	1	1
B	533	GLN	OE1-CD-NE2	4.63	117.97	122.60	1	1
A	51	GLN	OE1-CD-NE2	4.63	117.97	122.60	1	1
B	5	GLN	OE1-CD-NE2	4.55	118.05	122.60	1	1
B	123	ILE	C-N-CA	4.54	129.87	121.70	1	1
B	77	GLN	OE1-CD-NE2	4.51	118.09	122.60	1	1
B	417	HIS	CB-CG-CD2	4.50	125.35	131.20	1	1
A	222	GLN	OE1-CD-NE2	4.48	118.12	122.60	1	1
A	6	LEU	C-CA-CB	4.47	118.60	110.10	1	1
B	258	HIS	CB-CG-CD2	4.40	125.47	131.20	1	1
A	535	LYS	CB-CG-CD	4.37	101.25	111.30	1	1
A	530	GLY	C-N-CA	4.34	129.51	121.70	1	1
A	583	HIS	CB-CG-CD2	4.33	125.57	131.20	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	252	GLN	OE1-CD-NE2	4.33	118.27	122.60	1	1
A	246	ARG	CD-NE-CZ	4.33	130.46	124.40	1	1
A	364	ASP	CA-CB-CG	4.32	116.92	112.60	1	1
A	139	GLN	OE1-CD-NE2	4.26	118.34	122.60	1	1
A	297	GLN	OE1-CD-NE2	4.24	118.36	122.60	1	1
A	44	HIS	CB-CG-CD2	4.24	125.69	131.20	1	1
B	175	ARG	NE-CZ-NH2	4.22	123.00	119.20	1	1
B	313	ASP	CA-CB-CG	4.19	116.79	112.60	1	1
B	381	ARG	NH1-CZ-NH2	4.19	113.85	119.30	1	1
A	322	ASN	OD1-CG-ND2	4.18	118.42	122.60	1	1
A	441	PHE	CA-CB-CG	4.18	117.98	113.80	1	1
B	150	GLN	OE1-CD-NE2	4.11	118.49	122.60	1	1
B	238	GLN	OE1-CD-NE2	4.11	118.49	122.60	1	1
B	410	ASN	OD1-CG-ND2	4.08	118.52	122.60	1	1
A	283	ARG	NH1-CZ-NH2	4.06	114.03	119.30	1	1
B	529	GLN	OE1-CD-NE2	4.05	118.55	122.60	1	1
B	123	ILE	CA-CB-CG2	4.02	117.34	110.50	1	1
B	99	HIS	CB-CG-CD2	4.02	125.98	131.20	1	1
B	262	ASP	CA-CB-CG	4.01	108.59	112.60	1	1
B	423	ASN	OD1-CG-ND2	4.01	118.59	122.60	1	1
A	114	HIS	CB-CG-CD2	4.00	126.00	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	1.71	33

There are 33 clashes. The table below contains the detailed list of all clashes based on a MolProbity analysis. Bad clashes are  $\geq 0.4$  Angstrom.

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:5:TYR:CE2	B:127:VAL:HG23	0.78	1	1
A:5:TYR:CG	B:123:ILE:HG23	0.77	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:328:ARG:NH2	A:330:LEU:HD11	0.69	1	1
A:224:GLY:HA2	A:411:HIS:CD2	0.57	1	1
B:492:THR:HG23	B:497:ASP:HB2	0.55	1	1
A:5:TYR:CD2	B:123:ILE:HG23	0.54	1	1
A:500:PRO:HA	A:503:TYR:CE2	0.52	1	1
B:192:VAL:HA	B:491:MET:HE1	0.50	1	1
B:94:TYR:CZ	B:421:SER:HB2	0.50	1	1
B:227:LYS:HZ1	B:398:GLU:CD	0.49	1	1
A:505:ARG:HB2	A:549:MET:HE3	0.49	1	1
A:8:LEU:HD13	B:127:VAL:HG11	0.48	1	1
A:8:LEU:HD22	B:131:LEU:HD11	0.48	1	1
B:90:ARG:HH21	B:134:VAL:HG22	0.47	1	1
A:9:LEU:HB3	A:634:LEU:HD22	0.47	1	1
B:18:MET:HE2	B:49:ALA:HB1	0.46	1	1
A:5:TYR:CZ	B:123:ILE:C	0.46	1	1
A:8:LEU:HD22	B:127:VAL:HG11	0.46	1	1
A:5:TYR:CZ	B:127:VAL:HB	0.45	1	1
B:105:TRP:HB3	B:165:TYR:CZ	0.44	1	1
A:1:MET:SD	B:120:THR:HB	0.44	1	1
B:68:VAL:CG1	B:378:THR:HG23	0.43	1	1
A:221:ILE:O	A:398:GLY:HA2	0.43	1	1
A:5:TYR:CZ	B:123:ILE:O	0.43	1	1
B:280:ARG:HH22	B:296:THR:C	0.43	1	1
A:5:TYR:CD1	B:123:ILE:CG2	0.42	1	1
B:401:LYS:HE3	B:403:PHE:CE1	0.42	1	1
A:374:ILE:HA	A:374:ILE:HD12	0.41	1	1
A:5:TYR:CG	B:123:ILE:CG2	0.41	1	1
B:345:LEU:HB3	B:356:ILE:CG2	0.41	1	1
A:87:TYR:CD1	A:589:LYS:HE3	0.40	1	1
A:5:TYR:CD2	B:127:VAL:HG23	0.40	1	1
B:273:TYR:CE1	B:281:MET:HB3	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	1192	1156	33	3

There are 3 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	599	VAL	1
B	123	ILE	1
B	124	GLY	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	1040	990	29	21

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

Chain	Res	Type	Models (Total)
A	5	TYR	1
A	9	LEU	1
A	54	LEU	1
A	114	HIS	1
A	239	VAL	1
A	255	ASP	1
A	287	ASP	1
A	322	ASN	1
A	326	GLU	1
A	372	GLU	1
A	374	ILE	1
A	598	ASP	1
B	12	ASP	1
B	75	LEU	1
B	118	SER	1
B	239	LEU	1
B	257	ILE	1
B	382	LYS	1
B	480	LEU	1
B	506	LEU	1

Chain	Res	Type	Models (Total)
B	522	ASP	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*".

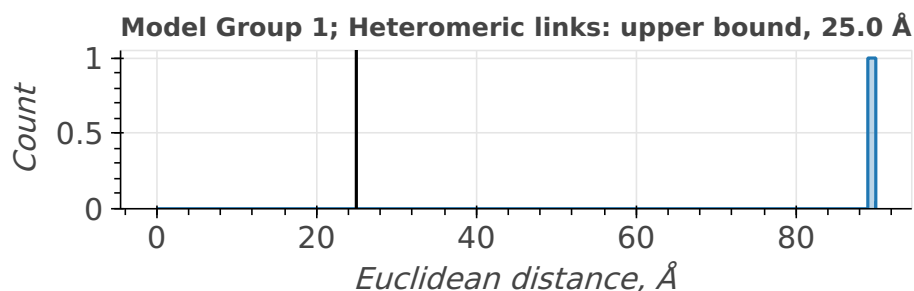
*Restraint group* represents a set of crosslinking restraints applied collectively in the modeling.

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

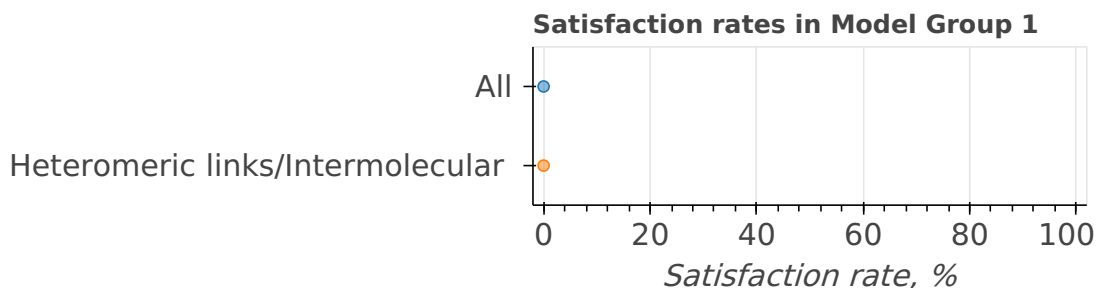
Satisfaction of restraints is calculated on a *restraint group* (a set of crosslinking restraints applied collectively in the modeling) level. Satisfaction of a restraint group depends on satisfaction of individual restraints in the group and the conditionality (all/any). A restraint group is considered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

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