

# Integrative Structure Validation Report

September 11, 2024 - 01:35 AM PDT

The following software was used in the production of this report:

*Python-IHM Version 1.3*

*MolProbity Version 4.5.2*

*Integrative Modeling Validation Version 1.2*

PDB ID	9A80
PDB-Dev ID	PDBDEV_00000365
Structure Title	Integrative model of CLPC-HOLB by crosslinking MS and deep learning
Structure Authors	Kolja Stahl; Oliver Brock; Juri Rappsilber

*This is a PDB-Dev IM Structure Validation Report for a publicly released PDB-Dev entry.*

*We welcome your comments at [pdb-dev@mail.wwpdb.org](mailto:pdb-dev@mail.wwpdb.org)*

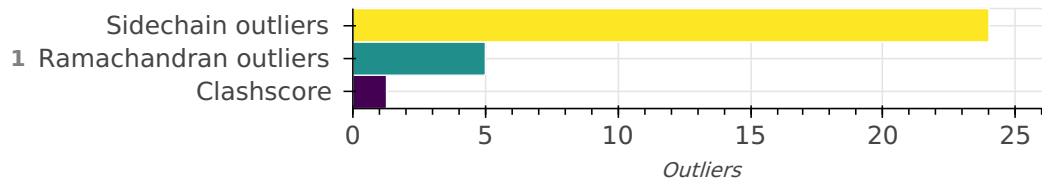
*A user guide is available at [https://pdb-dev.wwpdb.org/validation\\_help.html](https://pdb-dev.wwpdb.org/validation_help.html) with specific help available everywhere you see the  symbol.*

*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 assessment for SAS datasets and fit to model assessments for SAS 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 unique models, with 2 subunits in each model. A total of 1 datasets or restraints were used to build this entry. Each model is represented by 0 rigid bodies and 2 flexible or non-rigid units.

## Entry composition ?

There is 1 unique type of models in this entry. This model is titled None/None.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	CLPC_BACSU	A	A	810
1	2	2	HOLB_BACSU	B	B	329

## 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

## Representation ?

This entry has only one representation and includes 0 rigid bodies and 2 flexible units.

Chain ID	Rigid bodies	Non-rigid segments

Chain ID	Rigid bodies	Non-rigid segments
A	-	1-810
B	-	1-329

## 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>	1.0	model building	<a href="https://github.com/Rappsilber-Laboratory/AlphaLink2">https://github.com/Rappsilber-Laboratory/AlphaLink2</a>

## Data quality ?

### Crosslinking-MS

Validation for this section is under development.

## Model quality ?

For models with atomic structures, molprobit analysis is performed. For models with coarse-grained or multi-scale structures, excluded volume analysis is performed.

### Standard geometry: bond outliers ?

*There are 9136 bond outliers in this entry. A summary is provided below, and a detailed list of outliers can be found [here](#).*

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CD1--HD12	1.09	0.97	204

<b>Bond type</b>	<b>Observed distance (Å)</b>	<b>Ideal distance (Å)</b>	<b>Number of outliers</b>
CG1--HG12	1.09	0.97	151
CB--HB	1.09	0.97	204
CB--HB2	1.09	0.97	862
CG2--HG22	1.09	0.97	204
CA--HA	1.09	0.97	1066
CD2--HD22	1.09	0.97	127
CG--HG2	1.09	0.97	383
CD1--HD13	1.09	0.97	204
CD--HD2	1.09	0.97	187
CD--HD3	1.09	0.97	187
CA--HA3	1.09	0.97	73
CG--HG3	1.09	0.97	383
CD2--HD21	1.09	0.97	127
CB--HB3	1.09	0.97	862
CD2--HD23	1.09	0.97	127
CG--HG	1.09	0.97	127
CE--HE2	1.09	0.97	111
CG2--HG21	1.09	0.97	204
CG2--HG23	1.09	0.97	204
NZ--HZ2	1.01	0.89	83
CD1--HD11	1.09	0.97	204
CB--HB1	1.09	0.97	87
CE--HE3	1.09	0.97	111

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
OG--HG	0.96	0.84	67
NZ--HZ1	1.01	0.89	83
NZ--HZ3	1.01	0.89	83
CG1--HG13	1.09	0.97	151
OG1--HG1	0.96	0.84	53
CA--HA2	1.09	0.97	73
CG1--HG11	1.09	0.97	74
OH--HH	0.96	0.84	19
CE--HE1	1.09	0.97	28
N--H3	1.01	0.89	2
N--H1	1.01	0.89	2
N--H2	1.01	0.89	2
SG--HG	1.33	1.20	1
SG--HG	1.34	1.20	5
CE1--HE1	1.08	0.93	79
N--H	1.01	0.86	1104
ND2--HD21	1.01	0.86	43
NE2--HE22	1.01	0.86	62
NH1--HH12	1.01	0.86	71
NH2--HH22	1.01	0.86	71
NE2--HE21	1.01	0.86	62
NH2--HH21	1.01	0.86	71
NH1--HH11	1.01	0.86	71
ND2--HD22	1.01	0.86	43

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CE2--HE2	1.08	0.93	50
CD2--HD2	1.08	0.93	79
CZ--HZ	1.08	0.93	31
CH2--HH2	1.08	0.93	4
CD1--HD1	1.08	0.93	54
ND1--HD1	1.01	0.86	28
NE--HE	1.01	0.86	71
CZ3--HZ3	1.08	0.93	4
CE3--HE3	1.08	0.93	4
CZ2--HZ2	1.08	0.93	4
NE1--HE1	1.01	0.86	4
NE2--HE2	1.01	0.86	1

#### Standard geometry: angle outliers

There are 49 angle outliers in this entry. A summary is provided below, and a detailed list of outliers can be found [here](#).

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	118.03	1
OE1-CD-NE2	122.60	117.49	1
OE1-CD-NE2	122.60	117.73	3
OE1-CD-NE2	122.60	117.84	1
OE1-CD-NE2	122.60	117.85	1
OE1-CD-NE2	122.60	117.87	1
CB-CG-CD2	131.20	125.06	1
OE1-CD-NE2	122.60	117.96	1
CB-CG-CD2	131.20	125.17	1

<b>Angle type</b>	<b>Observed angle (°)</b>	<b>Ideal angle (°)</b>	<b>Number of outliers</b>
OE1-CD-NE2	122.60	118.00	2
CB-CG-CD2	131.20	125.23	1
NE-CZ-NH1	121.50	126.07	1
OE1-CD-NE2	122.60	118.04	1
OE1-CD-NE2	122.60	118.11	1
OE1-CD-NE2	122.60	118.17	1
CB-CG-CD2	131.20	125.46	1
OE1-CD-NE2	122.60	118.19	1
OE1-CD-NE2	122.60	118.20	2
OD1-CG-ND2	122.60	118.21	1
CA-CB-CG	112.60	116.97	1
OE1-CD-NE2	122.60	118.23	1
OE1-CD-NE2	122.60	118.24	1
OE1-CD-NE2	122.60	118.25	1
OE1-CD-NE2	122.60	118.28	1
CB-CG-CD2	131.20	125.59	1
OE1-CD-NE2	122.60	118.32	1
OE1-CD-NE2	122.60	118.33	1
OE1-CD-NE2	122.60	118.34	1
OE1-CD-NE2	122.60	118.36	3
CB-CG-CD2	131.20	125.70	1
CB-CG-CD2	131.20	125.71	1
OE1-CD-NE2	122.60	118.38	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.39	1
OD1-CG-ND2	122.60	118.43	1
CB-CG-CD2	131.20	125.79	1
OE1-CD-NE2	122.60	118.45	1
OE1-CD-NE2	122.60	118.52	2
OE1-CD-NE2	122.60	118.53	1
OE1-CD-NE2	122.60	118.55	1
OE1-CD-NE2	122.60	118.56	1
OD1-CG-ND2	122.60	118.58	1
HH11-NH1-HH12	105.76	120.00	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 the models in this entry.

Model ID	Clash score	Number of clashes
1	1.27	23

All 23 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:520:VAL:HG11	A:558:LEU:HD11	0.656
1	B:266:ILE:HD12	B:283:ILE:HG22	0.534
1	A:780:GLU:HB2	A:786:ILE:HD11	0.469
1	A:734:LEU:HD13	A:741:ILE:CD1	0.466
1	B:241:PRO:O	B:244:LYS:HE3	0.461
1	B:114:TYR:CZ	B:143:ALA:HB2	0.459
1	A:112:LEU:HD22	A:120:ALA:CB	0.454



Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:163:LEU:HD13	A:264:VAL:HG13	0.449
1	B:214:ARG:HH22	B:278:ASP:CG	0.447
1	A:436:PHE:HB3	B:303:LEU:HD11	0.446
1	B:189:ARG:NH1	B:277:GLN:HE21	0.443
1	B:11:LEU:HD11	B:177:ARG:NH2	0.437
1	A:780:GLU:CB	A:786:ILE:HD11	0.435
1	A:405:ARG:NH2	A:478:MET:HE1	0.433
1	A:752:ALA:O	A:756:VAL:HG23	0.430
1	A:387:LEU:HG	A:390:LYS:HE2	0.427
1	B:28:LEU:HD13	B:142:MET:HE1	0.426
1	A:174:ALA:HB3	A:226:ILE:CD1	0.416
1	A:95:ALA:HA	A:107:HIS:CD2	0.415
1	A:431:VAL:HG21	B:296:THR:HG23	0.414
1	A:257:PHE:CE1	A:294:ILE:HG21	0.412
1	A:624:PRO:HA	A:627:PHE:CD2	0.407
1	A:734:LEU:HD13	A:741:ILE:HD12	0.401

### 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	1135	1110	20	5

Detailed list of outliers are tabulated below.

### Torsion angles: Protein sidechains

In the following table, sidechain outliers are listed. The Analysed column shows the number of residues for which the sidechain conformation was analysed.

Model ID	Analysed	Favored	Allowed	Outliers
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<b>Model ID</b>	<b>Analyzed</b>	<b>Favored</b>	<b>Allowed</b>	<b>Outliers</b>
1	979	917	38	24

*Detailed list of outliers are tabulated below.*

<b>Model ID</b>	<b>Chain</b>	<b>Residue ID</b>	<b>Residue type</b>
1	A	145	ASN
1	A	147	THR
1	A	154	THR
1	A	171	THR
1	A	261	LEU
1	A	395	ILE
1	A	464	GLN
1	A	586	LEU
1	A	646	THR
1	A	654	LEU
1	A	682	HIS
1	A	720	THR
1	A	731	THR
1	A	781	LEU
1	A	786	ILE
1	A	794	LEU
1	A	805	THR
1	A	806	THR
1	A	809	THR
1	B	98	LEU
1	B	105	THR

Model ID	Chain	Residue ID	Residue type
1	B	107	LEU
1	B	274	LEU
1	B	293	GLN

### Fit of model to data used for modeling ?

#### Crosslinking-MS

Validation for this section is under development.

### Fit of model to data used for validation ?

Validation for this section is under development.

#### *Acknowledgements*

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