

# Integrative Structure Validation Report

September 11, 2024 - 12:59 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	9A7E
PDB-Dev ID	PDBDEV_00000343
Structure Title	Integrative model of CLPC-YPIB 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)*

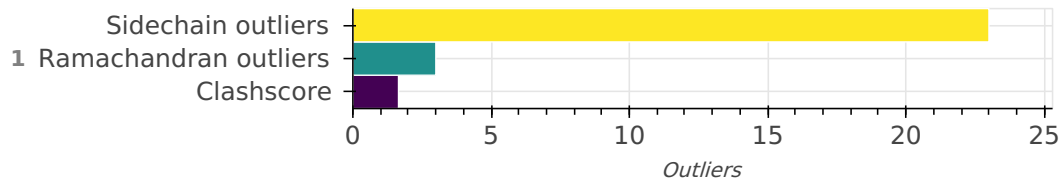
*A user guide is available at [https://pdb-dev.wwpdb.org/validation\\_help.html](https://pdb-dev.wwpdb.org/validation_help.html) with specific help available everywhere you see the  symbol.*

*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	YPIB_BACSU	B	B	179

## 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	-	1-179

## 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 7929 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
CG2--HG23	1.09	0.97	184

<b>Bond type</b>	<b>Observed distance (Å)</b>	<b>Ideal distance (Å)</b>	<b>Number of outliers</b>
CG2--HG21	1.09	0.97	184
CA--HA	1.09	0.97	927
CD1--HD12	1.09	0.97	167
NZ--HZ3	1.01	0.89	71
CB--HB2	1.09	0.97	743
CD2--HD21	1.09	0.97	100
CD--HD2	1.09	0.97	167
CG1--HG12	1.09	0.97	136
NZ--HZ2	1.01	0.89	71
CB--HB1	1.09	0.97	72
CB--HB3	1.09	0.97	743
CG1--HG13	1.09	0.97	136
CA--HA2	1.09	0.97	62
CG--HG3	1.09	0.97	332
CB--HB	1.09	0.97	184
CG1--HG11	1.09	0.97	69
CG--HG	1.09	0.97	100
CG--HG2	1.09	0.97	332
CD--HD3	1.09	0.97	167
CD1--HD13	1.09	0.97	167
CE--HE2	1.09	0.97	92
CE--HE3	1.09	0.97	92
OG--HG	0.96	0.84	58

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CG2--HG22	1.09	0.97	184
CD2--HD22	1.09	0.97	100
CA--HA3	1.09	0.97	62
CD1--HD11	1.09	0.97	167
CD2--HD23	1.09	0.97	100
OH--HH	0.96	0.84	18
NZ--HZ1	1.01	0.89	71
OG1--HG1	0.96	0.84	48
CE--HE1	1.09	0.97	21
N--H3	1.01	0.89	2
N--H2	1.01	0.89	2
N--H1	1.01	0.89	2
SG--HG	1.33	1.20	1
SG--HG	1.34	1.20	3
NH2--HH22	1.01	0.86	68
CD2--HD2	1.08	0.93	73
N--H	1.01	0.86	959
CD1--HD1	1.08	0.93	52
CZ--HZ	1.08	0.93	30
NE2--HE22	1.01	0.86	48
NH2--HH21	1.01	0.86	68
NH1--HH11	1.01	0.86	68
NH1--HH12	1.01	0.86	68
NE2--HE21	1.01	0.86	48

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
ND2--HD22	1.01	0.86	38
CE2--HE2	1.08	0.93	48
CE1--HE1	1.08	0.93	73
NE--HE	1.01	0.86	68
ND2--HD21	1.01	0.86	38
ND1--HD1	1.01	0.86	23
CZ3--HZ3	1.08	0.93	4
CE3--HE3	1.08	0.93	4
CH2--HH2	1.08	0.93	4
NE2--HE2	1.01	0.86	2
CZ2--HZ2	1.08	0.93	4
NE1--HE1	1.01	0.86	4

#### Standard geometry: angle outliers

There are 48 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
OE1-CD-NE2	122.60	116.86	1
CA-CB-CG	112.60	118.13	1
OD1-CG-ND2	122.60	117.08	1
CA-CB-CG	112.60	118.06	1
CB-CG-CD2	131.20	124.28	1
OE1-CD-NE2	122.60	117.37	1
OE1-CD-NE2	122.60	117.55	1
NH1-CZ-NH2	119.30	112.75	1
OE1-CD-NE2	122.60	117.72	1

<b>Angle type</b>	<b>Observed angle (°)</b>	<b>Ideal angle (°)</b>	<b>Number of outliers</b>
OE1-CD-NE2	122.60	117.75	1
OE1-CD-NE2	122.60	117.81	1
OE1-CD-NE2	122.60	117.84	2
OE1-CD-NE2	122.60	117.89	1
CB-CG-CD2	131.20	125.10	1
OE1-CD-NE2	122.60	117.93	1
OE1-CD-NE2	122.60	118.02	1
OG1-CB-CG2	109.30	100.15	1
OE1-CD-NE2	122.60	118.07	1
CB-CG-CD2	131.20	125.36	1
OE1-CD-NE2	122.60	118.11	1
OE1-CD-NE2	122.60	118.15	1
OE1-CD-NE2	122.60	118.19	1
OE1-CD-NE2	122.60	118.21	1
OE1-CD-NE2	122.60	118.23	1
OE1-CD-NE2	122.60	118.24	1
OE1-CD-NE2	122.60	118.26	1
OE1-CD-NE2	122.60	118.28	1
OE1-CD-NE2	122.60	118.30	1
OD1-CG-ND2	122.60	118.31	1
OD1-CG-ND2	122.60	118.34	1
OE1-CD-NE2	122.60	118.36	1
CA-CB-CG	113.80	109.58	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.42	2
OE1-CD-NE2	122.60	118.44	1
CA-CB-CG	113.80	117.94	1
OE1-CD-NE2	122.60	118.49	1
OE1-CD-NE2	122.60	118.50	2
OE1-CD-NE2	122.60	118.51	2
OE1-CD-NE2	122.60	118.52	1
CB-CG-CD2	131.20	125.90	1
OE1-CD-NE2	122.60	118.53	1
OE1-CD-NE2	122.60	118.59	1
CB-CG-ND1	122.70	128.71	1
HH11-NH1-HH12	101.95	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	1.65	26

All 26 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:92:MET:HE1	B:135:LEU:HD23	0.962
1	A:520:VAL:HG11	A:558:LEU:HD11	0.690
1	A:3:PHE:CZ	B:142:HIS:CD2	0.660
1	A:752:ALA:O	A:756:VAL:HG23	0.624
1	A:719:LEU:HD13	A:756:VAL:HG22	0.595



Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:147:THR:HG22	A:149:SER:O	0.560
1	A:544:LEU:HD23	A:658:SER:HB3	0.560
1	B:24:LYS:HA	B:63:HIS:CE1	0.553
1	A:23:ARG:NH2	A:61:GLN:HE21	0.540
1	A:257:PHE:CE1	A:294:ILE:HG21	0.534
1	A:741:ILE:CD1	A:777:LEU:HD11	0.518
1	A:88:ILE:HG13	B:140:LEU:HD21	0.511
1	A:520:VAL:HG11	A:558:LEU:CD1	0.498
1	B:58:ILE:HD11	B:89:ILE:HD11	0.488
1	A:53:LEU:HD11	A:134:ALA:HA	0.474
1	A:175:LYS:HE3	A:226:ILE:HD12	0.455
1	A:717:LYS:HE2	A:718:HIS:NE2	0.448
1	A:702:ILE:HG23	A:708:ILE:HD11	0.445
1	A:741:ILE:HD12	A:777:LEU:HD11	0.444
1	A:542:ILE:HG13	A:705:ILE:HD13	0.433
1	B:24:LYS:HE3	B:62:THR:O	0.431
1	B:103:PHE:CE2	B:106:ALA:HA	0.426
1	A:635:GLU:CD	A:704:ARG:NH1	0.413
1	A:28:ASN:OD1	A:79:HIS:CE1	0.412
1	A:80:TYR:CE2	B:140:LEU:HD22	0.408
1	A:387:LEU:HG	A:390:LYS:HE2	0.403

### 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	Analyzed	Favored	Allowed	Outliers
1	985	961	21	3

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	Analyzed	Favored	Allowed	Outliers
1	855	804	28	23

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	68	ILE
1	A	79	HIS
1	A	147	THR
1	A	149	SER
1	A	171	THR
1	A	261	LEU
1	A	408	THR
1	A	584	SER
1	A	586	LEU
1	A	587	VAL
1	A	679	THR
1	A	682	HIS
1	A	720	THR
1	A	725	LEU
1	A	781	LEU
1	A	794	LEU

Model ID	Chain	Residue ID	Residue type
1	A	805	THR
1	A	806	THR
1	A	809	THR
1	B	3	THR
1	B	126	LEU
1	B	135	LEU
1	B	178	LEU

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

#### Crosslinking-MS

Validation for this section is under development.

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Validation for this section is under development.

#### *Acknowledgements*

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