

# Integrative Structure Validation Report

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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	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

*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)*

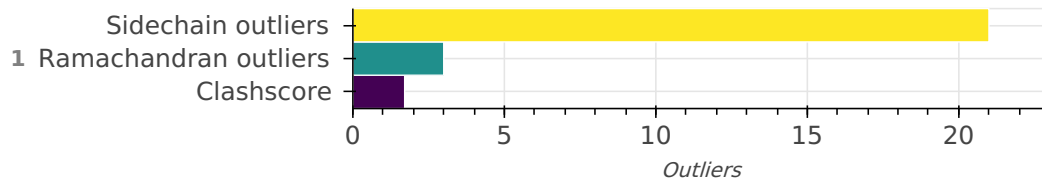
*A user guide is available at [https://pdb-dev.wwpdb.org/validation\\_help.html](https://pdb-dev.wwpdb.org/validation_help.html) with specific help available everywhere you see the  symbol.*

*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	F16PC_BACSU	A	A	641
1	2	2	GLPD_BACSU	B	B	555

## 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	-	1-641
B	-	1-555

### 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 9623 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
CB--HB3	1.09	0.97	900

<b>Bond type</b>	<b>Observed distance (Å)</b>	<b>Ideal distance (Å)</b>	<b>Number of outliers</b>
CD1--HD11	1.09	0.97	188
CG2--HG23	1.09	0.97	216
CD1--HD12	1.09	0.97	188
CA--HA	1.09	0.97	1116
NZ--HZ1	1.01	0.89	106
CB--HB	1.09	0.97	216
CG--HG2	1.09	0.97	383
CG--HG	1.09	0.97	109
CG2--HG22	1.09	0.97	216
CD1--HD13	1.09	0.97	188
CD--HD2	1.09	0.97	204
CE--HE3	1.09	0.97	140
CB--HB2	1.09	0.97	900
CD--HD3	1.09	0.97	204
NZ--HZ2	1.01	0.89	106
CG2--HG21	1.09	0.97	216
CD2--HD21	1.09	0.97	109
CG--HG3	1.09	0.97	383
CG1--HG11	1.09	0.97	72
CD2--HD22	1.09	0.97	109
CA--HA3	1.09	0.97	80
CD2--HD23	1.09	0.97	109
CA--HA2	1.09	0.97	80

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
OH--HH	0.96	0.84	58
CG1--HG13	1.09	0.97	151
OG1--HG1	0.96	0.84	65
CB--HB1	1.09	0.97	76
NZ--HZ3	1.01	0.89	106
CE--HE2	1.09	0.97	140
OG--HG	0.96	0.84	54
CE--HE1	1.09	0.97	34
CG1--HG12	1.09	0.97	151
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	3
SG--HG	1.34	1.20	5
N--H	1.01	0.86	1156
NH1--HH11	1.01	0.86	60
ND2--HD22	1.01	0.86	48
NH2--HH21	1.01	0.86	60
NH2--HH22	1.01	0.86	60
NH1--HH12	1.01	0.86	60
ND1--HD1	1.01	0.86	25
CZ3--HZ3	1.08	0.93	11
CD2--HD2	1.08	0.93	136
CZ--HZ	1.08	0.93	43

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NE2--HE21	1.01	0.86	33
CE1--HE1	1.08	0.93	136
NE--HE	1.01	0.86	60
ND2--HD21	1.01	0.86	48
CE2--HE2	1.08	0.93	101
CE3--HE3	1.08	0.93	11
CZ2--HZ2	1.08	0.93	11
NE2--HE22	1.01	0.86	33
NE2--HE2	1.01	0.86	10
CD1--HD1	1.08	0.93	112
NE1--HE1	1.01	0.86	11
CH2--HH2	1.08	0.93	11

### Standard geometry: angle outliers?

There are 56 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
O-C-OXT	118.00	168.30	1
CA-C-OXT	121.00	81.98	1
CA-C-O	121.00	86.36	1
C-N-CA	121.70	132.24	1
CA-CB-CG	112.60	118.15	1
OE1-CD-NE2	122.60	117.06	1
C-CA-CB	111.60	122.06	1
OE1-CD-NE2	122.60	117.43	1
CA-CB-CG	112.60	117.64	1

<b>Angle type</b>	<b>Observed angle (°)</b>	<b>Ideal angle (°)</b>	<b>Number of outliers</b>
CA-CB-CG	112.60	117.54	1
OE1-CD-NE2	122.60	117.68	1
NH1-CZ-NH2	119.30	112.91	1
OE1-CD-NE2	122.60	117.69	1
CA-CB-CG	112.60	117.44	1
OE1-CD-NE2	122.60	117.81	1
OE1-CD-NE2	122.60	117.83	1
CB-CG-CD2	131.20	125.02	1
CB-CG-CD2	131.20	125.03	1
CA-CB-CG	113.90	105.38	1
NE-CZ-NH2	119.20	123.43	1
NE-CZ-NH2	119.20	123.40	1
OE1-CD-NE2	122.60	117.97	2
OE1-CD-NE2	122.60	118.05	1
C-N-CA	121.70	129.87	1
OE1-CD-NE2	122.60	118.09	1
CB-CG-CD2	131.20	125.35	1
OE1-CD-NE2	122.60	118.12	1
C-CA-CB	110.10	118.60	1
CB-CG-CD2	131.20	125.47	1
CB-CG-CD	111.30	101.25	1
C-N-CA	121.70	129.51	1
CB-CG-CD2	131.20	125.57	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.27	1
CD-NE-CZ	124.40	130.46	1
CA-CB-CG	112.60	116.92	1
OE1-CD-NE2	122.60	118.34	1
OE1-CD-NE2	122.60	118.36	1
CB-CG-CD2	131.20	125.69	1
NE-CZ-NH2	119.20	123.00	1
CA-CB-CG	112.60	116.79	1
NH1-CZ-NH2	119.30	113.85	1
OD1-CG-ND2	122.60	118.42	1
CA-CB-CG	113.80	117.98	1
OE1-CD-NE2	122.60	118.49	2
OD1-CG-ND2	122.60	118.52	1
NH1-CZ-NH2	119.30	114.03	1
OE1-CD-NE2	122.60	118.55	1
CA-CB-CG2	110.50	117.34	1
CB-CG-CD2	131.20	125.98	1
CA-CB-CG	112.60	108.59	1
OD1-CG-ND2	122.60	118.59	1
CB-CG-CD2	131.20	126.00	1
HZ2-NZ-HZ3	96.91	109.00	1
HZ1-NZ-HZ2	96.48	109.00	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.*

<b>Model ID</b>	<b>Clash score</b>	<b>Number of clashes</b>
1	1.71	33

*All 33 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.*

<b>Model ID</b>	<b>Atom-1</b>	<b>Atom-2</b>	<b>Clash overlap (Å)</b>
1	A:5:TYR:CE1	B:127:VAL:HG23	0.779
1	A:5:TYR:CG	B:123:ILE:HG23	0.769
1	A:328:ARG:NH2	A:330:LEU:HD11	0.691
1	A:224:GLY:HA2	A:411:HIS:CD2	0.572
1	B:492:THR:HG23	B:497:ASP:HB2	0.548
1	A:5:TYR:CD1	B:123:ILE:HG23	0.537
1	A:500:PRO:HA	A:503:TYR:CE1	0.521
1	B:192:VAL:HA	B:491:MET:HE1	0.503
1	B:94:TYR:CZ	B:421:SER:HB2	0.498
1	B:227:LYS:HZ1	B:398:GLU:CD	0.491
1	A:505:ARG:HB2	A:549:MET:HE3	0.488
1	A:8:LEU:HD13	B:127:VAL:HG11	0.483
1	A:8:LEU:HD22	B:131:LEU:HD11	0.483
1	B:90:ARG:HH21	B:134:VAL:HG22	0.474
1	A:9:LEU:HB3	A:634:LEU:HD22	0.470
1	B:18:MET:HE2	B:49:ALA:HB1	0.462
1	A:5:TYR:CZ	B:123:ILE:C	0.459
1	A:8:LEU:HD22	B:127:VAL:HG11	0.457
1	A:5:TYR:CZ	B:127:VAL:HB	0.450
1	B:105:TRP:HB3	B:165:TYR:CZ	0.440

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:1:MET:SD	B:120:THR:HB	0.437
1	B:68:VAL:CG1	B:378:THR:HG23	0.435
1	A:221:ILE:O	A:398:GLY:HA2	0.432
1	A:5:TYR:CZ	B:123:ILE:O	0.429
1	B:280:ARG:HH22	B:296:THR:C	0.426
1	A:5:TYR:CD2	B:123:ILE:CG2	0.422
1	B:401:LYS:HE3	B:403:PHE:CE1	0.420
1	A:374:ILE:HA	A:374:ILE:HD12	0.407
1	A:5:TYR:CG	B:123:ILE:CG2	0.406
1	B:345:LEU:HB3	B:356:ILE:CG2	0.406
1	A:87:TYR:CD1	A:589:LYS:HE3	0.404
1	A:5:TYR:CD1	B:127:VAL:HG23	0.404
1	B:273:TYR:CE2	B:281:MET:HB3	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	Analysed	Favored	Allowed	Outliers
1	1192	1156	33	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	Analysed	Favored	Allowed	Outliers
1	1040	990	29	21

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
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Model ID	Chain	Residue ID	Residue type
1	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	B	522	ASP

Fit of model to data used for modeling 

### Crosslinking-MS

Validation for this section is under development.

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

Validation for this section is under development.

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#### *Acknowledgements*

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