

# 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	9A5D
PDB-Dev ID	PDBDEV_00000270
Structure Title	Integrative model of WALK-YYCH 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)*

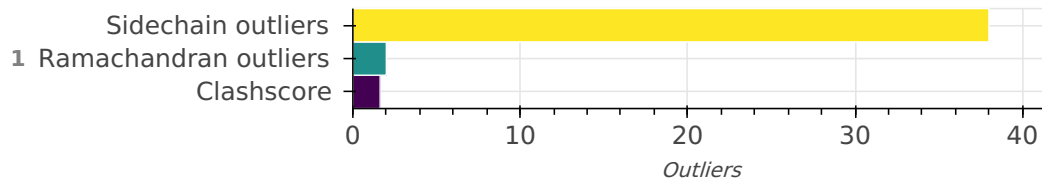
*A user guide is available at [https://pdb-dev.wwpdb.org/validation\\_help.html](https://pdb-dev.wwpdb.org/validation_help.html) with specific help available everywhere you see the  symbol.*

*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	WALK_BACSU	A	A	611
1	2	2	YYCH_BACSU	B	B	455

## 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	-	1-611
B	-	1-455

## 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 8591 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	230

<b>Bond type</b>	<b>Observed distance (Å)</b>	<b>Ideal distance (Å)</b>	<b>Number of outliers</b>
CD1--HD13	1.09	0.97	183
CA--HA	1.09	0.97	1016
CB--HB2	1.09	0.97	786
NZ--HZ2	1.01	0.89	77
CD1--HD11	1.09	0.97	183
CG1--HG12	1.09	0.97	159
CG2--HG21	1.09	0.97	230
CB--HB3	1.09	0.97	786
CD1--HD12	1.09	0.97	183
CG--HG3	1.09	0.97	313
CB--HB	1.09	0.97	230
CD2--HD22	1.09	0.97	96
CE--HE2	1.09	0.97	104
CG--HG	1.09	0.97	96
CD--HD3	1.09	0.97	152
CB--HB1	1.09	0.97	49
CE--HE3	1.09	0.97	104
CA--HA2	1.09	0.97	50
CG1--HG13	1.09	0.97	159
CD2--HD21	1.09	0.97	96
OG1--HG1	0.96	0.84	71
CG2--HG22	1.09	0.97	230
CG--HG2	1.09	0.97	313

<b>Bond type</b>	<b>Observed distance (Å)</b>	<b>Ideal distance (Å)</b>	<b>Number of outliers</b>
CD2--HD23	1.09	0.97	96
CA--HA3	1.09	0.97	50
CG1--HG11	1.09	0.97	72
NZ--HZ1	1.01	0.89	77
OH--HH	0.96	0.84	40
CD--HD2	1.09	0.97	152
CE--HE1	1.09	0.97	27
NZ--HZ3	1.01	0.89	77
OG--HG	0.96	0.84	83
N--H3	1.01	0.89	2
N--H1	1.01	0.89	2
N--H2	1.01	0.89	2
N--H	1.01	0.86	1036
CE2--HE2	1.08	0.93	90
ND2--HD22	1.01	0.86	54
NE--HE	1.01	0.86	47
CD1--HD1	1.08	0.93	103
CD2--HD2	1.08	0.93	104
CZ2--HZ2	1.08	0.93	13
NH1--HH12	1.01	0.86	47
CE3--HE3	1.08	0.93	13
CE1--HE1	1.08	0.93	104
NE2--HE21	1.01	0.86	53
NE2--HE22	1.01	0.86	53

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NH2--HH22	1.01	0.86	47
CZ--HZ	1.08	0.93	50
NH1--HH11	1.01	0.86	47
NH2--HH21	1.01	0.86	47
NE1--HE1	1.01	0.86	13
ND2--HD21	1.01	0.86	54
CH2--HH2	1.08	0.93	13
CZ3--HZ3	1.08	0.93	13
ND1--HD1	1.01	0.86	13
NE2--HE2	1.01	0.86	1

#### Standard geometry: angle outliers?

There are 57 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	118.90	1
CA-CB-CG	112.60	118.57	1
OE1-CD-NE2	122.60	117.10	1
CA-CB-CG	112.60	117.96	1
OE1-CD-NE2	122.60	117.44	1
CB-CG-CD2	131.20	124.59	1
OE1-CD-NE2	122.60	117.54	1
OE1-CD-NE2	122.60	117.64	1
OE1-CD-NE2	122.60	117.65	1
CA-CB-CG	113.80	118.72	1
CA-CB-CG	112.60	117.46	1

<b>Angle type</b>	<b>Observed angle (°)</b>	<b>Ideal angle (°)</b>	<b>Number of outliers</b>
OE1-CD-NE2	122.60	117.74	1
OE1-CD-NE2	122.60	117.79	1
OE1-CD-NE2	122.60	117.82	1
OE1-CD-NE2	122.60	117.83	1
OE1-CD-NE2	122.60	117.86	1
CG-CD2-CE3	133.90	129.20	1
NE-CZ-NH2	119.20	123.40	1
OE1-CD-NE2	122.60	117.96	1
OE1-CD-NE2	122.60	118.03	1
CB-CG-CD2	131.20	125.27	1
OD1-CG-ND2	122.60	118.05	1
OD1-CG-ND2	122.60	118.07	1
OE1-CD-NE2	122.60	118.08	1
OE1-CD-NE2	122.60	118.16	2
OE1-CD-NE2	122.60	118.18	3
OE1-CD-NE2	122.60	118.19	1
CB-CG-CD2	131.20	125.48	1
CA-CB-CG	112.60	116.98	1
OE1-CD-NE2	122.60	118.25	1
CA-CB-CG	112.60	116.95	1
CA-CB-CG	112.60	116.91	1
CB-CG-CD2	131.20	125.61	1
OE1-CD-NE2	122.60	118.31	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	116.89	1
C-CA-CB	110.10	118.24	1
CA-CB-CG	113.80	118.07	1
OE1-CD-NE2	122.60	118.34	1
OE1-CD-NE2	122.60	118.35	1
CB-CG-CD2	131.20	125.69	1
OE1-CD-NE2	122.60	118.40	1
CA-CB-CG	112.60	116.79	1
OE1-CD-NE2	122.60	118.42	1
OE1-CD-NE2	122.60	118.46	1
NH1-CZ-NH2	119.30	113.98	1
OE1-CD-NE2	122.60	118.52	1
OE1-CD-NE2	122.60	118.54	1
CB-CG-CD2	131.20	125.92	1
NE-CZ-NH1	121.50	125.56	1
OE1-CD-NE2	122.60	118.56	1
OE1-CD-NE2	122.60	118.57	1
OE1-CD-NE2	122.60	118.58	2
OE1-CD-NE2	122.60	118.60	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	1.63	28



All 28 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:91:ARG:HH11	A:144:ILE:HD11	0.666
1	B:231:VAL:HG23	B:375:ILE:HD11	0.662
1	A:285:ILE:HG21	A:288:LEU:HD11	0.620
1	A:390:THR:HG21	A:559:ARG:HH22	0.619
1	B:89:LEU:HD11	B:157:ILE:HD11	0.617
1	A:98:LYS:HE2	A:161:VAL:HA	0.579
1	A:390:THR:HG21	A:559:ARG:NH2	0.571
1	A:113:VAL:HG13	B:43:VAL:HG11	0.562
1	B:106:LYS:HA	B:176:GLN:HE22	0.558
1	A:185:ALA:HA	B:26:TRP:CZ3	0.524
1	A:16:LEU:HD22	B:11:LEU:HD23	0.512
1	A:295:LEU:HA	A:336:ARG:HH22	0.492
1	A:184:LEU:C	B:26:TRP:HZ3	0.481
1	B:82:TYR:C	B:82:TYR:CD1	0.480
1	A:56:LEU:CD2	A:93:ILE:HD11	0.478
1	A:586:SER:HB2	A:592:THR:HG23	0.458
1	B:157:ILE:HG21	B:192:MET:HE3	0.458
1	B:113:PHE:CD2	B:156:LEU:HD11	0.446
1	B:113:PHE:CE2	B:156:LEU:HD11	0.441
1	A:184:LEU:C	B:26:TRP:CZ3	0.439
1	B:278:GLN:CD	B:364:LYS:HE3	0.433
1	B:22:THR:O	B:26:TRP:CD1	0.422
1	A:66:SER:C	A:68:ASN:H	0.420

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:61:ARG:NH2	B:82:TYR:CE1	0.418
1	A:185:ALA:CA	B:26:TRP:CZ3	0.413
1	A:572:LYS:HA	A:582:ILE:HG21	0.407
1	A:185:ALA:N	B:26:TRP:CZ3	0.405
1	A:188:THR:HG1	B:26:TRP:HH2	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	1062	1030	30	2

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	967	893	36	38

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	71	THR
1	A	85	THR
1	A	99	SER
1	A	134	LEU
1	A	184	LEU
1	A	194	LEU
1	A	202	LEU
1	A	220	LEU

<b>Model ID</b>	<b>Chain</b>	<b>Residue ID</b>	<b>Residue type</b>
1	A	247	LEU
1	A	251	LEU
1	A	258	THR
1	A	299	SER
1	A	302	THR
1	A	340	LEU
1	A	392	LEU
1	A	425	GLU
1	A	437	LEU
1	A	527	LEU
1	A	602	GLU
1	A	610	GLU
1	B	1	MET
1	B	11	LEU
1	B	14	LEU
1	B	39	THR
1	B	89	LEU
1	B	134	ASP
1	B	177	LEU
1	B	209	SER
1	B	283	GLN
1	B	289	SER
1	B	341	THR
1	B	372	THR

Model ID	Chain	Residue ID	Residue type
1	B	375	ILE
1	B	377	THR
1	B	381	GLU
1	B	396	THR
1	B	404	ASP
1	B	455	GLU

### 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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