

# Integrative Structure Validation Report

September 11, 2024 - 12:16 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	9A6P
PDB-Dev ID	PDBDEV_00000318
Structure Title	Integrative model of RPOB-RPOC 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)*

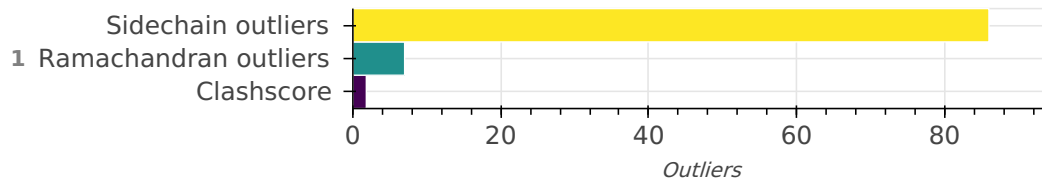
*A user guide is available at [https://pdb-dev.wwpdb.org/validation\\_help.html](https://pdb-dev.wwpdb.org/validation_help.html) with specific help available everywhere you see the  symbol.*

*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	RPOB_BACSU	A	A	1193
1	2	2	RPOC_BACSU	B	B	1199

## 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	-	1-1193
B	-	1-1199

## 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 19002 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	482

<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	482
CB--HB2	1.09	0.97	1718
CA--HA	1.09	0.97	2200
CE--HE1	1.09	0.97	65
CG--HG2	1.09	0.97	783
CB--HB3	1.09	0.97	1718
CE--HE2	1.09	0.97	215
CD--HD3	1.09	0.97	426
OG--HG	0.96	0.84	113
CD1--HD13	1.09	0.97	371
OG1--HG1	0.96	0.84	125
CD1--HD11	1.09	0.97	371
CG1--HG13	1.09	0.97	357
CG2--HG22	1.09	0.97	482
CD1--HD12	1.09	0.97	371
CG1--HG12	1.09	0.97	357
CD--HD2	1.09	0.97	426
CG--HG3	1.09	0.97	783
CA--HA2	1.09	0.97	192
CE--HE3	1.09	0.97	215
CB--HB1	1.09	0.97	147
CB--HB	1.09	0.97	482
NZ--HZ1	1.01	0.89	150

<b>Bond type</b>	<b>Observed distance (Å)</b>	<b>Ideal distance (Å)</b>	<b>Number of outliers</b>
CG--HG	1.09	0.97	218
CD2--HD22	1.09	0.97	218
OH--HH	0.96	0.84	71
CG1--HG11	1.09	0.97	204
NZ--HZ2	1.01	0.89	150
NZ--HZ3	1.01	0.89	150
CD2--HD23	1.09	0.97	218
CA--HA3	1.09	0.97	192
CD2--HD21	1.09	0.97	218
N--H1	1.01	0.89	2
N--H2	1.01	0.89	2
N--H3	1.01	0.89	2
SG--HG	1.33	1.20	1
SG--HG	1.34	1.20	14
N--H	1.01	0.86	2281
ND2--HD22	1.01	0.86	98
CE1--HE1	1.08	0.93	180
NH2--HH21	1.01	0.86	167
NH2--HH22	1.01	0.86	167
NH1--HH12	1.01	0.86	167
NH1--HH11	1.01	0.86	167
NE--HE	1.01	0.86	167
CE2--HE2	1.08	0.93	142
CZ--HZ	1.08	0.93	71

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CD1--HD1	1.08	0.93	155
ND1--HD1	1.01	0.86	32
CZ2--HZ2	1.08	0.93	13
CH2--HH2	1.08	0.93	13
ND2--HD21	1.01	0.86	98
NE2--HE22	1.01	0.86	84
NE2--HE21	1.01	0.86	84
CD2--HD2	1.08	0.93	180
CZ3--HZ3	1.08	0.93	13
NE1--HE1	1.01	0.86	13
CE3--HE3	1.08	0.93	13
NE2--HE2	1.01	0.86	6

### Standard geometry: angle outliers

There are 89 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
C-N-CA-CB-CG	112.60	120.50	1
C-N-CA-CB-CG	112.60	119.50	1
O-C-CA-CB-CG	112.60	119.44	1
C-N-CA-CB-CG	112.60	118.84	1
C-N-NE-CZ-NH2	119.20	124.70	1
CA-CB-CG	112.60	118.71	1
CA-C-C-N-NE-CZ-NH2	119.20	124.32	1
CA-CB-CG	112.60	118.23	1
OE1-CD-NE2	122.60	117.27	1

<b>Angle type</b>	<b>Observed angle (°)</b>	<b>Ideal angle (°)</b>	<b>Number of outliers</b>
CB-CG-CA-CB-CG	112.60	117.85	1
NE-CZ-NH1	121.50	126.68	1
OE1-CD-NE2	122.60	117.47	1
OD1-CG-ND2	122.60	117.48	1
CA-CB-CG	112.60	117.71	1
CB-CG-CD2	131.20	124.66	1
OD1-CG-ND2	122.60	117.64	1
CA-CB-CG	112.60	117.52	1
OE1-CD-NE2	122.60	117.70	1
CA-CB-CA-CB-CG	112.60	117.45	1
CA-CB-CG	112.60	117.45	1
CA-CB-CB-CG-CD2	131.20	124.94	1
NH1-CZ-NH2	119.30	113.05	1
OE1-CD-OE1-CD-NE2	122.60	117.82	1
CB-CG-CD2	131.20	124.98	1
CD-NE-OE1-CD-NE2	122.60	117.89	1
OE1-CD-NE2	122.60	117.93	1
OE1-CD-NE2	122.60	117.95	1
OE1-CD-NE2	122.60	117.98	1
CA-CB-CG	112.60	117.19	1
OD1-CG-ND2	122.60	118.02	1
OE1-CD-NE2	122.60	118.02	2
OE1-CD-NE2	122.60	118.03	1

<b>Angle type</b>	<b>Observed angle (°)</b>	<b>Ideal angle (°)</b>	<b>Number of outliers</b>
OE1-CD-NE2	122.60	118.05	1
CA-CB-CG	112.60	117.14	1
OE1-CD-NE2	122.60	118.08	1
OE1-CD-CB-CG-CD2	131.20	125.34	1
OE1-CD-NE2	122.60	118.13	2
CB-CG-CD2	131.20	125.40	1
OE1-CD-NE2	122.60	118.14	1
OE1-CD-NE2	122.60	118.16	1
OE1-CD-NE2	122.60	118.18	1
NH1-CZ-NH2	119.30	113.56	1
OD1-CG-ND2	122.60	118.20	1
CA-CB-OE1-CD-NE2	122.60	118.21	1
OE1-CD-NE2	122.60	118.21	1
OE1-CD-NE2	122.60	118.22	2
C-N-OE1-CD-NE2	122.60	118.23	1
OE1-CD-CA-CB-CG	112.60	116.96	1
OE1-CD-NE2	122.60	118.25	1
CA-CB-CG	112.60	116.94	1
OD1-CG-ND2	122.60	118.28	1
CB-CG-CD2	131.20	125.58	1
OE1-CD-NE2	122.60	118.29	3
OE1-CD-OE1-CD-NE2	122.60	118.34	1
OD1-CG-ND2	122.60	118.36	1
OE1-CD-NE2	122.60	118.37	2



Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-NE-CZ-NH2	119.20	123.00	1
N-CA-CA-CB-CG	112.60	116.80	1
CB-CG-CD2	131.20	125.76	1
CB-CG-CD2	131.20	125.78	1
N-CA-CA-CB-CG	112.60	116.75	1
NE-CZ-NH2	119.20	122.90	1
OE1-CD-N-CA-OD1-CG-ND2	122.60	118.52	1
NH1-CZ-NH2	119.30	114.00	1
OE1-CD-NE2	122.60	118.52	1
OE1-CD-CB-CG-CD2	131.20	125.90	1
NE-CZ-OE1-CD-NE2	122.60	118.54	1
OE1-CD-NE2	122.60	118.55	1
OD1-CG-ND2	122.60	118.55	1
CD-NE-CZ	124.40	130.07	1
OE1-CD-NE2	122.60	118.57	1
OE1-CD-NE2	122.60	118.58	2
OE1-CD-OD1-CG-ND2	122.60	118.60	1
C-N-H	112.29	124.30	1
CD-NE2-HE21	107.93	120.00	1
C-N-H	111.83	124.30	1
CZ-NH1-HH11	107.34	120.00	1
C-N-H	111.20	124.30	1
HH21-NH2-HH22	104.90	120.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CZ-NH1-HH12	104.58	120.00	1
C-N-H	108.22	124.30	1
HH11-NH1-HH12	98.26	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	1.82	69

All 69 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	B:752:ALA:HB3	B:942:GLY:HA3	0.771
1	A:510:HIS:CD2	A:514:MET:HE2	0.712
1	A:800:ARG:NH1	B:248:ARG:HH21	0.630
1	B:726:ILE:HG22	B:741:PHE:CE2	0.573
1	A:764:MET:HE1	A:869:ALA:HB2	0.540
1	B:808:ALA:HB3	B:170:MET:HE3	0.540
1	A:854:LEU:HD11	B:269:LYS:HG3	0.503
1	B:134:TYR:CD2	B:450:PHE:CE2	0.492
1	B:214:GLU:OE2	A:781:LEU:HD12	0.486
1	B:98:ALA:HB2	B:749:GLY:HA2	0.482
1	B:978:VAL:CG2	B:784:ARG:HH21	0.479
1	B:346:VAL:HG22	A:48:MET:HE2	0.471
1	A:791:HIS:CE1	B:615:PHE:CD2	0.466
1	A:777:MET:HG3	A:486:LEU:HD22	0.465

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:747:MET:HE2	A:965:ARG:HD2	0.465
1	A:516:PRO:C	B:723:LEU:HD22	0.464
1	B:915:VAL:HG12	A:510:HIS:CE1	0.463
1	A:48:MET:HA	B:887:ARG:HH21	0.462
1	B:503:THR:HG21	B:383:ILE:HG23	0.461
1	B:808:ALA:CB	A:578:ASN:H	0.452
1	A:409:LEU:HD21	A:345:GLN:CD	0.449
1	A:636:ARG:CZ	A:905:VAL:HG22	0.448
1	B:506:ARG:HH21	B:741:PHE:CE2	0.448
1	A:507:HIS:H	B:663:ILE:HD11	0.446
1	A:917:ARG:HH11	B:473:MET:HE3	0.445
1	B:820:THR:HG22	B:619:ILE:CD1	0.445
1	B:371:MET:HE2	A:409:LEU:HD22	0.438
1	B:5:ASN:HA	A:508:TYR:CE1	0.426
1	A:576:GLN:HG3	A:982:TYR:CZ	0.426
1	A:281:ILE:HD11	B:614:PRO:HG2	0.417
1	A:800:ARG:HE	A:924:LYS:HE2	0.416
1	B:726:ILE:CG2	A:48:MET:HA	0.413
1	A:968:ILE:HD11	B:762:PRO:HG3	0.413
1	B:469:ALA:HA	B:961:GLU:CD	0.413
1	B:581:PRO:HB2	B:729:MET:HE1	0.409
1	A:136:SER:HB3	B:619:ILE:HD12	0.404
1	B:978:VAL:HG22	A:712:LEU:HD23	0.403

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:643:MET:HE2	B:932:THR:HG22	0.403
1	A:947:LEU:CD2	A:223:LYS:HD3	0.402
1	B:895:PRO:HA	A:954:ASP:HB3	0.402
1	A:766:TRP:CZ2	A:924:LYS:HE2	0.402

### 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	2388	2319	62	7

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	2053	1848	119	86

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	2	THR
1	A	48	MET
1	A	52	ILE
1	A	59	THR
1	A	86	VAL
1	A	133	VAL
1	A	139	VAL
1	A	161	THR
1	A	174	THR

Model ID	Chain	Residue ID	Residue type
1	A	192	VAL
1	A	214	ASN
1	A	229	SER
1	A	255	LEU
1	A	319	LEU
1	A	353	THR
1	A	361	ILE
1	A	391	LEU
1	A	409	LEU
1	A	440	THR
1	A	576	GLN
1	A	578	ASN
1	A	603	VAL
1	A	613	VAL
1	A	645	ARG
1	A	737	VAL
1	A	753	LEU
1	A	838	ASP
1	A	846	VAL
1	A	852	THR
1	A	920	SER
1	A	942	GLU
1	A	953	ILE
1	A	968	ILE

<b>Model ID</b>	<b>Chain</b>	<b>Residue ID</b>	<b>Residue type</b>
1	A	1038	ILE
1	A	1169	LEU
1	A	1180	THR
1	B	2	LEU
1	B	36	TYR
1	B	55	THR
1	B	76	ASP
1	B	102	SER
1	B	107	PHE
1	B	125	LEU
1	B	135	VAL
1	B	159	LEU
1	B	190	MET
1	B	195	LEU
1	B	204	THR
1	B	256	ASP
1	B	287	MET
1	B	329	GLN
1	B	349	HIS
1	B	357	LEU
1	B	381	HIS
1	B	419	HIS
1	B	431	VAL

<b>Model ID</b>	<b>Chain</b>	<b>Residue ID</b>	<b>Residue type</b>
1	B	444	THR
1	B	451	ASP
1	B	488	VAL
1	B	489	VAL
1	B	490	THR
1	B	504	LEU
1	B	524	LEU
1	B	551	GLU
1	B	580	GLU
1	B	646	LEU
1	B	666	LEU
1	B	716	LEU
1	B	737	ASN
1	B	761	LEU
1	B	774	LEU
1	B	810	ASP
1	B	813	ILE
1	B	816	THR
1	B	938	THR
1	B	941	THR
1	B	974	ILE
1	B	977	THR
1	B	999	THR

Model ID	Chain	Residue ID	Residue type
1	B	1003	THR
1	B	1018	ILE
1	B	1041	THR
1	B	1042	THR
1	B	1143	THR
1	B	1171	VAL
1	B	1177	MET

### 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*

*Development of integrative model validation metrics, implementation of a model validation pipeline, and creation of a validation report for integrative structures, are funded by NSF ABI awards (DBI-1756248, DBI-2112966, DBI-2112967, DBI-2112968, and DBI-1756250). The [PDB-Dev team](#) and members of [Sali lab](#) contributed model validation metrics and software packages.*

*Implementation of validation methods for SAS data and SAS-based models are funded by [RCSB PDB](#) (grant number DBI-1832184). Dr. Stephen Burley, Dr. John Westbrook, and Dr. Jasmine Young from [RCSB PDB](#), Dr. Jill Trehwella, Dr. Dina Schneidman, and members of the [SASBDB](#) repository are acknowledged for their advice and support in implementing SAS validation methods.*

*Members of the [wwPDB Integrative/Hybrid Methods Task Force](#) provided recommendations and community support for the project.*