

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	9A6H
PDB-Dev ID	PDBDEV_00000310
Structure Title	Integrative model of MRPA-MRPD 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

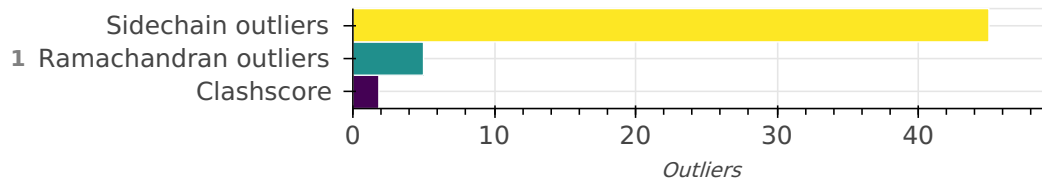
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the  symbol.

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	MRPA_BACSU	A	A	801
1	2	2	MRPD_BACSU	B	B	493

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	-	1-801
B	-	1-493

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	AlphaLink2	1.0	model building	https://github.com/Rappsilber-Laboratory/AlphaLink2

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 10578 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
OH--HH	0.96	0.84	54

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CG1--HG13	1.09	0.97	222
CB--HB2	1.09	0.97	877
CG--HG	1.09	0.97	190
CA--HA	1.09	0.97	1183
CD1--HD13	1.09	0.97	315
CE--HE2	1.09	0.97	107
CB--HB3	1.09	0.97	877
CD2--HD23	1.09	0.97	190
CD1--HD11	1.09	0.97	315
CG2--HG21	1.09	0.97	306
CD1--HD12	1.09	0.97	315
CG1--HG11	1.09	0.97	97
CG2--HG23	1.09	0.97	306
CG2--HG22	1.09	0.97	306
OG--HG	0.96	0.84	88
CB--HB	1.09	0.97	306
CE--HE3	1.09	0.97	107
CD2--HD22	1.09	0.97	190
CD2--HD21	1.09	0.97	190
CB--HB1	1.09	0.97	101
NZ--HZ3	1.01	0.89	57
CG--HG3	1.09	0.97	248
NZ--HZ1	1.01	0.89	57

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CA--HA3	1.09	0.97	111
NZ--HZ2	1.01	0.89	57
CG1--HG12	1.09	0.97	222
CG--HG2	1.09	0.97	248
OG1--HG1	0.96	0.84	84
CD--HD3	1.09	0.97	130
CD--HD2	1.09	0.97	130
CE--HE1	1.09	0.97	50
CA--HA2	1.09	0.97	111
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	2
CD1--HD1	1.08	0.93	175
CE1--HE1	1.08	0.93	184
N--H	1.01	0.86	1250
CE2--HE2	1.08	0.93	157
CD2--HD2	1.08	0.93	184
ND2--HD21	1.01	0.86	23
NE2--HE21	1.01	0.86	26
NE--HE	1.01	0.86	31
NE2--HE22	1.01	0.86	26
NH2--HH22	1.01	0.86	31
NE1--HE1	1.01	0.86	18

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CZ--HZ	1.08	0.93	103
NH1--HH11	1.01	0.86	31
CE3--HE3	1.08	0.93	18
NH1--HH12	1.01	0.86	31
ND2--HD22	1.01	0.86	23
CZ2--HZ2	1.08	0.93	18
CZ3--HZ3	1.08	0.93	18
ND1--HD1	1.01	0.86	25
NH2--HH21	1.01	0.86	31
CH2--HH2	1.08	0.93	18
NE2--HE2	1.01	0.86	2

Standard geometry: angle outliers?

There are 23 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	116.88	1
CA-CB-CG1	110.40	119.57	1
CA-CB-CG	113.80	108.55	1
NE-CZ-NH2	119.20	123.60	1
CB-CG-CD2	131.20	125.03	1
OE1-CD-NE2	122.60	117.89	1
OE1-CD-NE2	122.60	117.90	1
CB-CG-CD2	131.20	125.37	1
CB-CG-CD2	131.20	125.44	1
CB-CG-CD2	131.20	125.46	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.26	1
CB-CG-CD2	131.20	125.57	1
CB-CG-CD2	131.20	125.63	1
CB-CG-CD2	131.20	125.64	1
OE1-CD-NE2	122.60	118.39	1
OE1-CD-NE2	122.60	118.42	1
CA-CB-OG1	109.60	115.82	1
OE1-CD-NE2	122.60	118.46	1
OE1-CD-NE2	122.60	118.48	1
OE1-CD-NE2	122.60	118.55	1
OE1-CD-NE2	122.60	118.59	2
OD1-CG-ND2	122.60	118.59	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	1.84	38

All 38 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:598:ILE:HD11	B:165:PHE:CE1	0.889
1	B:374:PHE:CE1	B:378:ILE:HD11	0.644
1	A:598:ILE:HD11	B:165:PHE:CZ	0.629
1	A:364:THR:HB	A:462:LEU:HD22	0.614
1	A:441:THR:HA	A:444:TYR:CE1	0.607

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:376:MET:HE2	A:383:PHE:CZ	0.590
1	A:359:ILE:HG23	A:469:ALA:HB2	0.555
1	B:129:LEU:HD23	B:177:VAL:HG22	0.555
1	A:4:LEU:CD1	A:58:LEU:HD22	0.545
1	A:337:MET:HE3	A:407:MET:HE3	0.544
1	A:337:MET:CE	A:407:MET:HE3	0.503
1	A:319:VAL:HG13	A:415:VAL:CG2	0.502
1	A:583:THR:HA	A:586:TYR:CE1	0.500
1	A:507:TYR:HB3	A:510:LEU:HD12	0.496
1	A:760:ASN:O	A:764:VAL:HG22	0.463
1	A:408:PHE:CE1	A:434:ALA:HB1	0.462
1	A:337:MET:HE3	A:407:MET:CE	0.452
1	B:313:PHE:CD1	B:411:ILE:HD12	0.452
1	A:301:ILE:HD11	A:369:ILE:HD11	0.447
1	A:586:TYR:CE2	A:587:MET:HG2	0.445
1	A:137:MET:HA	B:384:PRO:HG2	0.441
1	A:139:TRP:CD2	A:177:MET:HE1	0.436
1	A:598:ILE:HD11	B:165:PHE:CD1	0.431
1	A:194:ARG:NH2	A:197:VAL:HG21	0.429
1	A:241:THR:HG21	A:358:GLY:HA3	0.429
1	B:169:SER:HA	B:218:MET:HE1	0.427
1	B:289:GLY:HA3	B:302:TYR:CD1	0.426
1	A:511:LEU:HD11	A:517:PHE:CD2	0.425

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:388:ILE:HG21	A:481:VAL:HG13	0.422
1	B:230:PRO:HA	B:301:ILE:HG21	0.422
1	B:320:PRO:HA	B:481:LEU:HD11	0.421
1	B:23:THR:HG21	B:108:PHE:CE1	0.419
1	B:370:GLY:HA2	B:430:PHE:CE1	0.413
1	A:475:VAL:HB	A:476:PRO:HD3	0.407
1	A:388:ILE:HG23	A:399:PHE:CE1	0.404
1	A:633:LEU:CD1	A:670:ILE:HD12	0.403
1	B:333:ASP:OD1	B:337:LYS:HE2	0.401
1	A:684:GLU:HA	A:684:GLU:OE2	0.400

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	1290	1262	23	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
1	1082	988	49	45

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	3	LEU
1	A	4	LEU
1	A	6	LEU

Model ID	Chain	Residue ID	Residue type
1	A	30	THR
1	A	46	LEU
1	A	92	SER
1	A	202	LEU
1	A	343	LEU
1	A	369	ILE
1	A	425	THR
1	A	467	HIS
1	A	483	LEU
1	A	522	SER
1	A	548	LEU
1	A	571	LEU
1	A	572	LEU
1	A	573	THR
1	A	596	LEU
1	A	606	ILE
1	A	610	PHE
1	A	630	GLU
1	A	649	SER
1	A	651	LEU
1	A	695	PHE
1	A	713	THR
1	A	717	ILE

Model ID	Chain	Residue ID	Residue type
1	A	728	LEU
1	A	749	SER
1	A	788	MET
1	B	4	PHE
1	B	10	LEU
1	B	26	LEU
1	B	28	LEU
1	B	43	ILE
1	B	129	LEU
1	B	139	LEU
1	B	141	ILE
1	B	154	ILE
1	B	165	PHE
1	B	294	SER
1	B	405	PHE
1	B	423	LEU
1	B	437	THR
1	B	450	TYR
1	B	460	LEU

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 ?

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Acknowledgements

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