

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	9A50
PDB-Dev ID	PDBDEV_00000257
Structure Title	Integrative model of RPSB-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

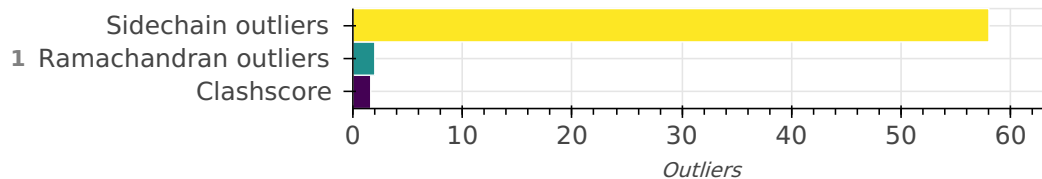
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the  symbol.

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	RPSB_BACSU	A	A	262
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	-	1-262
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	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 11822 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
CE--HE2	1.09	0.97	155

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CG2--HG23	1.09	0.97	301
CG2--HG21	1.09	0.97	301
CG--HG2	1.09	0.97	498
CA--HA	1.09	0.97	1358
CD1--HD13	1.09	0.97	235
CG--HG3	1.09	0.97	498
CB--HB3	1.09	0.97	1057
CE--HE3	1.09	0.97	155
CB--HB2	1.09	0.97	1057
CG--HG	1.09	0.97	142
CG1--HG13	1.09	0.97	216
CB--HB	1.09	0.97	301
CG1--HG11	1.09	0.97	123
CD1--HD12	1.09	0.97	235
NZ--HZ1	1.01	0.89	111
CD2--HD23	1.09	0.97	142
CD2--HD21	1.09	0.97	142
CG1--HG12	1.09	0.97	216
NZ--HZ3	1.01	0.89	111
CD1--HD11	1.09	0.97	235
OG--HG	0.96	0.84	71
CD--HD2	1.09	0.97	270
CD2--HD22	1.09	0.97	142

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CE--HE1	1.09	0.97	44
CG2--HG22	1.09	0.97	301
CD--HD3	1.09	0.97	270
CA--HA3	1.09	0.97	103
OH--HH	0.96	0.84	37
NZ--HZ2	1.01	0.89	111
CA--HA2	1.09	0.97	103
CB--HB1	1.09	0.97	93
OG1--HG1	0.96	0.84	85
N--H1	1.01	0.89	2
N--H3	1.01	0.89	2
N--H2	1.01	0.89	2
SG--HG	1.34	1.20	11
CD1--HD1	1.08	0.93	85
CZ3--HZ3	1.08	0.93	8
NH1--HH12	1.01	0.86	98
NE2--HE21	1.01	0.86	62
N--H	1.01	0.86	1398
NE--HE	1.01	0.86	98
CD2--HD2	1.08	0.93	103
ND1--HD1	1.01	0.86	23
NH2--HH21	1.01	0.86	98
NH1--HH11	1.01	0.86	98
ND2--HD21	1.01	0.86	50

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CZ--HZ	1.08	0.93	40
CE1--HE1	1.08	0.93	103
NH2--HH22	1.01	0.86	98
NE2--HE22	1.01	0.86	62
ND2--HD22	1.01	0.86	50
CE2--HE2	1.08	0.93	77
NE1--HE1	1.01	0.86	8
CE3--HE3	1.08	0.93	8
CH2--HH2	1.08	0.93	8
CZ2--HZ2	1.08	0.93	8
NE2--HE2	1.01	0.86	3

Standard geometry: angle outliers?

There are 45 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	117.43	1
OE1-CD-NE2	122.60	117.45	1
OD1-CG-ND2	122.60	117.62	1
OE1-CD-NE2	122.60	117.66	1
NE-CZ-NH2	119.20	123.62	1
OE1-CD-NE2	122.60	117.69	1
CA-CB-CG	112.60	117.50	1
CA-CB-CG	112.60	117.47	1
OE1-CD-NE2	122.60	117.76	1
OE1-CD-NE2	122.60	117.82	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD2	131.20	124.99	1
OE1-CD-NE2	122.60	117.88	2
OE1-CD-NE2	122.60	117.99	1
OD1-CG-ND2	122.60	118.00	1
OE1-CD-NE2	122.60	118.00	1
OE1-CD-NE2	122.60	118.01	1
OE1-CD-OE1-CD-NE2	122.60	118.03	1
CB-CG-CD2	131.20	125.26	1
OE1-CD-NE2	122.60	118.04	1
OE1-CD-OE1-CD-NE2	122.60	118.09	1
OD1-CG-ND2	122.60	118.12	1
OE1-CD-CB-CG-CD2	131.20	125.44	1
CB-CG-CB-CG-CD2	131.20	125.53	1
OE1-CD-NE2	122.60	118.26	1
OE1-CD-NE2	122.60	118.30	1
CB-CG-CD2	131.20	125.62	1
CA-CB-OE1-CD-NE2	122.60	118.34	1
OE1-CD-NE2	122.60	118.34	2
OE1-CD-NE2	122.60	118.36	1
OE1-CD-OE1-CD-NE2	122.60	118.39	1
CB-CG-CD2	131.20	125.74	2
CA-CB-CG	112.60	116.79	1
CA-C-CA-CB-CG2	110.50	117.58	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.46	1
OE1-CD-NE2	122.60	118.49	2
CA-CB-CG	112.60	116.69	1
NE-CZ-NH2	119.20	122.86	1
OE1-CD-NE2	122.60	118.59	1
CA-CB-CG	112.60	116.61	1
HZ2-NZ-HZ3	95.99	109.00	1
HH21-NH2-HH22	101.72	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	1.63	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	B:808:ALA:CB	B:36:TYR:CD1	0.691
1	B:978:VAL:CG2	B:495:MET:HE1	0.658
1	A:155:MET:HE3	B:428:PRO:HG2	0.648
1	B:441:LEU:HD21	B:749:GLY:HA2	0.634
1	B:405:ILE:HG23	B:114:MET:HE2	0.618
1	B:747:MET:HE2	B:321:LYS:HE2	0.614
1	B:808:ALA:HB2	B:723:LEU:HD22	0.587
1	B:107:PHE:HB2	B:383:ILE:HG23	0.548
1	B:317:SER:HB3	A:219:ILE:HD12	0.525

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:978:VAL:HG22	B:87:VAL:HG22	0.524
1	B:506:ARG:HH21	B:321:LYS:CE	0.519
1	B:978:VAL:HG23	B:741:PHE:CE1	0.511
1	B:371:MET:HE2	B:615:PHE:CD2	0.504
1	B:808:ALA:HB1	B:741:PHE:CD2	0.466
1	A:215:ASP:OD1	B:125:LEU:HD22	0.461
1	B:84:ARG:O	B:762:PRO:HG3	0.453
1	B:317:SER:HB3	B:565:LEU:HB3	0.452
1	B:720:LEU:HD11	B:644:LYS:HA	0.450
1	B:503:THR:HG21	A:60:ARG:HE	0.432
1	B:895:PRO:HA	B:383:ILE:HG23	0.432
1	B:726:ILE:HG21	B:242:VAL:HG11	0.426
1	B:114:MET:HE3	A:94:ILE:HG23	0.425
1	B:705:TRP:CD2	A:82:PHE:HA	0.425
1	B:519:THR:HG23	B:741:PHE:CZ	0.423
1	B:495:MET:HE3	B:614:PRO:HG2	0.418
1	A:43:ASP:CG	B:450:PHE:CE2	0.411

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	1457	1414	41	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	1265	1135	72	58

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	2	THR
1	A	7	THR
1	A	8	THR
1	A	104	SER
1	A	140	GLU
1	A	144	VAL
1	A	176	THR
1	A	180	LEU
1	A	199	LEU
1	A	241	LEU
1	A	261	LEU
1	B	2	LEU
1	B	76	ASP
1	B	107	PHE
1	B	125	LEU
1	B	159	LEU
1	B	195	LEU
1	B	204	THR
1	B	214	GLU
1	B	234	ILE
1	B	242	VAL

Model ID	Chain	Residue ID	Residue type
1	B	256	ASP
1	B	345	VAL
1	B	357	LEU
1	B	373	GLU
1	B	431	VAL
1	B	444	THR
1	B	449	ASP
1	B	453	ASP
1	B	488	VAL
1	B	490	THR
1	B	497	LEU
1	B	504	LEU
1	B	524	LEU
1	B	583	LYS
1	B	646	LEU
1	B	657	THR
1	B	692	ILE
1	B	716	LEU
1	B	761	LEU
1	B	774	LEU
1	B	780	THR
1	B	781	HIS
1	B	803	ARG

Model ID	Chain	Residue ID	Residue type
1	B	816	THR
1	B	932	THR
1	B	938	THR
1	B	974	ILE
1	B	977	THR
1	B	999	THR
1	B	1003	THR
1	B	1018	ILE
1	B	1041	THR
1	B	1042	THR
1	B	1107	LEU
1	B	1163	GLU
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

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