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	9A7I
PDB-Dev ID	PDBDEV_00000347
Structure Title	Integrative model of NUSA-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

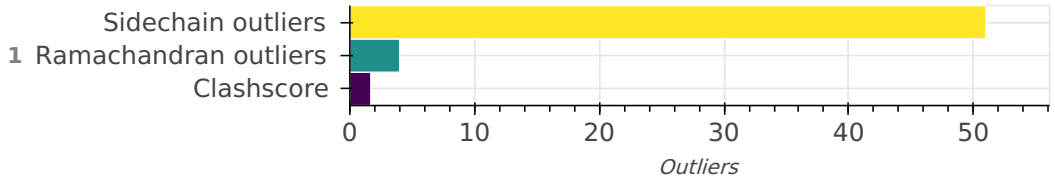
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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	NUSA_BACSU	A	A	371
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	-	1-371
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, molprobity analysis is performed. For models with coarse-grained or multi-scale structures, excluded volume analysis is performed.

Standard geometry: bond outliers

There are 12640 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
CD1--HD11	1.09	0.97	250

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CG2--HG23	1.09	0.97	333
CG2--HG22	1.09	0.97	333
CB--HB2	1.09	0.97	1127
CA--HA	1.09	0.97	1460
CB--HB3	1.09	0.97	1127
CG--HG2	1.09	0.97	530
OG1--HG1	0.96	0.84	86
CG--HG3	1.09	0.97	530
CG2--HG21	1.09	0.97	333
CE--HE3	1.09	0.97	153
CD2--HD22	1.09	0.97	142
CD2--HD21	1.09	0.97	142
CD--HD2	1.09	0.97	292
CG--HG	1.09	0.97	142
CD2--HD23	1.09	0.97	142
CD1--HD12	1.09	0.97	250
CG1--HG12	1.09	0.97	247
CE--HE2	1.09	0.97	153
CB--HB	1.09	0.97	333
CG1--HG11	1.09	0.97	139
CA--HA2	1.09	0.97	110
CB--HB1	1.09	0.97	107
CG1--HG13	1.09	0.97	247

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CD1--HD13	1.09	0.97	250
NZ--HZ2	1.01	0.89	115
CD--HD3	1.09	0.97	292
OH--HH	0.96	0.84	41
NZ--HZ1	1.01	0.89	115
OG--HG	0.96	0.84	72
CE--HE1	1.09	0.97	38
NZ--HZ3	1.01	0.89	115
CA--HA3	1.09	0.97	110
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	1
SG--HG	1.34	1.20	11
N--H	1.01	0.86	1497
NH2--HH22	1.01	0.86	106
NE2--HE21	1.01	0.86	58
NE1--HE1	1.01	0.86	9
CE2--HE2	1.08	0.93	84
NE--HE	1.01	0.86	106
CD1--HD1	1.08	0.93	93
CD2--HD2	1.08	0.93	108
NH1--HH11	1.01	0.86	106
CZ--HZ	1.08	0.93	43

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
ND2--HD21	1.01	0.86	59
CE1--HE1	1.08	0.93	108
NH1--HH12	1.01	0.86	106
ND2--HD22	1.01	0.86	59
NH2--HH21	1.01	0.86	106
ND1--HD1	1.01	0.86	22
NE2--HE22	1.01	0.86	58
CE3--HE3	1.08	0.93	9
CZ3--HZ3	1.08	0.93	9
CZ2--HZ2	1.08	0.93	9
NE2--HE2	1.01	0.86	2
CH2--HH2	1.08	0.93	9

Standard geometry: angle outliers

There are 64 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	121.70	134.31	1
C-N-CA	121.70	133.63	1
NE-CZ-NH2	119.20	124.94	1
N-CA-C	111.00	128.18	1
CA-CB-CA-C-N	116.20	127.84	1
CA-CB-CG	112.60	118.34	1
OE1-CD-NE2	122.60	117.15	1
N-CA-C	111.00	126.23	1
CA-CB-CG	112.60	118.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	117.25	1
OE1-CD-NE2	122.60	117.36	1
OE1-CD-NE2	122.60	117.43	1
OE1-CD-NE2	122.60	117.46	1
CA-CB-CG	112.60	117.67	1
OD1-CG-ND2	122.60	117.57	1
N-CA-C	111.00	124.94	1
CB-CG-CD2	131.20	124.74	1
OE1-CD-NE2	122.60	117.64	1
N-CA-C	111.00	124.63	1
OE1-CD-NE2	122.60	117.76	1
OE1-CD-NE2	122.60	117.82	3
OE1-CD-NE2	122.60	117.91	1
OE1-CD-NE2	122.60	117.96	3
OE1-CD-NE2	122.60	117.97	1
OE1-CD-NE2	122.60	117.99	1
NE-CZ-NH2	119.20	123.33	1
NE-CZ-NH2	119.20	123.30	1
CA-CB-CG	112.60	117.15	1
CA-C-N	116.90	123.71	1
OE1-CD-OE1-CD-NE2	122.60	118.12	1
OE1-CD-NE2	122.60	118.14	1
OD1-CG-ND2	122.60	118.16	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.18	1
OE1-CD-OD1-CG-ND2	122.60	118.20	1
OE1-CD-OE1-CD-CA-CB-CG2	110.50	103.09	1
OE1-CD-OE1-CD-NE2	122.60	118.30	1
OD1-CG-ND2	122.60	118.35	1
NE-CZ-NH2	119.20	115.38	1
OE1-CD-NE2	122.60	118.36	2
OE1-CD-NE2	122.60	118.38	1
CA-CB-CG	112.60	116.79	1
NH1-CZ-NH2	119.30	113.86	1
CB-CG-CB-CG-CD2	131.20	125.80	1
CB-CG-CD2	131.20	125.82	1
OE1-CD-NE2	122.60	118.47	1
OE1-CD-NE2	122.60	118.48	2
OE1-CD-NE2	122.60	118.50	1
CA-CB-CG	112.60	116.70	1
CA-CB-CB-CG-CD2	131.20	125.87	1
OE1-CD-NE2	122.60	118.52	1
CB-CG-CD2	131.20	125.93	1
OE1-CD-NE2	122.60	118.55	1
OD1-CG-ND2	122.60	118.57	2
CB-CG-CD2	131.20	125.99	1
OE1-CD-NE2	122.60	118.59	1
HZ1-NZ-HZ2	96.07	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HH21-NH2-HH22	101.28	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	1.68	42

All 42 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:113:ARG:HH11	B:212:VAL:HG22	0.881
1	B:808:ALA:HB2	B:495:MET:HE1	0.680
1	B:808:ALA:CB	B:741:PHE:CE2	0.658
1	B:441:LEU:HD21	B:316:LEU:HD21	0.616
1	B:726:ILE:HG21	B:383:ILE:HG23	0.616
1	B:234:ILE:HD11	B:212:VAL:HG22	0.613
1	B:371:MET:CE	B:7:PHE:HZ	0.570
1	B:113:ARG:NH1	B:887:ARG:HH21	0.563
1	B:2:LEU:HD22	B:741:PHE:CE1	0.559
1	B:930:PRO:HB3	B:321:LYS:HE2	0.539
1	B:820:THR:HG22	B:565:LEU:HD11	0.528
1	B:720:LEU:HD11	B:235:PRO:HD2	0.521
1	B:214:GLU:OE2	B:212:VAL:HG23	0.515
1	B:317:SER:HB3	A:102:PHE:CG	0.511
1	B:539:VAL:HG21	B:723:LEU:HD22	0.473
1	B:234:ILE:HG22	B:644:LYS:HA	0.468

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:208:LYS:O	A:4:GLU:OE2	0.467
1	A:99:PRO:HD2	B:495:MET:HE1	0.463
1	B:808:ALA:HB1	A:102:PHE:CD2	0.460
1	B:978:VAL:HG22	B:182:ILE:HD11	0.454
1	B:506:ARG:HH21	A:99:PRO:HD3	0.427
1	B:495:MET:HE3	B:741:PHE:HE2	0.426
1	A:1:MET:HA	B:321:LYS:HE2	0.419
1	B:978:VAL:CG2	B:450:PHE:CE2	0.416
1	B:441:LEU:CD2	B:209:ARG:CZ	0.413
1	B:895:PRO:HA	B:316:LEU:CD2	0.411
1	A:99:PRO:HG2	B:762:PRO:HG3	0.409

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	1566	1521	41	4

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	1353	1225	77	51

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	5	LEU
1	A	221	GLU

Model ID	Chain	Residue ID	Residue type
1	A	258	VAL
1	A	348	ILE
1	A	362	THR
1	A	366	THR
1	B	1	MET
1	B	24	SER
1	B	55	THR
1	B	76	ASP
1	B	107	PHE
1	B	125	LEU
1	B	159	LEU
1	B	195	LEU
1	B	234	ILE
1	B	287	MET
1	B	327	PHE
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	474	LEU

Model ID	Chain	Residue ID	Residue type
1	B	488	VAL
1	B	497	LEU
1	B	504	LEU
1	B	646	LEU
1	B	657	THR
1	B	666	LEU
1	B	692	ILE
1	B	716	LEU
1	B	761	LEU
1	B	780	THR
1	B	809	GLN
1	B	813	ILE
1	B	816	THR
1	B	949	ILE
1	B	957	GLN
1	B	974	ILE
1	B	977	THR
1	B	999	THR
1	B	1003	THR
1	B	1018	ILE
1	B	1040	LEU
1	B	1041	THR
1	B	1042	THR
1	B	1124	THR

Model ID	Chain	Residue ID	Residue type
1	B	1161	LEU
1	B	1171	VAL

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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