Integrative Structure Validation Report

September 11, 2024 - 04:44 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	9A7U
PDB-Dev ID	PDBDEV_00000359
Structure Title	Integrative model of RPOC-GREA 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

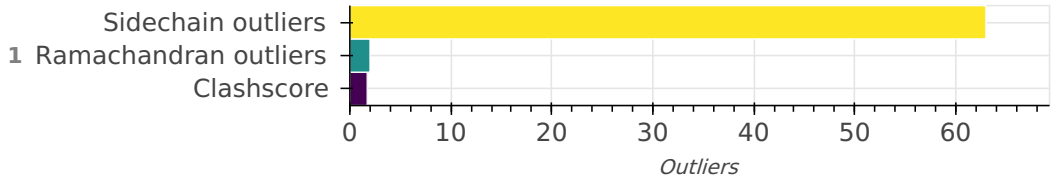
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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	RPOC_BACSU	A	A	1199
1	2	2	GREA_BACSU	B	B	157

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	-	1-1199
B	-	1-157

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 10901 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
CG--HG3	1.09	0.97	459

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CA--HA	1.09	0.97	1253
CG2--HG22	1.09	0.97	279
CE--HE2	1.09	0.97	143
CD2--HD22	1.09	0.97	127
CB--HB2	1.09	0.97	974
CE--HE3	1.09	0.97	143
CG2--HG21	1.09	0.97	279
CB--HB3	1.09	0.97	974
NZ--HZ2	1.01	0.89	105
NZ--HZ3	1.01	0.89	105
CD1--HD13	1.09	0.97	211
CD2--HD23	1.09	0.97	127
CG1--HG11	1.09	0.97	118
CG--HG	1.09	0.97	127
CD--HD3	1.09	0.97	252
OH--HH	0.96	0.84	33
CD--HD2	1.09	0.97	252
CB--HB	1.09	0.97	279
N--H2	1.01	0.89	2
CG--HG2	1.09	0.97	459
CG2--HG23	1.09	0.97	279
CG1--HG12	1.09	0.97	202
CD1--HD12	1.09	0.97	211

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CG1--HG13	1.09	0.97	202
CD2--HD21	1.09	0.97	127
CD1--HD11	1.09	0.97	211
CA--HA3	1.09	0.97	103
NZ--HZ1	1.01	0.89	105
OG--HG	0.96	0.84	62
CB--HB1	1.09	0.97	91
CA--HA2	1.09	0.97	103
OG1--HG1	0.96	0.84	77
CE--HE1	1.09	0.97	38
N--H3	1.01	0.89	2
N--H1	1.01	0.89	2
SG--HG	1.34	1.20	11
NH1--HH11	1.01	0.86	88
ND2--HD21	1.01	0.86	52
N--H	1.01	0.86	1295
NH2--HH21	1.01	0.86	88
CD1--HD1	1.08	0.93	80
CZ--HZ	1.08	0.93	40
ND1--HD1	1.01	0.86	19
NE--HE	1.01	0.86	88
NE2--HE22	1.01	0.86	49
CE1--HE1	1.08	0.93	94
CZ3--HZ3	1.08	0.93	7

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
ND2--HD22	1.01	0.86	52
CD2--HD2	1.08	0.93	94
CE2--HE2	1.08	0.93	73
NH1--HH12	1.01	0.86	88
NE2--HE21	1.01	0.86	49
NH2--HH22	1.01	0.86	88
CZ2--HZ2	1.08	0.93	7
NE1--HE1	1.01	0.86	7
CH2--HH2	1.08	0.93	7
CE3--HE3	1.08	0.93	7
NE2--HE2	1.01	0.86	2

Standard geometry: angle outliers

There are 52 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	113.80	124.66	1
OD1-CG-ND2	122.60	117.20	1
CA-CB-CG	112.60	117.74	1
CA-CB-CG	112.60	117.73	1
CA-CB-CG	112.60	117.62	1
OE1-CD-NE2	122.60	117.59	1
OE1-CD-NE2	122.60	117.60	1
CA-CB-CG	112.60	117.58	1
NE-CZ-NH2	119.20	123.64	1
OE1-CD-NE2	122.60	117.67	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	113.80	108.91	1
CB-CG-CD2	131.20	124.87	1
OE1-CD-OE1-CD-NE2	122.60	117.84	1
OE1-CD-NE2	122.60	117.92	1
OE1-CD-NE2	122.60	117.93	1
OE1-CD-CA-CB-CG	112.60	117.24	1
OE1-CD-NE2	122.60	118.00	1
OD1-CG-ND2	122.60	118.04	1
OE1-CD-NE2	122.60	118.07	1
OE1-CD-NE2	122.60	118.08	1
OE1-CD-NE2	122.60	118.10	1
CB-CG-CD2	131.20	125.40	1
OD1-CG-ND2	122.60	118.17	1
OE1-CD-NE2	122.60	118.17	1
OE1-CD-NE2	122.60	118.23	1
OE1-CD-OD1-CG-ND2	122.60	118.27	1
NE-CZ-NH2	119.20	123.09	1
OE1-CD-NE2	122.60	118.29	1
CB-CG-CD2	131.20	125.61	1
OE1-CD-NE2	122.60	118.33	1
OE1-CD-NE2	122.60	118.34	2
C-N-CA	121.70	129.32	1
C-N-CA	121.70	129.28	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	116.81	1
CB-CG-CD2	131.20	125.76	1
OE1-CD-NE2	122.60	118.43	1
OD1-CG-ND2	122.60	118.46	1
C-N-CA	121.70	129.15	1
OE1-CD-NE2	122.60	118.49	1
CA-CB-CG	112.60	116.70	1
NE-CZ-NH2	119.20	122.89	1
CA-CB-CG	112.60	116.68	1
CB-CG-CD2	131.20	125.92	2
HH21-NH2-HH22	107.54	120.00	1
HZ1-NZ-HZ3	95.90	109.00	1
CA-CB-HB2	87.57	109.00	1
CG-CB-HB2	85.40	108.00	1
CA-CB-HB3	82.53	109.00	1
CG-CB-HB3	76.81	108.00	1
HB2-CB-HB3	149.38	110.00	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	1.72	37

All 37 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Model ID	Atom-1	Atom-2	Clash overlap (Å)

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:808:ALA:CB	A:316:LEU:HD21	0.709
1	A:808:ALA:HB2	A:741:PHE:CE2	0.693
1	A:234:ILE:HD11	A:741:PHE:CD2	0.679
1	A:978:VAL:CG2	A:321:LYS:HE2	0.622
1	A:726:ILE:HG21	A:316:LEU:CD2	0.621
1	A:726:ILE:HG21	A:383:ILE:HG23	0.603
1	A:317:SER:HB3	A:615:PHE:CD2	0.589
1	A:234:ILE:HD11	A:596:LEU:HD11	0.582
1	A:371:MET:HE3	A:749:GLY:HA2	0.573
1	A:978:VAL:HG22	A:495:MET:HE1	0.571
1	A:503:THR:HG21	A:87:VAL:HG22	0.534
1	A:559:ILE:HD11	A:596:LEU:CD1	0.523
1	A:747:MET:HE2	A:321:LYS:CE	0.500
1	A:441:LEU:HD21	A:723:LEU:HD22	0.483
1	A:978:VAL:HG23	A:619:ILE:CD1	0.473
1	A:84:ARG:O	A:887:ARG:HH21	0.465
1	A:991:ILE:HD11	A:146:LYS:HE3	0.463
1	A:559:ILE:HD11	A:741:PHE:CE1	0.454
1	A:895:PRO:HA	A:644:LYS:HA	0.450
1	A:808:ALA:HB1	A:383:ILE:HG23	0.439
1	A:317:SER:HB3	A:782:GLY:HA3	0.430
1	A:506:ARG:HH21	A:723:LEU:CD2	0.428
1	A:581:PRO:HB2	A:114:MET:CE	0.426

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:820:THR:HG22	A:762:PRO:HG3	0.422
1	A:137:THR:O	B:151:VAL:HG11	0.418
1	A:720:LEU:HD11	A:764:LYS:HE2	0.416
1	A:495:MET:HE3	A:450:PHE:CE2	0.406

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	1352	1307	43	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	1162	1023	76	63

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	2	LEU
1	A	55	THR
1	A	76	ASP
1	A	107	PHE
1	A	125	LEU
1	A	135	VAL
1	A	159	LEU
1	A	187	GLU
1	A	195	LEU

Model ID	Chain	Residue ID	Residue type
1	A	260	ARG
1	A	287	MET
1	A	345	VAL
1	A	352	MET
1	A	357	LEU
1	A	363	LEU
1	A	373	GLU
1	A	381	HIS
1	A	382	ASN
1	A	385	SER
1	A	412	LEU
1	A	431	VAL
1	A	438	LEU
1	A	444	THR
1	A	453	ASP
1	A	474	LEU
1	A	497	LEU
1	A	504	LEU
1	A	519	THR
1	A	531	VAL
1	A	583	LYS
1	A	634	THR
1	A	641	ASP
1	A	646	LEU

Model ID	Chain	Residue ID	Residue type
1	A	706	SER
1	A	716	LEU
1	A	751	MET
1	A	753	ASN
1	A	761	LEU
1	A	765	SER
1	A	774	LEU
1	A	781	HIS
1	A	809	GLN
1	A	810	ASP
1	A	816	THR
1	A	869	ASP
1	A	932	THR
1	A	935	THR
1	A	950	THR
1	A	974	ILE
1	A	977	THR
1	A	999	THR
1	A	1003	THR
1	A	1018	ILE
1	A	1041	THR
1	A	1042	THR
1	A	1130	THR

Model ID	Chain	Residue ID	Residue type
1	A	1171	VAL
1	A	1177	MET
1	B	46	SER
1	B	89	LEU
1	B	141	THR
1	B	150	LEU
1	B	151	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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