

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	9A78
PDB-Dev ID	PDBDEV_00000337
Structure Title	Integrative model of SYFB-CGOX 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

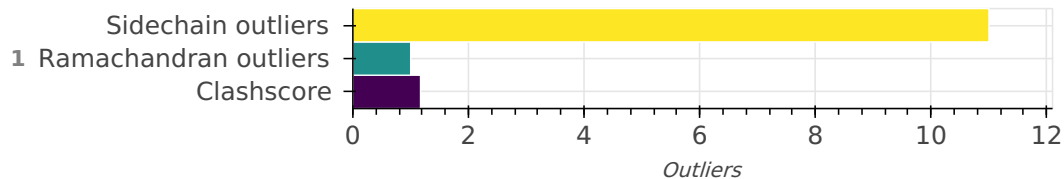
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the  symbol.

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	SYFB_BACSU	A	A	804
1	2	2	CGOX_BACSU	B	B	470

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	-	1-804
B	-	1-470

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 9945 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--HG2	1.09	0.97	370

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CA--HA	1.09	0.97	1174
CB--HB	1.09	0.97	260
CD1--HD12	1.09	0.97	208
CB--HB3	1.09	0.97	914
CB--HB2	1.09	0.97	914
CD1--HD11	1.09	0.97	208
CB--HB1	1.09	0.97	112
CD--HD3	1.09	0.97	192
CD2--HD22	1.09	0.97	134
CG1--HG12	1.09	0.97	182
CE--HE3	1.09	0.97	121
CG1--HG13	1.09	0.97	182
CG--HG3	1.09	0.97	370
CG2--HG23	1.09	0.97	260
CD--HD2	1.09	0.97	192
CE--HE2	1.09	0.97	121
CD1--HD13	1.09	0.97	208
NZ--HZ1	1.01	0.89	96
NZ--HZ3	1.01	0.89	96
CA--HA2	1.09	0.97	100
CG--HG	1.09	0.97	134
CG2--HG21	1.09	0.97	260
CG2--HG22	1.09	0.97	260

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
OH--HH	0.96	0.84	37
OG--HG	0.96	0.84	78
NZ--HZ2	1.01	0.89	96
CD2--HD21	1.09	0.97	134
CD2--HD23	1.09	0.97	134
OG1--HG1	0.96	0.84	78
CG1--HG11	1.09	0.97	108
CA--HA3	1.09	0.97	100
CE--HE1	1.09	0.97	25
N--H2	1.01	0.89	2
N--H3	1.01	0.89	2
N--H1	1.01	0.89	2
SG--HG	1.33	1.20	1
SG--HG	1.34	1.20	6
CZ--HZ	1.08	0.93	35
ND2--HD22	1.01	0.86	42
CD1--HD1	1.08	0.93	79
N--H	1.01	0.86	1222
ND2--HD21	1.01	0.86	42
NH1--HH11	1.01	0.86	46
NE2--HE21	1.01	0.86	46
NE2--HE22	1.01	0.86	46
CD2--HD2	1.08	0.93	99
CE2--HE2	1.08	0.93	72

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NH2--HH22	1.01	0.86	46
NH1--HH12	1.01	0.86	46
NH2--HH21	1.01	0.86	46
CE1--HE1	1.08	0.93	99
NE2--HE2	1.01	0.86	4
NE--HE	1.01	0.86	46
NE1--HE1	1.01	0.86	7
CH2--HH2	1.08	0.93	7
ND1--HD1	1.01	0.86	23
CZ3--HZ3	1.08	0.93	7
CE3--HE3	1.08	0.93	7
CZ2--HZ2	1.08	0.93	7

Standard geometry: angle outliers

There are 27 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
NE-CZ-NH2	119.20	125.23	1
CA-CB-CG	112.60	107.11	1
OE1-CD-NE2	122.60	117.52	1
OE1-CD-NE2	122.60	117.55	1
NE-CZ-NH1	121.50	126.22	1
OE1-CD-NE2	122.60	117.95	1
OE1-CD-NE2	122.60	118.00	1
CB-CG-CD2	131.20	125.26	1
OE1-CD-NE2	122.60	118.03	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OD1-CG-ND2	122.60	118.08	1
OE1-CD-NE2	122.60	118.14	1
CB-CG-CD2	131.20	125.46	1
OD1-CG-ND2	122.60	118.24	1
OE1-CD-NE2	122.60	118.26	1
OE1-CD-NE2	122.60	118.34	1
CA-CB-CG	112.60	116.84	1
OE1-CD-NE2	122.60	118.36	1
OE1-CD-NE2	122.60	118.37	1
OE1-CD-NE2	122.60	118.38	1
OD1-CG-ND2	122.60	118.39	1
N-CA-CB	103.00	107.63	1
CB-CG-CD2	131.20	125.82	1
OE1-CD-NE2	122.60	118.49	1
C-N-CA	121.70	129.02	1
OD1-CG-ND2	122.60	118.57	1
OE1-CD-NE2	122.60	118.59	1
HZ2-NZ-HZ3	96.48	109.00	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	1.17	23

All 23 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:7:TRP:CD1	A:245:LYS:HZ3	0.598
1	B:23:TYR:CE2	B:458:LYS:HE2	0.594
1	B:187:MET:HE1	B:194:TYR:CD1	0.577
1	B:187:MET:HE1	B:194:TYR:CG	0.564
1	A:218:ASP:OD2	A:289:LYS:HE3	0.556
1	B:294:LEU:HD12	B:440:MET:CE	0.540
1	B:173:LEU:HD22	B:190:PHE:CE2	0.522
1	B:325:MET:SD	B:347:TRP:CZ2	0.515
1	B:52:THR:HG21	B:233:GLY:HA3	0.512
1	A:65:LYS:HE3	A:77:GLN:CD	0.495
1	A:502:LYS:HB3	A:697:LEU:HD22	0.494
1	B:23:TYR:CZ	B:458:LYS:HE2	0.491
1	A:758:MET:HE2	A:763:LYS:CA	0.467
1	A:65:LYS:HE3	A:77:GLN:OE1	0.461
1	A:660:ILE:HD12	A:691:LEU:HD21	0.460
1	A:758:MET:HE2	A:763:LYS:HA	0.459
1	A:206:GLU:HB2	A:398:LEU:HD22	0.453
1	A:749:VAL:HG22	A:767:PHE:CE1	0.450
1	B:157:ARG:HH12	B:182:ASP:CG	0.441
1	B:294:LEU:HD12	B:440:MET:HE3	0.413
1	B:112:MET:HE1	B:190:PHE:CE1	0.409
1	A:215:LYS:HA	A:404:GLU:OE2	0.405
1	B:425:LYS:HE2	B:429:GLU:OE1	0.401

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	1270	1238	31	1

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	1062	1030	21	11

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	493	THR
1	A	704	LEU
1	A	802	LEU
1	B	3	ASP
1	B	129	LEU
1	B	146	THR
1	B	203	LEU
1	B	205	LEU
1	B	210	THR
1	B	219	LEU
1	B	431	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 ?

Validation for this section is under development.

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