

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	9A71
PDB-Dev ID	PDBDEV_00000330
Structure Title	Integrative model of BUK-SYGB 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

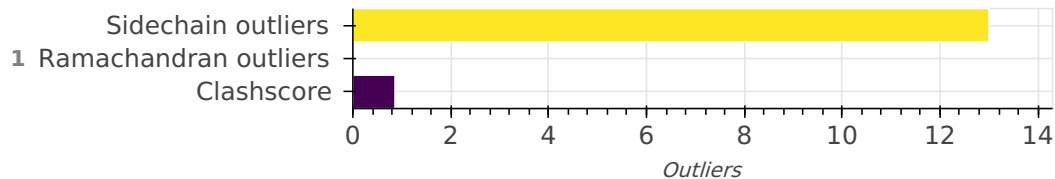
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the  symbol.

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	BUK_BACSU	A	A	363
1	2	2	SYGB_BACSU	B	B	679

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	-	1-363
B	-	1-679

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 8172 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
CD--HD2	1.09	0.97	152

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CG1--HG12	1.09	0.97	148
CG--HG	1.09	0.97	97
CB--HB3	1.09	0.97	774
CA--HA	1.09	0.97	963
OG--HG	0.96	0.84	60
CD1--HD11	1.09	0.97	170
NZ--HZ1	1.01	0.89	73
CA--HA3	1.09	0.97	79
CG--HG2	1.09	0.97	316
CD2--HD23	1.09	0.97	97
CB--HB	1.09	0.97	189
CB--HB2	1.09	0.97	774
CD1--HD12	1.09	0.97	170
CG2--HG22	1.09	0.97	189
CG1--HG11	1.09	0.97	75
CG2--HG23	1.09	0.97	189
NZ--HZ2	1.01	0.89	73
CG--HG3	1.09	0.97	316
CB--HB1	1.09	0.97	91
CE--HE3	1.09	0.97	98
CD1--HD13	1.09	0.97	170
CG2--HG21	1.09	0.97	189
NZ--HZ3	1.01	0.89	73

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CE--HE1	1.09	0.97	25
CD2--HD22	1.09	0.97	97
CG1--HG13	1.09	0.97	148
CE--HE2	1.09	0.97	98
OH--HH	0.96	0.84	31
CD--HD3	1.09	0.97	152
CD2--HD21	1.09	0.97	97
OG1--HG1	0.96	0.84	41
CA--HA2	1.09	0.97	79
N--H3	1.01	0.89	2
N--H1	1.01	0.89	2
N--H2	1.01	0.89	2
SG--HG	1.34	1.20	2
NE2--HE21	1.01	0.86	43
NH1--HH12	1.01	0.86	47
NE--HE	1.01	0.86	47
CD2--HD2	1.08	0.93	99
CD1--HD1	1.08	0.93	80
CE1--HE1	1.08	0.93	99
ND2--HD22	1.01	0.86	44
N--H	1.01	0.86	1008
ND2--HD21	1.01	0.86	44
NH2--HH22	1.01	0.86	47
NH2--HH21	1.01	0.86	47

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NH1--HH11	1.01	0.86	47
CZ--HZ	1.08	0.93	42
CH2--HH2	1.08	0.93	7
CE2--HE2	1.08	0.93	73
CE3--HE3	1.08	0.93	7
ND1--HD1	1.01	0.86	25
CZ3--HZ3	1.08	0.93	7
NE2--HE22	1.01	0.86	43
NE1--HE1	1.01	0.86	7
CZ2--HZ2	1.08	0.93	7
NE2--HE2	1.01	0.86	1

Standard geometry: angle outliers?

There are 38 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	116.90	1
OE1-CD-NE2	122.60	117.06	1
OD1-CG-ND2	122.60	117.09	1
CB-CG-CD2	131.20	125.07	1
OE1-CD-NE2	122.60	117.90	1
OE1-CD-NE2	122.60	117.96	2
OE1-CD-NE2	122.60	117.99	1
OE1-CD-NE2	122.60	118.02	1
OE1-CD-NE2	122.60	118.03	1
CB-CG-CD2	131.20	125.29	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OD1-CG-ND2	122.60	118.07	1
OE1-CD-NE2	122.60	118.09	1
OE1-CD-NE2	122.60	118.11	1
CD-NE-CZ	124.40	130.67	1
OE1-CD-NE2	122.60	118.13	1
OE1-CD-NE2	122.60	118.14	1
OE1-CD-NE2	122.60	118.18	1
OE1-CD-NE2	122.60	118.19	1
CA-CB-CG	112.60	116.98	1
OE1-CD-NE2	122.60	118.25	2
OE1-CD-NE2	122.60	118.27	1
CB-CG-CD2	131.20	125.60	1
OE1-CD-NE2	122.60	118.29	1
CB-CG-CD2	131.20	125.62	1
OE1-CD-NE2	122.60	118.32	2
OE1-CD-NE2	122.60	118.34	1
CA-CB-CG	112.60	116.85	1
OD1-CG-ND2	122.60	118.36	1
OE1-CD-NE2	122.60	118.38	1
CA-C-N	116.90	123.23	1
OE1-CD-NE2	122.60	118.39	1
OE1-CD-NE2	122.60	118.41	1
OD1-CG-ND2	122.60	118.52	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.54	1
CA-CB-CG2	110.50	117.31	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	0.86	14

All 14 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:433:HIS:CE1	B:434:TYR:CE2	0.520
1	B:11:GLY:HA3	B:162:TRP:CD2	0.509
1	A:179:TYR:CE1	A:201:GLY:HA2	0.499
1	B:64:LYS:HE2	B:124:GLY:O	0.492
1	A:159:PHE:HA	A:194:THR:HG21	0.491
1	B:11:GLY:HA3	B:162:TRP:CE2	0.470
1	A:187:THR:HG23	A:195:ILE:HG13	0.469
1	B:193:HIS:CE1	B:210:GLN:HE22	0.467
1	B:184:THR:HG21	B:194:GLU:OE1	0.444
1	B:262:PHE:CZ	B:296:PRO:HA	0.433
1	B:445:SER:C	B:494:ARG:HH22	0.432
1	B:282:GLN:HB3	B:284:TYR:CZ	0.426
1	A:29:ARG:CZ	B:322:ALA:HB1	0.423
1	B:244:LEU:HD22	B:279:LYS:HG2	0.404

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	1038	1018	20	0

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	872	842	17	13

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	4	LEU
1	A	50	ILE
1	A	144	LEU
1	A	232	LEU
1	A	243	ILE
1	A	248	VAL
1	B	41	THR
1	B	102	VAL
1	B	246	ASP
1	B	358	LEU
1	B	372	LEU
1	B	407	GLU
1	B	678	VAL

[Fit of model to data used for modeling !\[\]\(faf942dc3e59ce8eb64b4ac481eca7e0_img.jpg\)](#)

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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