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	9A4E
PDB-Dev ID	PDBDEV_00000235
Structure Title	Integrative model of ATPA-ATPF 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

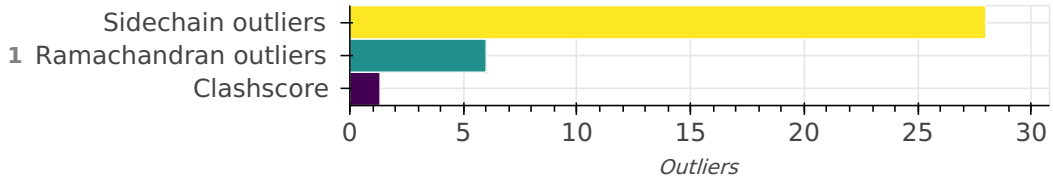
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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	ATPA_BACSU	A	A	502
1	2	2	ATPF_BACSU	B	B	170

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	-	1-502
B	-	1-170

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 5316 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--HD12	1.09	0.97	127

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CG--HG3	1.09	0.97	219
CA--HA	1.09	0.97	621
CG2--HG23	1.09	0.97	125
CB--HB2	1.09	0.97	496
CB--HB3	1.09	0.97	496
CG2--HG21	1.09	0.97	125
CD2--HD21	1.09	0.97	75
CG--HG2	1.09	0.97	219
OG1--HG1	0.96	0.84	26
CD--HD3	1.09	0.97	104
NZ--HZ1	1.01	0.89	43
CB--HB1	1.09	0.97	64
CD2--HD23	1.09	0.97	75
CG2--HG22	1.09	0.97	125
CD--HD2	1.09	0.97	104
CD1--HD11	1.09	0.97	127
CG1--HG11	1.09	0.97	47
CE--HE2	1.09	0.97	57
CG--HG	1.09	0.97	75
CA--HA3	1.09	0.97	51
NZ--HZ3	1.01	0.89	43
CE--HE3	1.09	0.97	57
CD1--HD13	1.09	0.97	127

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CB--HB	1.09	0.97	125
CG1--HG12	1.09	0.97	99
CD2--HD22	1.09	0.97	75
CG1--HG13	1.09	0.97	99
NZ--HZ2	1.01	0.89	43
CA--HA2	1.09	0.97	51
OH--HH	0.96	0.84	18
OG--HG	0.96	0.84	39
CE--HE1	1.09	0.97	14
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	2
N--H	1.01	0.86	644
NH1--HH11	1.01	0.86	35
CE1--HE1	1.08	0.93	42
NH1--HH12	1.01	0.86	35
ND2--HD22	1.01	0.86	19
NE2--HE21	1.01	0.86	41
CD2--HD2	1.08	0.93	42
NE2--HE22	1.01	0.86	41
ND2--HD21	1.01	0.86	19
NE--HE	1.01	0.86	35
CD1--HD1	1.08	0.93	35

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CZ--HZ	1.08	0.93	17
CE2--HE2	1.08	0.93	35
NH2--HH21	1.01	0.86	35
ND1--HD1	1.01	0.86	7
NH2--HH22	1.01	0.86	35

Standard geometry: angle outliers

There are 39 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	133.61	1
OE1-CD-NE2	122.60	117.50	1
OE1-CD-NE2	122.60	117.58	1
OE1-CD-NE2	122.60	117.62	1
OE1-CD-NE2	122.60	117.67	1
OD1-CG-ND2	122.60	117.72	1
OE1-CD-NE2	122.60	117.85	1
OE1-CD-NE2	122.60	117.89	1
OE1-CD-NE2	122.60	117.90	1
OE1-CD-NE2	122.60	117.93	1
OE1-CD-NE2	122.60	117.97	1
OE1-CD-NE2	122.60	117.98	1
OE1-CD-NE2	122.60	118.03	1
OE1-CD-NE2	122.60	118.07	1
OE1-CD-NE2	122.60	118.11	1
OE1-CD-NE2	122.60	118.14	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.22	1
OE1-CD-NE2	122.60	118.24	1
OE1-CD-NE2	122.60	118.26	1
OE1-CD-NE2	122.60	118.27	1
CA-CB-CG	112.60	116.92	1
OE1-CD-NE2	122.60	118.29	1
OE1-CD-NE2	122.60	118.33	1
OE1-CD-NE2	122.60	118.35	3
OE1-CD-NE2	122.60	118.39	1
OE1-CD-NE2	122.60	118.43	1
OE1-CD-NE2	122.60	118.45	1
CB-CG-CD2	131.20	125.85	1
OE1-CD-NE2	122.60	118.48	1
OD1-CG-ND2	122.60	118.50	1
OE1-CD-NE2	122.60	118.51	2
OE1-CD-NE2	122.60	118.53	1
CB-CG-CD2	131.20	125.97	1
OE1-CD-NE2	122.60	118.60	1
HH11-NH1-HH12	107.56	120.00	1
HH21-NH2-HH22	106.75	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

Model ID	Clash score	Number of clashes
1	1.33	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	A:348:LEU:HD11	A:390:ARG:HH22	0.844
1	A:95:MET:HE1	A:237:LEU:HD13	0.610
1	A:41:VAL:HG21	A:73:ILE:HD12	0.549
1	A:348:LEU:HD11	A:390:ARG:NH2	0.525
1	A:53:VAL:HG21	A:73:ILE:HD13	0.497
1	A:107:ILE:HD11	A:209:VAL:HG11	0.476
1	A:389:TYR:CD2	A:413:GLY:HA3	0.459
1	A:32:ILE:HD11	A:42:HIS:HB2	0.450
1	B:146:ILE:HA	B:150:LEU:HD13	0.447
1	A:129:ILE:HG23	A:240:TYR:HB3	0.427
1	A:217:ALA:HA	A:220:TYR:CE1	0.426
1	A:41:VAL:CG2	A:73:ILE:HD12	0.422
1	A:55:PHE:CD1	A:88:VAL:HG22	0.409
1	A:74:VAL:CG1	A:233:PRO:CG	0.408

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	668	650	12	6

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	557	494	35	28

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	10	THR
1	A	11	LEU
1	A	19	TYR
1	A	157	ILE
1	A	273	LEU
1	A	386	LEU
1	A	407	GLN
1	A	410	LEU
1	A	487	PHE
1	B	4	LEU
1	B	6	LEU
1	B	8	LEU
1	B	10	LEU
1	B	18	LEU
1	B	22	LEU
1	B	27	LEU
1	B	31	LEU
1	B	36	LEU
1	B	39	LEU
1	B	67	LEU
1	B	75	LEU

Model ID	Chain	Residue ID	Residue type
1	B	84	THR
1	B	85	LEU
1	B	111	LEU
1	B	137	LEU
1	B	156	GLU
1	B	158	LEU
1	B	162	TYR

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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