Integrative Structure Validation Report

September 10, 2024 - 11:08 PM 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	9A5I
PDB-Dev ID	PDBDEV_00000275
Structure Title	Integrative model of MTNK-DHOM 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

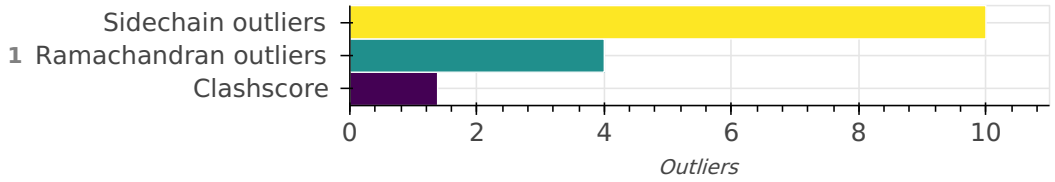
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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	MTNK_BACSU	A	A	397
1	2	2	DHOM_BACSU	B	B	433

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	-	1-397
B	-	1-433

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 6517 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
CG1--HG13	1.09	0.97	132

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CD1--HD11	1.09	0.97	135
CD2--HD21	1.09	0.97	79
CB--HB3	1.09	0.97	591
CD1--HD13	1.09	0.97	135
CB--HB2	1.09	0.97	591
CA--HA	1.09	0.97	773
CD--HD3	1.09	0.97	116
CG--HG2	1.09	0.97	230
CG--HG3	1.09	0.97	230
CB--HB	1.09	0.97	182
NZ--HZ1	1.01	0.89	58
CA--HA2	1.09	0.97	57
CG2--HG23	1.09	0.97	182
CD--HD2	1.09	0.97	116
CD2--HD23	1.09	0.97	79
CG2--HG22	1.09	0.97	182
CD1--HD12	1.09	0.97	135
CG1--HG12	1.09	0.97	132
CD2--HD22	1.09	0.97	79
CE--HE3	1.09	0.97	75
CG2--HG21	1.09	0.97	182
N--H3	1.01	0.89	2
NZ--HZ3	1.01	0.89	58

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CG--HG	1.09	0.97	79
CA--HA3	1.09	0.97	57
OG1--HG1	0.96	0.84	50
CE--HE2	1.09	0.97	75
CG1--HG11	1.09	0.97	76
OG--HG	0.96	0.84	52
NZ--HZ2	1.01	0.89	58
CE--HE1	1.09	0.97	17
OH--HH	0.96	0.84	24
CB--HB1	1.09	0.97	52
N--H1	1.01	0.89	2
N--H2	1.01	0.89	2
SG--HG	1.33	1.20	3
SG--HG	1.34	1.20	2
NH1--HH11	1.01	0.86	29
N--H	1.01	0.86	799
CD2--HD2	1.08	0.93	87
CD1--HD1	1.08	0.93	68
CE1--HE1	1.08	0.93	87
NE--HE	1.01	0.86	29
ND2--HD22	1.01	0.86	25
CE2--HE2	1.08	0.93	63
ND1--HD1	1.01	0.86	23
CZ--HZ	1.08	0.93	39

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NE2--HE22	1.01	0.86	25
NH2--HH22	1.01	0.86	29
NH1--HH12	1.01	0.86	29
NH2--HH21	1.01	0.86	29
ND2--HD21	1.01	0.86	25
NE2--HE21	1.01	0.86	25
CH2--HH2	1.08	0.93	5
CZ3--HZ3	1.08	0.93	5
NE1--HE1	1.01	0.86	5
CE3--HE3	1.08	0.93	5
NE2--HE2	1.01	0.86	1
CZ2--HZ2	1.08	0.93	5

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
CA-CB-CG	112.60	119.22	1
CA-CB-CG	112.60	118.11	1
OE1-CD-NE2	122.60	117.43	1
CB-CG-CD2	131.20	124.62	1
OE1-CD-NE2	122.60	117.72	1
CB-CG-CD2	131.20	125.03	1
CA-CB-CG	112.60	117.29	1
OE1-CD-NE2	122.60	117.96	1
OE1-CD-NE2	122.60	118.12	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OD1-CG-ND2	122.60	118.13	1
OE1-CD-NE2	122.60	118.14	1
OE1-CD-NE2	122.60	118.20	1
CB-CG-CD2	131.20	125.52	1
OE1-CD-NE2	122.60	118.25	1
OE1-CD-NE2	122.60	118.29	1
OE1-CD-NE2	122.60	118.32	1
CA-CB-CG	112.60	116.87	1
C-N-CA	121.70	129.30	1
OD1-CG-ND2	122.60	118.46	1
NE-CZ-NH2	119.20	122.92	1
OE1-CD-NE2	122.60	118.48	1
OE1-CD-NE2	122.60	118.49	1
OE1-CD-NE2	122.60	118.50	1
OE1-CD-NE2	122.60	118.51	1
CB-CG-CD2	131.20	125.92	1
CB-CG-CD2	131.20	125.95	1
HZ1-NZ-HZ3	96.99	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	1.38	18

All 18 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:141:THR:HG21	B:296:PHE:CZ	0.668
1	B:90:LEU:HD22	B:100:VAL:HG11	0.565
1	A:211:VAL:HG21	A:372:THR:HG23	0.535
1	B:19:VAL:HG22	B:39:ILE:HD13	0.517
1	B:51:ARG:HH12	B:60:LEU:HD13	0.506
1	B:51:ARG:HH12	B:60:LEU:CD1	0.497
1	B:168:LYS:HZ1	B:182:GLU:CD	0.488
1	B:13:THR:HG22	B:303:SER:HB2	0.479
1	A:178:GLU:OE1	A:223:LEU:HD21	0.471
1	B:90:LEU:HD22	B:100:VAL:CG1	0.469
1	A:69:VAL:HG13	A:70:VAL:HG23	0.435
1	A:211:VAL:CG2	A:372:THR:HG23	0.423
1	A:101:ARG:HH21	B:381:GLN:NE2	0.422
1	A:201:PHE:CZ	A:365:ARG:HD2	0.421
1	B:68:ILE:O	B:98:LYS:HE2	0.414
1	A:8:LEU:HD21	B:271:HIS:CE1	0.408
1	A:149:PHE:CD1	A:303:ALA:HB1	0.407
1	B:231:ILE:HD11	B:265:PRO:HB3	0.405

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	826	802	20	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	721	685	26	10

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	4	THR
1	A	8	LEU
1	A	58	LEU
1	A	161	LYS
1	A	190	ASP
1	A	360	ARG
1	A	393	LEU
1	B	13	THR
1	B	66	ASP
1	B	240	LYS

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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