

Integrative Structure Validation Report ?

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The following software was used in the production of this report:

Integrative Modeling Validation Version 2.0

Python-IHM Version 1.8

MolProbity Version 4.5.2

PDB ID	9A8A
PDB-Dev ID	PDBDEV_00000375
Structure Title	Dipeptide repeat designed model, 4x DPR1, verified with CD and NMR data.
Structure Authors	Moyer, A.P.; Baker, D.; Ramelot, T.A.; Montelione, G.T.
Deposited on	2024-03-08

This is a PDB-IHM IM Structure Validation Report for a publicly released PDB-IHM entry.

We welcome your comments at helpdesk@pdb-ihm.org

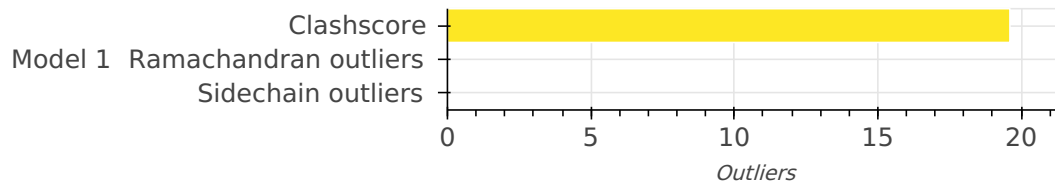
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 and fit to model assessments for SAS and crosslinking-MS 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 model(s). A total of 4 datasets were used to build this entry.

Representation ?

This entry has 1 representation(s).

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
1	1	1	ACE-PHE-CPI-PHE-CPI-PHE-CPI-NME peptide	A	10	-	1-10	100.00 / 0.00	Atomic

Datasets used for modeling ?

There are 4 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
2	NMR data	BMRB	52496
3	Other	Not available	Not available
4	NMR data	BMRB	52497
5	NMR data	BMRB	52500

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	None	None	AIMNet(SMD)-D4 used for energy minimizations and scoring	None	False	False

There are 5 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
4	PDBStat	5.21	restraint analysis and structure quality assessment	https://github.rpi.edu/RPIBioinformatics/PDBStat_public
5	Poky	build 20220114	NMR data analysis	https://sites.google.com/view/pokynmr
1	AIMNet	AIMNet(SMD)-D4	energy minimization and scoring	https://github.com/aiqm/aimnet
2	Cambridge Structural Database (CSD) ConfGen	Not available	initial conformation generator	http://confgen.net
3	SciPy	1.12.0	code for model building	https://scipy.org/

Data quality ?

NMR

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 no bond length outliers.

Standard geometry: angle outliers ?

There are no bond angle outliers.

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 atomic models in this entry.

Model ID	Clash score	Number of clashes
1	19.61	3

There are 3 clashes. The table below contains the detailed list of all clashes based on a MolProbity analysis. Bad clashes are ≥ 0.4 Angstrom.

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:4:PHE:HA	A:5:CPI:HE2	0.43	1	1
A:8:PHE:HA	A:9:CPI:HE2	0.42	1	1
A:6:PHE:HA	A:7:CPI:HE2	0.42	1	1

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	Analysed	Favored	Allowed	Outliers
1	0	0	0	0

Torsion angles : Protein sidechains ?

In the following table, sidechain rotameric outliers are listed. The Analysed column shows the number of residues for which the sidechain conformation was analysed.

Model ID	Analysed	Favored	Allowed	Outliers
1	4	4	0	0

Fit of model to data used for modeling ?

NMR

Validation for this section is under development.

Fit of model to data used for validation ?

Validation for this section is under development.

Acknowledgments

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