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	9A8B
PDB-Dev ID	PDBDEV_00000376
Structure Title	Dipeptide repeat designed model, 4x DPR2, verified with CD and NMR data.
Structure Authors	Moyer, A.P.; Baker, D.; Ramelot, T.A.; Montelione, G.T.

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

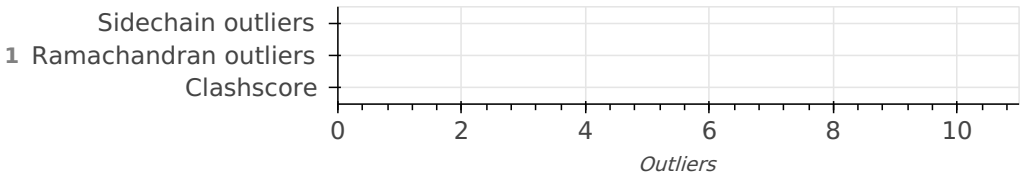
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 1 subunits in each model. A total of 3 datasets or restraints were used to build this entry. Each model is represented by 0 rigid bodies and 1 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	ACE-ZTR-PRO-ZTR-PRO-ZTR-PRO-ZTR-PRO-NME peptide	A	A	10

Datasets used for modeling

There are 3 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
2	NMR data	BMRB	52499
3	Other	Not available	Not available
4	NMR data	BMRB	52504

Representation

This entry has only one representation and includes 0 rigid bodies and 1 flexible units.

Chain ID	Rigid bodies	Non-rigid segments
A	-	1-10

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	Computational model produced with in-house monomer and dimer sampling protocols using AIMnet(SMD)-D4 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	Not available	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 28 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
CB--HB2	1.09	0.97	4
CG--HG3	1.09	0.97	4
CB--HB3	1.09	0.97	4
CA--HA	1.09	0.97	4
CG--HG2	1.09	0.97	4
CD--HD3	1.09	0.97	4
CD--HD2	1.09	0.97	4

Standard geometry: angle outliers

Bond angle outliers do not exist or can not be evaluated for this model

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	0.00	0

All 0 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

Model ID	Analyzed	Favored	Allowed	Outliers
1	0	0	0	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	4	4	0	0

Detailed list of outliers are tabulated below.

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.

Acknowledgements

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