Integrative Structure Validation Report

July 22, 2024 - 04:48 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	9A22
PDB-Dev ID	PDBDEV_00000139
Structure Title	Photoinduced intermediate J' of bacteriorhodopsin from 0.5 to 2 picosecond immediately after photoisomerization
Structure Authors	Ren, Z.

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

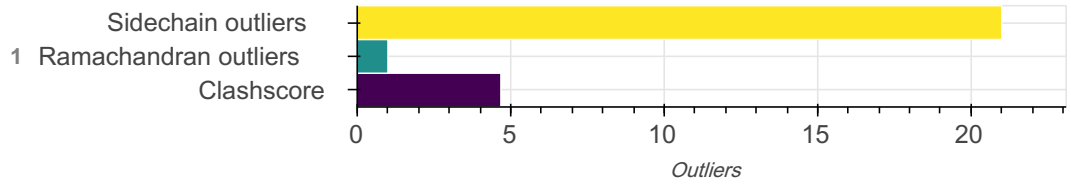
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 3 subunits in each model. A total of 21 datasets or restraints were used to build this entry. Each model is represented by 0 rigid bodies and 3 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	BACTERIORHODOPSIN	A	A	248
1	2	2	RETINAL	B	A	Not available
1	3	3	water	C	A	6

Datasets used for modeling

There are 21 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Experimental model	PDB	6g7h
2	Other	PDB	6g7h
3	Other	PDB	6g7i

ID	Dataset type	Database name	Data access code
4	Other	PDB	6g7j
5	Other	PDB	6g7k
6	Other	PDB	6ga2
7	Other	PDB	6ga4
8	Other	PDB	6ga5
9	Other	PDB	6ga6
10	Other	PDB	6ga7
11	Other	PDB	6ga8
12	Other	PDB	6ga9
13	Other	PDB	6gaa
14	Other	PDB	6gab
15	Other	PDB	6gac
16	Other	PDB	6gad
17	Other	PDB	6gae
18	Other	PDB	6gaf
19	Other	PDB	6gag
20	Other	PDB	6gah
21	Other	PDB	6gai

Representation

This entry has only one representation and includes 0 rigid bodies and 3 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	-	1-248

Chain ID	Rigid bodies	Non-rigid segments
B	-	None-None
C	-	1-6

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	Singular value decomposition	Singular value decomposition analysis of difference Fourier maps	None	1	False	False

There are 2 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	PHENIX	(1.13_2998: ???)	refinement	Not available
2	dynamiX	Not available	Data reduction	Not available

Data quality

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

Bond length outliers can not be evaluated for this model

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	4.68	17

All 17 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:159:LYS:O	A:162:SER:OG	0.710
1	A:156:PHE:HB3	A:171:PHE:CZ	0.620
1	A:121:THR:HG23	A:137:TRP:HE3	0.539
1	A:194:GLU:OE2	C:5:HOH:O	0.482
1	A:153:PHE:CE1	A:179:VAL:HG21	0.477
1	A:98:ALA:HB1	A:108:ILE:HG12	0.458
1	A:104:ASP:OD1	A:107:THR:OG1	0.447
1	A:16:GLY:O	A:20:MET:HG2	0.441
1	A:152:LEU:O	A:157:THR:HG22	0.439
1	A:107:THR:O	A:111:LEU:HB2	0.427
1	A:111:LEU:HA	A:111:LEU:HD12	0.409
1	A:156:PHE:HB3	A:171:PHE:HZ	0.407
1	A:87:LEU:HD23	A:88:PHE:CE2	0.406
1	A:15:LEU:HD23	A:209:MET:HE1	0.404
1	A:174:LEU:HD21	A:222:ILE:HB	0.404
1	A:69:VAL:HG12	A:71:PHE:HD2	0.404
1	A:12:TRP:CZ2	A:206:LEU:HD12	0.403

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	228	219	8	1

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	181	148	12	21

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	11	ILE
1	A	20	MET
1	A	28	LEU
1	A	29	VAL
1	A	30	LYS
1	A	40	LYS
1	A	55	THR
1	A	61	LEU
1	A	66	LEU
1	A	78	ILE
1	A	111	LEU
1	A	119	ILE
1	A	127	LEU
1	A	128	THR
1	A	129	LYS
1	A	145	MET

Model ID	Chain	Residue ID	Residue type
1	A	157	THR
1	A	169	SER
1	A	173	VAL
1	A	222	ILE
1	A	229	ILE

Fit of model to data used for modeling

Fit of model to data used for validation

Validation for this section is under development.

Acknowledgements

Development of integrative model validation metrics, implementation of a model validation pipeline, and creation of a validation report for integrative structures, are funded by NSF ABI awards (DBI-1756248, DBI-2112966, DBI-2112967, DBI-2112968, and DBI-1756250). The PDB-Dev team and members of Sali labcontributed model validation metrics and software packages.

Implementation of validation methods for SAS data and SAS-based models are funded byRCSB PDB (grant number DBI-1832184). Dr. Stephen Burley, Dr. John Westbrook, and Dr. Jasmine Young from RCSB PDB, Dr. Jill Trewhella, Dr. Dina Schneidman, and members of the SASBDB repository are acknowledged for their advice and support in implementing SAS validation methods.

Members of the wwPDB Integrative/Hybrid Methods Task Force provided recommendations and community support for the project.