

Integrative Structure Validation Report ?

February 18, 2025 - 08:33 AM PST

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	9A21
PDB-Dev ID	PDBDEV_00000138
Structure Title	Photoinduced intermediate I of bacteriorhodopsin at ~400 femtosecond with an expanded retinal binding pocket
Structure Authors	Ren, Z.
Deposited on	2022-07-15

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

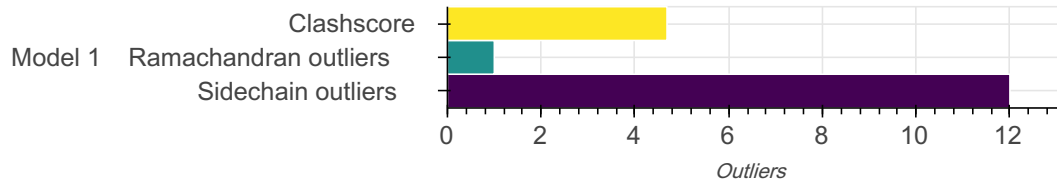
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 21 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	BACTERIORHODOPSIN	A	248	-	1-248	100.00 / 100.00	Atomic
		2	RETINAL	B [A]	Non-polymeric	-	-	Not available / Not available	Atomic
		3	water	C [A]	Non-polymeric	-	-	Not available / Not available	Atomic

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	X-ray diffraction data	PDB	6g7h

ID	Dataset type	Database name	Data access code
3	X-ray diffraction data	PDB	6g7i
4	X-ray diffraction data	PDB	6g7j
5	X-ray diffraction data	PDB	6g7k
6	X-ray diffraction data	PDB	6ga2
7	X-ray diffraction data	PDB	6ga4
8	X-ray diffraction data	PDB	6ga5
9	X-ray diffraction data	PDB	6ga6
10	X-ray diffraction data	PDB	6ga7
11	X-ray diffraction data	PDB	6ga8
12	X-ray diffraction data	PDB	6ga9
13	X-ray diffraction data	PDB	6gaa
14	X-ray diffraction data	PDB	6gab
15	X-ray diffraction data	PDB	6gac
16	X-ray diffraction data	PDB	6gad
17	X-ray diffraction data	PDB	6gae
18	X-ray diffraction data	PDB	6gaf
19	X-ray diffraction data	PDB	6gag
20	X-ray diffraction data	PDB	6gah
21	X-ray diffraction data	PDB	6gai

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 analysis of difference Fourier maps	Singular value decomposition	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	https://phenix-online.org/
2	dynamiX	Not available	Data reduction	Not available

Data quality ?

X-ray diffraction

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	4.68	17

There are 17 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:159:LYS:O	A:162:SER:OG	0.78	1	1
A:20:MET:HE2	A:213:VAL:HG22	0.76	1	1
A:157:THR:OG1	A:175:ARG:NH1	0.71	1	1
A:149:LEU:HD13	A:179:VAL:HG13	0.63	1	1
A:176:ASN:O	A:180:VAL:HG23	0.63	1	1
A:141:SER:HB3	B:1:RET:H41	0.57	1	1
A:156:PHE:HB3	A:171:PHE:CZ	0.55	1	1
A:153:PHE:CE2	A:179:VAL:HG21	0.52	1	1
A:181:LEU:HD13	A:215:ALA:HB2	0.49	1	1
A:68:MET:HB3	A:75:GLN:HG3	0.46	1	1
A:141:SER:CB	B:1:RET:H41	0.46	1	1
A:5:THR:OG1	A:6:GLY:N	0.43	1	1
A:156:PHE:HB3	A:171:PHE:HZ	0.43	1	1
A:218:GLY:O	A:222:ILE:HG13	0.42	1	1
A:66:LEU:HD11	A:77:PRO:HB2	0.41	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:83:TYR:CD1	A:83:TYR:N	0.41	1	1
A:157:THR:HA	A:171:PHE:HE2	0.41	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	228	218	9	1

There are 1 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	161	GLU	1

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	181	154	15	12

There are 12 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	29	VAL	1
A	34	VAL	1
A	46	THR	1
A	87	LEU	1
A	107	THR	1
A	128	THR	1
A	141	SER	1
A	164	ARG	1
A	166	GLU	1
A	173	VAL	1
A	177	VAL	1
A	178	THR	1

Fit of model to data used for modeling ?

X-ray diffraction

Validation for this section is under development.

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Acknowledgments

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