

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	9A26
PDB-Dev ID	PDBDEV_00000144
Structure Title	Photoinduced intermediate K of bacteriorhodopsin from 3 picosecond to 2 microsecond with a lifetime of more than five decades
Structure Authors	Ren, Z.
Deposited on	2022-07-28

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

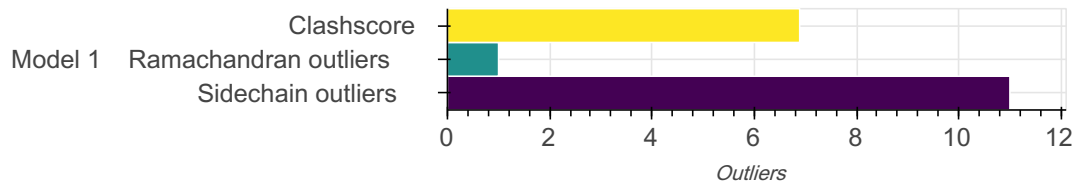
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 25 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	-	5-234	92.74 / 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 25 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	5b6v

ID	Dataset type	Database name	Data access code
3	X-ray diffraction data	PDB	5b6w
4	X-ray diffraction data	PDB	5b6x
5	X-ray diffraction data	PDB	5b6y
6	X-ray diffraction data	PDB	5b6z
7	X-ray diffraction data	PDB	5h2h
8	X-ray diffraction data	PDB	5h2i
9	X-ray diffraction data	PDB	5h2j
10	X-ray diffraction data	PDB	5h2k
11	X-ray diffraction data	PDB	5h2l
12	X-ray diffraction data	PDB	5h2m
13	X-ray diffraction data	PDB	5h2n
14	X-ray diffraction data	PDB	5h2o
15	X-ray diffraction data	PDB	5h2p
16	X-ray diffraction data	PDB	6g7h
17	X-ray diffraction data	PDB	6g7l
18	X-ray diffraction data	PDB	6ga1
19	X-ray diffraction data	PDB	6ga2
20	X-ray diffraction data	PDB	6ga3
21	X-ray diffraction data	PDB	6rmk
22	X-ray diffraction data	PDB	6rnj
23	X-ray diffraction data	PDB	6rph
24	X-ray diffraction data	PDB	6rqo
25	X-ray diffraction data	PDB	6rqp

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	None	None

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 1 bond length outliers in this entry (0.05% of 1839 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	121	THR	CB-CG2	4.80	1.36	1.52	1	1

Standard geometry: angle outliers ?

There are 2 bond angle outliers in this entry (0.08% of 2512 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	89	THR	C-N-CA	5.16	112.42	121.70	1	1
A	90	THR	CA-C-N	4.06	122.99	116.90	1	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 atomic models in this entry.

Model ID	Clash score	Number of clashes
1	6.89	25

There are 25 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:121:THR:HG22	A:141:SER:HB2	0.77	1	1
A:55:THR:HG23	A:56:MET:HE3	0.70	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:117:ILE:O	A:121:THR:HB	0.64	1	1
A:159:LYS:HG2	A:163:MET:HE1	0.62	1	1
A:156:PHE:HB3	A:171:PHE:CZ	0.61	1	1
A:160:ALA:HA	A:163:MET:HE2	0.55	1	1
A:157:THR:HA	A:171:PHE:HE2	0.54	1	1
A:52:ILE:O	A:55:THR:HG22	0.52	1	1
A:49:VAL:HB	A:50:PRO:HD3	0.51	1	1
A:157:THR:HG21	A:175:ARG:HH11	0.49	1	1
A:141:SER:HB3	B:1:RET:H41	0.48	1	1
A:37:PRO:O	A:41:LYS:HG3	0.45	1	1
A:29:VAL:HA	A:32:MET:HG3	0.44	1	1
A:157:THR:CG2	A:175:ARG:HH11	0.44	1	1
A:60:MET:HG3	A:81:ALA:HB3	0.44	1	1
A:101:VAL:HA	A:163:MET:HE3	0.44	1	1
A:55:THR:HG23	A:56:MET:CE	0.43	1	1
A:203:ILE:HA	A:203:ILE:HD13	0.42	1	1
A:218:GLY:O	A:222:ILE:HG13	0.42	1	1
A:93:LEU:HD13	C:8:HOH:O	0.42	1	1
A:56:MET:HA	A:56:MET:HE2	0.42	1	1
A:229:ILE:HG13	A:230:PHE:CD1	0.42	1	1
A:166:GLU:O	A:170:THR:OG1	0.42	1	1
A:49:VAL:HG13	A:89:THR:HB	0.41	1	1
A:85:ASP:C	A:85:ASP:OD1	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	223	4	1

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

Chain	Res	Type	Models (Total)
A	85	ASP	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	153	17	11

There are 11 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	5	THR	1
A	55	THR	1
A	61	LEU	1
A	66	LEU	1
A	100	LEU	1
A	111	LEU	1
A	121	THR	1
A	157	THR	1
A	164	ARG	1
A	170	THR	1
A	177	VAL	1

Fit of model to data used for modeling ?

X-ray diffraction

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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