

# Integrative Structure Validation Report ?

February 18, 2025 - 08:34 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	9A29
PDB-Dev ID	PDBDEV_00000147
Structure Title	Photoinduced intermediate M2 of bacteriorhodopsin from 0.5 to 5 millisecond
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](mailto:helpdesk@pdb-ihm.org)*

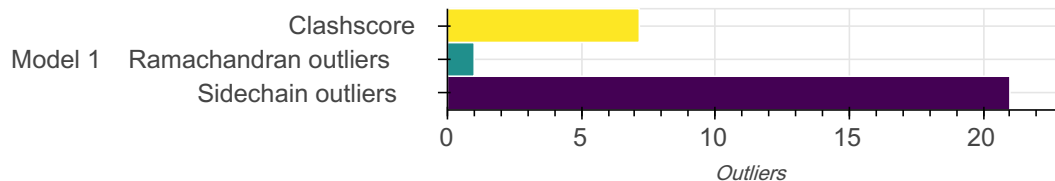
*A user guide is available at [https://pdb-ihm.org/validation\\_help.html](https://pdb-ihm.org/validation_help.html) with specific help available everywhere you see the ? symbol.*

*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	<a href="#">6g7h</a>
2	X-ray diffraction data	PDB	<a href="#">5b6v</a>

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

### 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	<a href="#">PHENIX</a>	(1.13_2998: ???)	refinement	<a href="https://phenix-online.org/">https://phenix-online.org/</a>
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	7.16	26

*There are 26 clashes. The table below contains the detailed list of all clashes based on a MolProbity analysis. Bad clashes are  $\geq 0.4$  Angstrom.*

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:124:VAL:O	A:128:THR:HG22	0.66	1	1
B:1:RET:H8	B:1:RET:H161	0.64	1	1
A:100:LEU:HD22	A:167:VAL:HG13	0.60	1	1
A:153:PHE:CZ	A:179:VAL:HG11	0.58	1	1
A:174:LEU:O	A:178:THR:OG1	0.57	1	1
A:82:ARG:HA	C:1:HOH:O	0.54	1	1
A:77:PRO:HG2	A:201:LEU:HD22	0.53	1	1
A:160:ALA:HB1	A:168:ALA:HA	0.52	1	1
A:42:PHE:O	A:46:THR:HG23	0.52	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:141:SER:HB3	B:1:RET:H41	0.51	1	1
A:38:ASP:HA	A:41:LYS:NZ	0.51	1	1
A:100:LEU:HD13	A:171:PHE:HB2	0.50	1	1
A:153:PHE:CE2	A:179:VAL:HG11	0.50	1	1
A:38:ASP:HA	A:41:LYS:HZ3	0.49	1	1
A:173:VAL:HG12	A:174:LEU:HD23	0.48	1	1
A:159:LYS:O	A:162:SER:OG	0.48	1	1
A:186:PRO:HB3	B:1:RET:H183	0.48	1	1
B:1:RET:C8	B:1:RET:H161	0.47	1	1
A:156:PHE:HB3	A:171:PHE:CZ	0.46	1	1
A:45:ILE:HD11	A:95:LEU:HD23	0.46	1	1
A:41:LYS:HE2	A:99:LEU:HD13	0.46	1	1
A:57:TYR:HA	A:60:MET:HE2	0.44	1	1
A:97:LEU:O	A:101:VAL:HG22	0.43	1	1
A:43:TYR:CE1	A:224:LEU:HD13	0.43	1	1
A:100:LEU:HA	A:100:LEU:HD23	0.42	1	1
B:1:RET:H7	B:1:RET:H181	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	219	8	1

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

Chain	Res	Type	Models (Total)
A	102	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	145	15	21

There are 21 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	5	THR	1

Chain	Res	Type	Models (Total)
A	11	ILE	1
A	15	LEU	1
A	35	SER	1
A	38	ASP	1
A	45	ILE	1
A	55	THR	1
A	66	LEU	1
A	68	MET	1
A	82	ARG	1
A	100	LEU	1
A	107	THR	1
A	111	LEU	1
A	128	THR	1
A	163	MET	1
A	169	SER	1
A	173	VAL	1
A	179	VAL	1
A	199	VAL	1
A	222	ILE	1
A	223	LEU	1

### Fit of model to data used for modeling ?

#### X-ray diffraction

Validation for this section is under development.

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Validation for this section is under development.

#### *Acknowledgments*

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