

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 | 9A27 |
| PDB-Dev ID | PDBDEV_00000145 |
| Structure Title | Photoinduced intermediate L of bacteriorhodopsin from 1 to 100 microsecond with a flattened 13-cis retinal |
| 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

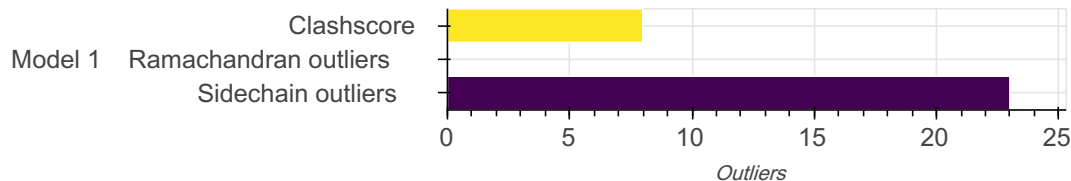
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 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 | 7.99 | 29 |

There are 29 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:160:ALA:HA | A:163:MET:HE2 | 0.77 | 1 | 1 |
| A:101:VAL:HA | A:163:MET:HE1 | 0.74 | 1 | 1 |
| A:157:THR:HG21 | A:175:ARG:HH11 | 0.68 | 1 | 1 |
| A:42:PHE:O | A:46:THR:OG1 | 0.62 | 1 | 1 |
| A:9:GLU:OE2 | A:79:TYR:OH | 0.58 | 1 | 1 |
| A:118:MET:HE1 | A:182:TRP:HZ3 | 0.55 | 1 | 1 |
| A:102:ASP:O | A:159:LYS:NZ | 0.54 | 1 | 1 |
| A:45:ILE:HG23 | A:92:LEU:HD22 | 0.54 | 1 | 1 |
| A:164:ARG:O | A:167:VAL:HG22 | 0.53 | 1 | 1 |

| Atom 1 | Atom 2 | Clash(Å) | Model ID (Worst) | Models (Total) |
|---------------|----------------|----------|------------------|----------------|
| A:156:PHE:HB3 | A:171:PHE:CZ | 0.52 | 1 | 1 |
| A:82:ARG:NE | C:2:HOH:O | 0.52 | 1 | 1 |
| A:163:MET:HE3 | A:167:VAL:HG21 | 0.52 | 1 | 1 |
| B:1:RET:H8 | B:1:RET:H171 | 0.52 | 1 | 1 |
| A:20:MET:HE1 | A:213:VAL:HA | 0.49 | 1 | 1 |
| A:77:PRO:HG2 | A:201:LEU:HD22 | 0.49 | 1 | 1 |
| A:153:PHE:CE2 | A:179:VAL:HG21 | 0.47 | 1 | 1 |
| A:194:GLU:N | A:194:GLU:OE1 | 0.45 | 1 | 1 |
| A:43:TYR:CE1 | A:224:LEU:HD13 | 0.45 | 1 | 1 |
| B:1:RET:H7 | B:1:RET:H181 | 0.45 | 1 | 1 |
| A:86:TRP:O | A:90:THR:OG1 | 0.45 | 1 | 1 |
| A:153:PHE:CD2 | A:179:VAL:HG21 | 0.44 | 1 | 1 |
| A:131:TYR:O | A:134:ARG:HB2 | 0.44 | 1 | 1 |
| A:66:LEU:HD23 | A:79:TYR:CD2 | 0.44 | 1 | 1 |
| A:166:GLU:CD | A:166:GLU:H | 0.43 | 1 | 1 |
| A:20:MET:CE | A:213:VAL:HA | 0.43 | 1 | 1 |
| A:56:MET:HG3 | A:85:ASP:HB2 | 0.43 | 1 | 1 |
| A:19:LEU:HA | A:19:LEU:HD12 | 0.41 | 1 | 1 |
| A:174:LEU:O | A:178:THR:OG1 | 0.41 | 1 | 1 |
| A:163:MET:HE3 | A:167:VAL:CG2 | 0.40 | 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 | 220 | 8 | 0 |

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 | 13 | 23 |

There are 23 unique sidechain outliers. Detailed list of outliers are tabulated below.

| Chain | Res | Type | Models (Total) |
|-------|-----|------|----------------|
| A | 7 | ARG | 1 |
| A | 11 | ILE | 1 |

| Chain | Res | Type | Models (Total) |
|-------|-----|------|----------------|
| A | 19 | LEU | 1 |
| A | 28 | LEU | 1 |
| A | 46 | THR | 1 |
| A | 61 | LEU | 1 |
| A | 66 | LEU | 1 |
| A | 68 | MET | 1 |
| A | 100 | LEU | 1 |
| A | 101 | VAL | 1 |
| A | 111 | LEU | 1 |
| A | 119 | ILE | 1 |
| A | 128 | THR | 1 |
| A | 132 | SER | 1 |
| A | 153 | PHE | 1 |
| A | 157 | THR | 1 |
| A | 159 | LYS | 1 |
| A | 164 | ARG | 1 |
| A | 166 | GLU | 1 |
| A | 187 | VAL | 1 |
| A | 199 | VAL | 1 |
| A | 211 | LEU | 1 |
| A | 223 | LEU | 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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