

**Summary of integrative structure determination of Parathyroid hormone receptor type 1 in complex with a long-acting parathyroid hormone analog and arrestin 2 (6pwc-based template) (PDB ID: 9A3M, PDB-Dev ID: PDBDEV\_00000207)**

| <b>1. Model Composition</b>                                           |                                                                                                                                                                                                                                                                                                                                           |
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| <a href="#">Entry composition</a>                                     | <ul style="list-style-type: none"> <li>- Arrestin2: chain(s) A (357 residues)</li> <li>- Long-acting parathyroid hormone analog: chain(s) B (32 residues)</li> <li>- PTH1R: chain(s) C [P] (504 residues)</li> </ul>                                                                                                                      |
| <a href="#">Datasets used for modeling</a>                            | <ul style="list-style-type: none"> <li>- Crosslinking-MS data, Not available</li> <li>- Experimental model, PDB: <a href="#">6NBF</a></li> <li>- Experimental model, PDB: <a href="#">6PWC</a></li> <li>- Comparative model, Not available</li> <li>- Comparative model, Not available</li> <li>- De Novo model, Not available</li> </ul> |
| <b>2. Representation</b>                                              |                                                                                                                                                                                                                                                                                                                                           |
| <a href="#">Number of representations</a>                             | 1                                                                                                                                                                                                                                                                                                                                         |
| <a href="#">Scale</a>                                                 | Atomic                                                                                                                                                                                                                                                                                                                                    |
| Number of <a href="#">rigid</a> and <a href="#">flexible</a> segments | 0, 3                                                                                                                                                                                                                                                                                                                                      |
| <b>3. Restraints</b>                                                  |                                                                                                                                                                                                                                                                                                                                           |
| <a href="#">Physical principles</a>                                   | Information about physical principles was not provided                                                                                                                                                                                                                                                                                    |
| <a href="#">Experimental data</a>                                     | - 1 unique CrossLinkRestraint: BrEtY, 136 crosslinks                                                                                                                                                                                                                                                                                      |
| <b>4. Validation</b>                                                  |                                                                                                                                                                                                                                                                                                                                           |
| <a href="#">Number of ensembles</a>                                   | 0                                                                                                                                                                                                                                                                                                                                         |
| <a href="#">Number of models in ensembles</a>                         | Not applicable                                                                                                                                                                                                                                                                                                                            |
| <a href="#">Number of deposited models</a>                            | 1                                                                                                                                                                                                                                                                                                                                         |
| <a href="#">Model precision (uncertainty of models)</a>               | Not available                                                                                                                                                                                                                                                                                                                             |
| <a href="#">Data quality</a>                                          | Data quality has not been assessed                                                                                                                                                                                                                                                                                                        |
| <a href="#">Model quality: assessment of atomic segments</a>          | <ul style="list-style-type: none"> <li>- Clashscore: 1.54</li> <li>- Ramachandran outliers: 9</li> <li>- Sidechain outliers: 12</li> </ul>                                                                                                                                                                                                |
| <a href="#">Fit to data used for modeling</a>                         | Satisfaction of crosslinks: 45.16%                                                                                                                                                                                                                                                                                                        |

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|-------------------------------------------------|----------------------------------------------------------------------------|
| <a href="#">Fit to data used for validation</a> | Fit of model to information not used to compute it has not been determined |
| <b>5. Methodology and Software</b>              |                                                                            |
| 1. <a href="#">Name</a>                         | None                                                                       |
| <a href="#">Software</a>                        | <a href="#">ICM-Pro</a> (version v.3.9.2c)                                 |