

**Summary of integrative structure determination of Parathyroid hormone receptor type 1 in complex with a long-acting parathyroid hormone analog and arrestin 2 (6u1n-based template)**  
(PDB ID: 9A3I | pdb\_00009a3i, PDB-Dev ID: PDBDEV\_00000203 )

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| <b>1. Model Composition</b>                                       |                                                                                                                                                                                                                                                                                                                                                           |
| <a href="#">1.1. 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="#">1.2. Datasets used for modeling</a>                   | <ul style="list-style-type: none"> <li>- Crosslinking-MS data, Not available</li> <li>- Experimental model, PDB: <a href="#">pdb_00006nbf</a></li> <li>- Experimental model, PDB: <a href="#">pdb_00006u1n</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="#">2.1. Number of representations</a>                    | 1                                                                                                                                                                                                                                                                                                                                                         |
| <a href="#">2.2. Scale</a>                                        | Atomic                                                                                                                                                                                                                                                                                                                                                    |
| <a href="#">2.3. Number of rigid and flexible segments</a>        | 0, 3                                                                                                                                                                                                                                                                                                                                                      |
| <b>3. Restraints</b>                                              |                                                                                                                                                                                                                                                                                                                                                           |
| <a href="#">3.1. Physical principles</a>                          | Information about physical principles was not provided                                                                                                                                                                                                                                                                                                    |
| <a href="#">3.2. Experimental data</a>                            | - 1 unique CrossLinkRestraint: BrEtY, 136 crosslinks                                                                                                                                                                                                                                                                                                      |
| <b>4. Validation</b>                                              |                                                                                                                                                                                                                                                                                                                                                           |
| <a href="#">4.2. Number of ensembles</a>                          | 0                                                                                                                                                                                                                                                                                                                                                         |
| <a href="#">4.3. Number of models in ensembles</a>                | Not applicable                                                                                                                                                                                                                                                                                                                                            |
| <a href="#">4.4. Number of deposited models</a>                   | 1                                                                                                                                                                                                                                                                                                                                                         |
| <a href="#">4.5. Model precision</a>                              | Not available                                                                                                                                                                                                                                                                                                                                             |
| <a href="#">4.6. Data quality</a>                                 | Data quality has not been assessed                                                                                                                                                                                                                                                                                                                        |
| <a href="#">4.7. Model quality: assessment of atomic segments</a> | <ul style="list-style-type: none"> <li>- Clashscore: 3.85</li> <li>- Ramachandran outliers: 15</li> <li>- Sidechain outliers: 19</li> </ul>                                                                                                                                                                                                               |
| <a href="#">4.8. Fit to data used for modeling</a>                | Satisfaction of crosslinks: 51.61%                                                                                                                                                                                                                                                                                                                        |
| <a href="#">4.9. 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>                                |                                                                                                                                                                                                                                                                                                                                                           |

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| 1. <a href="#">5.1. Method name</a> | Not available                              |
| <a href="#">5.5. Software</a>       | <a href="#">ICM-Pro</a> (version v.3.9.2c) |