

Summary of integrative structure determination of Parathyroid hormone receptor type 1 in complex with a long-acting parathyroid hormone analog and arrestin 2 (6up7-based template) (PDB ID: 9A3J, PDB-Dev ID: PDBDEV_0000204)

| 1. Model Composition | |
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| Entry composition | <ul style="list-style-type: none"> - PTH1R: Chain C (504 residues) - Long-acting parathyroid hormone analog: Chain B (32 residues) - Arrestin2: Chain A (357 residues) |
| Datasets used for modeling | <ul style="list-style-type: none"> - Crosslinking-MS data, Linker name and number of cross-links: BrEtY, 136 cross-links - Experimental model, PDB ID: 6NBF - Experimental model, PDB ID: 6UP7 - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - De Novo model, Not available |
| 2. Representation | |
| Resolution | Atomic |
| Number of rigid bodies , flexible units | 0, 3 |
| Flexible units | <ul style="list-style-type: none"> - C: 1-504 - A: 1-357 - B: 1-32 |
| Structural coverage (rigid bodies) | 100% |
| 3. Restraints | |
| Physical principles | Information about physical principles was not provided |
| Experimental data | - 1 unique CrossLinkRestraint: BrEtY, 136 cross-links |
| 4. Validation | |
| Number of ensembles | 0 |
| Number of models in ensembles | Not applicable |
| Number of deposited models | 1 |
| Model precision (uncertainty of models) | Model precision can not be calculated with one structure |
| Data quality | Data quality has not been assessed |

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| <i>Model quality: assessment of atomic segments</i> | Model-1: Clashscore = 3.38, Number of Ramachandran outliers = 19, Number of sidechain outliers = 28 |
| <i>Model quality: assessment of excluded volume</i> | Not applicable |
| <i>Fit to data used for modeling</i> | Fit of model to information used to compute it has not been determined |
| <i>Fit to data used for validation</i> | Fit of model to information not used to compute it has not been determined |
| 5. Methodology and Software | |
| 1. <i>Method</i> | None |
| <i>Name</i> | None |
| <i>Software</i> | ICM-Pro (version v.3.9.2c) |