

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-Dev ID: PDBDEV_00000203)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - Long-acting parathyroid hormone analog: Chain B (32 residues) - PTH1R: Chain C (504 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: 6U1N - 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

<i>Model quality: assessment of atomic segments</i>	Model-1: Clashscore = 3.85, Number of Ramachandran outliers = 15, Number of sidechain outliers = 19
<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)