

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"> - Arrestin2: chain(s) A (357 residues) - Long-acting parathyroid hormone analog: chain(s) B (32 residues) - PTH1R: chain(s) C [P] (504 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - Crosslinking-MS data, Not available - Experimental model, PDB: 6NBF - Experimental model, PDB: 6U1N - Comparative model, Not available - Comparative model, Not available - De Novo model, Not available
2. Representation	
Number of representations	1
Scale	Atomic
Number of rigid and flexible segments	0, 3
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique CrossLinkRestraint: BrEtY, 136 crosslinks
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	1
Model precision (uncertainty of models)	Not available
Data quality	Data quality has not been assessed
Model quality: assessment of atomic segments	<ul style="list-style-type: none"> - Clashscore: 3.84 - Ramachandran outliers: 15 - Sidechain outliers: 19
Fit to data used for modeling	Satisfaction of crosslinks: 51.61%

Fit to data used for validation	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
1. Name	None
Software	ICM-Pro (version v.3.9.2c)