

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)

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

<u>Model quality: assessment of atomic segments</u>	Model-1: Clashscore = 1.54, Number of Ramachandran outliers = 9, Number of sidechain outliers = 12
<u>Model quality: assessment of excluded volume</u>	Not applicable
<u>Fit to data used for modeling</u>	Fit of model to information used to compute it has not been determined
<u>Fit to data used for validation</u>	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
1. <u>Method</u>	None
<u>Name</u>	None
<u>Software</u>	ICM-Pro (version v.3.9.2c)