

Summary of integrative structure determination of Modeling of the GLP-1 receptor-Gs complex (PDB ID: 9A3F, PDB-Dev ID: PDBDEV_0000200)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - GB: Chain D (340 residues) - GLP1: Chain B (31 residues) - GA: Chain C (394 residues) - GG: Chain E (71 residues) - NB: Chain F (129 residues) - GLP1R: Chain A (440 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - Crosslinking-MS data, Linker name and number of cross-links: BS3, 228 cross-links - Experimental model, PDB ID: Not available - Experimental model, PDB ID: Not available - Experimental model, PDB ID: Not available - Experimental model, PDB ID: Not available - Experimental model, PDB ID: Not available - Experimental model, PDB ID: Not available - Experimental model, PDB ID: Not available - Other, File: 10.5281/zenodo.13325078 - Other, File: 10.5281/zenodo.13325078 - Other, File: 10.5281/zenodo.13325078 - Other, File: 10.5281/zenodo.13325078 - Experimental model, PDB ID: 6X18
2. Representation	
Resolution	Atomic
Number of rigid bodies , flexible units	0, 14
Flexible units	<ul style="list-style-type: none"> - B: 1-31 - A: 1-400, 401-440 - C: 1-10, 11-391, 392-394 - E: 1-6, 7-45, 46-71 - F: 1-1, 2-127, 128-129 - D: 1-2, 3-340
Structural coverage (rigid bodies)	100%
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	<ul style="list-style-type: none"> - 1 unique CrossLinkRestraint: BS3, 228 cross-links - 1 unique CrossLinkRestraint: DSG, 203 cross-links - 1 unique CrossLinkRestraint: EDC, 126 cross-links - 1 unique CrossLinkRestraint: KARGO, 40 cross-links
4. Validation	

<i>Number of ensembles</i>	1
<i>Number of models in ensembles</i>	29999
<i>Number of deposited models</i>	7
<i>Model precision (uncertainty of models)</i>	None, Å
<i>Data quality</i>	Data quality has not been assessed
<i>Model quality: assessment of atomic segments</i>	<ul style="list-style-type: none"> - Model-1: Clashscore = 158.69, Number of Ramachandran outliers = 117, Number of sidechain outliers = 74 - Model-2: Clashscore = 182.34, Number of Ramachandran outliers = 138, Number of sidechain outliers = 94 - Model-3: Clashscore = 158.34, Number of Ramachandran outliers = 139, Number of sidechain outliers = 60 - Model-4: Clashscore = 154.41, Number of Ramachandran outliers = 123, Number of sidechain outliers = 89 - Model-5: Clashscore = 204.24, Number of Ramachandran outliers = 164, Number of sidechain outliers = 115 - Model-6: Clashscore = 144.74, Number of Ramachandran outliers = 120, Number of sidechain outliers = 81 - Model-7: Clashscore = 227.11, Number of Ramachandran outliers = 139, Number of sidechain outliers = 81
<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. Method	Sampling
<i>Name</i>	Replica exchange monte carlo
<i>Number of computed models</i>	844020
<i>Software</i>	<ul style="list-style-type: none"> - IMP PMI module (version Not available) - Integrative Modeling Platform (IMP) (version Not available) - MODELLER (version Not available)