

Summary of integrative structure determination of Rosetta model of human LRH-1 nuclear receptor generated with XL-MS, HDX-MS, and SAXS data (PDB ID: 8ZZZ, PDB-Dev ID: PDBDEV_00000035)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - LRH-1 DNA-binding domain: chain(s) A (102 residues) - LRH-1 Ligand-binding domain: chain(s) B (240 residues) - LRH-1 full length polypeptide: chain(s) C (538 residues) - PGC1-alpha coactivator peptide: chain(s) D (10 residues) - DNA strand 1: chain(s) E (12 residues) - DNA strand 2: chain(s) F (12 residues) - Phospholipid ligand: chain(s) X - Zinc ion: chain(s) Y, Z
Datasets used for modeling	<ul style="list-style-type: none"> - Experimental model, PDB: 2A66 - Experimental model, PDB: 1YOK - Comparative model, Zenodo: 10.5281/zenodo.3405545 - Comparative model, Zenodo: 10.5281/zenodo.3405545 - Crosslinking-MS data, Zenodo: 10.5281/zenodo.3405545 - H/D exchange data, Zenodo: 10.5281/zenodo.3405545 - Integrative model, Zenodo: 10.5281/zenodo.3405545 - Crosslinking-MS data, Zenodo: 10.5281/zenodo.3405545 - SAS data, SASBDB: SASDG85
2. Representation	
Number of representations	2
Scale	<ul style="list-style-type: none"> - Atomic - Atomic
Number of rigid and flexible segments	<ul style="list-style-type: none"> - 2, 3 - 3, 1
3. Restraints	
Physical principles	Information about physical principles was not provided

Experimental data	<ul style="list-style-type: none"> - 1 unique CrossLinkRestraint: BS3, 3 crosslinks - 1 unique CrossLinkRestraint: BS3, 10 crosslinks - 1 unique SASRestraint: Assembly name: Assembly of full-length LRH-1 with DNA, coactivator and P6L Ligand Fitting method: CRY SOL Multi-state: True
4. Validation	
Number of ensembles	1
Number of models in ensembles	10
Number of deposited models	11
Model precision (uncertainty of models)	Not available
Data quality	SASDG85: Rg from Gunier is 3.82nm and Rg from p(r) is 3.91nm
Model quality: assessment of atomic segments	<ul style="list-style-type: none"> - Clashscore: 0.00-0.00 - Ramachandran outliers: 0-12 - Sidechain outliers: 0-2
Fit to data used for modeling	Satisfaction of crosslinks: 70.00-100.00%
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	Loop modeling
Method	RosettaRemodel
Number of computed models	100
2. Name	Docking
Method	RosettaDock
Number of computed models	40000
3. Name	Linker modeling
Method	Ranch and RosettaMinimize
Number of computed models	45000
Software	<ul style="list-style-type: none"> - Rosetta (version 3.10) - ATSAS (version 2.8.4) - REMO (version 1)