

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"> - Zinc ion: Chain Z (Not available residues) - LRH-1 DNA-binding domain: Chain A (102 residues) - Zinc ion: Chain Y (Not available residues) - LRH-1 full length polypeptide: Chain C (538 residues) - LRH-1 Ligand-binding domain: Chain B (240 residues) - PGC1-alpha coactivator peptide: Chain D (10 residues) - DNA strand 1: Chain E (12 residues) - DNA strand 2: Chain F (12 residues) - Phospholipid ligand: Chain X (Not available residues)
Datasets used for modeling	<ul style="list-style-type: none"> - Experimental model, PDB ID: 2A66 - Experimental model, PDB ID: 1YOK - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Crosslinking-MS data, Linker name and number of cross-links: BS3, 3 cross-links - H/D exchange data, File: 10.5281/zenodo.3405545 - Integrative model, File: 10.5281/zenodo.3405545 - Crosslinking-MS data, Linker name and number of cross-links: BS3, 10 cross-links - SAS data, SASBDB: SASDG85
2. Representation	
Resolution	Atomic
Number of <i>rigid bodies</i>, <i>flexible units</i>	10, 5
<i>Rigid bodies</i>	<ul style="list-style-type: none"> - A: - - B: - - C: - - D: 1-10 - E: 1-121-12 - F: 1-121-12 - X: None-None - Y: None-NoneNone-None - Z: None-NoneNone-None

<i>Flexible units</i>	<ul style="list-style-type: none"> - A: 1-102 - B: 1-240 - C: 1-538 - D: 1-10 - E: - - F: - - X: None-None - Y: - - Z: -
<i>Structural coverage (rigid bodies)</i>	100%
3. Restraints	
<i>Physical principles</i>	Information about physical principles was not provided
<i>Experimental data</i>	<ul style="list-style-type: none"> - 1 unique CrossLinkRestraint: BS3, 3 cross-links - 1 unique CrossLinkRestraint: BS3, 10 cross-links - 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	
<i>Number of ensembles</i>	1
<i>Number of models in ensembles</i>	10
<i>Number of deposited models</i>	11
<i>Model precision (uncertainty of models)</i>	None, Å
<i>Data quality</i>	SASDG85: Rg from Guinier is 3.82nm and Rg from p(r) is 3.91nm

<p><i>Model quality: assessment of atomic segments</i></p>	<ul style="list-style-type: none"> - Model-1: Clashscore = 0.0, Number of Ramachandran outliers = 8, Number of sidechain outliers = 0 - Model-2: Clashscore = 0.0, Number of Ramachandran outliers = 6, Number of sidechain outliers = 1 - Model-3: Clashscore = 0.0, Number of Ramachandran outliers = 7, Number of sidechain outliers = 1 - Model-4: Clashscore = 0.0, Number of Ramachandran outliers = 12, Number of sidechain outliers = 1 - Model-5: Clashscore = 0.0, Number of Ramachandran outliers = 7, Number of sidechain outliers = 0 - Model-6: Clashscore = 0.0, Number of Ramachandran outliers = 8, Number of sidechain outliers = 1 - Model-7: Clashscore = 0.0, Number of Ramachandran outliers = 9, Number of sidechain outliers = 1 - Model-8: Clashscore = 0.0, Number of Ramachandran outliers = 3, Number of sidechain outliers = 1 - Model-9: Clashscore = 0.0, Number of Ramachandran outliers = 8, Number of sidechain outliers = 0 - Model-10: Clashscore = 0.0, Number of Ramachandran outliers = 4, Number of sidechain outliers = 0 - Model-11: Clashscore = 0.0, Number of Ramachandran outliers = 11, Number of sidechain outliers = 0
<p><i>Model quality: assessment of excluded volume</i></p>	<p>Not applicable</p>
<p><i>Fit to data used for modeling</i></p>	<p>Fit of model to information used to compute it has not been determined</p>
<p><i>Fit to data used for validation</i></p>	<p>Fit of model to information not used to compute it has not been determined</p>
<p>5. Methodology and Software</p>	
<p>1. <i>Method</i></p>	<p>Loop modeling</p>
<p><i>Name</i></p>	<p>RosettaRemodel</p>
<p><i>Number of computed models</i></p>	<p>100</p>
<p>2. <i>Method</i></p>	<p>Docking</p>
<p><i>Name</i></p>	<p>RosettaDock</p>
<p><i>Number of computed models</i></p>	<p>40000</p>
<p>3. <i>Method</i></p>	<p>Linker modeling</p>
<p><i>Name</i></p>	<p>Ranch and RosettaMinimize</p>

<i>Number of computed models</i>	45000
<i>Software</i>	<ul style="list-style-type: none">- Rosetta (version 3.10)- ATSAS (version 2.8.4)- REMO (version 1)