

**Summary of integrative structure determination of Integrative structure
of P450-Ferredoxin Complex (PDB ID: 8ZZD, PDB-Dev ID:
PDBDEV_00000013)**

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - CYP199A2: chain(s) A [A1] (399 residues) - HaPux: chain(s) B [C1] (106 residues) - PROTOPORPHYRIN IX CONTAINING FE: chain(s) C [A1] - 4-METHOXYBENZOIC ACID: chain(s) D [A1] - CHLORIDE ION: chain(s) E [A1] - FE2/S2 (INORGANIC) CLUSTER: chain(s) F [C1]
Datasets used for modeling	<ul style="list-style-type: none"> - Experimental model, PDB: 4DNJ - Experimental model, PDB: 4LTU - EPR data, Not available: 10.5287/bodleian:5zqPg5yVe - EPR data, Not available: 10.5287/bodleian:5zqPg5yVe - EPR data, Not available: 10.5287/bodleian:5zqPg5yVe - EPR data, Not available: 10.5287/bodleian:5zqPg5yVe - EPR data, Not available: 10.5287/bodleian:5zqPg5yVe - EPR data, Not available: 10.5287/bodleian:5zqPg5yVe
2. Representation	
Number of representations	1
Scale	Atomic
Number of rigid and flexible segments	2, 0
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	<ul style="list-style-type: none"> - 1 unique DerivedDistanceRestraint: Upper Bound Distance: 41.2 - 1 unique DerivedDistanceRestraint: Upper Bound Distance: 23.0 - 1 unique DerivedDistanceRestraint: Upper Bound Distance: 35.2 - 1 unique DerivedDistanceRestraint: Upper Bound Distance: 26.8 - 1 unique DerivedDistanceRestraint: Upper Bound Distance: 44.2 - 1 unique DerivedDistanceRestraint: Upper Bound Distance: 31.0

4. Validation	
<i>Number of ensembles</i>	1
<i>Number of models in ensembles</i>	6
<i>Number of deposited models</i>	6
<i>Model precision (uncertainty of models)</i>	Not available
<i>Data quality</i>	Data quality has not been assessed
<i>Model quality: assessment of atomic segments</i>	<ul style="list-style-type: none"> - Clashscore: 2.45-3.10 - Ramachandran outliers: 10-15 - Sidechain outliers: 11-18
<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. <i>Name</i>	Integrative Modeling
<i>Software</i>	<ul style="list-style-type: none"> - PatchDock (version Beta1.3) - FireDock (version develop-5abded4c39) - MMM (version 2017.1) - Matlab (version R2017a) - Gromacs (version Not available)