

Summary of integrative structure determination of Structure of the human myeloid-derived growth factor (hMYDGF) engaging the chicken KDEL receptor 2 (cKDELR2) (PDB ID: 9A00, PDB-Dev ID: PDBDEV_00000036)

1. Model Composition	
Entry composition	- Myeloid-derived growth factor: Chain B (142 residues) - ER lumen protein-retaining receptor 2: Chain A (207 residues)
Datasets used for modeling	- Experimental model, PDB ID: 6O6W - Experimental model, PDB ID: 6I6H
2. Representation	
Resolution	Atomic
Number of <i>rigid bodies</i>, <i>flexible units</i>	2, 0
Rigid bodies	- B: 1-142 - A: 1-207
Structural coverage (<i>rigid bodies</i>)	100%
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 36 unique DerivedDistanceRestraint: Upper Bound Distance: 3.0
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	2
Model precision (<i>uncertainty of models</i>)	Model precision can not be calculated with one structure
Data quality	Data quality has not been assessed
Model quality: <i>assessment of atomic segments</i>	- Model-1: Clashscore = 4.8, Number of Ramachandran outliers = 1, Number of sidechain outliers = 23 - Model-2: Clashscore = 4.09, Number of Ramachandran outliers = 1, Number of sidechain outliers = 19
Model quality: <i>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. <i>Method</i>	?
<i>Name</i>	?
<i>Number of computed models</i>	?
<i>Software</i>	HADDOCK (version Not available)