## Summary of integrative structure determination of structure of the human myeloid-derived growth factor (hmydgf) engaging the chicken kdel receptor 2 (ckdelr2) (PDBDEV00000036)

| 1. Model Composition                                  |   |
|---|---|
| Entry composition                                     | - ER lumen protein-retaining receptor 2: Chain A (207 residues) - Myeloid-derived growth factor: Chain B (142 residues) |
| Datasets used for modeling                            | - Experimental model, PDB ID: 606W<br>- Experimental model, PDB ID: 616H  |
| 2. Representation                                     |   |
| Atomic structural coverage                            | 100%  |
| Number of <u>rigid bodies</u> , <u>flexible units</u> | 2, 0  |
| Rigid bodies  | - B: 1-142:Experimental model/6O6W.<br>- A: 1-207:Experimental model/6I6H.  |
| Flexible units  | - B: -<br>- A: -  |
| Resolution  | - Rigid bodies: 1 residue per bead.<br>- Flexible regions: N/A  |
| 3. Restraints   |   |
| Physical principles                                   | Information about physical principles was not provided  |
| Experimental data                                     | - 36 unique DerivedDistanceRestraint: Upper Bound Distance: 3.0   |
| 4. Validation   |   |
| Sampling validation                                   | - Information related to sampling validation has not been provided  |
| Clustering algorithm ,clustering feature              | Distance threshold-based clustering used if ensembles are deposited, Not applicable                                     |
| Number of ensembles                                   | 0   |
| Number of models in ensembles                         | Not applicable  |
| Model precision (uncertainty of models)               | Model precision can not be calculated with one structure  |
| Quality of data                                       | - Quality of input data has not be assessed   |
| Model quality: assessment of atomic segments          | Clashscore: 5.16, Ramachandran outliers: 0.29%, Sidechain outliers: 6.95%   |
| Model quality: assessment of excluded volume          | - Not applicable  |

| Fit of the model to information used to compute it     | - Fit of model to information used to compute it has not been determined     |
|--|--|
| Fit of the model to information not used to compute it | - Fit of model to information not used to compute it has not been determined |
| 5. Methodology and Software                            |  |
| <u>Method</u>  | ?  |
| <u>Name</u>  | ?  |
| <u>Details</u>   | - Method details unspecified   |
| <u>Software</u>  | - HADDOCK (version None) - No location specified                             |