

**Summary of integrative structure determination of Structure
determination of the HgcAB complex using metagenome sequence data,
coevolution analysis, and ab initio structure calculations (PDB ID: 9A0B,
PDB-Dev ID: PDBDEV_00000047)**

1. Model Composition	
<i>Entry composition</i>	<ul style="list-style-type: none"> - HgcA: chain(s) A (329 residues) - HgcB: chain(s) B (95 residues) - COBALAMIN: chain(s) C [A] - IRON/SULFUR CLUSTER: chain(s) D [B], E [B]
<i>Datasets used for modeling</i>	<ul style="list-style-type: none"> - Predicted contacts, Not available - De Novo model, Not available - De Novo model, Not available - De Novo model, Not available - Experimental model, PDB: 2FDN - Experimental model, PDB: 8C7P
2. Representation	
<i>Number of representations</i>	1
<i>Scale</i>	Atomic
<i>Number of rigid and flexible segments</i>	0, 3
3. Restraints	
<i>Physical principles</i>	Information about physical principles was not provided
	<ul style="list-style-type: none"> - 18 unique DerivedDistanceRestraint: restraint type HarmonicDistanceRestraintExperimental model - 2 unique PredictedContactRestraint: Distance: 10.16 - 1 unique PredictedContactRestraint: Distance: 11.145 - 1 unique PredictedContactRestraint: Distance: 10.303 - 6 unique PredictedContactRestraint: Distance: 8.72 - 1 unique PredictedContactRestraint: Distance: 7.083 - 4 unique PredictedContactRestraint: Distance: 6.904 - 4 unique PredictedContactRestraint: Distance: 6.957 - 5 unique PredictedContactRestraint: Distance: 6.929 - 1 unique PredictedContactRestraint: Distance: 7.114 - 1 unique PredictedContactRestraint: Distance: 7.484 - 5 unique PredictedContactRestraint: Distance: 6.166

[Experimental data](#)

- 2 unique PredictedContactRestraint:
Distance: 8.037
- 1 unique PredictedContactRestraint:
Distance: 9.738
- 2 unique PredictedContactRestraint:
Distance: 10.45
- 3 unique PredictedContactRestraint:
Distance: 8.603
- 1 unique PredictedContactRestraint:
Distance: 6.592
- 7 unique PredictedContactRestraint:
Distance: 7.812
- 1 unique PredictedContactRestraint:
Distance: 8.402
- 1 unique PredictedContactRestraint:
Distance: 9.088
- 2 unique PredictedContactRestraint:
Distance: 6.864
- 3 unique PredictedContactRestraint:
Distance: 11.076
- 2 unique PredictedContactRestraint:
Distance: 12.244
- 1 unique PredictedContactRestraint:
Distance: 6.451
- 1 unique PredictedContactRestraint:
Distance: 8.168
- 1 unique PredictedContactRestraint:
Distance: 7.683
- 1 unique PredictedContactRestraint:
Distance: 8.215
- 2 unique PredictedContactRestraint:
Distance: 6.801
- 1 unique PredictedContactRestraint:
Distance: 8.961
- 1 unique PredictedContactRestraint:
Distance: 7.361
- 2 unique PredictedContactRestraint:
Distance: 9.542
- 3 unique PredictedContactRestraint:
Distance: 5.778
- 1 unique PredictedContactRestraint:
Distance: 8.367
- 1 unique PredictedContactRestraint:
Distance: 9.294
- 1 unique PredictedContactRestraint:
Distance: 8.068
- 2 unique PredictedContactRestraint:
Distance: 6.328
- 6 unique PredictedContactRestraint:
Distance: 7.832
- 2 unique PredictedContactRestraint:
Distance: 8.393
- 1 unique PredictedContactRestraint:
Distance: 7.115
- 3 unique PredictedContactRestraint:
Distance: 9.85
- 2 unique PredictedContactRestraint:
Distance: 5.643
- 2 unique PredictedContactRestraint:
Distance: 9.5
- 1 unique PredictedContactRestraint:
Distance: 10.027
- 1 unique PredictedContactRestraint:
Distance: 6.12

- 1 unique PredictedContactRestraint:
Distance: 6.677
 - 1 unique PredictedContactRestraint:
Distance: 5.739
 - 1 unique PredictedContactRestraint:
Distance: 10.267
 - 1 unique PredictedContactRestraint:
Distance: 11.507
 - 1 unique PredictedContactRestraint:
Distance: 11.061
 - 1 unique PredictedContactRestraint:
Distance: 9.6
 - 1 unique PredictedContactRestraint:
Distance: 7.914
 - 1 unique PredictedContactRestraint:
Distance: 8.711
 - 1 unique PredictedContactRestraint:
Distance: 10.43
 - 1 unique PredictedContactRestraint:
Distance: 9.987
 - 2 unique PredictedContactRestraint:
Distance: 10.241
 - 1 unique PredictedContactRestraint:
Distance: 10.276
 - 1 unique PredictedContactRestraint:
Distance: 9.303
 - 1 unique PredictedContactRestraint:
Distance: 8.185
 - 1 unique PredictedContactRestraint:
Distance: 7.89
 - 1 unique PredictedContactRestraint:
Distance: 9.299
 - 1 unique PredictedContactRestraint:
Distance: 7.259
 - 1 unique PredictedContactRestraint:
Distance: 10.236
 - 1 unique PredictedContactRestraint:
Distance: 6.679
 - 1 unique PredictedContactRestraint:
Distance: 7.831
 - 1 unique PredictedContactRestraint:
Distance: 6.36
 - 2 unique PredictedContactRestraint:
Distance: 8.552
 - 1 unique PredictedContactRestraint:
Distance: 10.181
 - 1 unique PredictedContactRestraint:
Distance: 8.009
 - 1 unique PredictedContactRestraint:
Distance: 9.462

4. Validation	
<i>Number of ensembles</i>	0
<i>Number of models in ensembles</i>	Not applicable
<i>Number of deposited models</i>	1
<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: 0.00 - Ramachandran outliers: 3 - Sidechain outliers: 0
<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>	modeling with restraints from coevolution analysis
<i>Method</i>	ab initio modeling
<i>Number of computed models</i>	1500
<i>Software</i>	<ul style="list-style-type: none"> - HH-Suite (version Not available) - HMMER (version 3.1b1) - GREMLIN (version Not available) - ROSETTA (version Not available)