

## Supplemental Information S10

### HDOCK results for BvrR docked to DNA

#### Your HDOCK results for job *BvrR*

NOTE: No template was used for the **Ligand** Molecule!

You may **bookmark this page** and come back later to view the results.

##### Template Information

Molecule	PDB ID	Chain ID	Align_length	Coverage	Seq_ID (%)
Receptor	<a href="#">4B09</a>	A	230	0.962	37.8
Ligand					

##### Summary of the top 10 models

Rank	1	2	3	4	5	6	7	8	9	10
Docking Score	-485.79	-484.78	-481.22	-458.31	-453.66	-450.74	-448.30	-447.17	-446.14	-440.93
Ligand rmsd (Å)	108.93	142.58	91.94	89.52	144.00	90.35	126.84	91.31	138.27	128.13

- (a) Row 1: The ranks of the models.
- (b) Row 2: The docking energy scores.
- (c) Row 3: The ligand RMSDs from the input structures or modeled structures by homology modeling.