Reviewer Report

Title: eModel-BDB: A database of comparative structure models of drug-target interactions from the Binding Database

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Reviewer name: Michael K Gilson

Reviewer Comments to Author:

This manuscript describes the assignment of computed 3D ligand-protein structures to a vast set of ligand-protein interactions for which affinity data are available in the BindingDB database. The project appears to be thoughtfully executed, and is notable for its inclusion of a validation step based on new structures deposited in the PDB subsequent to the initial processing. The structural RMSD values listed at the bottom of page 7 are impressively good. I am confident that many users will find the computed structures provided her to be useful in their own work, as indicated by the authors. I have only a few small suggestions for the paper.Although the title is "A database...", the format of the database is not clear. Will the models be searchable and browse-able, for example? Also, it would be interesting to know if there is a plan to expand the database as more data enter BindingDB.Page 3, line 30, delete "a" before "high-throughput"Page 4, last line: it would be helpful to provide information on how good a GDT-score of >0.4 is. (Perhaps this is in the text and I missed it.)Page 5, line 4: "Confident structure models...": does this mean those models with a GDT-score of >0.4? If not, then how was confidence defined here?

Level of Interest

Please indicate how interesting you found the manuscript: An article of importance in its field

Quality of Written English

Please indicate the quality of language in the manuscript: Acceptable

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The present manuscript describes a project that makes extensive use of the BindingDB database, which my lab developed and maintains.

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