Reviewer Report

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

Version: **Revision 1** **Date:** 4/12/2018

Reviewer name: **Michael K Gilson**

Reviewer Comments to Author:

I havThis paper describes a new database that is likely to be of substantial interest and value to the scientific community. The work appears basically sound, but might benefit from some clarification and enhancements, including in relation to the validation statistics, as now detailed.

The attention to validation of the modeled structures is very welcome, but perhaps a little unclear. For example, text on page 8 says the models were tested against 7,012 experimental structures, but I am not sure what the results of these tests were. The text does says the results were validated for 952 reaction set IDs, but I'm not sure how this relates to the 7,012 cases. What fraction of tests were passed, and what was the definition of passing? Perhaps this is stated, and I missed it.

Also, on page 9, a median distance between predicted and actual pocket locations of 6 A does not sound that good, but the ligand RMSDs reported in Figure 8 seem quite good. It might be helpful to clarify the relationship between these figures of merit. Also, please clarify the dataset plotted in Figure 8. Is this for the 7,012 structures mentioned above?

Finally, regarding the database itself, I think that entries, such as http://www.brylinski.org/pub/eModelBDB.php?reactant_set_id=00267770, would be improved by including the source organism and common name of the protein and possibly its amino acid sequence; a SMILES and/or INCHI string of the compound; and possibly the IDs of the PDB structure(s) used to build the model. This added information would make each entry more self-contained, rather than requiring users to refer back to the PDB and BindingDB for this basic information.e no further comments.

Methods

Are the methods appropriate to the aims of the study, are they well described, and are necessary controls included? Yes

Conclusions

Are the conclusions adequately supported by the data shown? Yes

Reporting Standards

Does the manuscript adhere to the journal's guidelines on minimum standards of reporting? No

Choose an item.

Statistics

Are you able to assess all statistics in the manuscript, including the appropriateness of statistical tests used? No, and I do not feel adequately qualified to assess the statistics.

Quality of Written English

Please indicate the quality of language in the manuscript: Acceptable

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