Fig. S4  Chemical space plots of the top 500 hit lists from Glide SP, Prime MM-GBSA, and consensus for Structure 4 based on the various ligand preparation protocols

A. Ionizer – Ligand Strain included.

B. Ionizer – Ligand Strain not included.

C. Ionizer – Go Nuts – Ligand strain included
D. Ionizer – Go Nuts – Ligand strain not included

E. Epik – Ligand Strain included

F. Epik – Ligand Strain not included

G. Epik – Go Nuts – Ligand Strain included
Compounds at the edges are chemically unrelated to other compounds in the dataset (singletons). Compounds in the center are chemically related to each other, and the distance between points is a measure of chemical similarity. Actives are indicated by squares, inactives by circles. Compounds that only scored in the Top 500 by Glide SP are shown in red; compounds that only scored in the Top 500 by Prime MM-GBSA are shown in green; compounds that scored in the Top 500 of both the Consensus score and Glide SP are shown in black; compounds that scored in the Top 500 of both the Consensus score and Prime MM-GBSA are shown in cyan; compounds that scored in the Top 500 of all three functions, Glide SP, Prime MM-GBSA, and Consensus are shown in dark blue; compounds that scored in the Top 500 of the Consensus score but not in the Top 500 of either Glide SP or Prime MM-GBSA are shown in dark blue.