|  |  |
| --- | --- |
| **HADDOCK Score b** | -130 (7) |
| **RMSD (Å) c** | 1.8 (0.9) |
| **Number of structures** | 71 |
| **BSA (Å2) d** | 1968 (106) |
| **EAIR e** | 30.5 (15.2) |
| **Einterf** | -398(50) |
| **Enbg** | -431(46) |

Statistics on the top-ranking cluster of the structural models of CNBD and TRIP8bnano complex obtained through HADDOCK2.2 calculations and in agreement with previous experimental data (Deberg *et al*, 2015). Averages (standard deviations are reported in parenthesis) were calculated over the best ten structures.

a Cluster rank according to the HADDOCK score. b HADDOCK score defined as a weighted sum of different energetic terms, such as: van der Waals energy, electrostatic energy, distance restraints energy, buried surface area, binding energy and desolvation energy. c Backbone RMSD from the lowest HADDOCK score structure in each cluster. Some individual energy terms are also reported: d Buried surface area, e distance restraints energy, f binding energy, g non-bonded interaction energy.

Deberg HA, Bankston JR, Rosenbaum JC, Brzovic PS, Zagotta WN & Stoll S (2015) Structural mechanism for the regulation of HCN ion channels by the accessory protein TRIP8b. *Structure* **23:** 734–744. Retrieved from https://doi.org/10.1016/j.str.2015.02.007.