

Structure / Ensemble size

Supplementary figure 5. Energy-ordered rmsd profiles and total energies for the 50 calculated structures of Hrp1-PEE complex. Filled black circles represent the total XPLOR Energy values (scale on the right vertical axis). Rmsd values were calculated for the overall structure (residues 160-318; open circles) and separately for the RBD1 (160-234; diamonds) and RBD2 (234-318; up triangles) domains (scale on the left vertical axis). The red line represents the chosen cut-off for the final ensemble of structures (Table 1).