**Supplementary Material**

# Mapping the Encounter State of a Transient Protein Complex by PRE NMR Spectroscopy

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Supplementary File **10858_2010_9452_MOESM2_ESM.tar.gz** contains the scripts for generating the conformational space grid and encounter state mapping, example startup files, and an instructions file (readme.txt).

**Movie S1. Spatiotemporal map of Cc-CcP encounter state.** Interaction grid isosurface $\theta, \varphi, r_{(\chi,\psi,\xi=0)}$ colored according to $p_{max}(\theta, \varphi)$, ranging from 0 (blue) to 0.3 (red). See the legend to Fig. 2B for details.

**Movie S2. Comparison of the encounter map and the encounter ensembles.** Overlay of the Cc-CcP interaction isosurface colored according to the experimental PREs at p = 0.03 and CMs of Cc molecules from 100 PRE-based ensemble simulations (N = 10, green spheres). See the legend to Fig. 5B for details.

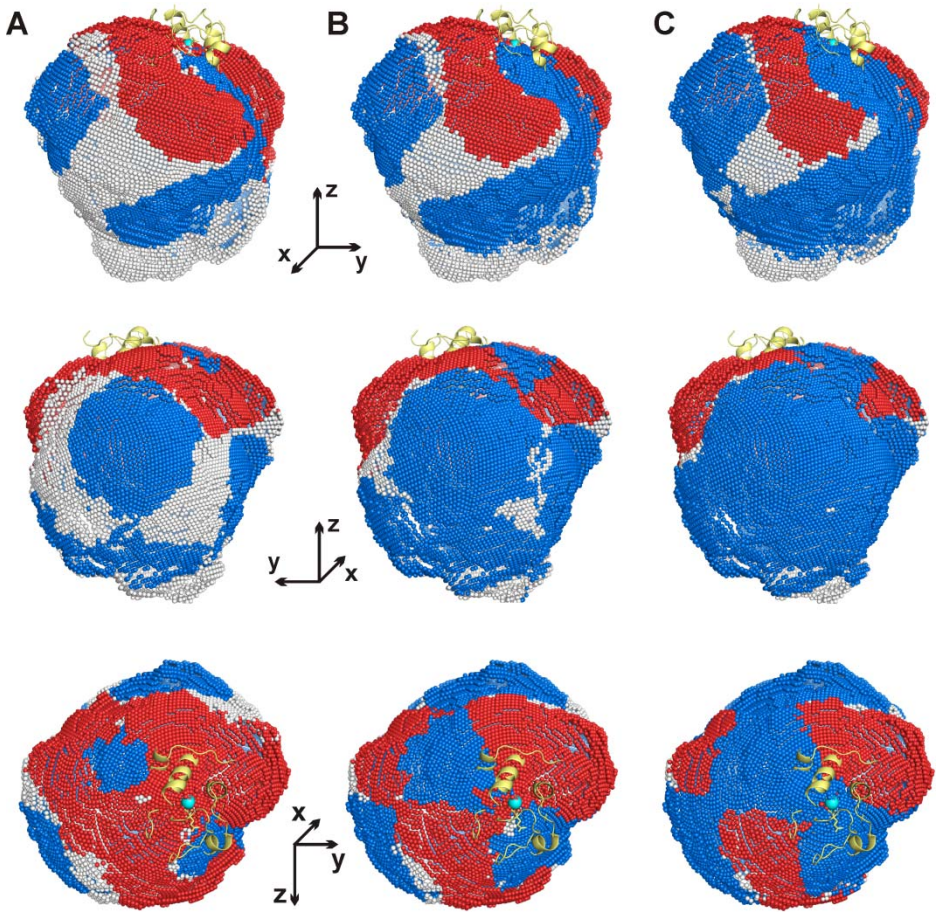


**Figure S1. Experimental coverage of the conformational space of Cc-CcP encounter state.** Cc CMs for the orientations that, respectively, violate experimental PREs (blue) or contribute ≥ 5 Hz to $\Gamma_2^*$ (red) at (**A**) $p = 0.05$, (**B**) $p = 0.15$, and (**C**) $p = 0.3$. Combination of the blue and red areas defines the total conformational space covered by the effects from the introduced SLs. See the legend to Fig. 3 for more details.

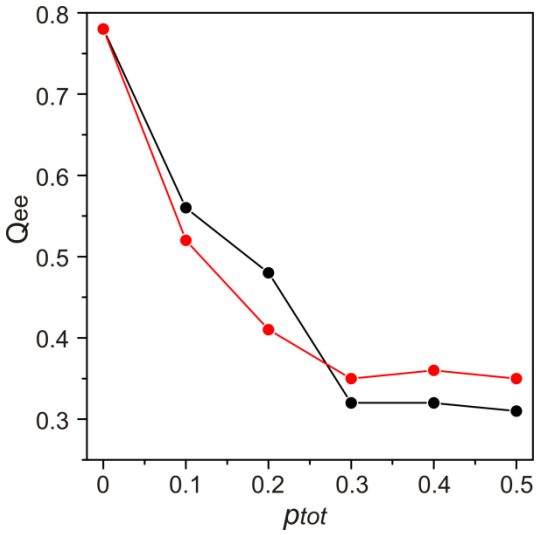


**Figure S2. Intermolecular $Q_{ee}$ factors for ensemble refinement runs at different $p_{tot}$.** Ensemble size N = 5 (red) and N = 10 (black). For each point 100 independent structure calculations were performed.

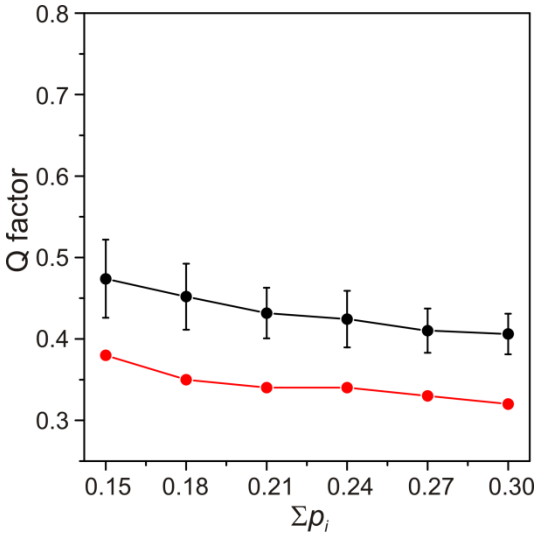


**Figure S3. Intermolecular Q factors for ensemble refinement at different $\sum_i p_i$.** The Q factors $Q_e$ (black) and $Q_{ee}$ (red) are plotted. For each point 100 independent structure calculations were performed.

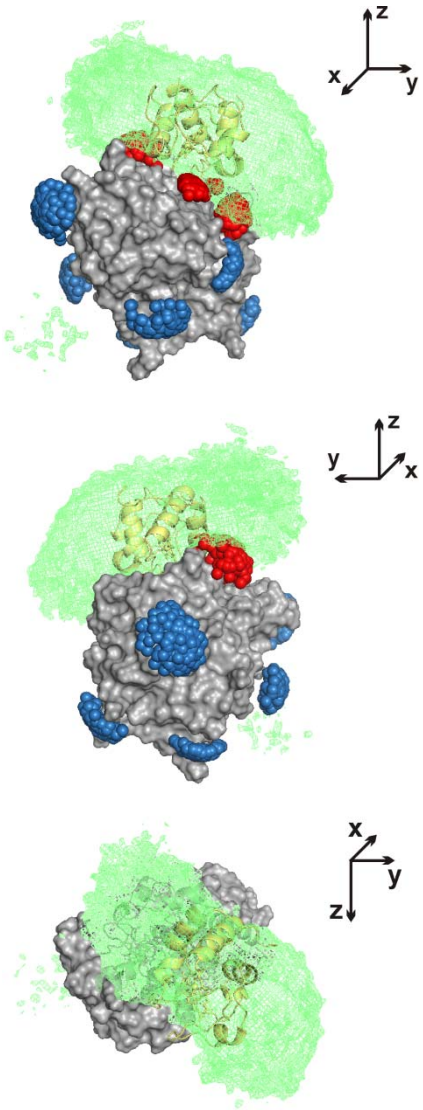


**Figure S4. Spatial distribution of the encounter ensembles with $\sum_i p_i$ = 0.21**. Reweighted atomic probability density maps for the overall distribution of Cc molecules obtained from 100 PRE-based ensemble calculations (N = 7, $\sum_i p_i$. = 0.21 plotted at a threshold of 20 % maximum). In the bottom view, SL atoms are removed for clarity. See the legend to Fig. 5A for details.