Supplementary Information

The exact NOE as an alternative in ensemble structure determination

Beat Vögeli[1*], Simon Olsson[1,2], Peter Güntert[1,3,4] & Roland Riek[1]

[1]Laboratory of Physical Chemistry, Vladimir-Prelog-Weg 2, Swiss Federal Institute of Technology, ETH-Hönggerberg, CH-8093 Zürich, Switzerland

[2] Institute for Research in Biomedicine, Via Vincenzo Vela 6, CH-6500 Bellinzona, Switzerland

[3] Institute of Biophysical Chemistry, Center for Biomolecular Magnetic Resonance, and Frankfurt Institute for Advanced Studies, J.W. Goethe-Universität, Max-von-Laue-Str. 9, 60438 Frankfurt am Main, Germany

[4] Graduate School of Science, Tokyo Metropolitan University, Hachioji, Tokyo 192-0397, Japan

*Correspondence should be addressed to:

Beat Vögeli, Laboratory of Physical Chemistry, HCI F217, Vladimir-Prelog-Weg, Swiss Federal Institute of Technology, ETH-Hönggerberg, CH-8093 Zürich, Switzerland, Tel: (+41)-44-633-4405, beat.voegeli@phys.chem.ethz.ch

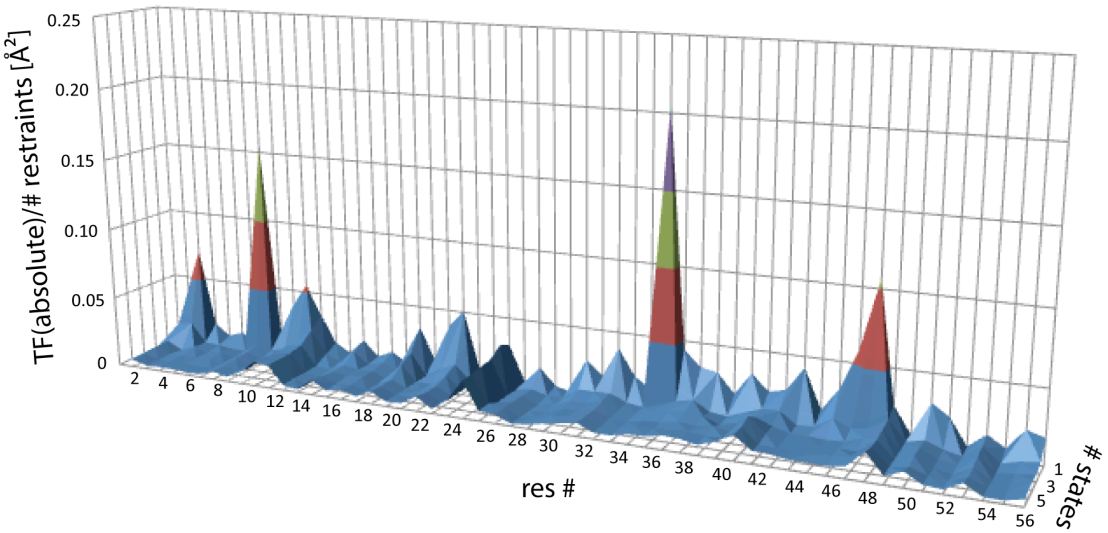

Figure S1, related to Figure 2. Residue-specific target function values normalized to the number of restraints on the residues. The individual contributions are plotted versus the residue number and the number of states on the x and y axes, respectively.

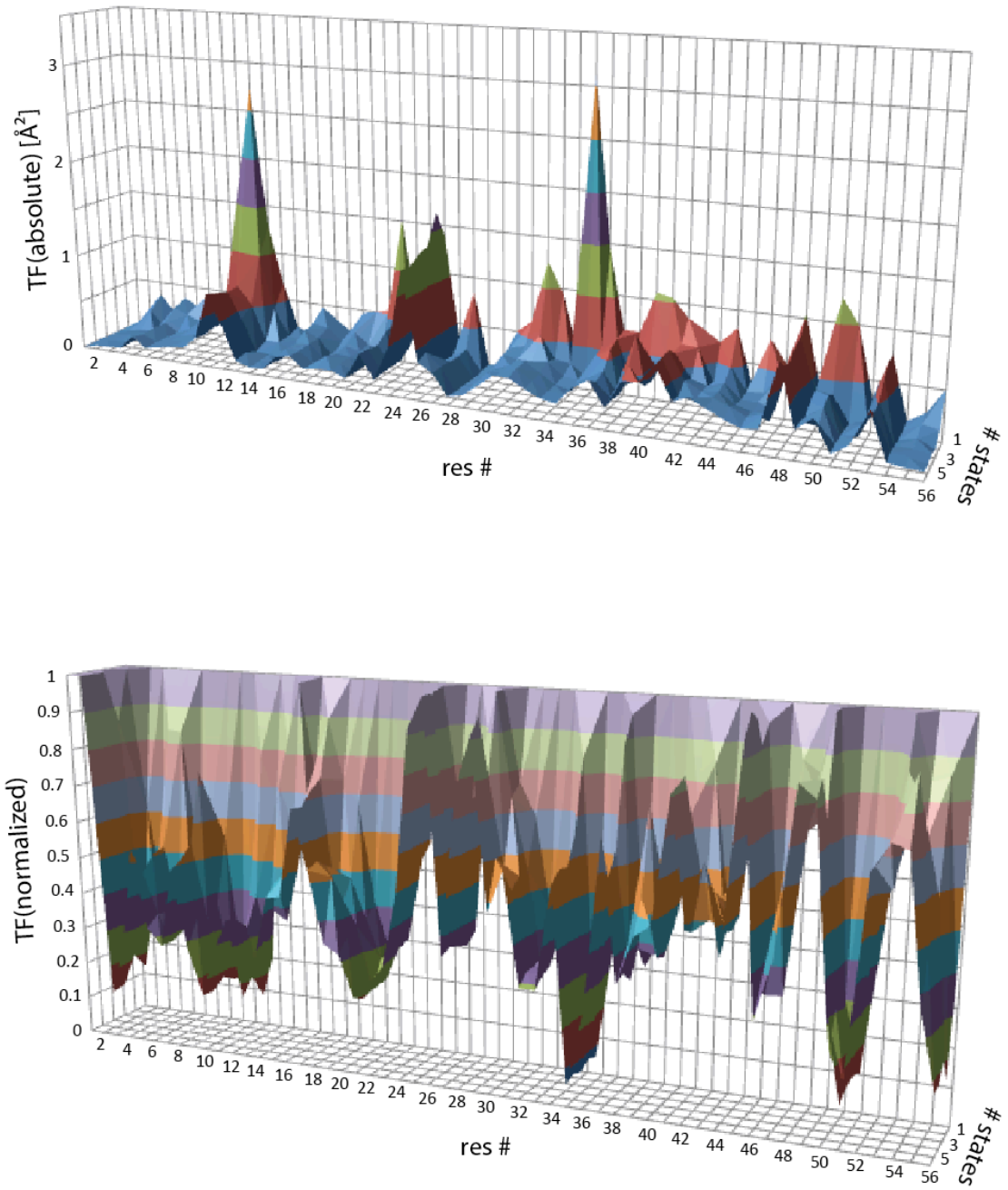

Figure S2, related to Figures 2 and 3. Contributions to residue-specific target function values from the backbone. The individual contributions are plotted versus the residue number and the number of states on the x and y axes, respectively. The target function values are shown in absolute values and normalized to the values for the single-state structure in the top and bottom panels.

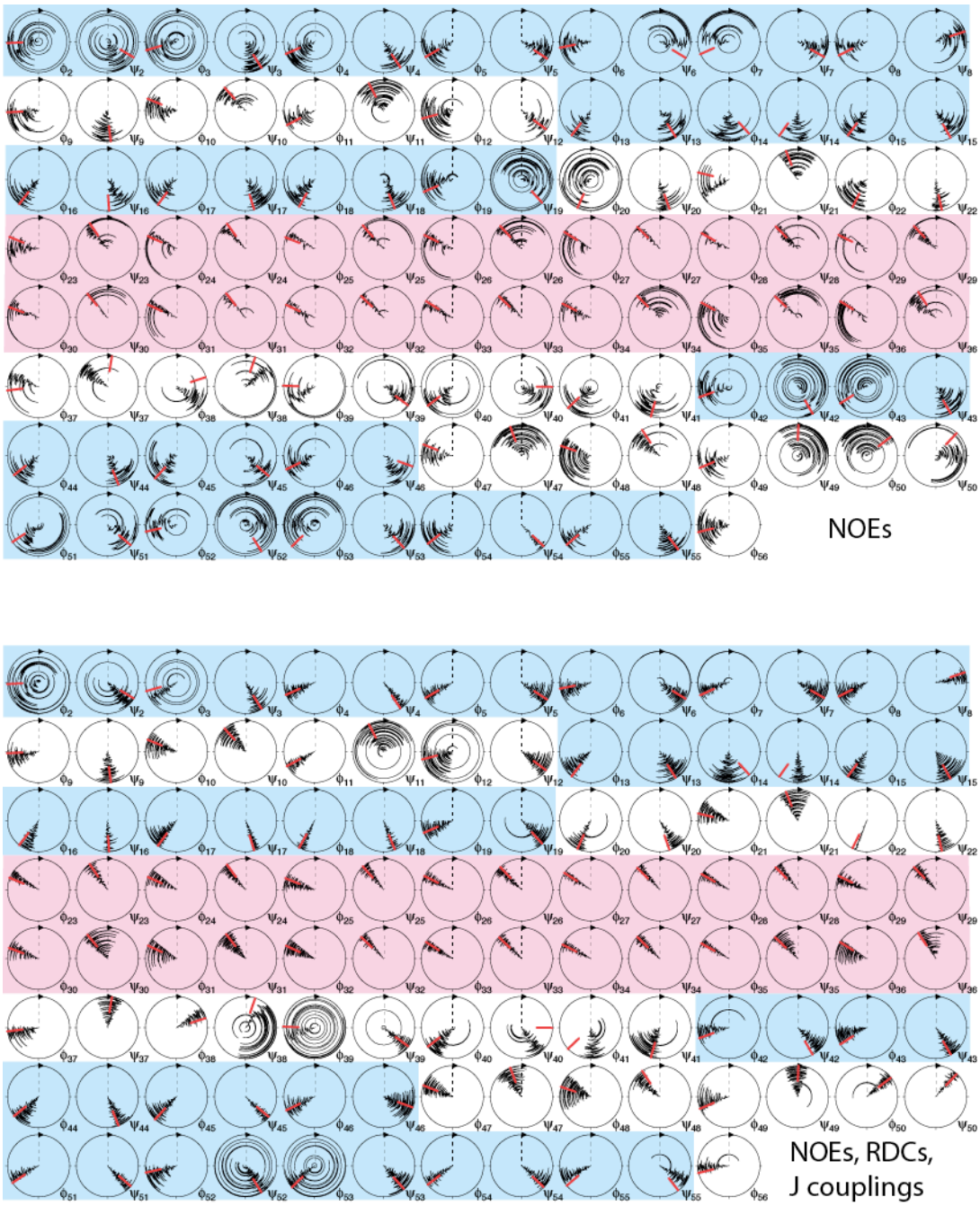

Figure S3, related to Figure 6. Circle diagrams of backbone φ and ψ torsion angles. The four states of 20 ensembles are plotted from the center to the outer circle. Angles obtained from ensembles calculated from conventional NOEs exclusively are shown on the top, and ensembles calculated from conventional NOEs, RDCs and *J* couplings at the bottom, respectively. The red bars indicate angles extracted from the high-resolution X-ray structure 1IGD [41]. Diagrams of residues that are located in a β strand and the α helix are shaded in blue and pink, respectively. The figure was generated in MolMol [55].

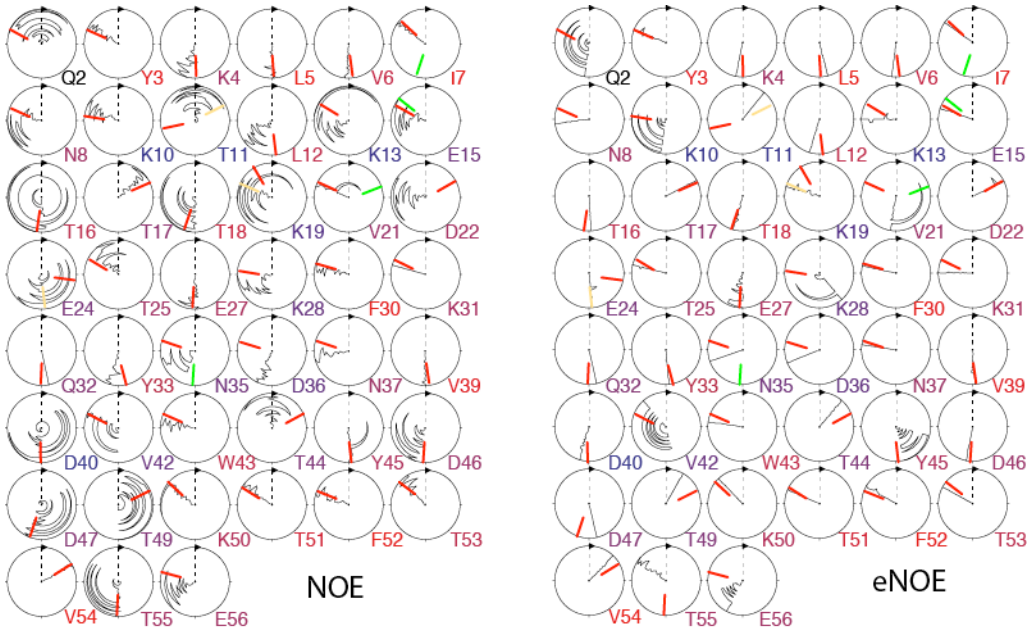

Figure S4, related to Figure 7. Impact of exact NOE evalution on χ^1 angles in single-state bundles. Angles obtained from bundles calculated from conventional NOEs exclusively are shown on the left, and bundles calculated from eNOEs on the right, respectively. The single states of 20 structures are plotted from the center to the outer circle in the circle diagrams. In most cases, identical main rotamer states are obtained. Exceptions are residues 2, 21 and 55. Typically, the eNOEs produce considerably smaller standard deviations from the mean values (overall standard deviations are 46.8° versus 19.6°). The red bars indicate angles extracted from the high-resolution X-ray structure 1IGD [41], and the green and yellow bars different states and additional states from an anisotropic re-evaluation. The single-letter amino acid codes and residue numbers are colored according to the solvent accessible surface area of the residue (red for 0%; blue for 50% or more). For nearly all angles, the NOE and eNOE ensembles reproduce the X-ray rotamer states by their most populated states. Exceptions are residues 10, 21, 28 and 55 for the eNOEs, 22 and 36 for the conventional NOEs, and 2 for both. The figure was generated in MolMol [55].

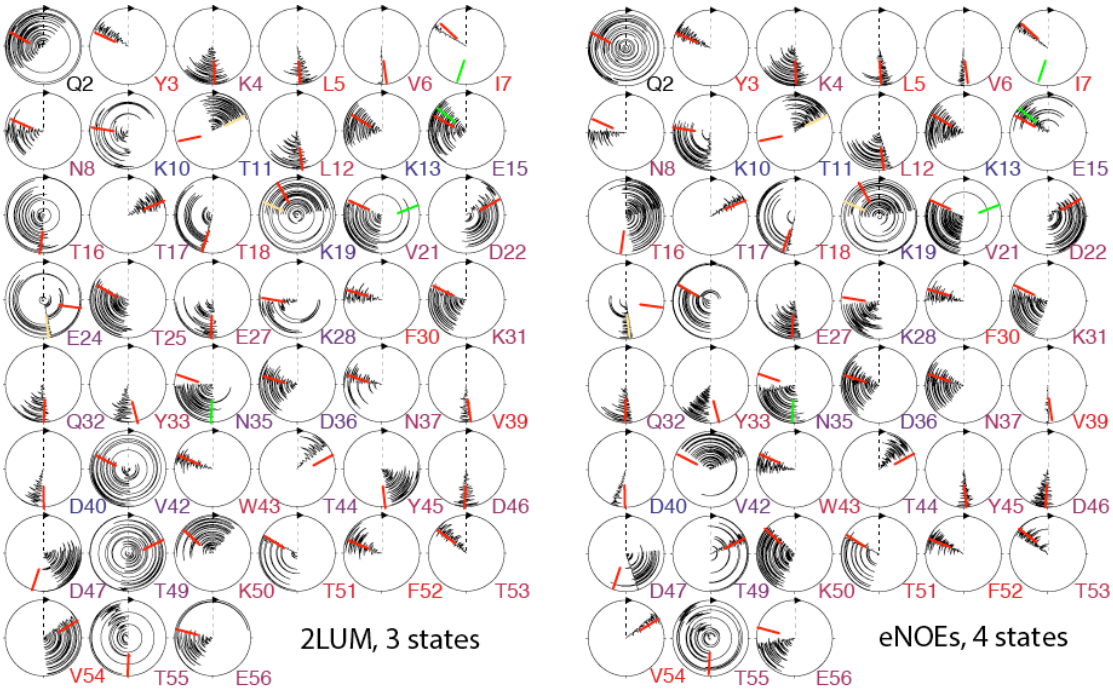

Figure S5, related to Figure 7. Comparison of the χ^1 angle sampling to the one of the previously determined three-state ensemble (pdb access code: 2LUM) [31,32]. Angles obtained from ensembles calculated from 2LUM are shown on the left, and four-state ensembles calculated from eNOEs (as shown in Figure 7) on the right, respectively. The three/four states of 20 ensembles are plotted from the center to the outer circle in the circle diagrams. The red bars indicate angles extracted from the high-resolution X-ray structure 1IGD [41], and the green and yellow bars different states and additional states from an anisotropic re-evaluation. The single-letter amino acid codes and residue numbers are colored according to the solvent accessible surface area of the residue (red for 0%; blue for 50% or more). The figure was generated in MolMol [55].

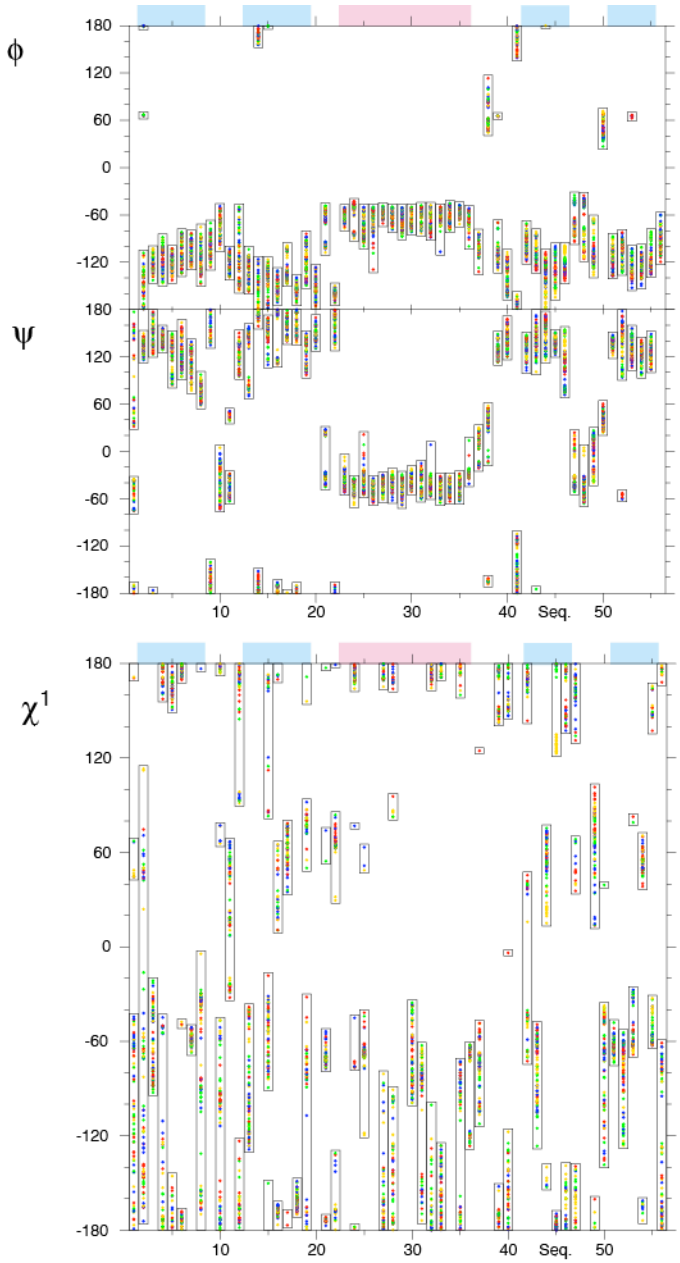

Figure S6, related to Figure 9. Correlations in four-state ensembles of GB3 calculated from eNOEs, RDCs and *J* couplings. Shown are φ, ψ and χ^1 angles in the top, middle and bottom panels, respectively. The states are grouped in residues 45 and 46 and the colors are the same as used in Figure 5. β strands and the α helix are indicated by blue and pink shades above the plots, respectively. The figure was generated in MolMol [55].

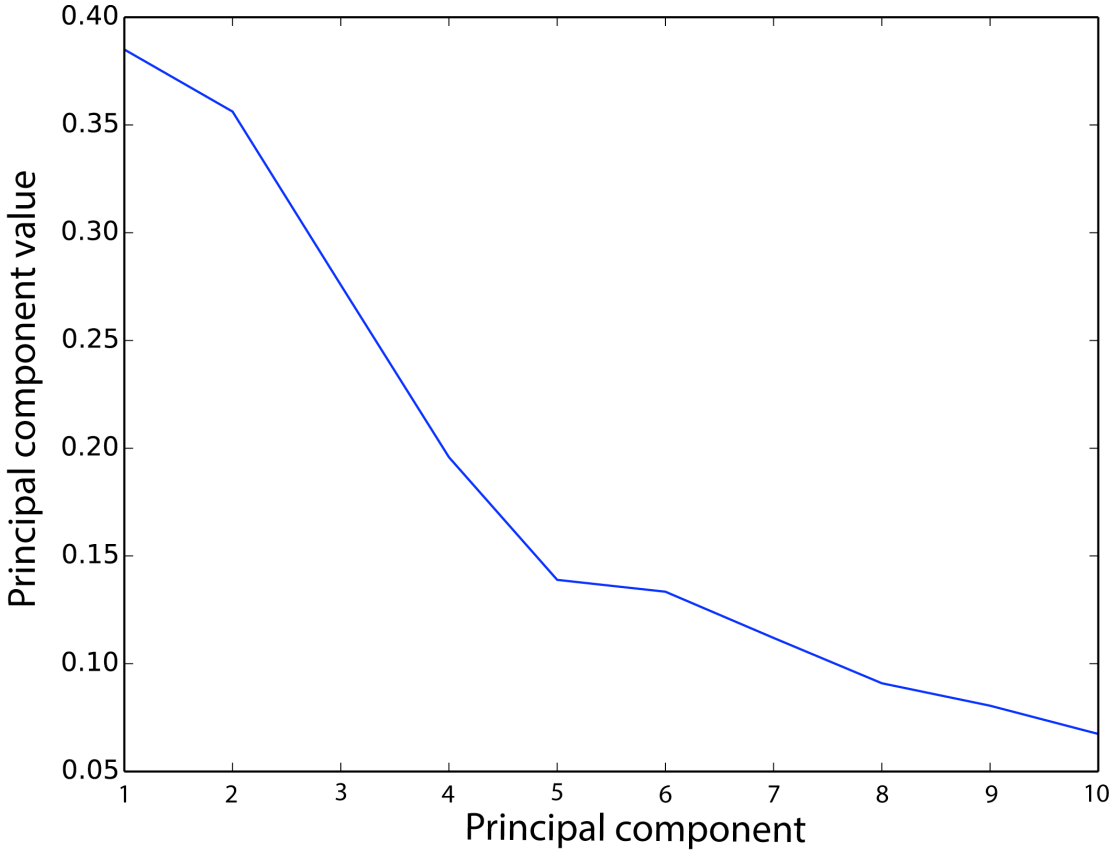

Figure S7, related to Principal component analysis. 10 largest principal components of the 20 four-state ensembles of GB3. The ensemble was calculated from the complete set of eNOEs, RDCs and *J* couplings.

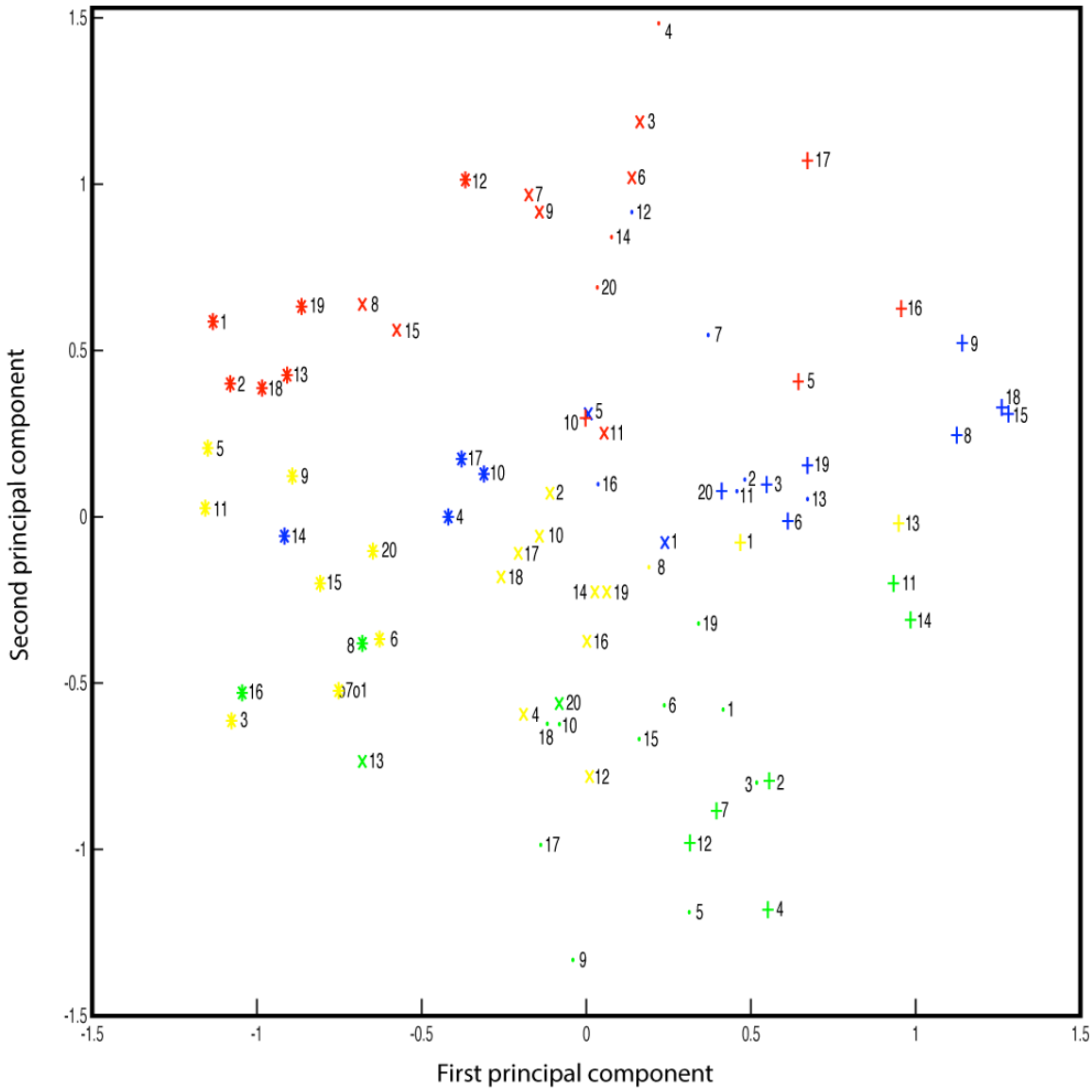

Figure S8, related to Principal component analysis. Correlation plot of the first and second principal components of the four-state ensemble of GB3 calculated from eNOEs, RDCs and *J* couplings. The symbols '*', 'x', '.' and '+' represent the grouping according to the first principal component, and the colors red, blue, yellow and green to the second principal component.