Supplementary Material

Automated error-tolerant macromolecular structure determination from multidimensional nuclear Overhauser enhancement spectra and chemical shift assignments: Improved robustness and performance of the PASD algorithm

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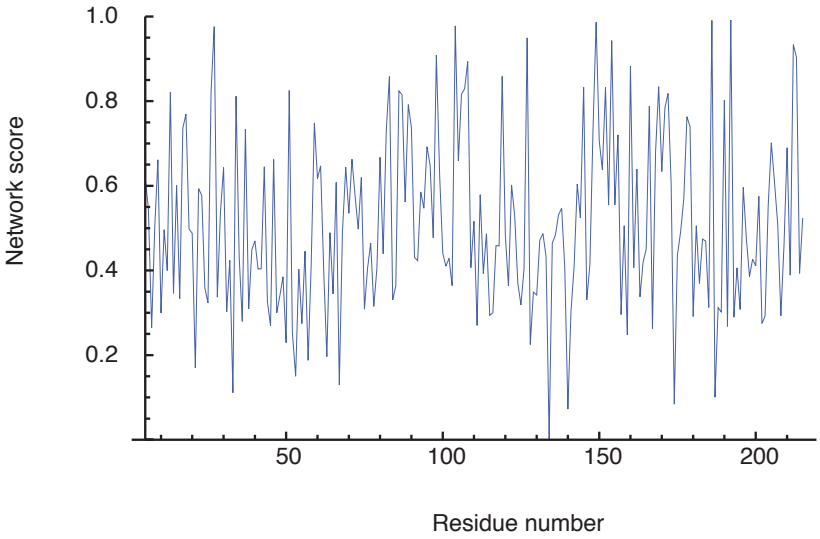

Figure 1: Intraresidue network residue pair scores $R(a, a)$ (defined in Eq. 1) for ThTP as a function of residue number. These scores were calculated on the basis of the set of peak assignments generated by the two-step NOE peak matching algorithm (Section 2.1.2). It can be see that there is large variation in $R(a, a)$ along the sequence.

Table 1: Performance of Shift Correction Procedure[a]

Spectrum	shift assignments with no target (%)	shift assignments with no consistent target (%)	overall score (%)	Shift Correction (ppm) ^{1}H from	heavy from	^{1}H to	heavy to
CVN							
3dC	8	15	48	0.012	0.137	0.012	
3dN	25	64	13	0.016	0.222	0.018	
IL-4							
3dC	4	20	44	0.015	0.129	0.015	
3dN	39	56	6	0.014	0.085	0.013	
4dCC	48	45	11	0.034	0.249	0.021	0.240
YmoA							
3dC	2	3	74	0.016	0.158	0.015	
3dN	43	47	17	0.010	0.220	0.016	
4dCC	6	20	53	0.013	0.112	0.016	0.108
4dCN	41	6	88	0.022	0.233	0.009	0.156
mth1743							
3dC	34	31	40	0.016	0.059	0.016	
3dN	24	75	1	0.008	0.040	0.005	
NiRD							
3dC aliph.	41	35	31	0.013	0.100	0.014	
3dC arom.	86	9	17	0.008	0.051	0.016	
3dN	28	64	12	0.013	0.116	0.024	
4dCC	25	31	36	0.015	0.131	0.014	0.114
ThTP							
3dC aliph.	6	21	45	0.014	0.145	0.015	
3dC arom.	91	3	37	0.007	0.029	0.020	
3dN	26	72	3	0.014	0.224	0.011	

[a] For each NOESY spectrum, the fraction of shift assignments without any possible targets is shown in the first column. The fraction of shift assignments for which there is no target consistent with the others is shown in the second column. The third column corresponds to the fraction of possible calibration peaks for which there are assignments. The last four columns give the standard deviation of the difference between the raw chemical shifts and the corrected chemical shifts for shift assignments along each dimension of the spectrum.

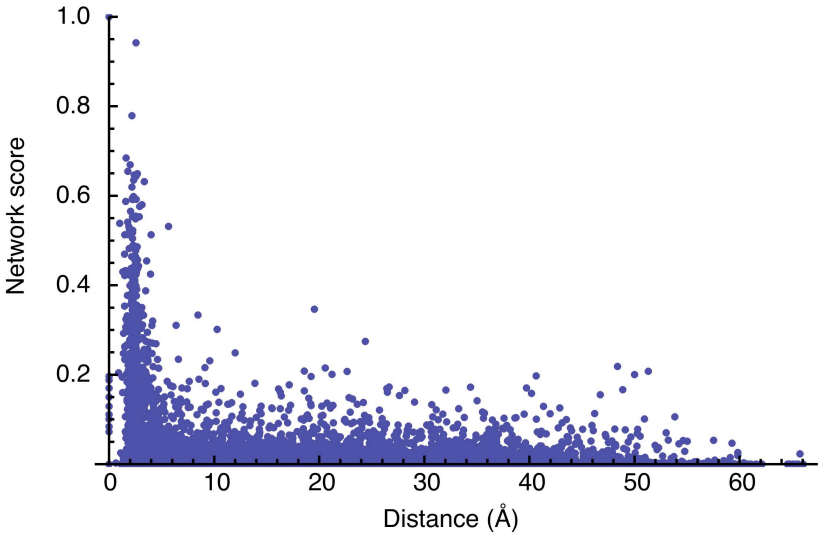

Figure 2: Normalized network residue pair scores $R'(a, b)$ (defined in Eq. 2) for ThTP as a function of the distance in space between the residues in the reference structure. R' is calculated on the basis of the peak assignments generated by the two-step matching procedure (Section 2.1.2) using the NOE spectra of ThTP (Table 2), as described in Section 2.1.3. One can see that at the chosen cutoff value of $R' = 0.2$, a reasonable number of bad contacts are selected along with a large number of true contacts.

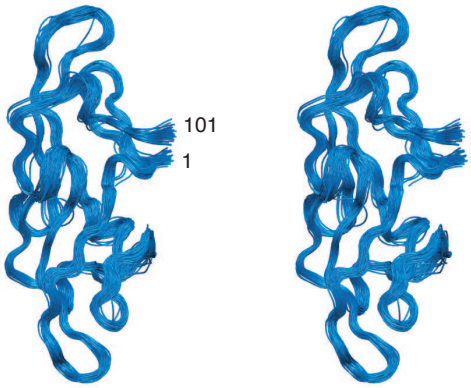

Figure 3: Ensemble of 50 structures of CVN resulting from the second structure calculation pass.

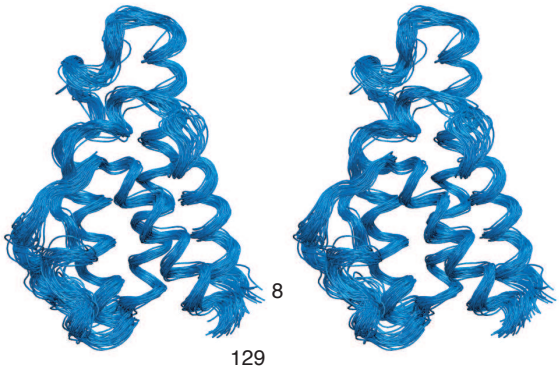

Figure 4: Ensemble of 50 structures of IL-4 resulting from the second structure calculation pass.

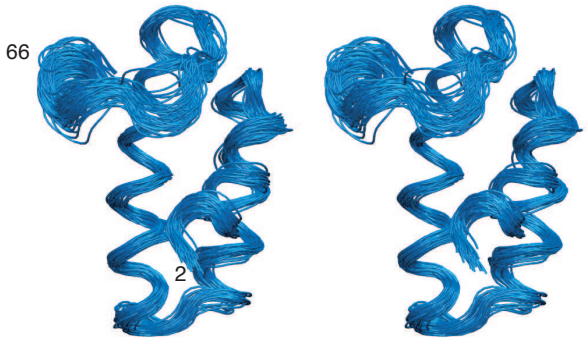

Figure 5: Ensemble of 50 structures of YmoA resulting from the second structure calculation pass.

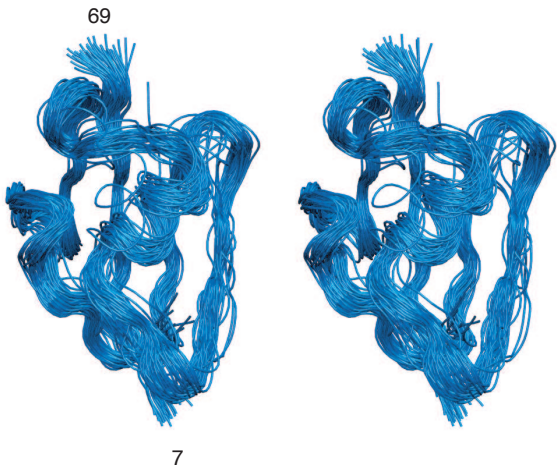

Figure 6: Ensemble of 50 structures of mth1743 resulting from the second structure calculation pass.

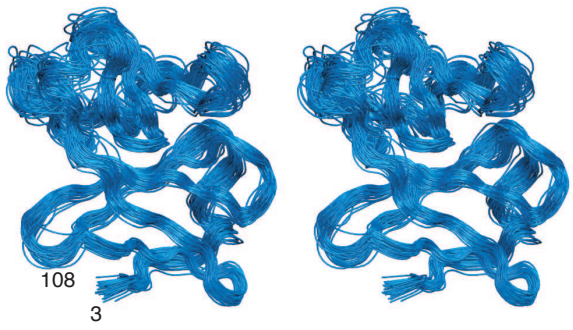

Figure 7: Ensemble of 50 structures of NiRD resulting from the second structure calculation pass.

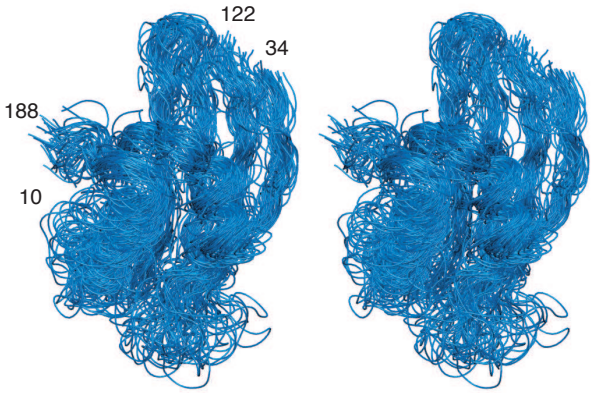

Figure 8: Ensemble of 50 structures of ThTp, domain 1 resulting from the second structure calculation pass.

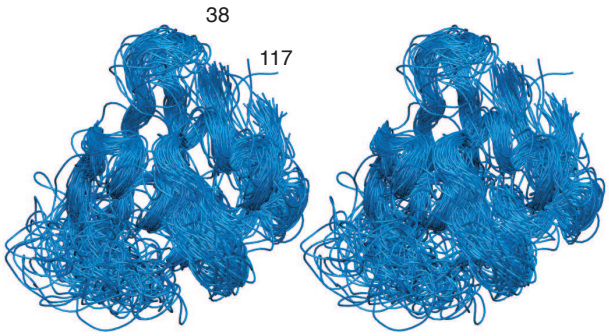

Figure 9: Ensemble of 50 structures of ThTp, domain 2 resulting from the second structure calculation pass.

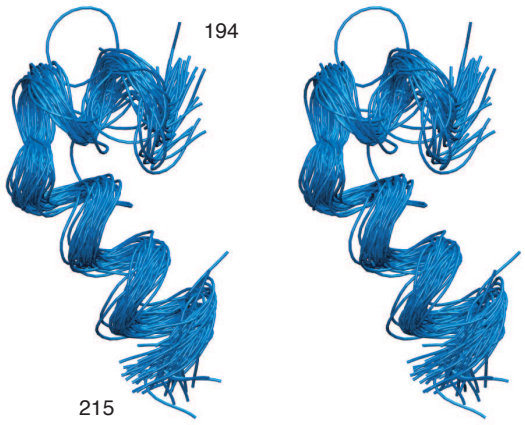

Figure 10: Ensemble of 50 structures of ThTP, domain 3 resulting from the second structure calculation pass.