Table 6. Statistical analysis of the energy minimized family of conformers and of the mean structure of Cu(I)DR1885

	REM[a]	**<REM>**[a]
RMS violations per meaningful distance constraint (Å) [b]		
Intraresidue (306)	0.0135 ± 0.0030	0.0119
Sequential (788)	0.0120 ± 0.0014	0.0136
Medium range (312) [c]	0.0124 ± 0.0020	0.0126
Long range (1200)	0.0108 ± 0.0013	0.0114
Total (2606)	0.0118 ± 0.0010	0.0123
RMS violations per meaningful dihedral angle constraints (deg) [b]		
Phi (60)	2.02 ± 0.37	2.42
Psi (60)	1.62 ± 0.41	1.53
Average number of violations per structure		
Intraresidue	6.5 ± 2.0	6
Sequential	12.8 ± 2.5	13
Medium range	6.9 ± 1.9	7
Long range	18.1 ± 3.1	20
Total	44.2 ± 5.1	46
Phi	8.6 ± 1.8	11
Psi	3.8 ± 1.5	3
Average no. of NOE violations larger than 0.3 Å	0.0 ± 0.0	0
Average no. of NOE violations between 0.1 Å and 0.3 Å	10.1 ± 3.0	9

Structural analysis[d]

% of residues in most favorable regions	59.7	60.6
% of residues in allowed regions	35.0	35.4
% of residues in generously allowed regions	3.6	4.0
% of residues in disallowed regions	1.8	0.0
H-bond energy (kJ mol^{-1})	-	3.10
Overall G-factor	-	-0.41

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[a]REM indicates the energy minimized family of 20 structures and <REM> is the energy minimized mean structure obtained from the coordinates of the individual REM structures.

[b]The number of meaningful constraints for each class is reported in parentheses.

[c]Medium range distance constraints are those between residues (i,i+2), (i,i+3), (i,i+4), and (i,i+5).

[d]As it results from the Ramachandran plot analysis. For the PROCHECK statistics, an average H-bond energy in the range of 2.5-4.0 kJ·mol^{-1}, and an overall G-factor larger than -0.5 are expected for a good quality structure.