Table 5. Statistical analysis of the energy minimized family of conformers and of the mean structure of apoDR1885

	REM[a]	**<REM>**[a]
RMS violations per meaningful distance constraint (Å) [b]		
Intraresidue (225)	0.0224 ± 0.0048	0.0234
Sequential (588)	0.0143 ± 0.0040	0.0108
Medium range (186) [c]	0.0133 ± 0.0035	0.0157
Long range (733)	0.0160 ± 0.0027	0.0097
Total (1732)	0.0165 ± 0.0005	0.0133
RMS violations per meaningful dihedral angle constraints (deg) [b]		
Phi (57)	2.03 ± 0.48	1.91
Psi (60)	1.94 ± 1.67	1.20
Average number of violations per structure		
Intraresidue	9.2 ± 2.6	7
Sequential	10.2 ± 3.5	9
Medium range	4.3 ± 1.6	4
Long range	21.9 ± 4.6	13
Total	45.6 ± 7.7	33
Phi	7.9 ± 1.8	10
Psi	3.6 ± 1.5	2
Average no. of NOE violations larger than 0.3 Å	0.1 ± 0.3	0
Average no. of NOE violations between 0.1 Å and 0.3 Å	15.6 ± 4.8	7

Structural analysis[d]

% of residues in most favorable regions	55.4	54.9
% of residues in allowed regions	39.2	42.2
% of residues in generously allowed regions	3.9	2.9
% of residues in disallowed regions	1.5	0.0
H-bond energy (kJ mol^{-1})	-	3.14
Overall G-factor	-	-0.40

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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.