Table 9. Statistical analysis of the energy minimized family of conformers and of the mean structure of MMP12-NNGH adduct

	REM (20 structures)	<REM> (mean)
RMS violations per meaningful distance constraint, Å[*]		
Intraresidue (426)	0.0229 ± 0.0027	0.0239
Sequential (778)	0.0079 ± 0.0011	0.0089
Medium range (672)[†]	0.0086 ± 0.0011	0.0097
Long range (765)	0.0119 ± 0.0013	0.0099
Total (2,641)	0.0128 ± 0.0008	0.0129
NOEs per residue	16.6	16.6
RMS violations per meaningful dihedral angle constraints (deg)[*]		
Phi (81)	1.14 ± 0.32	0.91
Psi (86)	0.64 ± 0.33	1.46
Average no. of violations per structure		
Intraresidue	15.2 ± 1.7	15
Sequential	10.9 ± 2.2	17
Medium range	10.5 ± 2.7	13
Long range	13.6 ± 2.1	10
Total (meaningful NOEs)	50.2 ± 4.2	55
Phi	4.2 ± 1.3	4
Psi	1.4 ± 0.8	1
Average no. of NOE violations larger than 0.3 Å	0.85 ± 0.36	1
Average no. of NOE violations between 0.1 and 0.3 Å	8.2 ± 1.8	5
RMSD to the mean structure (Å) (BB)[‡]	0.74 ± 0.10	-
RMSD to the mean structure (Å) (HA)[‡]	1.23 ± 0.11	-
Target function ($Å^2$)	1.07 ± 0.10	-
Structural analysis[§]		
% of residues in most favorable regions	85.2 ± 1.6	87.8
% of residues in allowed regions	13.4 ± 1.4	9.8
% of residues in generously allowed regions	1.0 ± 0.8	1.6
% of residues in disallowed regions	0.5 ± 0.6	0.8
Bad contact / 100 residues	0.55 ± 0.83	1
H-bond energy standard deviation (ref. 1)	0.82 ± 0.04	0.84
Overall *G* factor	-0.31 ± 0.03	-0.29

REM and <REM> indicate the energy minimized family of 20 structures and the energy minimized mean structure, respectively.

[*] The number of meaningful constraints for each class is reported in parenthesis.

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

[‡] The RMSD to the mean structure for residues 113-259.

[§] The results from the Ramachandran plot analysis for residues 113-259, which are connected to the range of RMSD calculated.

1. Morris, A. L., MacArthur, M. W., Hutchinson, E. G. & Thornton, J. M. (1992) *Proteins Struct. Funct. Genet.* **12**, 345-364.