

Supplementary Table 1. Structural statistics for the 20 lowest energy structures.

# Restraints	Z2-DPC-d ₃₈	Z8-DPC-d ₃₈	Z8-SDS-d ₂₅	Z9-DPC-d ₃₈	Z9-SDS-d ₂₅
Unambiguous nOes	296	455	358	343	374
Ambiguous nOes	27	52	81	56	70
Unassigned nOes	0	0	0	0	0
Total nOes	323	507	439	399	444
# Dihedral Restraints	20	20	20	20	20
RMSD from ideal ^a					
Bonds (Å)	$8.97 \times 10^{-4} \pm 7.81 \times 10^{-5}$	$5.97 \times 10^{-3} \pm 9.22 \times 10^{-5}$	$3.85 \times 10^{-3} \pm 5.46 \times 10^{-5}$	$8.84 \times 10^{-4} \pm 5.1 \times 10^{-5}$	$3.96 \times 10^{-3} \pm 3.1 \times 10^{-4}$
Angles (Å)	$0.29 \pm 2.82 \times 10^{-3}$	$0.54 \pm 1.17 \times 10^{-2}$	$0.393 \pm 5.27 \times 10^{-3}$	$0.274 \pm 2.2 \times 10^{-3}$	$0.420 \pm 1.9 \times 10^{-2}$
Impropers (deg)	$0.128 \pm 6.66 \times 10^{-3}$	$0.45 \pm 1.54 \times 10^{-2}$	$0.21 \pm 4.82 \times 10^{-3}$	$9.93 \times 10^{-2} \pm 7.3 \times 10^{-3}$	$0.256 \pm 2.5 \times 10^{-2}$
VDW (kcal·mol ⁻¹)	6.90 ± 0.69	39.03 ± 2.45	9.56 ± 0.66	4.98 ± 0.6	14.7 ± 0.92
Distance Restraints					
Unambiguous	$6.37 \times 10^{-2} \pm 3.90 \times 10^{-2}$	$6.67 \times 10^{-2} \pm 1.91 \times 10^{-2}$	$6.10 \times 10^{-2} \pm 2.48 \times 10^{-2}$	$8.84 \times 10^{-2} \pm 1.7 \times 10^{-2}$	$4.60 \times 10^{-2} \pm 1.8 \times 10^{-2}$
Ambiguous	$6.09 \times 10^{-3} \pm 1.33 \times 10^{-2}$	$1.05 \times 10^{-2} \pm 1.84 \times 10^{-3}$	$5.97 \times 10^{-3} \pm 9.12 \times 10^{-3}$	$8.05 \times 10^{-3} \pm 1.1 \times 10^{-2}$	$6.673 \times 10^{-3} \pm 5.1 \times 10^{-3}$
All dist. restraints	$6.09 \times 10^{-2} \pm 3.69 \times 10^{-2}$	$6.34 \times 10^{-2} \pm 1.80 \times 10^{-2}$	$5.55 \times 10^{-2} \pm 2.22 \times 10^{-2}$	$8.20 \times 10^{-2} \pm 1.6 \times 10^{-2}$	$4.228 \times 10^{-2} \pm 1.6 \times 10^{-2}$
Dihedral restraints (deg)	$2.08 \times 10^{-2} \pm 3.33 \times 10^{-2}$	0.66 ± 0.25	$2.63 \times 10^{-2} \pm 4.00 \times 10^{-2}$	$1.00 \times 10^{-2} \pm 2.5 \times 10^{-2}$	-
Nonbonded energies					
Elect. (kcal·mol ⁻¹)	-543.54 ± 36.94	-467.98 ± 52.09	-513.94 ± 34.36	-458.82 ± 49.8	-493.37 ± 35.6
VDW (kcal·mol ⁻¹)	-150.63 ± 4.02	-173.70 ± 3.67	-165.41 ± 2.83	-156.41 ± 4.0	-166.84 ± 2.0
Ramachandran (%) ^{b, c}					
Most favoured	54.5	55.8	87.4	58.4	49.7
Additionally allowed	45.5	44.2	12.6	41.6	50.3
Generously allowed	0	0	0	0	0
Disallowed	0	0	0	0	0
Global RMSD ^d					
Backbone	(res. 3-19) 0.991	(res. 2-20) 0.514	(res. 4-17) 0.996	(res. 4-19) 0.849	(res. 4-19) 0.633
Heavy atoms	(res. 3-19) 1.364	(res. 2-20) 0.928	(res. 4-17) 1.587	(res. 4-19) 1.428	(res. 4-19) 1.027

a) The data in the Table are taken directly from the PROCHECK (41, 42) software output and do not imply an extremely high level of accuracy in the RMSD; b) Determined using PROCHECK (41,42); c) The relatively large number of residues that have backbone conformations in the additionally allowed regions, is quite frequently seen for structural ensembles of such linear helical peptides; typically these arise from residues near the N- and C-termini of the peptide, where the backbone structure is less well defined; d) Determined using MOLMOL (40).