

Table S1. Statistical analysis of pezadeftide structures. All statistics are given as mean \pm SD.

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|---|-------------------|
| Experimental restraints | |
| Total no. distance restraints | 419 |
| Intraresidue | 128 |
| Sequential | 132 |
| Medium range, $i-j < 5$ | 53 |
| Long range, $i-j \geq 5$ | 106 |
| Hydrogen bond restraints | 24 |
| Dihedral angle restraints | |
| Phi | 38 |
| psi | 25 |
| chi1 | 19 |
| Deviations from idealized geometry | |
| Bond lengths (Å) | 0.011 \pm 0.000 |
| Bond angles (deg) | 1.076 \pm 0.041 |
| Impropers (deg) | 1.36 \pm 0.11 |
| NOE (Å) | 0.010 \pm 0.002 |
| cDih (deg) | 0.056 \pm 0.053 |
| Mean energies (kcal/mol) | |
| Overall | -1626 \pm 35 |
| Bonds | 20.2 \pm 1.4 |
| Angles | 58.4 \pm 5.3 |
| Improper | 23.3 \pm 3.4 |
| van Der Waals | -216.2 \pm 7.2 |
| NOE | 0.04 \pm 0.01 |
| cDih | 0.06 \pm 0.09 |
| Electrostatic | -1738 \pm 35 |
| Violations | |
| NOE violations exceeding 0.2 Å | 0 |
| Dihedral violations exceeding 2.0 Å | 0 |
| Rms deviation from mean structure, Å | |
| Backbone atoms | 1.59 \pm 0.44 |
| All heavy atoms | 2.35 \pm 0.45 |
| Backbone atoms, residues 18-26,5-7,32-37,43-48 | 0.61 \pm 0.14 |
| All heavy atoms, residues 18-26,5-7,32-37,43-48 | 1.30 \pm 0.23 |
| Stereochemical quality (according to MolProbity) | |
| Residues in most favoured Ramachandran region, % | 94.7 \pm 2.2 |
| Ramachandran outliers, % | 0.6 \pm 1.3 |
| Unfavourable sidechain rotamers, % | 0.3 \pm 0.7 |
| Clashscore, all atoms | 14.6 \pm 4.1 |
| Overall MolProbity score | 2.1 \pm 0.1 |