**S1 Table. NMR and refinement statistics for integrin 2 TMD monomer**

|  |  |
| --- | --- |
|  | **Protein (PDB** 5ZAZ**)** |
| **NMR distance and dihedral constraints** |  |
| Distance constraints |  |
|  Total NOE | 452 |
|  Intraresidue | 161 |
|  Inter-residue | 291 |
|  Sequential (|*i* – *j*| = 1) | 178 |
|  Medium range (2 ≤ |*i* – *j*| ≤ 4) | 113 |
|  Long range (|*i* – *j*| ≥ 5) | 0 |
|  Hydrogen bonds | 50 |
| Total dihedral-angle restraints |  |
|  *φ* | 33 |
|  *ψ* | 33 |
|  |  |
| **Structure statistics** |  |
| CYANA target function valueViolations (mean ± s.d.) | 0.20 |
|  Distance constraints (Å)  | 0 |
|  Dihedral-angle constraints (°) | 0 |
|  Max. dihedral-angle violation (°)  |  |
|  Max. distance-constraint violation (Å)  |  |
| Average pairwise r.m.s. deviation (Å)a  |  |
|  Heavy | 0.66 |
|  Backbone  | 0.31 |

aPairwise r.m.s.d. was calculated for the -helix region (I679-E712) for the final 20 structures with the lowest target function values.