Table S4. NMR validation tables for designs D9.16, D8.31, and D8.21. RMSD calculated for 20 lowest energy structures out of 100. Related to Figure 4.

| NMR restraints   | D9.16         | D9.16         | D9.16         | D8.31         | D8.31         | D8.31         |
|------------------|---------------|---------------|---------------|---------------|---------------|---------------|
|                  | DMSO trans-cis| CDCl3 trans-cis| trans-trans   | DMSO cis-cis  | CDCl3 cis-cis | trans-trans   |
| Total NOEs       | 106           | 89            | 99            | 111           | 84            | 82            |
| Intra-residue    | 38            | 35            | 41            | 38            | 26            | 24            |
| Sequential [i-j]=1| 48            | 31            | 38            | 59            | 48            | 47            |
| Medium 1<i-j<5   | 20            | 23            | 20            | 14            | 10            | 11            |
| Long [i-j]>5     | 0             | 0             | 0             | 73            | 0             | 0             |
| Hydrogen bonds   | 0             | 0             | 0             | 0             | 0             | 0             |
| PHI dihedral restraints | 5 | 5 | 5 | 4 | 4 | 4 |

**Structure Statistics**

**Violations (mean and s.d.)**

|                      | D9.16 | D9.16 | D9.16 | D8.31 | D8.31 | D8.31 |
|----------------------|-------|-------|-------|-------|-------|-------|
| Max. distance restraint (Å) | 0.10  | 0.14  | 0.41  | 0.35  | 0.07  | 0.74  |
| Ave. distance restraints viol. (Å) | 0.02 ± 0.02 | 0.03 ± 0.03 | 0.07 ± 0.10 | 0.19 ± 0.15 | 0.02 ± 0.02 | 0.09 ± 0.15 |
| Max. dihedral angle (°) | 2.53  | 2.45  | 1.18  | 1.26  | 0.30  | 3.68  |
| Ave. dihedral viol (°) | 0.86 ± 0.73 | 0.78 ± 0.67 | 0.36 ± 0.26 | 1.18 ± 0.06 | 0.19 ± 0.07 | 1.27 ± 1.19 |

**Average pairwise RMSD**

|                      | D9.16 | D9.16 | D9.16 | D8.31 | D8.31 | D8.31 |
|----------------------|-------|-------|-------|-------|-------|-------|
| backbone (Å)         | 0.21 ± 0.07 | 0.24 ± 0.09 | 0.20 ± 0.05 | 0.21 ± 0.10 | 0.14 ± 0.12 | 0.48 ± 0.09 |
| heavy (Å)            | 0.53 ± 0.08 | 0.68 ± 0.12 | 0.73 ± 0.07 | 0.52 ± 0.22 | 0.54 ± 0.16 | 1.15 ± 0.16 |

| NMR restraints   | D8.21         | D8.21         | D8.21         | D8.21         | D8.21         | D8.21         |
|------------------|---------------|---------------|---------------|---------------|---------------|---------------|
|                  | DMSO trans-trans| DMSO50 trans-trans| cis-cis | DMSO trans-trans| DMSO50 trans-trans| cis-cis |
| Total NOEs       | 84            | 94            | 66            | 144           | 94            | 94            |
| Intra-residue    | 22            | 38            | 24            | 48            | 30            | 30            |
| Sequential [i-j]=1| 48            | 36            | 32            | 56            | 38            | 38            |
| Medium 1<i-j<5   | 14            | 20            | 10            | 40            | 26            | 26            |
| Long [i-j]>5     | 0             | 0             | 0             | 0             | 0             | 0             |
| Hydrogen bonds   | 0             | 0             | 0             | 0             | 0             | 0             |
| PHI dihedral restraints | 4 | 4 | 4 | 4 | 4 | 4 |

**Structure Statistics**

**Violations (mean and s.d.)**

|                      | D8.21 | D8.21 | D8.21 | D8.21 | D8.21 |
|----------------------|-------|-------|-------|-------|-------|
| Max. distance restraint (Å) | 0.19  | 0.45  | 0.01  | 0.30  | 0.57  |
| Ave. distance restraints viol. (Å) | 0.06 ± 0.06 | 0.08 ± 0.08 | 0.01 ± 0.00 | 0.08 ± 0.08 | 0.12 ± 0.16 |
| Max. dihedral angle (°) | 2.23  | 2.80  | 1.23  | 3.12  | 4.25  |
| Ave. dihedral viol (°) | 0.46 ± 0.59 | 2.17 ± 0.52 | 0.35 ± 0.47 | 2.56 ± 0.34 | 1.53 ± 1.37 |

**Average pairwise RMSD**

|                      | D8.21 | D8.21 | D8.21 | D8.21 | D8.21 |
|----------------------|-------|-------|-------|-------|-------|
| backbone (Å)         | 0.39 ± 0.18 | 0.25 ± 0.19 | 0.13 ± 0.03 | 0.21 ± 0.13 | 0.30 ± 0.11 |
| heavy (Å)            | 1.02 ± 0.25 | 0.74 ± 0.23 | 0.68 ± 0.13 | 0.64 ± 0.28 | 0.76 ± 0.17 |