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.

	D9.16 DMSO trans-cis	D9.16 CDCl3 trans-cis	D9.16 CDCl3 trans-trans	D8.31 CDCl3 cis-cis	D8.31 DMSO cis-cis	D8.31 DMSO cis-trans
NMR restraints						
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.)						
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 (º)	2.53	2.45	1.18	1.26	0.30	3.68
Ave. dihedral viol (º)	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						
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

	D8.21 DMSO trans-trans	D8.21 DMSO50 trans-trans	D8.21 DMSO50 cis-cis	D8.21 CDCl3 trans-trans	D8.21 CDCl3 trans-cis
NMR restraints					
Total NOEs	84	94	66	144	94
Intra-residue	22	38	24	48	30
Sequential |i-j|=1	48	36	32	56	38
Medium 1<|i-j|<5	14	20	10	40	26
Long |i-j|>=5	0	0	0	0	0
Hydrogen bonds	0	0	0	0	0
PHI dihedral restraints	4	4	4	4	4
Structure Statistics					
Violations (mean and s.d.)					
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 (º)	2.23	2.80	1.23	3.12	4.25
Ave. dihedral viol (º)	0.46 ± 0.59	2.17 ± 0.52	0.35 ± 0.47	2.56± 0.34	1.53 ±1.37
Average pairwise RMSD					
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