Table S1. Structural statistics for the 10 best structures of alvinellacin showing the lowest target functions. None of the distance constraints was violated by more than 0.5 Å in any structure.

Distance restraints	*Number*
Intraresidual ($\|i-j\| = 0$)	38
Sequential ($\|i-j\| = 1$)	40
Medium range ($2 \leq \|i-j\| \leq 4$)	0
Long range ($\|i-j\| \geq 5$)	14
Disulfide bonds (included)	12
Total	104
Pairwise rmsd	
Mean global backbone rmsd to mean*	0.49 ± 0.20 Å
Mean global heavy rmsd to mean*	1.47 ± 0.20 Å
Ramachandran plot	
Most favored regions	73.5 %
Additional allowed regions	18.8 %
Generously allowed regions	6.5 %
Disallowed regions	1.2 %

* Residues considered: 4-9, 14-19