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The structure determination of biological peptides like antibiotics and microproteins is complicated by unique factors. There are only a few crystallisation screens available that are directed to this substance class, and the asymmetric unit is usually comparable to that in average protein structures, which constitutes a significant barrier when trying to overcome the phase problem. In addition, refinement of these structures is complicated by unusual residues and requires high-resolution data.

Three structures belonging to this class have recently been determined using *ab initio* direct methods. Viscotoxin B2 is a thionin with 46 amino acid residues, but with two independent molecules that correspond to about 800 atoms. Asymmetric unit of the antibiotic feglymycin was thought to consist of about 500 independent atoms with oxygen as the heaviest element present. The amphomycin-analogue tsushimycin is an 11-residue Ca^{2+}-binding cyclopeptide with a long fatty acid sidechain, and contains about 1300 atoms in 12 independent molecules.

In all cases, data were available to atomic resolution, but resolution limit varied from higher than 1.0 Å to barely atomic with 3σ intensity between 1.1-1.2 Å. SHELXD [1] was employed by first locating heavier elements (viscotoxin: 6 S, tsushimycin: 24 Ca^{2+}) and then expanding the structure with peaklist optimisation. For feglymycin, where there is no element heavier than oxygen, a portion of the structure was searched that was thought to be large enough to give an indication for success. Solution was achieved in all cases with varying success rates, which were considerably dependent on the number of heavier atoms and was the highest for tsushimycin and the lowest for the equal-atom structure feglymycin. In the refinement, feglymycin proved to be merohedrally twinned, and taking the twin operation into account, the size of the asymmetric unit corresponds to more than 1000 atoms with that feglymycin is by far the largest equal-atom structure solved so far.

[1] Sheldrick, G. M., Hauptman, H. A., Weeks, C. M., Miller, M. & Usón, I. (2001). International Tables for Crystallography, Vol. F, edited by E. Arnold & M. G. Rossmann, pp. 333-351. Kluwer Academic Publishers, Dordrecht.