Molecular replacement using *ab initio* polyalanine models generated with *ROSETTA*

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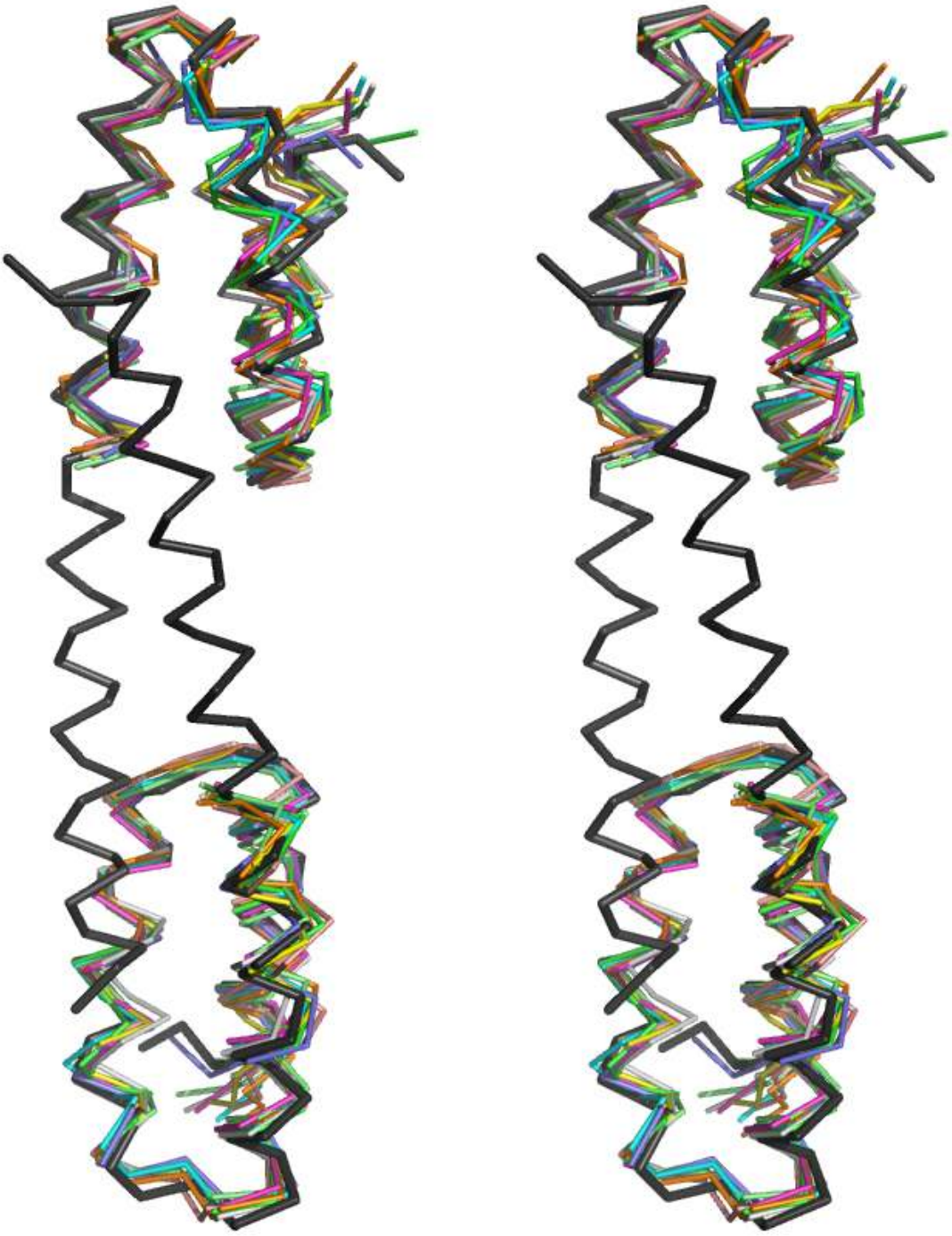
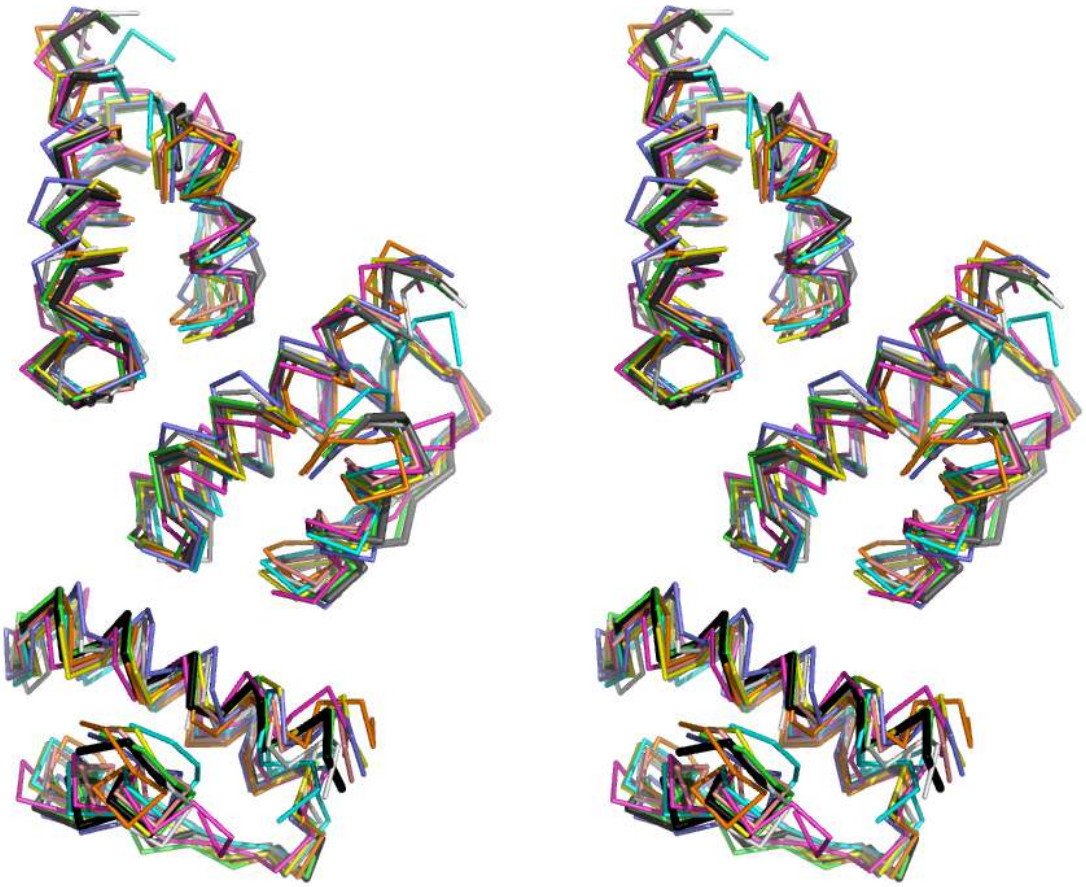
Supplementary material

Supplementary Figure 1. Cross-eyed stereo representations of the most accurate solutions found for a) 2fzt, b) 2nn4, c) 2o3l, d) 2pmr and e) 2duy (see also Table 1). In each case the crystal structure is shown as a Cα trace, in shades of dark grey or black to differentiate between chains. The solutions are shown as single structures (2pmr) or ensembles (see Table 1) with different colours indicating members of the ensemble. This figure and Supp. Fig 2 were made with *PyMOL* [Delano, W. L. (2002), *The PyMOL Molecular Graphics System*, DeLano Scientific LLC, San Carlos, California, USA, http://www.pymol.org]. PDB files of these structures are available on request.

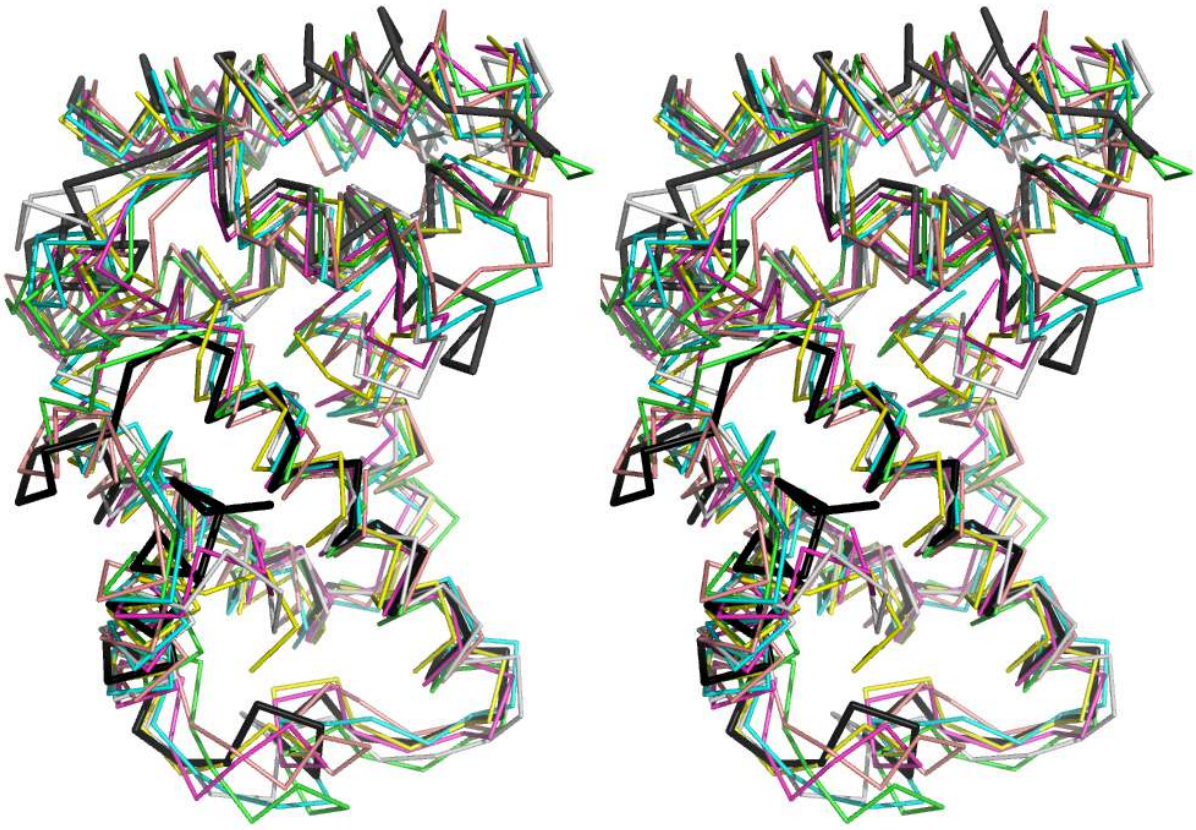
a)



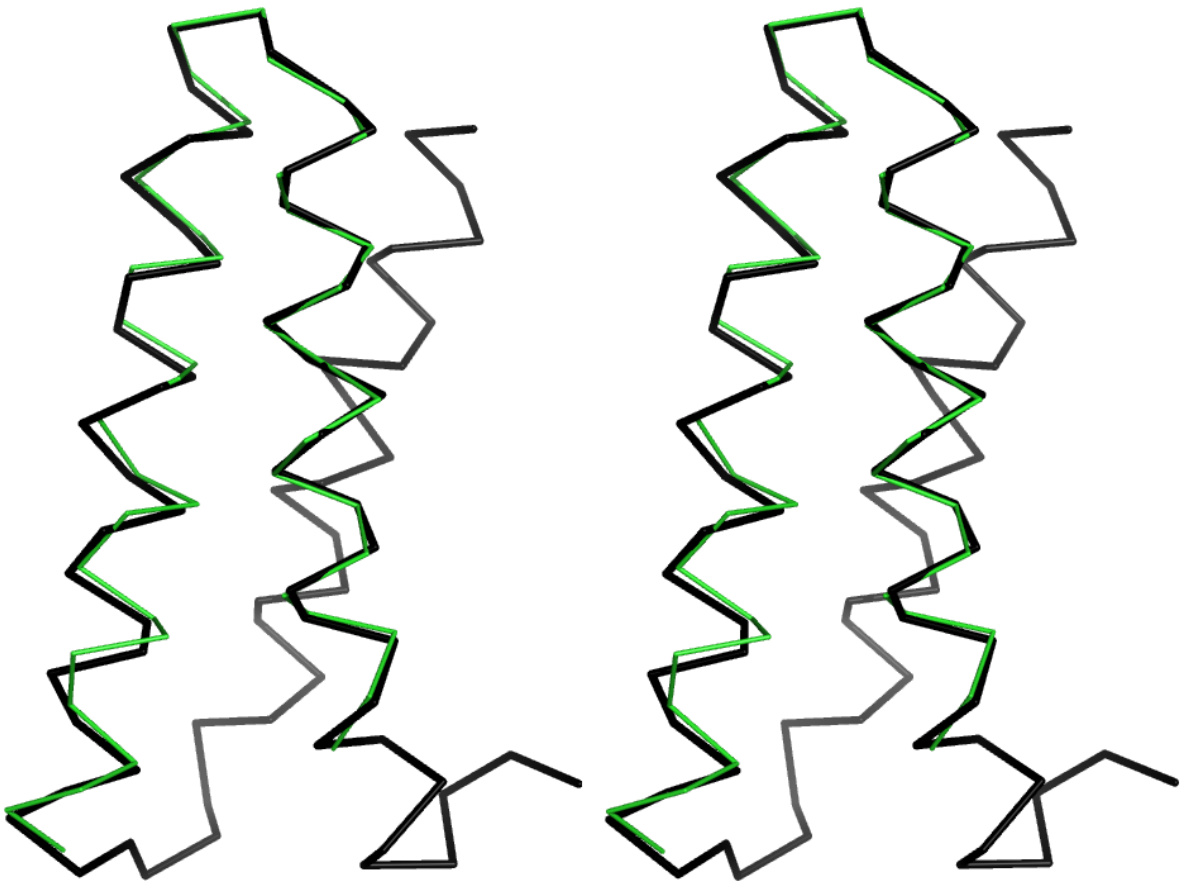
b)



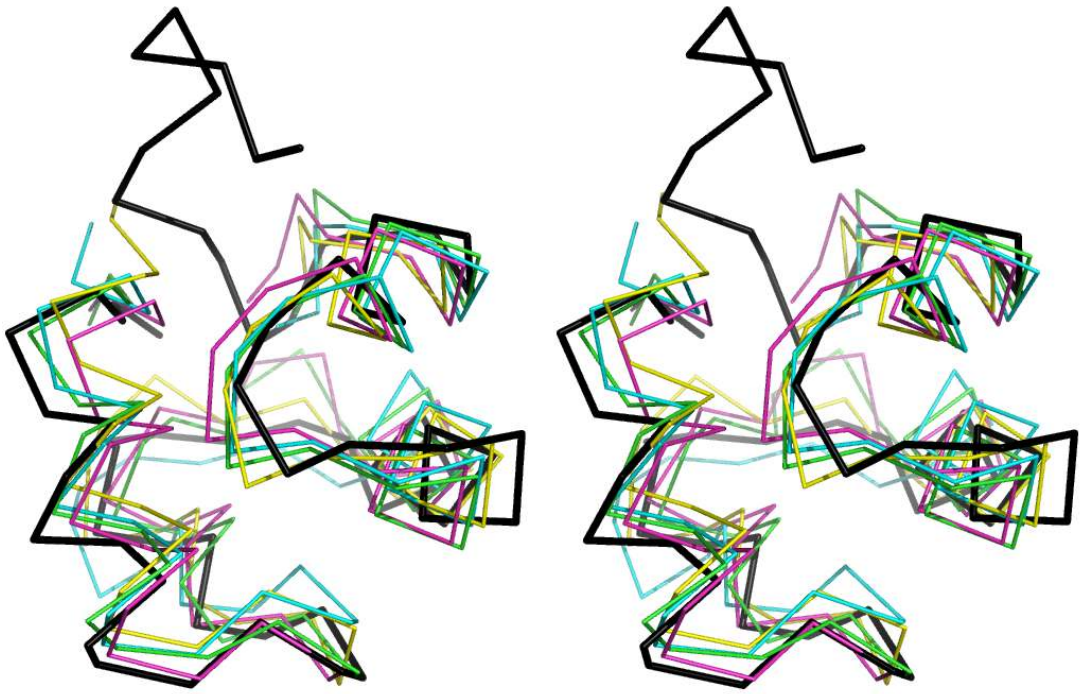
c)



d)



e)



Supplementary Figure 2. Cross-eyed stereo representations of the most accurate solution found for 2pmr, drawn as in Supp. Fig 1, but including side chains. Note that certain residues in the crystal structure were modelled with alternative side chain conformations. PDB files of these structures are available on request.