Table 2. Anisotropic refinement statistics

	MMP12-NNGH	MMP12-AHA-HR
Resolution, Å	46.4 – 1.3	14.0 – 1.0
Total reflections used	36,256	70,800
Reflections in working set	33,678	65,283
Reflections in test set, 8%	2,578	5,517
R_{cryst} / R_{free}, %	17.8 / 21.4	15.5 / 16.7
Protein atoms	1,249	2,417 (including hydrogens)
Ligand atoms	26	8 (including hydrogens)
Water molecules	236	291
RMSD bonds, Å	0.014	0.009
RMSD angles, °	1.66	1.3
Average *B* factor (including ligand), $Å^2$	18.2	8.7