ESRF	Experiment title: The peripheral anionic site of Mouse Acetylcholinesterase	Experiment number: LS1657
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Report:

We used a new crystal form of mouse acetylcholinesterase (AchE) that permits more accurate studies of the peripheral anionic site of this enzyme. This new crystal form diffracts up to 2.2 Å resolution and contains two molecules in the asymmetric unit, with the catalytic gorge entrance being freely solvent accessible in each subunit. This differs from the previous 3 Å resolution structure (1) for which only one molecule out of two possessed a solvent-accessible gorge entrance. In addition, the previous crystal form grew with a high salt concentration compared to a low salt concentration required for the new crystal form, a critical parameter to study ligands directed to the peripheral anionic site. We thus used two compounds (A & B) that display high affinity for this site and performed co-crystallization experiments with AChE. Previous data from similar crystals soaked with these two compounds showed only partial occupancies for these compounds. Data obtained from these crystals are of excellent quality (Table 1). For these two structures, rigid-body refinement was then performed on each subunit with CNS using data between 30 Å and 3 Å and gave an R-factor and R-free values of 22.8 and 23% for compound A and B, respectively. For 2% of the reflections against which the two models were not refined, R-free was 23.5% and 22.6%. Refinement of these two structures is underway.

Table 1. Data collection and refinement statistics

	compound A	compound B
Resolution (Å)	2.35	2.35
No. observations	366 789	359 483
No. unique	81 919	24 748
R_{sym} (%)	4.6 (18)	4.6 (25)
I/σ(I)	8.3 (4.1)	9.4 (2.8)
Redundancy	2.9	3.0
Completeness (%)	97.6 (84)	93.5 (93.5)
Resolution (Å)	20- 2.35	20 – 2.35
R-factor - R free (%)	22.4 - 25	20 - 24

References

1 Bourne, Y., Taylor, P. & Marchot, P. (1999) *J. Biol. Chem.* **274**, 2963-70.