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online data

SUPPLEMENTARY ONLINE DATA

How the biotin–streptavidin interaction was made even stronger: investigation via crystallography and a chimaeric tetramer

Claire E. CHIVERS, Apurba L. KONER, Edward D. LOWE and Mark HOWARTH[1]

Department of Biochemistry, Oxford University, South Parks Road, Oxford OX1 3QU, U.K.

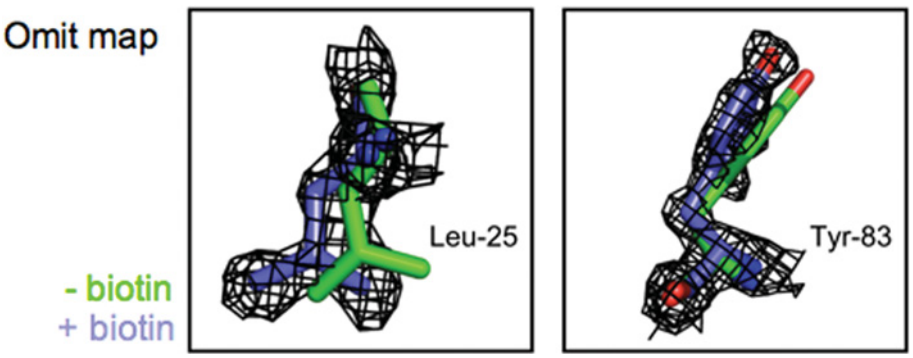

Figure S1 Testing for bias in the biotin–Tr structure caused by the search model for molecular replacement

Apo-Tr was used as the search model for molecular replacement to solve the structure of biotin–Tr. Simulated annealing composite omit maps, with starting phases from the apo-Tr structure, are shown in black mesh for Leu^{25} (left-hand panel) and Tyr^{83} (right-hand panel), contoured at 1.3 σ. The apo-Tr backbone structure is overlaid in green and the biotin–Tr structure in blue. The final biotin–Tr structure fitted the omit map much better (correlation coefficient 0.73 for side-chain atoms) than the apo-Tr structure (correlation coefficient 0.47 for side-chain atoms). Leu^{25} and Tyr^{83} were chosen because they illustrate that the biotin–Tr structure fits the omit map better than the apo-Tr structure does. Overall, the alignment clearly shows that the apo-Tr model does not fit the composite omit maps, which indicates that the solution of the biotin–Tr structure was not biased by the search model.

[1] To whom correspondence should be addressed (email mark.howarth@bioch.ox.ac.uk).

The structural co-ordinates reported will appear in the PDB under accession codes 2Y3E and 2Y3F.

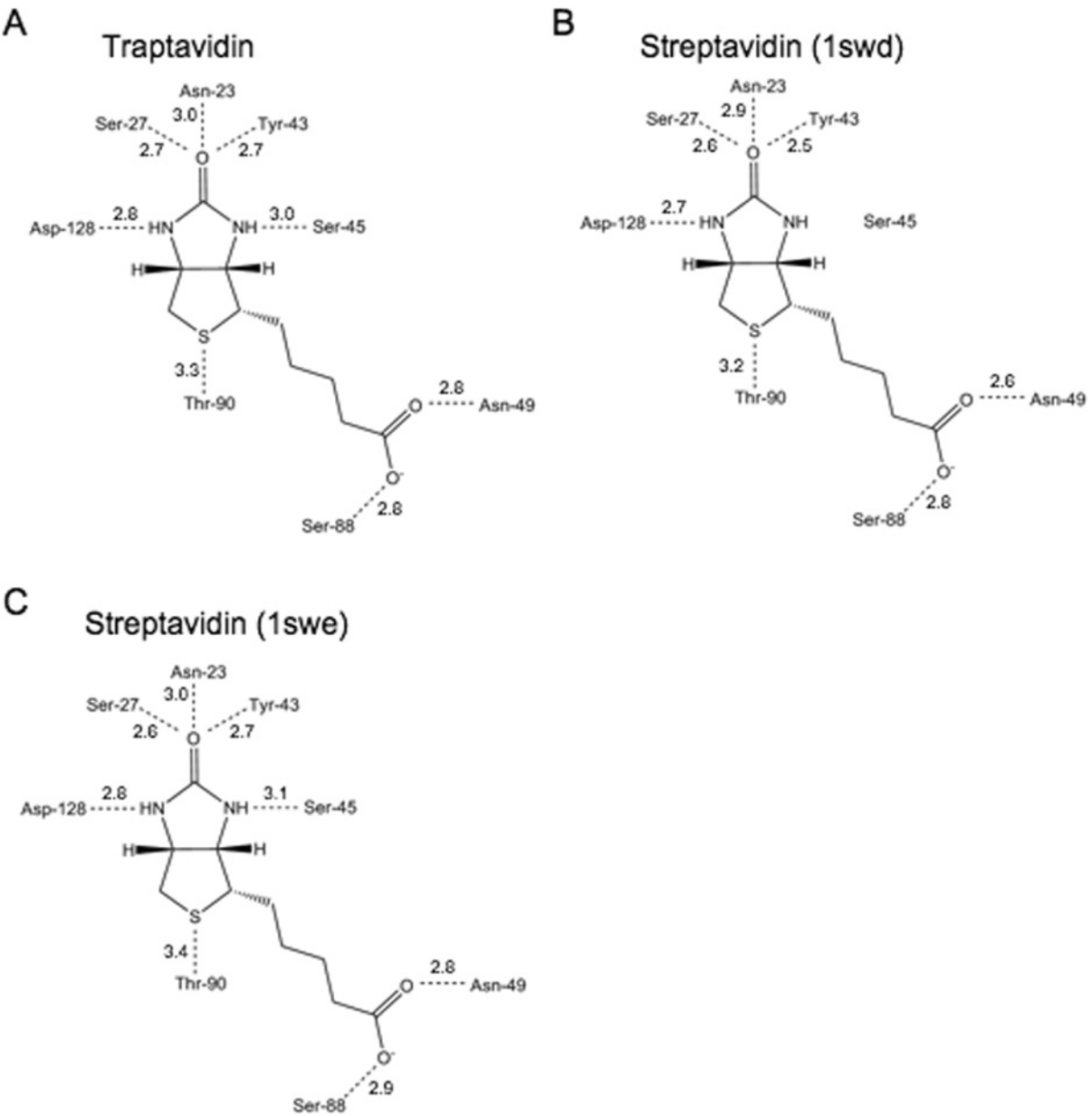

Figure S2 Hydrogen-bond lengths to biotin for Tr and SA

(**A**) Hydrogen bond lengths (in Å) for Tr (only one subunit shown, since all subunits are equivalent). The DPI gave an estimated co-ordinate error for biotin–Tr of 0.051 Å. (**B**) Hydrogen-bond lengths for SA, 1SWD (mean bond lengths for the two biotins bound per tetramer). Ser[45] here does not form a hydrogen bond to biotin. (**C**) Hydrogen-bond lengths to biotin for SA from an alternative crystal structure, 1SWE (mean bond lengths for the four biotins bound per tetramer).

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