



STRUCTURAL BIOLOGY
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Supporting information for article:

Structures of *Brucella ovis* leucine-, isoleucine-, valine-, threonine- and alanine-binding protein reveal a conformationally flexible peptide-binding cavity

Graham Chakafana, Reghan Boswell, Andrew Chandler, Krishelle A. Jackson, Senai Neblett, Tyler Postal, Sandhya Subramanian, Jan Abendroth, Peter J. Myler and Oluwatoyin A. Asojo

Ligands bound in the binding site are crystallization artifacts and usurped from the crystallization solution.

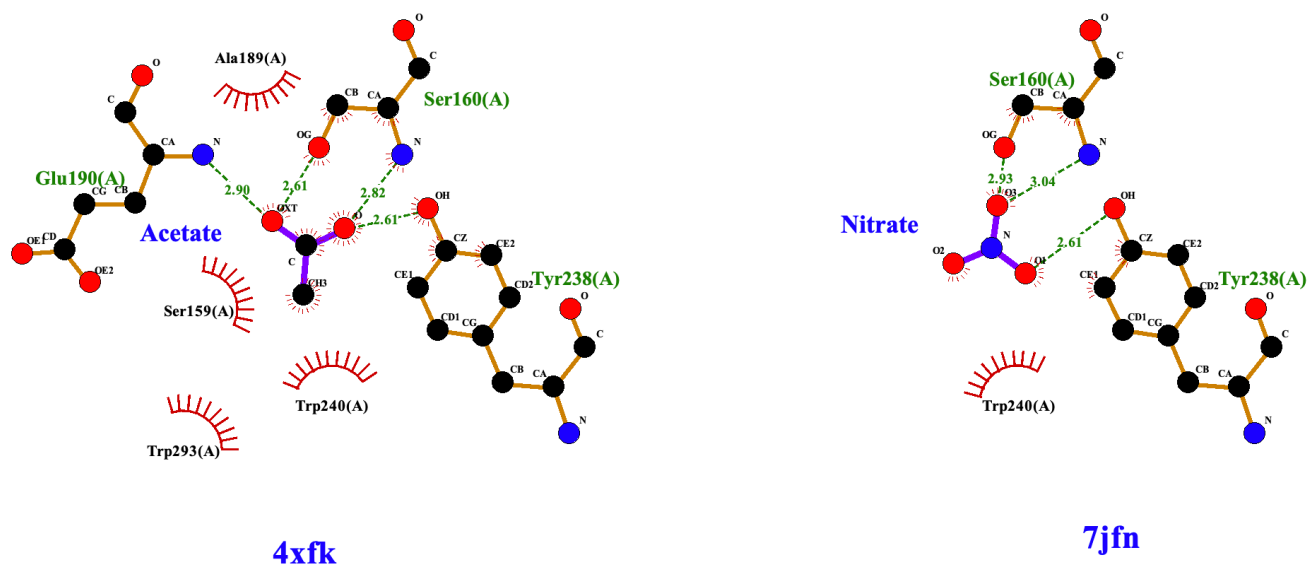


Figure S1a: Ligplus map of the interactions of acetate and nitrate atoms in the binding cavities of 4xfk and 7jfn, respectively.

These ligands have well-ordered electron density maps, as shown below.

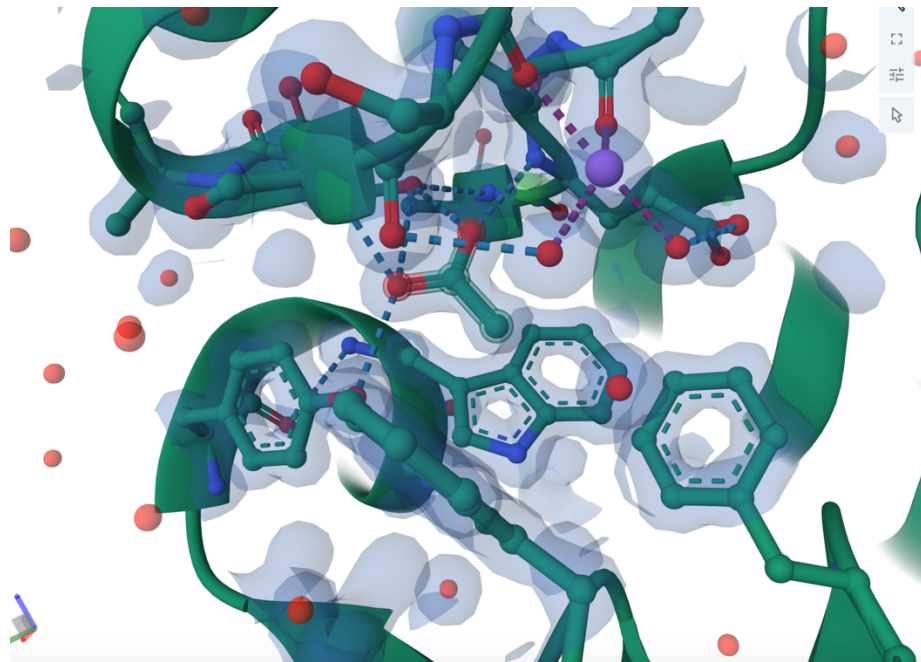


Figure S1b Acetate in the binding cavity of PDB entry 4xfk. Image generated with pdb viewer and 2Fo-F map electron density contoured at 1.6σ

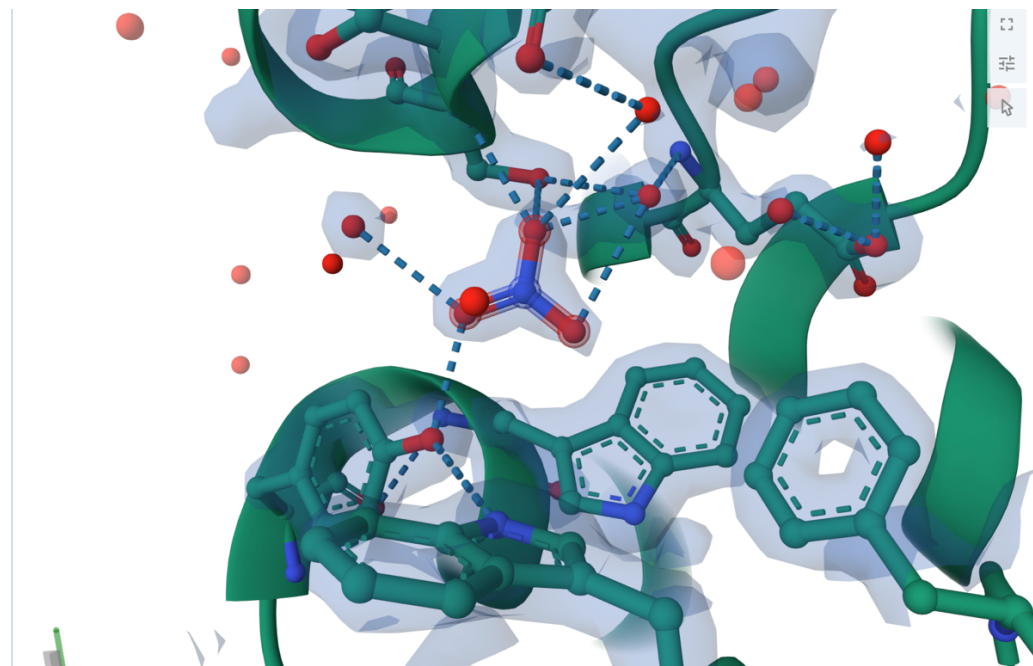


Figure S1c: Nitrate in the binding cavity of PDB entry 7jfn. Image generated with pdb viewer and 2Fo-F map electron density contoured at 1.74σ

S2. DynDom Analysis

Domain Pairs

Property	Value
Fixed Domain (blue)	1
Moving Domain (red)	2
Rotation Angle (deg)	12.0
Translation (A)	0.2
Closure (%)	99.1
Bending Residues (green)	211 - 212
	316 - 322
	326 - 335
	339 - 340
	426 - 429
	448 - 449
	456 - 457

[Bending Region Analysis](#)

Dynamic Contact Graph

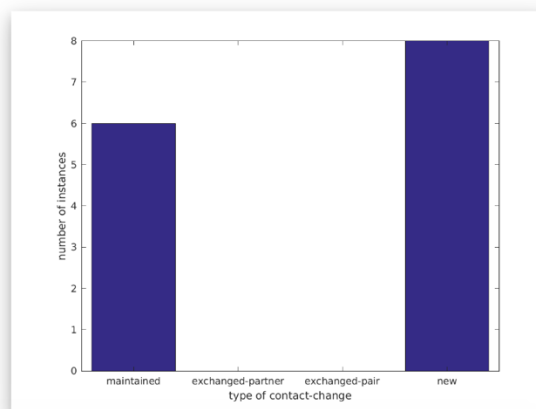
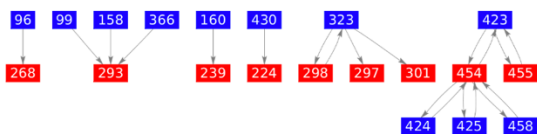
Conformer 1 Contact:

Residue 1 \dashrightarrow **Residue 2**

Conformer 2 Contact:

Residue 2 \dashrightarrow **Residue 1**

Movement classification: Hinge

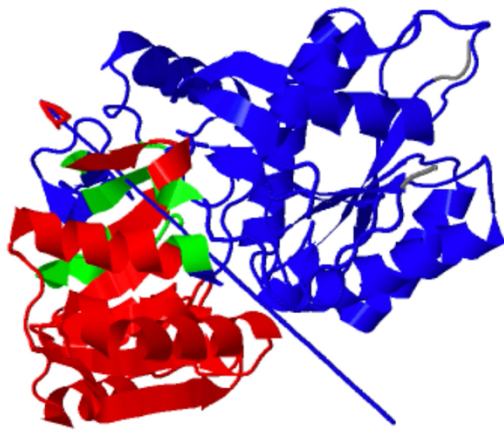


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4XFK (A) : AEPLKIALVETLSGPQASTGLLYRAAVLYQLGKINEAGGFNGEKIQILEYDNQGGPVGAAADRVKAAIADGAQIIVQGSS:
:
7JFN (A) : AEPLKIALVETLSGPQASTGLLYRAAVLYQLGKINEAGGFNGEKIQILEYDNQGGPVGAAADRVKAAIADGAQIIVQGSS:
:
      211
4XFK (A) : FYHFRFSPNAAIRFKTVAQGMKDKGILGERAYSINQNSWGVVDVENTVVANAKEIGYEVVDKTLHEVNKIQDFSPYVAK:
:
7JFN (A) : FYHFRFSPNAAIRFKTVAQGMKDKGILGERAYSINQNSWGVVDVENTVVANAKEIGYEVVDKTLHEVNKIQDFSPYVAK:
:
      211
      326      339
4XFK (A) : PGNIGNAGAI AEGHIVSTPFNPEANGEASMAFAEDYK KVTGHYPSYVEPAAV FGLQLFGEALKNV KPEGKINTTDIAL:
:
7JFN (A) : PGNIGNAGAI AEGHIVSTPFNPEANGEASMAFAEDYK KVTGHYPSYVEPAAV FGLQLFGEALKNV KPEGKINTTDIAL:
:
      326      339
      448      456
4XFK (A) : GTEYGFLPFKTF TGDESIDPVQESCSMKRPG
:
7JFN (A) : GTEYGFLPFKTF TGDESIDPVQESCSMKRP*
:
      448      456

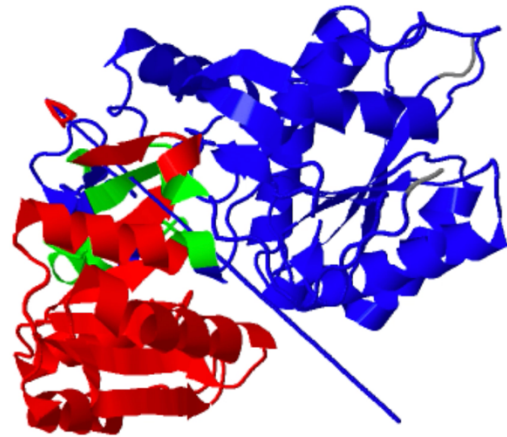
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DynDom



4XFK (A)

DynDom



JSmol 7JFN (A)

JSmol

The conformational plasticity is more evident in the movie than in still images.