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The controlled relay of multiple protons required at the active site of nitrogenase.

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Supplementary material

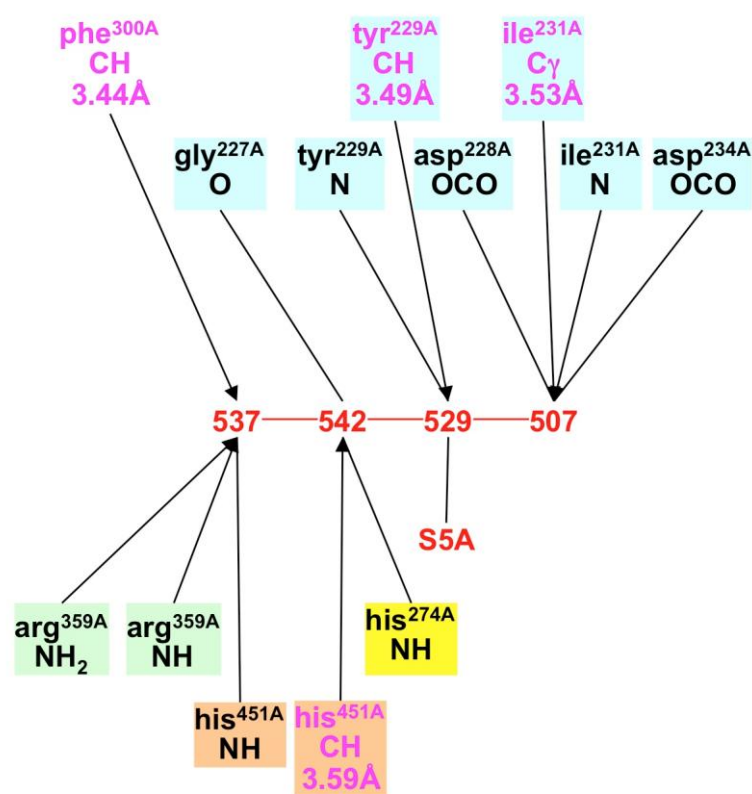


Fig S1. Schematic presentation of the hydrogen bonding of the four water molecules W537, W542, W529, W507 (PDB 3U7Q labels) with S5A and surrounding amino-acids: see Fig 3. Lines are possible hydrogen bonds, similarly coloured residues are in the same chain section, and possible C-H → O hydrogen bonds are marked in magenta.

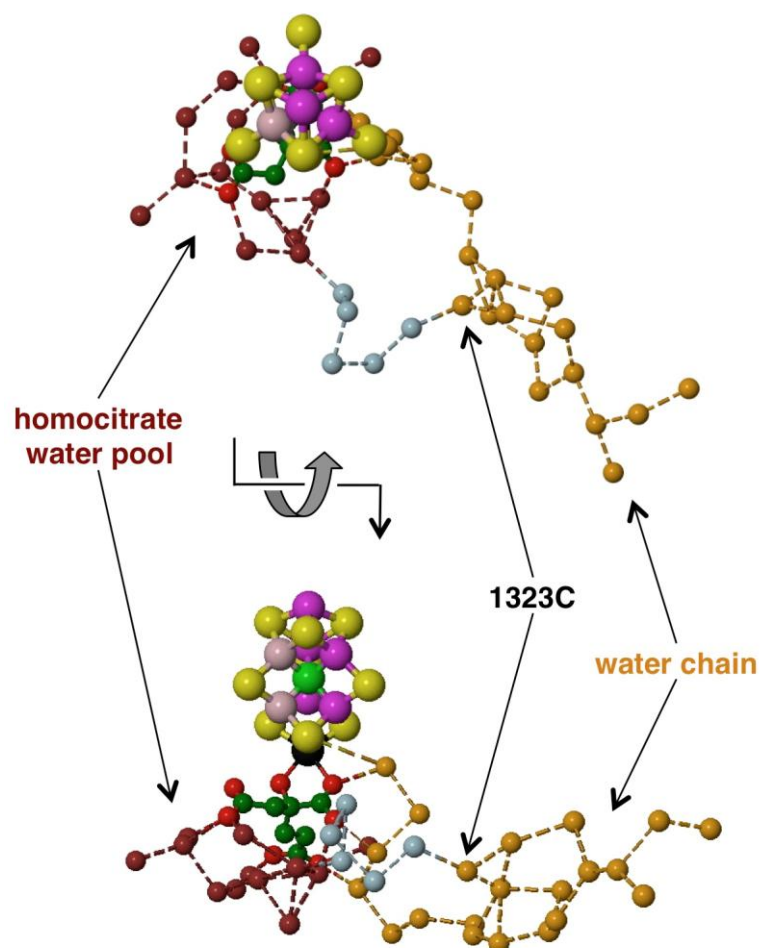


Fig S2. Top and front views of five water molecules, grey, chaining between water 1323C of PDB 3U7Q and the pool of water molecules (dark brown) around homocitrate. This chain is not near the proton wire. Water 1323C is in the branched proton bay section of the water chain.

Supplementary Table T1. Details of the numbering and hydrogen bonding connections of the first nine water molecules in the twelve high quality instances of the water chain

structure	W1	W2	W3	W4	W5	W6	W7	W8	insertion	W9
	Arg C γ	Arg C α					Arg C γ ,C δ			Ala C β
	His O	Arg N	Gly O	Arg NH $_2$	Arg NH	Gly O		Ala O		
1M1N #1	679	15	259	24	50	370	120	261		1806
	HCA O5		HCA O6	HCA O3	Tyr OH		Val O	Val N, Leu N		Leu N
	Ile C δ	Ser C α				Tyr ringC	Val C β , Tyr ringC			Asp C α
	Arg C γ	Arg C α					Arg C γ ,C δ			Ala C β
	His O	Arg N	Gly O	Arg NH $_2$	Arg NH	Gly O		Ala O		
1M1N #2	381	363	533	86	53	271	59	265		1549
	HCA O5		HCA O6	HCA O3	Tyr OH		Val O	Val N, Leu N		Leu N
	Ile C δ	Ser C α				Tyr ringC	Val C β , Tyr ringC			Asp C α
	Arg C γ	Arg C α					Arg C γ ,C δ			Ala C β
	His O	Arg N	Gly O	Arg NH $_2$	Arg NH	Gly O		Ala O		
1M1N #3	3220	2552	2796	2561	2587	2909	2657	2798		4321
	HCA O5		HCA O6	HCA O3	Tyr OH		Val O	Val N, Leu N		Leu N
	Ile C δ	Ser C α				Tyr ringC	Val C β , Tyr ringC			Asp C α
	Arg C γ	Arg C α					Arg C γ ,C δ			Ala C β
	His O	Arg N	Gly O	Arg NH $_2$	Arg NH	Gly O		Ala O		
1M1N #4	2920	2901	3072	2623	2590	2808	2596	2802		4079
	HCA O5		HCA O6	HCA O3	Tyr OH		Val O	Val N, Leu N		Leu N
	Ile C δ	Ser C α				Tyr ringC	Val C β , Tyr ringC			Asp C α
		Arg C α					Arg C γ ,C δ	Imid edge		Ala C β
	His O	Arg N	Gly O	Arg NH $_2$	Arg NH	Gly O		Ala O		
3U7Q #1	519A	506A	536A	534A	503A	510A	676D	511A		698D
	HCA O5		HCA O6	HCA O3	Tyr OH		Val O	Leu N		Leu N
		Ser C α				Tyr ringC	Val C β , Tyr ringC			Asp C α

		Arg C α					Arg C γ ,C δ		Ala C β
	His O	Arg N	Gly O	Arg NH ₂	Arg NH	Gly O		Ala O	
3U7Q #2	479C	514C	537C	517C	522C	521C	657B	502C	887B
	HCA O5		HCA O6	HCA O3	Tyr OH		Val O	Val N, Leu N	Leu N
		Ser C α	Ser C β			Tyr ringC	Val C β , Tyr ringC		Asp C α
							Arg C γ ,C δ		
	His O	Arg N	Gly O	Arg NH ₂	Arg NH	Gly O		Ala O	
2AFH #1	99	265	309	1456	341	648	1503	179	557
	HCA O5		HCA O6	HCA O3	Tyr OH		Val O	Val N, Leu N	Leu N
		Ser C α	Ser C β				Val C β , Tyr ringC		Asp C α
							Arg C γ ,C δ		Ala C β
	His O	Arg N	Gly O	Arg NH ₂	Arg NH	Gly O		Ala O	
2AFH #2	259	96	1074	314	1491	357	59	405	895
	HCA O5		HCA O6	HCA O3	Tyr OH		Val O	Val N, Leu N	Leu N
		Ser C α	Ser C β				Tyr ringC		
	Arg C γ	Arg C α					Arg C γ ,C δ		
	His O	Arg N	Gly O	Arg NH ₂	Arg NH	Gly O		Ala O	OCH₂CH₂O
1QGU #1	10	12	9	609	7	23	1967	19	138
	HCA O5		HCA O6	HCA O4*	Tyr OH		Val O	Val N, Leu N	Leu N
		Ser C α			Tyr ringC		Val C β , Tyr ringC		Asp C α
	Arg C γ						Arg C γ ,C δ		
	His O	Arg N	Gly O	Arg NH ₂	Arg NH	Gly O		Ala O	
1QGU #2	1396	1410	1393	1963	1376	1405	615	1384	802
	HCA O5		HCA O6	HCA O4*	Tyr OH		Val O	Val N	Val N
		Ser C α			Tyr ringC		Val C β , Tyr ringC		Asp C α
							Arg C γ ,C δ		
	His O	Arg N	Gly O	Arg NH ₂	Arg NH	Gly O		Ala O	OCH₂CH₂O
1QH1 #1	13	12	2	584	3	17	1861	15	126
	HCA O5		HCA O6	HCA O4*	Tyr OH		Val O	Leu N	Leu N
		Ser C α							

	Arg C γ , Ile C δ						Arg C γ ,C δ			
	His O	Arg N	Gly O	Arg NH ₂	Arg NH	Gly O		Ala O		
1QH1 #2	1335	1339	1344	1865	1311	1346	600	1319	1441	690
	HCA O5		HCA O6	HCA O4*	Tyr OH		Val O	Val N, Leu N		Leu N
		Ser C α					Tyr ringC			

* O3 in Av structures is labelled O4 in crystals 1QGU and 1QH1 of Kp.