

CHEM**BIO**CHEM

Supporting Information

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Supporting Information

for

Parallel Pathways and Free-Energy Landscapes for Enzymatic Hydride Transfer Probed by Hydrostatic Pressure

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Table S1. Data collection and refinement statistics of N189A MR - NADH₄ bound structure.

Data collection	
Space Group	$I2_12_12_1$
Unit Cell (Å)	$a=49.7$ $b=122.9$ $c=179.6$
Resolution (Å)	2.3 (2.4-2.3)
Total Reflections	104,562
Unique Reflections	23,517
Completeness (%)	92.1 (94.6)
Redundancy	4.4 (4.4)
Refinement	
R_{merge}	7.7 (29.1)
$\ \sigma \ $	7.4 (2.5)
R_{work}	18.1 (27.3)
R_{free}	23.1(46)
rmsd angle (°)	1.83
rmsd bond length (Å)	0.02

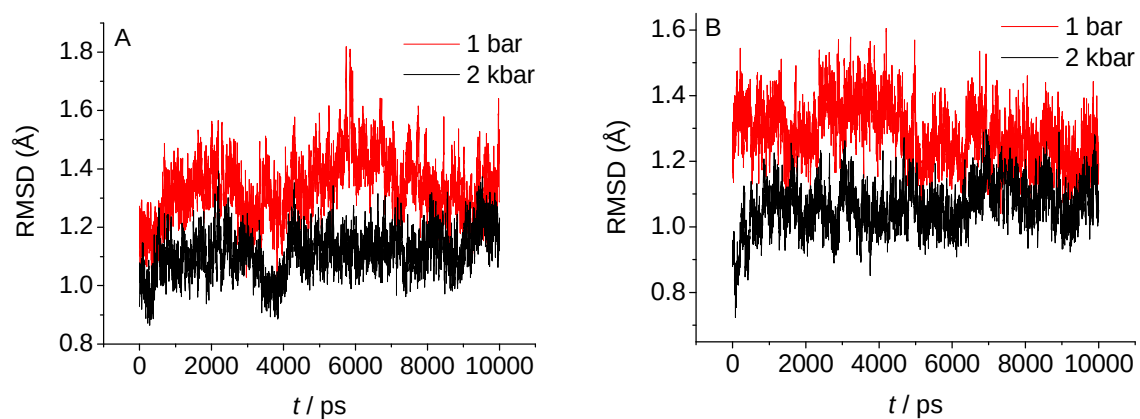


Figure S1. Root mean square deviations (RMSDs) of the backbone heavy atoms of wild-type MR (A) and N189A MR (B) along the stimulated trajectories at 1 bar (red) and 2 kbar (black).

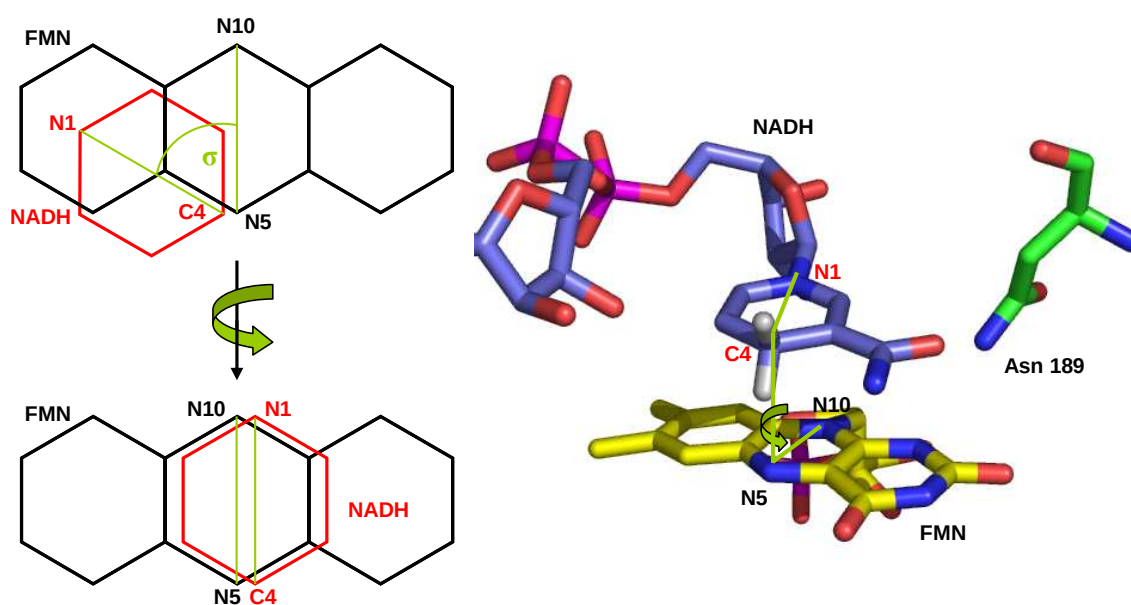


Figure S2. Structure of the N189A MR-NADH complex illustrating the dihedral angle NADH N1 – NADH C4 – FMN N5 – FMN N10.