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Supplementary Material

Structural basis of stereospecific reduction by quinuclidinone reductase

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Table S1. Statistics of the data collection of the RrQR crystal in the resolution range 2.98 Å to 2.20 Å. The diffraction data up to 2.2 Å resolution were used for the structural refinement.

Resolution (Å)	R_{merge} (%) [a]	Redundancy	Completeness (%)
2.98 – 2.77	11.7	12.5	99.4
2.77 – 2.61	12.8	12.6	98.9
2.61 – 2.48	14.3	12.7	98.8
2.48 - 2.37	16.1	12.2	98.6
2.37 – 2.28	20.9	9.9	93.1
2.28 – 2.20	23.9	8.9	81.0

[a] $R_{merge} = \Sigma_{hkl} \Sigma_i |I_i(hkl) - \langle I(hkl) \rangle| / \Sigma_{hkl} \Sigma_i I_i(hkl)$, where $I_i(hkl)$ is the *i*-th intensity measurement of reflection *hkl*, including symmetry-related reflections, and $\langle I(hkl) \rangle$ is its average.

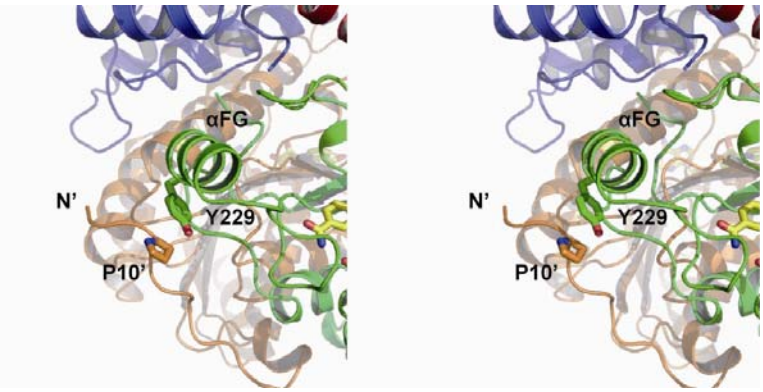

Fig. S1 Residues P10 and Y229 of a neighboring subunit shown by the stick model form a stacking interaction. Protomers in the tetramer are colored green, orange, blue, and red.

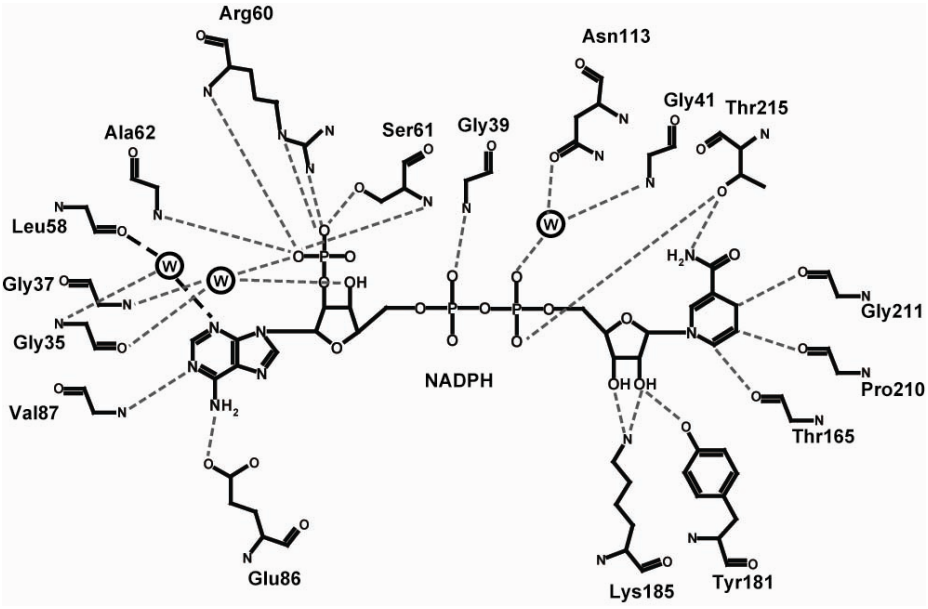

Fig. S2 The recognition of NADPH by RrQR. Hydrogen bonds are indicated by dotted lines. Water molecules involved in NADPH binding are shown.

Fig. S3 Residues interacting with the substrate. The schematic was prepared by the program Ligplot (Laskowski et al. 2011) using the catalytic model in Fig. 4.