Supplement Table 1: Diffraction data collection and refinement statistics (complete list)

Data collection and processing			
Data set	GatDH	GatDH with 1,2-pentanediol	GatDH with erythritol
PDB entry	2WSB	2WDZ	2LQF
Crystallization condition	100 mM sodium cacodylate, pH 6.5 200 mM sodium acetate 30 % PEG8000 4 % (v/v) n-propanole 1 mM GatDH 1 mM NAD^+	100 mM MES, pH 5.5 200 mM MgCl2 12.5 % MPEG5000 1 mM GatDH 8.3 mM NAD^+ 50 mM 1,2-(*R,S*)-pentanediol	100 mM MES, pH 5.7 200 mM MgCl2 14 % MPEG5000 1 mM GatDH 1 mM NAD^+
X-Ray source	ID 14.3, ESRF	BL 14.2, BESSY	BL 14.2, BESSY
Detector	Mar165 CCD	MARmosaic225	MARmosaic225
Wavelength (Å)	0.93	0.92	0.92
Temperature (K)	100	100	100
Crystal-to-film distance (mm) [a]	150/95/90 (lr/mr/hr)	290/180 (lr/hr)	200
Exposure time (sec) [a]	3/6/50 (lr/mr/hr)	3.5/7.2 (lr/hr)	3.5
Oscillation range (deg.)	0.4	1	0.5
total oscillation range (deg.) [a]	100/100/52.7 (lr/mr/hr)	180	180
Space group	P2(1)2(1)2(1)	C222(1)	P2(1)2(1)2(1)
Cell dimensions (Å, deg.)			
a / b / c	97.8/106.6/109.3	60.8 / 113.6 / 257.3	63.8 / 113.8 / 123.2
α / β / γ	90/90/90	90 / 90 / 90	90 / 90 / 90
Resolution limit (Å) [b]	20-1.25 (1.28-1.25)	20-1.95 (2.06-1.95)	33.3 – 1.8 (1.85-1.8)
Completeness (%) [b]	99.9 (99.8)	98.5 (98.5)	99.9 (99.3)
No. observations (overall / unique)	2111884/313320	572842 / 64019	614280 / 83822
Average redundancy	6.7 (2.5)	8.9 (4.8)	7.3 (6.8)
$\langle I/\sigma(I)\rangle$ [b]	8.4 (2.0)	15.1 (1.8)	17.65 (2.9)
$R_{p.i.m.}$ [b,c]	3.7 (34.8)	4.0 (31.6)	8.4 (74.7)
B-factor from Wilson plot ($Å^2$)	10.5	32	28.5
Refinement statistics			
Resolution limit (Å)	20-1.25	20-1.95	30 – 1.8
Number of unique reflections [b]	297654	60703	83814
R_{cryst} (%) [b, d]	13.4 (28.4)	18.9 (26.8)	17.9 (26.1)
R_{free} (%) [b, e]	17.7 (31.2)	24.0 (33.2)	22.2 (30.3)
No. of non-H atoms			
Protein	8177	7631	7828
Solvent	1765	495	509
Ramachandran plot (%)			
Favoured / allowed / generous [f]	98.8 / 1.2/ 0	98.1 / 1.8/ 0.1	98.1 / 1.7 / 0.2
Coordinate error [g]	0.04	0.07	0.05
Rms deviations from ideal values			
Bond lengths (Å)	0.03	0.02	0.014
Bond angles (deg.)	2.4	1.86	1.403
Mean *B*-factor ($Å^2$) per protein chain			
Backbone	15.6 / 15.9 / 15.7 / 16.9	23.0 / 23.7 / 29.1 / 26.4	22.9 / 20.5 / 22.8 / 24.6

Side chain	18.6 / 19.9 / 18.9 /21.0	25.8 / 26.6 / 31.5 / 29.1	25.9 / 23.2 / 25.2 / 26.7
Solvent	38.7 / 38.7 / 38.0 / 39.1	31.2 / 31.2 / 33.7 / 32.2	31.3 / 29.2 / 30.6 / 31.1

[a] lr, low-resolution data set; mr, medium-resolution date set; hr, high-resolution data set

[b] Values in parentheses are for the high-resolution bin.

[c] $$R_{p.i.m} = 100 \times \sum_{hkl} \sqrt{\frac{1}{N-1}} \sum_i \left| I_i(hkl) - \langle I_i(hkl) \rangle \right| / \sum_{hkl} \sum_i I_i(hkl)$$

where $I_i(hkl)$ is the intensity of the ith individual measurement of the reflection with Miller indices hkl and $\langle I_i(hkl) \rangle$ is the mean intensity of all measurements of $I(hkl)$, calculated for $I \geq 3\sigma(I)$; N is the redundancy or multiplicity of the observed reflection (1,2).

[d] $$R_{cryst} = 100 \times \sum \left(\left| |F_{obs}| - k|F_{calc}| \right| \right) / \sum |F_{obs}|$$

where F_{obs} and F_{calc} are the observed and calculated structure factor amplitudes, respectively.

[e] R_{free} is equivalent to R_{cryst} but calculated with reflections (5 %) omitted from the refinement process (3,4).

[f] Calculated using the program *PROCHECK* (5).

[g] Calculated based on a Luzzati plot using the program *SFCHECK* (6).

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