Supplementary Material for:

Single Wavelength Phasing Strategy for Quasi-Racemic Protein Crystal Diffraction Data

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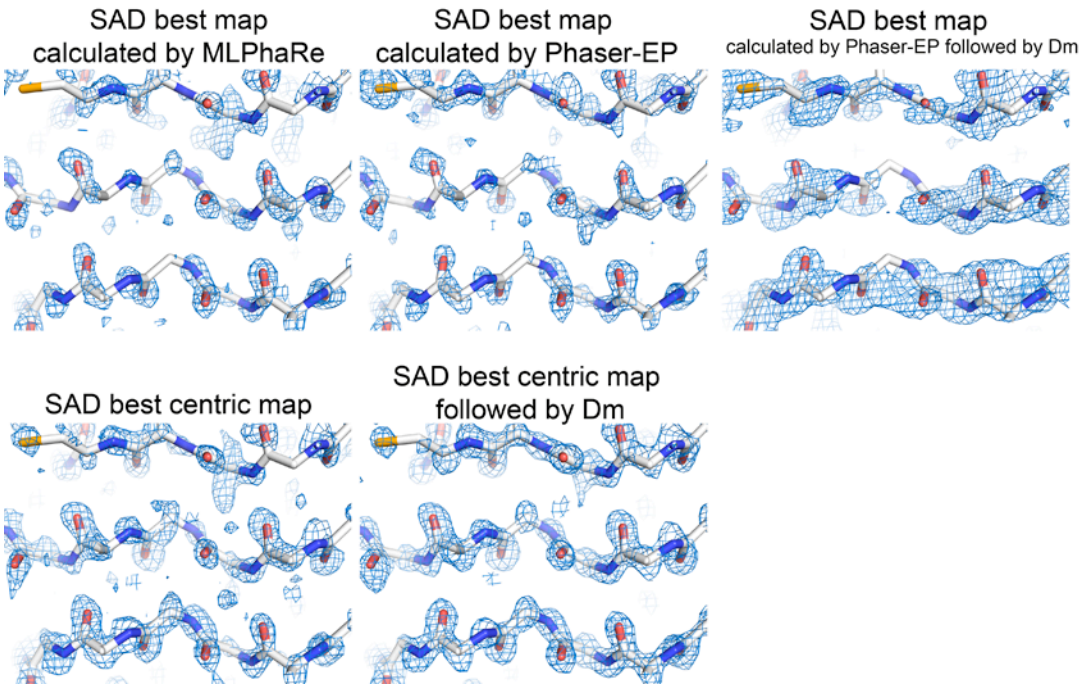

Supplementary Figure S1. Comparison of electron density maps calculated using different phasing strategies and programs. 'SAD best map' indicates that initial phases were obtained by the traditional single wavelength anomalous dispersion method, using either of the two programs MLPhaRe or Phaser-EP. 'SAD best centric' refers to the optimal strategy presented in this work for exploiting the expectation of near-centric phases. 'DM' indicates that density modification was performed. The final atomic model is shown for comparison. Correlation coefficients between the maps and the final model are given in Table 1 in the text.

Table S1. Diffraction data quality and atomic refinement statistics from Pentelute *et al.* (2008). *J. Am. Chem. Soc.* **130**, 9695-9701.

Space group	P1
Cell parameters	a = 28.64 Å
	b = 32.36 Å
	c = 59.70 Å
	α = 88.62°
	β = 89.31°
	γ = 72.84°
Beamline/Detector	APS 23ID D/MARCCD
Wavelength (Å)	0.9793
Resolution range (Å)	50.00 − 1.20 (1.24 − 1.20)[a]
Reflections measured	856855
Unique reflections measured[b]	60583
Completeness (%)	94.7 (91.7)
Average Redundancy	8.0 (7.9)
<I>/<σ(I)>	37.9 (9.9)
R_{merge}[c]	0.068 (0.21)
Resolution range (Å)	27.37 − 1.20 (1.23 − 1.20)
R_{work}[d]	0.160 (0.137)
R_{free}[e]	0.192 (0.195)

[a]Values for highest resolution shell are given in parentheses.
[b]Friedel mates merged.

[c] $R_{merge} = \left(\sum_{hkl} \sum_i \left| I_i(hkl) - \left\langle I\ (hkl) \right\rangle \right| \right) \Big/ \sum_{hkl} \sum_i I_i(hkl)$, where $I_i(hkl)$ is the intensity of an observation and $\langle I(hkl) \rangle$ is the mean value for that reflection.

[d] $R_{work} = \sum_{hkl} \left\| F_{obs} \right| - \left| F_{calc} \right\| \Big/ \sum_{hkl} \left| F_{obs} \right|$, where F_{obs} and F_{calc} are the observed and calculated structure-factor amplitudes, respectively. This calculation excludes the 5% of the reflections used as the "free" set.
[e] R_{free} is calculated as above, but only with the 5% of the data which were excluded from the refinement.