Table 1: Crystallographic data, phasing, and refinement

A. Data collection statistics

	No. of unique refl.	Redundancy	Completeness (%)	I/σ	R_{sym} [1] (%)
SeMet λ_1 (1.06883 Å)	24057	5.44 (2.03)	93.6 (68.3)	25.3 (2.8)	5.6 (20.2)
97984 Å)	25278	5.82 (3.07)	98.4 (88.2)	20.5 (2.2)	7.1 (40.0)
SeMet λ_3 (0.97961Å)	25300	5.89 (3.05)	98.4 (89.0)	20.8 (2.3)	7.2 (40.5)
SeMet λ_4 (0.92526 Å)	25598	6.01 (3.83)	99.6 (97.1)	17. (1.9)	8.3 (57.2)

B. Phasing statistics

Overall isomorphous and dispersive differences[2] Phasing power as defined in CNS[3]

Wavelength	λ_1	λ_2	λ_3	λ_4	$\mathbf{F}^+$ Friedel mate	$\mathbf{F}^-$ Friedel mate
λ_1 (remote)	0.0427	0.0766	0.0916	0.0569	(reference)	0.51
λ_2 (inflection)		0.0570	0.0484	0.0859	2.67	2.79
λ_3 (peak)			0.0707	0.0967	3.80	3.31
λ_4 (remote)				0.0843	0.69	1.06

C.Figure-of-merit[3]

Bragg Spacing Limits (Å)	Overall (43.14-1.79)	3.58	2.84	2.48	2.26	2.09	1.97	1.87	1.79
Figure of Merit (FOM)	0.72	0.92	0.91	0.85	0.77	0.69	0.58	0.46	0.33

D.Refinement

Resolution range	Overall										
Resolution (Å)	500-1.8Å	500-3.88	3.08	2.69	2.44	2.27	2.13	2.03	1.94	1.86	1.80
R-value[4]	20.6	20.8	20.4	21.3	18.1	20.7	20.1	20.2	20.5	23.6	25.2
R_{free} [5]	22.5	22.5	22.0	22.3	19.0	22.8	23.4	23.0	24.2	27.4	24.6
Luzzati coordinate error	0.21 Å										
Cross-validated Luzzati coord. error	0.23 Å										
Bond-length deviation	0.005 Å										
Bond-angle deviation	1.12°										
Improper-angle deviation	0.68°										
Dihedrals	18.0°										
Average B-factor	20.9 $Å^2$										
RMSD for bonded main chain atoms	1.87 $Å^2$										
RMSD for bonded side chain atoms	3.32 $Å^2$										
Minimum B-factor	7.46 $Å^2$										
Maximum B-factor	62.3 $Å^2$										
% Residues in core ϕ-ψ region	91.1%										
% Residues in disallowed regions	0.0 %										

Captions for Table 1

Values in parentheses are for the high-resolution bin (SPECIFY BIN???).

[1]$R_{sym} = \Sigma_{\mathbf{h}}\Sigma_i|I_i(\mathbf{h}) - \langle I(\mathbf{h})\rangle|/ \Sigma_{\mathbf{h}}\Sigma_i I_i(\mathbf{h})$ where $I_i(\mathbf{h})$ is the i-th measurement and $\langle I(\mathbf{h})\rangle$ is the mean of all measurements of $I(\mathbf{h})$ for Miller indices **h**.

[2]Values are $\langle(\Delta|\mathbf{F}|)^2\rangle^{1/2}/\langle|\mathbf{F}|^2\rangle^{1/2}$, where $\Delta|\mathbf{F}|$ is the dispersive (off-diagonal element), or Bijvoet difference (diagonal elements), computed between 500 and 1.8 Å resolution.

[3]MAD phasing power is defined as $[\langle|\,|\mathbf{F}_{\lambda 1}{}^{+}|-|\mathbf{F}_{\lambda i}{}^{(+/-)}|\,|^2\rangle/\int_\phi P(\phi)(||\mathbf{F}_{\lambda 1}{}^{+}|e^{i\phi}+\Delta\mathbf{F}|-|\mathbf{F}_{\lambda i}{}^{(+/-)}|)^2 d\phi]^{1/2}$ where $P(\phi)$ is the experimental phase probability distribution, *i* is any wavelength. $\mathbf{F}^+$ and $\mathbf{F}^-$ correspond to a Bijvoet pair of structure factors. $\Delta\mathbf{F}$ is the anomalous scatterer structure factor difference for a particular lack of closure expression.

[4]$R = \Sigma(|\mathbf{F}_{obs}|-k|\mathbf{F}_{calc}|)/\Sigma|\mathbf{F}_{obs}|$.

[5]Free *R* value is the *R* value obtained for a test set of reflections, consisting of a randomly selected 10 % subset of the diffraction data, not used during refinement.