

MAD data for the ternary complex (1:1:1) BMP-2:BMPR-IA_{ECD}:ActR-IIB_{ECD}

Crystal	BMP-2:BMPR-IA _{ECD} (F35M, L73M, L95M):ActR-IIB _{ECD}		
Space group	P2 ₁ 2 ₁ 2 ₁		
Cell constants	a = 64.36Å, b = 65.68Å, c = 113.97Å α = β = γ = 90°		
Wavelength	Se-Met (λ.1) 0.9799 Å	Se-Met (λ.2) 0.9796 Å	Se-Met (λ.3) 0.9079 Å
Resolution (Å) ^a	30.0 – 2.75 Å (2.90 – 2.75 Å) λ.1 (inflection)	30.0 – 2.75 Å (2.90 – 2.75 Å) λ.2 (peak)	30.0 – 2.75 Å (2.90 – 2.75 Å) λ.3 (remote high)
Number of measured reflections ^b	183773 (26598)	185933 (26610)	188670 (27520)
Number of unique reflections ^b	13130 (1874)	13134 (1872)	13137 (1879)
Completeness	99.9 (99.9)	99.9 (99.9)	99.9 (99.9)
Multiplicity	14.0 (14.2)	14.2 (14.2)	14.4 (14.9)
R _{sym} for all reflections ^c <Intensity/σ>	6.1 (16.6) % 38.3 (14.8)	7.1 (18.7) % 33.6 (13.2)	6.7 (17.4) % 35.7 (14.8)
Phasing	7 out of 10 Se-sites identified		
R _{cullis} (a/c) ^d	0.469/0.401	0.586/0.590	-
R _{Kraut} ^e	0.025	0.022	0.039
Phasing power (a/c) ^f	3.07/3.30	2.26/2.31	1.50/1.72
Figure of merit after DM		0.75	

- a) Numbers in parentheses indicate highest resolution shell
b) Cut-off for reflections $F > 0\sigma$
c) $R_{sym} = \sum_{hkl} |I_{hkl} - \langle I_{hkl} \rangle| / \sum_{hkl} \langle I_{hkl} \rangle$ where $\langle I_{hkl} \rangle$ is the mean intensity of symmetry related observations of a unique reflection
d) $R_{cullis} = \langle \text{phase-integrated lack of closure} \rangle / \langle F_{PH} - F_P \rangle$
(a/c) denotes acentric and centric reflections
e) $R_{Kraut} = \sum (|(F_P + F_H) - F_{PH}|) / \sum |F_P|$
f) Phasing power = $(\sqrt{|F_H|^2}) / (\sqrt{|\text{lack-of-closure}^2|})$, (a/c) denotes acentric and centric reflections