	α0-1 + β16-17	SeMet α0-1 + SeMet β16-17	α0-1 A99C + β16-17, EMP Derivative	α0-1 A131C + β16-17, EMP Derivative
Data Collection				
Detector Type/Source	MarCCD/APS	MarCCD/APS	ADSC-Q315 CCD/NSLS	ADSC-Q315 CCD/NSLS
Wavelength (Å)	0.97872	0.97872	1.00630	1.00710
Resolution[a]	40.0-2.80 (2.92-2.80)	40.0-3.50 (3.66-3.50)	40.0-3.30 (3.36-3.30)	40.0-3.80 (3.87-3.80)
Measured Reflections	54695 (6817)	44105 (5370)	152440 (6182)	55224 (1747)
Unique Reflections	18015 (2195)	9318 (1089)	11245 (552)	7360 (364)
Completeness	98.6 (99.3)	99.7 (100.0)	100.0 (100.0)	99.3 (94.1)
Multiplicity	3.0 (3.1)	4.7 (4.9)	13.6 (11.2)	7.5 (4.8)
Intensity (I/σ)	13.5 (3.4)	17.5 (5.2)	30.7 (3.2)	25.8 (2.4)
R_{sym} (%)[b]	5.7 (29.7)	5.9 (28.2)	12.1 (87.9)	14.4 (83.4)
R_{meas} (%)[c]	7.0 (35.8)	7.5 (35.7)	–	–
Phasing[d]				
Resolution	25.0-2.80	25.0-3.50	25.0-3.30	25.0-3.80
Phasing Power$_{isomorphous}$ (acentric/centric)	–	0.651/0.629	0.565/0.552	0.400/0.511
Phasing Power$_{anomalous}$	–	0.848	0.503	0.190
$R_{cullis-anomalous}$ (acentric/centric)	–	0.799/0.923	0.853/0.859	0.867/0.831
$R_{cullis-isomorphous}$	–	0.898	0.965	0.998
FOM (acentric/centric)	–	0.20/0.22	Together with SeMet HEα01 + SeMet HEβ1617	
Refinement				
Resolution	35.0-2.80 (2.87-2.80)			
Number of Reflections working/test	17085/922 (1251/76)			
R-factor (%)[e]	26.8 (40.9)			
R-free (%)[f]	29.9 (40.5)			
Protein Atoms	2673			
Bond lengths	0.011			
Bond angles	1.235			

[a]Numbers in parenthesis correspond to the highest resolution shell throughout.
[b]$R_{sym}=\sum|I-<I>|/\sum I$, where I is the observed intensity and $<I>$ the average intensity obtained from multiple measurements.
[c]R_{meas} as described in Diederichs and Karplus.
[d]Extracted from autoSHARP log files.
[e]R-factor=$\sum|F_o|-|F_c|/\sum|F_o|$, where $|F_o|$ is the observed structure factor amplitude and $|F_c|$ the calculated structure factor amplitude.
[f]R_{free}: R-factor based on 5% of the data excluded from refinement.
Note: Data collection statistics for native and seleno-methionine datasets were extracted from SCALA log files. Data collection statistics for mercury derivative datasets were extracted from HKL2000 log files.