

Table 3. Refinement statistics

	K4me3	R2me1/K4me3	R2me2a/K4me3	R2me2s/K4me3	R2me2s/K4me2
Space group	$P2_1$	$C2$	$C222_1$	$P2_1$	$P2_1$
Unit cell					
$a, b, c, \text{Å}$	54.8, 46.8, 57.0	76.7, 46.9, 57.0	62.9, 66.6, 87.5	40.4, 46.6, 57.0	36.2, 46.7, 56.9
$\alpha, \beta, \gamma, ^\circ$	90, 101.5, 90	90, 103.7, 90	90, 90, 90	90, 95.1, 90	90, 97.2, 90
Resolution range, Å	30–2.4 (2.49–2.4)	30–2.0 (2.07–2)	30–2.05 (2.12–2.05)	20–1.8 (1.86–1.8)	30–2.0 (2.07–2)
R_{merge}^*	0.150 (0.487)	0.074 (0.180)	0.182 (0.516)	0.056 (0.206)	0.101 (0.359)
Completeness, %	99.4 (95.7)	98.5 (89.6)	99.8 (99.9)	96.5 (87.9)	98.8 (92.7)
$I/\sigma(I)$	8.1 (1.8)	18.9 (5.0)	9.9 (3.0)	25.5 (3.9)	16.0 (2.9)
Unique reflections	11,048	13,424	11,827	19,094	12,678
Protein plus peptide atoms	1,937	1,405	1,448	1,430	1,381
Metal plus solvent atoms	242	181	348	241	256
R factor (R_{free}), % [†]	19.6 (23.0)	18.7 (19.7)	18.5 (20.9)	18.1 (20.8)	19.6 (23.2)
Rmsd bond length, Å	0.0071	0.01205	0.0063	0.0074	0.0152
rmsd bond angle, °	1.504	1.821	1.3259	1.8109	1.7993
Average B value (Wilson), Å ²	30.5 (14.6)	19.9 (11.0)	18.5 (10.0)	27.2 (19.4)	24.7 (16.7)

Data of the highest-resolution shell are shown in parentheses.

* $R_{\text{merge}} = \sum_h \sum_i |I_{hi} - \langle I_h \rangle| / \sum_i \langle I_h \rangle$, where I_{hi} is the intensity of the i th observation of reflection h and $\langle I_h \rangle$ is the average intensity of redundant measurements of the h reflections.

† R factor = $\sum |F_o| - |F_c| / \sum |F_o|$, where F_o and F_c are the observed and calculated structure-factor amplitudes. R_{free} is monitored with 5% of the reflections excluded from refinement.