Table 2. Crystallographic data collection and refinement statistics for the medium-dose data set

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Protein Data	2j5m
Bank ID code	
Space group	C222 ₁
Unit cell	59.0, 150.4, 99.6
dimensions	
a, b, c, Å	
Beamline/	SLS X10SA
x-ray source	
Wavelength, Å	1.008
Resolution of	20-1.75
data, Å	(1.80-1.75)
(high-resolution	
bin)	
No. of	185,241/
observations/	44,178
unique reference	
Completeness	95.6 (89.3)
total (high), %	
$I/\sigma I$ total (high)	10.9 (3.6)
R_{sym} total (high),	11.1 (41.3)
%	
Wilson B factor,	26.6
$ A^2$	
Refinement	
$R_{\rm work}$ / $R_{\rm free}$, %	19.7/21.0
Protein residues	298 (2,316)
(no. of atoms)	
Sugar residues	18(213)
(no. of atoms)	
Water molecules	356
Ligands (total	1 hydroperoxoanion
no. of atoms)	(2)
	1 EG (4), 1 acetate
	(4)
	1 Mn, heme (43)
Overall <i>B</i> factor,	21.6
\mathring{A}^2	
rms deviations	
Bond length, Å	0.006
Bond angles. °	1.04