

**Table 2. Data collection and refinement statistics**

Data collection				
Dataset	FEHR	FE0	FE30	FE120
X-ray source	ID29	ID29	PX06	ID29
X-ray wavelength, Å	0.976	1.731	1.731	1.731
Space group	P321	P321	P321	P321
Cell dimensions ( <i>a</i> , <i>b</i> , <i>c</i> ), Å	91.11	90.95	92.17	90.56
	91.11	90.95	92.17	90.56
	150.04	149.39	152.10	148.57
Resolution, Å	1.6	2.2	2.9	2.2
Observations	397,354	226,621	116,390	386,210
Unique reflections	92,251	36,571	30,227	345,72
Mosaicity, °	0.23	0.23	0.23	0.28
Wilson <i>B</i> -factor, Å <sup>2</sup>	28.6	37.7	61.5	18.9
<i>I</i> / $\sigma$ ( <i>I</i> )*, <i>R</i> <sub>merge</sub> <sup>†</sup>	10.07, 0.074	11.11, 0.109	9.75, 0.093	8.99, 0.079
Completeness, %	96.5	98.7	94.2	97.6
Refinement statistics (CNS/REFMAC)				
Space group	P321	P321	P321	P321
Resolution, Å	30-1.6	30-2.2	20-2.9	15-2.2
Reflections ( <i>F</i> >0)	56,417	34,298	17,102	34,572
<i>R</i> factor, <i>R</i> <sub>free</sub> <sup>‡</sup>	0.16, 0.21	0.17/0.23	0.21/0.23	0.18/0.23
Mean <i>B</i> value, Å <sup>2</sup>	21.5	31.2	58.0	46.4
rms deviation bonds, Å; angles, °	0.017, 1.55	0.023, 1.56	0.030, 1.67	0.033, 2.2
Total no. of atoms	6,766	5,741	5,550	5,735
No. of protein residues	705	705	705	705
No. of waters	796	270	40	312
No. of ions (Fe/Mg/Na)	6/4/2	6/4/2	38/0/2	30/0/2
Iron content <sup>§</sup>	Low (0 min)	Low (0 min)	High (30 min)	High (120 min)
No. of irons in TS <sup>¶</sup>	0	0	3 (T1-T3)	3 (T1-T3)
No. of irons is FOC <sup>¶</sup>	1 (F1)	1 (F1)	3 (F1-F3)	1 (F1)
No. of irons in NI <sup>¶</sup>	0	0	3 (N11-N13)	3 (N11-N13)
No. of irons in NII <sup>¶</sup>	1 (N21)	1 (N21)	5 (N21-N25)	5 (N21-N25)

FEHR, low-iron high-resolution dataset.

\*As calculated with the XSCALE (1).

<sup>†</sup> $R_{\text{merge}} = \frac{\sum_{\text{hkl}} \sum_i |I_i(\text{hkl}) - \langle I(\text{hkl}) \rangle|}{\sum_{\text{hkl}} \sum_i I_i(\text{hkl})}$ ; values in parentheses correspond to the highest-resolution shell.

<sup>‡</sup> $R$  factor =  $\frac{\sum |F_{\text{obs}} - F_{\text{calc}}|}{\sum F_{\text{obs}}}$ ; *R*<sub>free</sub> calculated with 7% of the data.

<sup>§</sup>Incubation time of crystals with Fe<sup>2+</sup> solutions is given in parentheses.

<sup>¶</sup>Definition of the subsites used in the text is given in parentheses.

1. Kabsch, W. J. (1988) *Appl. Crystallogr.* **21**, 67-71.