**Table 2. Statistics on data collection, phasing, and model refinement**

| | | | | | |
|---|---|---|---|---|---|
| **Data collection** | | | | | |
| Data set | SeMet (in complex with $NAD^+$) | | | Native 1 (binary complex) | Native 2 (ternary complex) |
| X-ray source | PF (BL-18B) | | | PF (BL-18B) | Cu $K\alpha$ |
| Temperature | 100 K | | | 100 K | 298 K |
| Space group | I4 | | | $P3_221$ | I4 |
| Unit cell axes, Å | $a = b = 120.02$, $c = 140.00$ | | | $a = b = 70.38$, $c = 148.93$ | $a = b = 122.16$, $c = 141.25$ |
| Wavelength, Å | 0.9798 | 0.9801 | 0.9500 | 1.0000 | 1.5418 |
| Resolution, Å | 20.0–2.1 | 20.0–2.1 | 20.0–2.1 | 20.0–1.8 | 20.0–2.4 |
| Reflections, total / unique | 328,553 / 57,609 | 312,172 / 57,655 | 288,652 / 57,609 | 280,336 / 40,259 | 133,031 / 40,358 |
| Completeness*, % | 99.9 (100) | 99.9 (100) | 99.9 (100) | 99.7 (99.7) | 99.5 (99.9) |
| $I / \sigma_I$ | 8.5 (2.6) | 9.3 (2.8) | 8.7 (2.4) | 10.2 (2.2) | 18.7 (3.4) |
| $R_{merge}$† | 7.3 (26.7) | 7.1 (25.9) | 7.5 (27.1) | 6.3 (34.5) | 8.4 (39.8) |
| **Phasing** | | | | | |
| Number of Se sites | 20 (5 per monomer × 4 monomers) | | | | |
| Figure of merit | 0.57 / 0.83 (before / after DM) | | | | |
| **Model refinement** | | | | | |
| $R_{work}$ / $R_{free}$‡ (%) | | | 20.3 / 23.6 | 16.4 / 19.9 | 16.0 / 18.7 |
| rms deviation in bond lengths / angles, Å / ° | | | 0.0060 / 1.30 | 0.0052 / 1.29 | 0.0067 / 1.36 |
| No. of nonhydrogen atoms / average B-factor, $Å^2$ | | | | | |
| Protein (residues 2–245) | | | 4 × 1,780 / 20.4 | 2 × 1,780 / 16.8 | 4 × 1,780 / 36.4 |
| Cofactor ($NAD^+$ or NADH) | | | 4 × 44 / 19.4 | 2 × 44 / 16.0 | 4 × 44 / 40.1 |
| Water | | | 385 / 25.9 | 432 / 31.8 | 238 / 40.4 |
| Substrate (androsterone) | | | – | – | 4 × 21 / 52.9 |

*Values in parentheses refer to the highest resolution shell.

†$R_{merge} = \Sigma_h\Sigma_i|I(h)_i - \langle I(h)\rangle|/\Sigma_h\Sigma_i I(h)_i$

‡$R = \Sigma||F_{obs}| - |F_{calc}|| / \Sigma|F_{obs}|$