Table 3. Data collection and refinement statistics

Data collection	Se used for refinement	Se (peak)	Se (inflection)	Se (remote)
Space group	P222$_1$	P222$_1$		
Unit cell dimensions, Å	$a = 40.9$, $b = 46.8$, $c = 283.1$	$a = 41.0$, $b = 47.2$, $c = 283.2$		
Wavelength, Å	1.0000	0.9796	0.9794	0.9719
Resolution limit, Å	2.2	2.4	2.4	2.4
R_{sym},* %	16.8%	10.8	9.8	10.5
R_{sym}, % (last shell)	34.2	35.6	43.8	42.6
I/σ (last shell)	2.1 (15.1)†	2.0	1.8	1.5
Total observations	233,050	120,481	58,582	112,996
Unique reflections	27,342 (20,050)	18,561	17,315	18,154
Completeness, %	92.7 (63.6)	80.8	74.7	78.3
Completeness, % (last shell)	78.6 (30.0)	46.3	35.5	41.9

Phase determination‡	Se (peak)	Se (inflection)	Se (remote)
R_{cullis},§ % (20–2.4 Å, acentric/centric, isomorphous)	0.97/0.95	–	0.92/0.85
R_{cullis},¶ % (20–2.4 Å, anomalous)	0.76	0.94	0.85
Phasing power$^{\parallel}$ (20–2.6 Å, acentric/centric)	0.50/0.35	–	0.72/0.55
Number of sites	11		
Mean overall figure of merit (before/after DM)	0.39/0.60		

Model refinement	Native
R_{work}** (20–2.1 Å)	24.7
R_{free}†† (20–2.1 Å)	31.2
Protein Data Bank ID code	2G38
Number of residues (protein/water)	499/73
Average B (main chain/side chain)	20.7/22.3
rmsd bonds, Å	0.007
rmsd angles, °	1.4
B values, Å^2 bonded	1.6

*$R_{sym} = \Sigma|I - <I>|^2/\Sigma I^2$.

†Values in parentheses correspond to statistics after elliptical truncation prompted by severe anisotropy.

[‡]The inflection data set was treated as a reference for phasing. Statistics are reported to 3.3-Å resolution.

[§]$R_{Cullis} = \Sigma\varepsilon/\Sigma|F_{PH} - F_P|$, where ε=lack of closure.

[¶]$R_{Cullis} = \Sigma\varepsilon/\Sigma|F^+ - F^-|$, where ε=lack of closure.

[∥]Phasing power = $<F_H/\varepsilon>$.

[**]$R_{work} = \Sigma|F_{obs} - F_{calc}|/\Sigma F_{obs}$.

[††]$R_{work} = \Sigma|F_{obs} - F_{calc}|/\Sigma F_{obs}$, where all reflections belong to a test set of 5% randomly selected data.