

Table 2. Data collection and refinement of the PD-1/PD-L1 complex

Data collection	
X-ray source	19-BM (Argonne)
Wavelength, Å	0.97943
Resolution limits, Å	50-2.65 (2.74-2.65)
Space group	P212121
Unit cell dimensions, Å	56.5 x 63.9 x 159.9
Completeness, %	98.9 (91.4)
Average redundancy	6.0 (3.8)
R _{sym} , %	7.5 (43.4)
I/σ	19.4 (2.9)
No. of observations/unique reflections	103,838/17,320
Refinement statistics	
Resolution limits, Å	20-2.65 (2.72-2.65)
No. of reflections in working set	16,327 (1050)
No. of reflections in (5%) test set	898 (52)
R _{work} , %	21.4
R _{free} , %	26.8
No. of atoms: Protein; glycerol; water	3,562; 6; 78
Bond lengths, rmsd, Å	0.01
Bond angles, rmsd, °	1.40
Average B factor, Å ²	68
Ramachandran, % (favored, allowed, generous, forbidden)	89.8, 9.2, 1.0, 0.0

Highest resolution shell is shown in parentheses.