## Table 1. Data collection and refinement statistics for the mouse DRD4 and L745870 complex.

|  |  |
| --- | --- |
| Number of crystals | 28 |
| Resolution range (Å) | 28–3.5 (3.6–3.5)a |
| Space group | P21221 |
| Unit cell: *a, b, c* (Å) | 46.7, 142, 146 |
| Total reflections | 73,140 |
| Unique reflections | 12,812 (1,227) |
| Multiplicity | 5.7 |
| Completeness (%) | 98.7 (95.6) |
| Mean I/sigma (I) | 3.2 (1.3) |
| Wilson B-factor (Å2) | 162 |
| Rmerge | 0.230 (0.827) |
| CC1/2\*\* | 0.985 (0.656) |
| No. of reflections used in refinement | 12,812 (1,210) |
| No. of reflections used for Rfree | 636 (56) |
| Rwork/Rfree | 0.305/0.335 |
| No. of non-hydrogen atoms: all | 5,020 |
|  proteins | 4,974 |
|  ligands | 46 |
| RMS deviations |  |
|  bonds (Å) | 0.004 |
|  angles (°) | 1.03 |
| Ramachandran plot |  |
|  favored (%) | 92.78 |
|  allowed (%) | 6.47 |
|  outliers (%)b | 0.75 |
| Rotamer outliers (%) | 0.2 |
| Average B-factor (Å2) all | 182 |
|  proteins | 182 |
|  ligands | 209 |

a. Values in parentheses present the highest resolution shell. CC1/2\*\* [66].

b. All outliers are located in loops not involved in ligand binding.