

Extended Data Table 1 | Data collection and refinement statistics for C5aR1 StaR

Data collection	
Number of crystals	11
Space group	<i>P1211</i>
Cell dimensions	
a, b, c (Å)	83.1, 51.1, 119.0
α , β , γ (°)	90.0, 106.7, 90.0
Number of reflections measured	131919
Number of unique reflections	26541
Resolution (Å)	34.60 – 2.70 (2.83 – 2.70)
R_{merge}	0.195 (0.923)
$CC_{1/2}$	0.987 (0.631)
Mean $I/\sigma(I)$	7.0 (1.7)
Completeness (%)	99.3 (99.6)
Redundancy	5.0 (5.1)
Refinement	
Resolution (Å)	19.89 – 2.70
Number of reflections (test set)	26440 (1352)
$R_{\text{work}}/R_{\text{free}}$	0.2079 / 0.2385
Number of atoms	
All	5349
Protein	4662
Ligand (NDT9513727)	86
Others (Lipids, ions, waters)	601
Average B factors (Å ²)	
All	46.24
C5aR	45.02
Ligand	28.41
Others (Lipid, ion, water)	58.19
RMSD	
Bond lengths (Å)	0.004
Bond angles (°)	1.035
Ramachandran statistics	
Favored regions (%)	98.62
Allowed regions (%)	1.38
Outliers (%)	0.0
<i>MolProbity</i> overall score (percentile)	1.33 (98 th)

Values in parentheses indicate highest resolution shell.