

Table X. X-ray Crystal Structure Data Collection and Structure Refinement Statistics.

Values in parentheses are for the outer shell

Structure	TYK2-JH2 + Compound 18	PDE4 + Compound 30
PDB ID Code	5TKD	5TKB
Diffraction source	APS 17-ID	APS 17-ID
Wavelength (Å)	1.0	1.0
Temperature (K)	100	100
Detector	Dectris Pilatus 6M	Dectris Pilatus 6M
Crystal-to-detector distance (mm)	350.0	400.0
Rotation range per image (°)	0.2	0.2
Total rotation range (°)	180	180
Exposure time per image (s)	0.2	0.2
Space group	P2(1)	P2(1)2(1)2(1)
<i>a, b, c</i> (Å)	69.6, 65.7, 74.7	99.0, 112.7, 159.9
α, β, γ (°)	90.0, 112.4, 90.0	90.0, 90.0, 90.0
Mosaicity (°)	0.15-0.42	0.07
Resolution range (Å)	47.60-1.92 (2.02-1.92)	112.71-2.16 (2.28-2.16)
Total No. of reflections	159023 (23557)	650368 (94884)
No. of unique reflections	47129 (6829)	96469 (13924)
Completeness (%)	98.9 (99.1)	100.0 (100.0)
Multiplicity	3.4 (3.4)	6.7 (6.8)
(<i>I</i> / σ (<i>I</i>))	9.5 (2.4)	12.2 (2.3)
<i>R</i> _{sym}	0.077 (0.467)	0.104 (0.759)
Structure Refinement		
Resolution range (Å)	28.11-1.92 (1.97-1.92)	31.62-2.16 (2.22-2.16)
Completeness (%)	98.6 (98.8)	100.0 (99.9)
Sigma Cutoff	0	0
No. of reflections, working set	44690 (3265)	91578 (6671)
No. of reflections, test set	2371 (189)	4770 (363)
Final <i>R</i> _{cryst}	0.192 (0.197)	0.188 (0.202)
Final <i>R</i> _{free}	0.215 (0.233)	0.209 (0.231)
No. of non-H atoms		
Protein	3753	10441
Ion	15 (SO4)	19 (MGSO4)
Ligand	46	124
Water	189	471
Total	4003	11055
R.m.s. deviations		
Bonds (Å)	0.010	0.010
Angles (°)	0.9	1.0
Average <i>B</i> factors (Å ²)		
Protein	28.7	40.3
Ion	44.8 (SO4)	66.2 (MGSO4)
Ligand	20.4	58.6
Water	35.6	41.6

Ramachandran plot		
Most favored (%)	94.9	93.1
Allowed (%)	5.1	6.9