

	AAGAB psGD E144K	psGD:AP1σ3
Data Collection		
Wavelength (Å)	0.99228	0.97918
Resolution range (Å)	45.14 – 1.78 (1.844 – 1.78)	46.43 – 1.68 (1.74 – 1.68)
Space group	P 21 21 21	P 21 21 21
Unit cell (a, b, c, Å) (α, β, γ, °)	39.268 94.349 102.796 90 90 90	50.294 61.608 92.854 90 90 90
Unique reflections	34572 (2096)	33173 (3112)
Multiplicity	9.6 (2.9)	12.9 (11.9)
Completeness (%)	93 (63)	98.68 (94.16)
Mean I/sigma(I)	14.4 (0.7)	18.51 (2.39)
Wilson B-factor	23.70	26.20
R-merge	0.119 (0.841)	0.07416 (0.8291)
R-meas	0.125 (0.985)	0.07728 (0.8663)
R-pim	0.037 (0.494)	0.02136 (0.2458)
CC1/2	1.004 (0.508)	0.999 (0.872)
CC*		1 (0.965)
Refinement		
Reflections used in refinement	34542 (2082)	33173 (3111)
Reflections used for R-free	1980 (119)	1995 (187)
R-work	0.1883 (0.3501)	0.1825 (0.2267)
R-free	0.2071 (0.3737)	0.2113 (0.2546)
Number of non-hydrogen atoms	2942	2669
macromolecules	2569	2346
solvent	373	323
Protein residues	330	288
RMS (bonds, Å)	0.009	0.008
RMS (angles, °)	1.20	1.07
Ramachandran favored (%)	99.07	99.29
Ramachandran allowed (%)	0.93	0.71
Ramachandran outliers (%)	0.00	0.00
Rotamer outliers (%)	1.03	0.38
Clashscore	0.98	4.06
Average B-factor	28.49	30.40
macromolecules	27.49	29.44
solvent	35.34	37.44
Number of TLS groups	1	1

Table S1. Crystallography data collection and refinement statistics. Values in parentheses are for the highest resolution shell.