	WT+L-ser	N100Y + L-ser	N100Y	N100C	N100W$^-$
Data collection					
Space group	$C222_1$	$C222_1$	$C222_1$	$C222_1$	$C222_1$
Cell dimensions (Å)	*a*= 74.3, *b*= 108.4, *c*= 91.2	*a*= 73.6, *b*= 107.1, *c*= 89.9	*a*= 71.7, *b*= 109.7, *c*= 91.4	*a*= 75.2, *b*= 107.4, *c*= 88.8	*a*=71.9 *b*=109.8, *c*=91.7
Resolution (Å)* (high resolution)	34.9-1.50 (1.54-1.5)	28.5-2.14 (2.2-2.14)	27.4 -1.50 (1.54-1.5)	29.1-1.25 (1.28-1.25)	27.4 – 1.43 (1.47-1.43)
R_{merge} (%)	8.5 (51.9)	6.2 (47.3)	3.9 (40.7)	5.9 (51.8)	4.2 (38.6)
$I/\sigma I$	8.6 (1.6)	17.8 (2.9)	22 (3.4)	15.6 (2.8)	21.7 (3.1)
Completeness (%)	98.8 (88.9)	99.5 (97)	99.7 (98.3)	99.7 (99.6)	98 (88)
Aver. redundancy	8 (3.2)	4 (4)	4.2 (4.3)	4.0 (3.9)	4.7 (3.3)
Beamline	BM14	BM14	BM14	Id14-4	BM14
Wavelength	0.87260	0.97626	0.97626	0.97900	0.99996
Refinement					
Unique reflections	55582	79794	54786	94021	62574
R_{work} / R_{free}	15.7 / 18.8	19.5/24.9	15.7/ 18.7	14.8 /16.4	16.1 / 18.9
No. atoms					
Protein	3062	3000	3036	3030	3029
Water	354	150	420	479	399
PLP / ald	22	22	17	17	17
B-factors (Å^2)**					
Protein	20.7	32.4	16.8	11.0	15.9
Water	20.8	20.6	16.9	15.1	16.3
PLP	12.6	25.3	17.0	8.9	16.9
Rmsd bonds (Å) / angles (°)	0.008 / 1.2	0.008 / 1.1	0.008 / 1.2	0.006 / 1.2	0.008 / 1.2
B-factor deviation Bond/angle (Å^2)					
Main chain	0.6 / 1.1	0.3/0.6	0.7 / 1.1	0.5 / 0.9	0.7 / 1.1
Side chain	1.8 / 2.9	1.0/1.7	1.8 / 2.8	1.5 / 2.4	1.8 / 2.8
PDB code	2w8j	2w8w	2w8u	2w8t	2w8v

- Numbers in parenthesis refer to highest resolution shell
- ** These B's have the TLS factors added back in using TLSANAL, the deposited coordinates are residual B-factors only.

Supplementary Table