

Table S2

Crystal parameters	AafB	AggA	AggB
Space group	P6 ₁ 22	C222 ₁	P2 ₁ 2 ₁ 2
Cell dimensions	<i>a</i> = <i>b</i> =81.76, <i>c</i> =222.70	<i>a</i> =77.832, <i>b</i> =80.172, <i>c</i> =91.42	<i>a</i> =130.80, <i>b</i> =163.97, <i>c</i> =58.63
Number of molecules per asymmetric unit	2	2	8
Data collection			
Beamline	DLS I24	BM-14	ID23-1
Wavelength (Å)	0.97780	0.954	0.98034
Resolution (Å)	43.77-3.00 (3.16-3.00)	47.66-1.55 (1.63-1.55)	58.63-2.40 (2.53-2.40)
Unique observations	9081 (768)	40475 (5758)	50214 (7238)
<i>R</i> _{merge}	0.111 (0.374)	0.038 (0.787)	0.062 (0.565)
<i><I>/σI</i>	6.5 (2.6)	19.0 (2.1)	14.8 (2.8)
Completeness (%)	97.0 (98.2)	97.2 (95.8)	99.9 (99.9)
Redundancy	2.9 (2.9)	4.2 (4.3)	5.2 (5.4)
Overall <i>B</i> factor from Wilson plot (Å ²)	74.4	22.9	55.1
Refinement			
<i>R</i> _{work} / <i>R</i> _{free} (%)	21.8/24.6	15.6/23.2	22.8/27.2
Number of protein residues	263	155	142
Number of ligands/ions	1 sulphate ion, 1 acetate ion	2 glycerol molecules	0
rmsd stereochemistry			
Bond lengths (Å)	0.009	0.008	0.009
Bond angles (°)	1.181	1.344	1.352
Ramachandran analysis*			
Residues in outlier regions	0	0	0.3%
Residues in favoured regions	95.5%	98%	93.0%
Residues in allowed regions	100%	100%	99.7%

Values for high resolution shells in parenthesis.

$R_{merge} = \sum_h \sum_i |I(h)_i - \langle I \rangle| / \sum_h \sum_i I(h)_i$, where $I(h)$ is the intensity of a reflection h , \sum_h is the sum over all reflections and \sum_i is the sum over i measurements of reflection h .

$R_{work} = \sum |F_O - F_C| / \sum F_O$ where F_O and F_C are the observed and calculated structure factors respectively. R_{free} is calculated for a test set of reflections randomly excluded from refinement.

R.m.s.d. stereochemistry is the deviation from ideal values. R.m.s.d. B-factors is deviation between bonded atoms.

*Output from Molprobit