Electronic Supplementary Material (ESI) for Medicinal Chemistry Communications

Supplementary Material for "Optimization of a Series of Dipeptides with a P3 - Neopentyl asparagine residue as potent non-covalent Inhibitors of the Chymoptrypsin-like activity of the Human 20S Proteasome"

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Crystallographic data and refinement statistics

	Compound	
	20	34
PDB ID	3SDI	3SDK
Space group	$P2_1$	$P2_1$
Unit cell dimensions (Å, °)	a= 136.6 b= 299.5 c= 145.5 β= 113.2	136.1 299.4 146.2 112.9
Wavelength (Å)	0.97958	0.97958
Resolution (Å)	50 - 2.65	50 - 2.7
R_{sym}[a] (%)	9.9 (37.8)[b]	8.3 (36.1)
Total observations	1097554	1044183
Unique reflections	297624	280182
Average redundancy	3.7	3.7
<I/σ>	9.5 (1.9)	8.9 (2.5)
Completeness (%)	95.8 (78.8)	95.3 (71.6)
Refinement resolution (Å)	50 – 2.65	50 - 2.7
Reflections (working/test)	290919/ 5996	274063/ 5652
R_{cryst}/R_{free} (%)[c]	21.9/25.3	22.3/25.8
Protein atoms	48900	49137
ligand atoms	84	86
MES atoms	24	24
Mg^{2+} atoms	20	10

Water atoms	1	0
rmsd bond lengths (Å)	0.010	0.009
rmsd bond angles (°)	1.26	1.18
Ramachandran analysis		
most-favored (%/#)	90.9/5038	90.9/5050
additional allowable (%/#)	8.6/478	8.4/468
generously allowed (%/#)	0.3/16	0.4/21
disallowed (%/#)	0.2/12	0.3/16

[a]$R_{sym} = (\Sigma_{hkl} \Sigma_i |I_i(hkl) - \langle I(hkl)\rangle|) / \Sigma_{hkl}\Sigma_i I_i(hkl)$ for n independent reflections and i observations of a given reflection. $\langle I(hkl)\rangle$ is the average intensity of the i^{th} observation.
[b]numbers in parenthesis are for highest resolution shell.
[c]$R_{cryst} = \Sigma_h ||F_o(h)| - |F_c(h)|| / \Sigma_h |F_o(h)|$, where F_o and F_c are the observed and calculated structure factors, respectively.