

Pogacic *et al.*, Supplementary Table 1.

Supplementary table 1: Diffraction data and refinement

Data Collection & Refinement	2C3I
Space group	P6 ₅
Cell dimensions [Å] [a=b,c]	98.439, 80.843
Resolution (last shell) [Å]	1.9 (1.9 – 1.97)
Unique observations (R_{free} set 5%)*	34063 (1709)
Completeness* [%]	97.2 (92.0)
Redundancy*	3.5 (2.6)
R_{merge} *	8.9 (59)
I/σ *	2.39 (2.39)
$R_{\text{work}} / R_{\text{free}}$ [%]	18.6/21.8
Atoms (Protein/Ligand/Water)	2246 / 23 / 153
B-factors (Protein/Ligand/Water) [Å ²]	32.4/36.0/39.4
r.m.s.d. bonds [Å]	0.018
r.m.s.d. angles [°]	1.59
Ramachandran	
Favourable [%] / allowed [%]	93.2 / 6.8

*values in brackets refer to last resolution shell used