CODE	3HV8 (PDB)	Resolution	1.45
Name		Ring size	12
Formula	$C_{20}H_{22}N_{10}O_{14}P_2^{2-}$	# Ligand atoms	46
Type	macrocycle	Scorpion Score	17.4

Mol. Weight (Da)	688.40	Saturated/ Unsaturated	S
cLogP	-14.813		
tPSA	342.92	Chiral centres.ring	4
#HBD's	6	Chiral centres.sub	4
#HBA's	20		
$N_{RB\ (RING)}$	10	$N_{RB\ (SUBSTITUENT)}$	2

Number of substituents	2	P/NP balance, substituents	16/14
Large (≥5HA)	2	P/NP balance, peripheral groups	4/0
Small (2-4HA)	-		
Proportion HA in substituents	65.5%	Degrees of unsaturation ring	16
Number of peripheral groups	4	N:O ratio	10:14
		Chiral centres	8

Polarity distribution ligand atoms

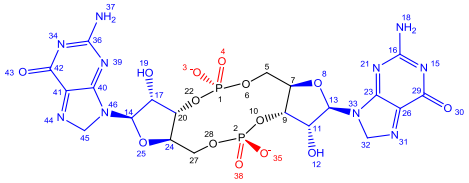
	All		Contact	
	Polar	*Nonpolar*	*Polar*	*Nonpolar*
Ring	6	6	-	-
Substituent	16	14	10	12
Peripheral groups	4	0	3	-
Total	26	20	13	12

Protein name	FimX EAL domain
Organism	Pseudomonas aeruginosa
Classification	Hydrolase
Binding mode	Face-on
Receptor secondary structure topology	
Number of residue 'hotspots'	12

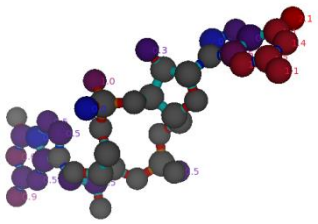
Number of protein-ligand interactions* ('Database link')

Hydrogen bond	8	Hydrogen donor-π	
Ionic interaction	3	π-π	8
Cation-dipole	1	VdW interaction	8
Cation-π	7	Unfavourable	2
Dipolar interaction		Poor-angle	1
Halogen bond		Unclassified	1
Water-mediated interaction			

2D-STRUCTURE LIGAND



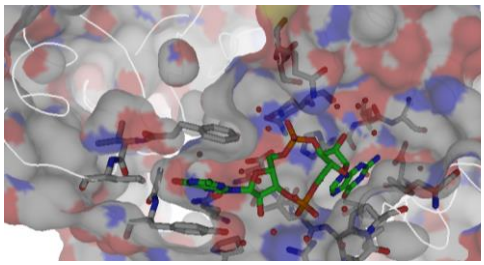
3D-STRUCTURE LIGAND +SCORPIONSCORE ('Scorpion link')



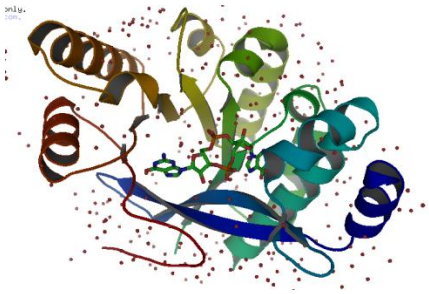
Physicochemical properties

'click for publication'

LIGAND-PROTEIN COMPLEX (I) ('Pymol link')



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis