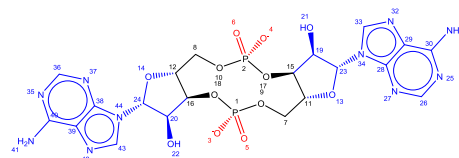


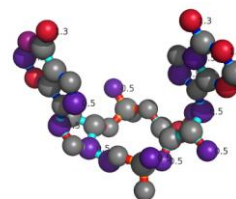
CODE	3C21 (PDB)	Resolution	2.7	
Name		Ring size	12	
Formula	C20H22N10O12P2 <sup>2-</sup>	# Ligand atoms	44	
Type		Scorpion Score	14.6	
Mol. Weight (Da)	656	Saturated/ Unsaturated	S	
cLogP	-15.0	Chiral centres.ring	4	
tPSA	315	Chiral centres.sub	4	
#HBD's	6	NRB (SUBSTITUENT)		
#HBA's	22	NRB (PERIPHERAL)		
NRB (RING)				
Number of substituents	2	P/NP balance, substituents	14/14	
<i>Large (≥5HA)</i>	2	P/NP balance, peripheral groups	4/0	
<i>Small (2-4HA)</i>	-	Degrees of unsaturation ring	15	
Proportion HA in substituents	63.6%	N:O ratio	5:6	
Number of peripheral groups	4	Chiral centres	8	
Polarity distribution ligand atoms				
	All		Contact	
	<i>Polar</i>	<i>Nonpolar</i>	<i>Polar</i>	<i>Nonpolar</i>
Ring	4	8	1	2
Substituent	14	14	9	7
Peripheral groups	4	-	2	-
Total	22	22	12	9

Protein name	*bacterial DNA damage sensor protein*		
Organism	Thermotoga maritima		
Classification	DNA binding protein		
Binding mode	Compact		
Receptor secondary structure topology			
Number of residue 'hotspots'	11		
Number of protein-ligand interactions* ('Database link')			
Hydrogen bond	13	Hydrogen donor-π	1
Ionic interaction	1	π-π	1
Cation-dipole	2	VdW interaction	12
Cation-π		Unfavourable	1
Dipolar interaction		Poor-angle	4
Halogen bond		Unclassified	4
Water-mediated interaction	0		

## 2D-STRUCTURE LIGAND



## 3D-STRUCTURE LIGAND +SCORPIONSORE ('Scorpion link')

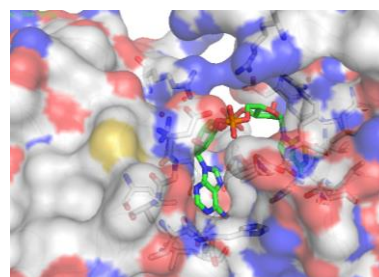


## Physicochemical properties

'click for publication'

## LIGAND-PROTEIN COMPLEX (I)

('Pymol link')



## LIGAND-PROTEIN COMPLEX (II)

