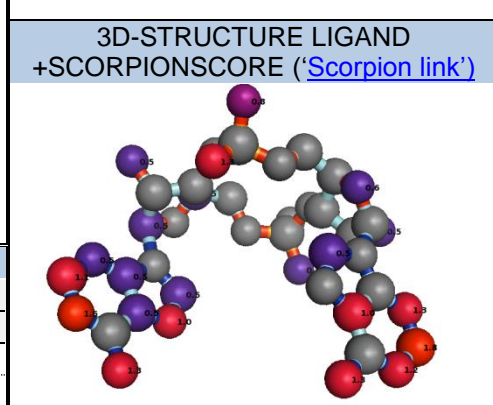
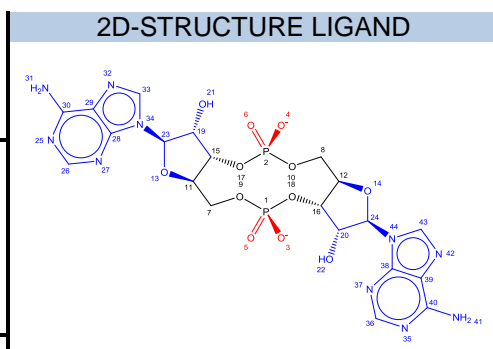
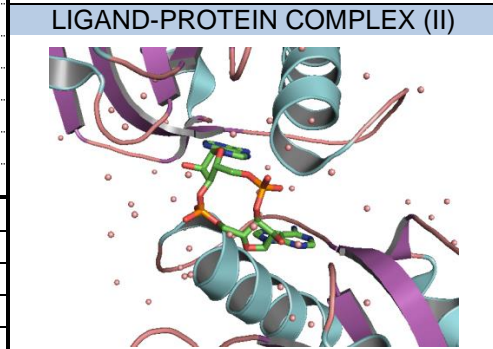
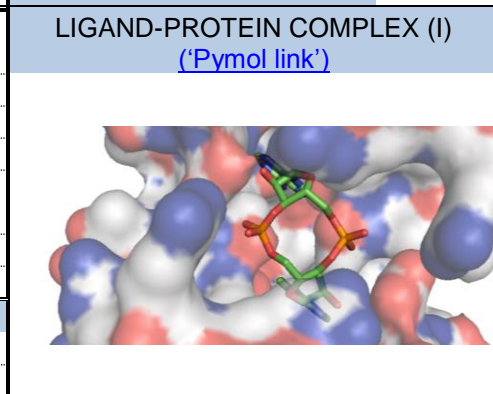


CODE	3C1Y(PDB)	Resolution	2.1	
Name		Ring size	12	
Formula	C20H22N10O12P2 <sup>2-</sup>	# Ligand atoms	44	
Type	Cyclic peptide	Scorpion Score	19.2	
Mol. Weight (Da)		Saturated/Unsaturated	S	
cLogP		Chiral centres.ring	4	
tPSA		Chiral centres.sub	4	
#HBD's		NRB (SUBSTITUENT)		
#HBA's		NRB (PERIPHERAL)		
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	10:12	
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	6	6	-	-
Substituent	14	14	7	6
Peripheral groups	4	-	2	-
Total	24	20	9	6

Protein name	DisA		
Organism	Thermotoga maritima		
Classification	DNA BINDING PROTEIN		
Binding mode	Compact		
Receptor secondary structure topology			
Number of residue 'hotspots'	8		
Number of protein-ligand interactions* ('Database link')			
Hydrogen bond	5	Hydrogen donor-π	
Ionic interaction		π-π	2
Cation-dipole	2	VdW interaction	14
Cation-π		Unfavourable	
Dipolar interaction		Poor-angle	2
Halogen bond		Unclassified	3
Water-mediated interaction	2		



Physicochemical properties  
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\*Based on Scorpion® analysis