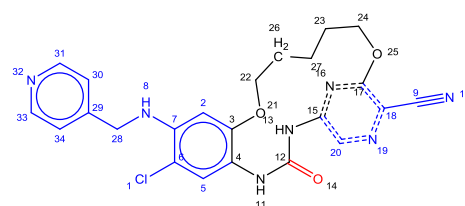


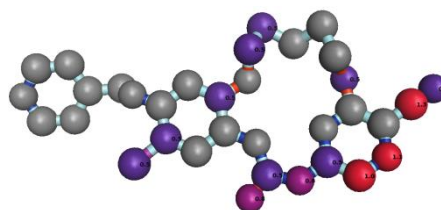
| | | | | |
|------------------------------------|------------------------------|---------------------------------|--------------|-----------------|
| CODE | 2E9V (PDB) | Resolution | 2.0 | |
| Name | | Ring size | 15 | |
| Formula | C23H22ClN7O3 | # Ligand atoms | 31 | |
| Type | Macrocyclic | Scorpion Score | 9.5 | |
| Mol. Weight (Da) | 480 | Saturated/Unsaturated | U | |
| cLogP | 3.7 | Chiral centres.ring | 0 | |
| tPSA | 134 | Chiral centres.sub | 0 | |
| #HBD's | 3 | | | |
| #HBA's | 9 | | | |
| N _{RB} (RING) | 10 | N _{RB} (SUBSTITUENT) | 4 | |
| Number of substituents | 2 | P/NP balance, substituents | 4/14 | |
| <i>Large (≥5HA)</i> | 2 | P/NP balance, peripheral groups | 1/0 | |
| <i>Small (2-4HA)</i> | - | Degrees of unsaturation ring | 16 | |
| Proportion HA in substituents | 58,1% | N:O ratio | 7:3 | |
| Number of peripheral groups | 1 | Chiral centres | 0 | |
| Polarity distribution ligand atoms | | | | |
| | All | | Contact | |
| | <i>Polar</i> | <i>Nonpolar</i> | <i>Polar</i> | <i>Nonpolar</i> |
| Ring | 5 | 10 | 1 | 4 |
| Substituent | 4 | 14 | 3 | 5 |
| Peripheral groups | 1 | - | 1 | - |
| Total | 10 | 24 | 5 | 9 |
| | | | | |
| | | | | |

| | | | |
|--|--------------|------------------|----|
| Protein name | h-CHK1 | | |
| Organism | Homo Sapiens | | |
| Classification | Transferase | | |
| Binding mode | Edge-on | | |
| Receptor secondary structure topology | | | |
| Number of residue 'hotspots' | 13 | | |
| Number of protein-ligand interactions* (Database link) | | | |
| Hydrogen bond | 3 | Hydrogen donor-π | - |
| Ionic interaction | - | π-π | 1 |
| Cation-dipole | - | VdW interaction | 13 |
| Cation-π | - | Unfavourable | 5 |
| Dipolar interaction | - | Poor-angle | 3 |
| Halogen bond | - | Unclassified | |
| Water-mediated interaction | 2 | | |
| | | | |
| | | | |
| | | | |

2D-STRUCTURE LIGAND



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

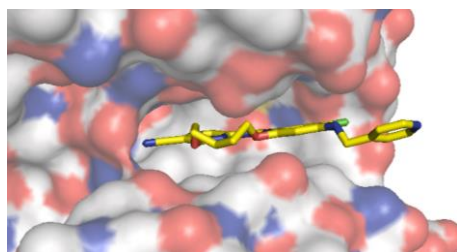


Physicochemical properties

'click for publication'

LIGAND-PROTEIN COMPLEX (I)

([Pymol link](#))



LIGAND-PROTEIN COMPLEX (II)

