

Features of Ligand	Detailed Name
nHeavyAtom	Number of Heavy Atoms
nH	Number of Hydrogen Atoms
nC	Number of Carbon Atoms
nN	Number of Nitrogen Atoms
nO	Number of Oxygen Atoms
nS	Number of Sulphur Atoms
nP	Number of Phosphorous Atoms
nF	Number of Fluorine Atoms
nI	Number of Iodine Atoms
nX	Number of Halogen (Cl, Br) Atoms
nBonds	Number of bonds (excluding bonds with hydrogen)
nBonds2	Total number of bonds (including bonds to hydrogens)
nBondsS	Number of single bonds (including bonds with hydrogen)
nBondsS2	Total number of single bonds (including bonds to hydrogens, excluding aromatic bonds)
nBondsS3	Total number of single bonds (excluding bonds to hydrogens and aromatic bonds)
nBondsD	Number of double bonds
nBondsD2	Total number of double bonds (excluding bonds to aromatic bonds)
nBondsT	Number of triple bonds
nBondsM	Total number of bonds that have bond order greater than one (aromatic bonds have bond order 1.5).
nRing	Number of rings
n3Ring	Number of 3-membered rings
n4Ring	Number of 4-membered rings
n5Ring	Number of 5-membered rings
n6Ring	Number of 6-membered rings
n7Ring	Number of 7-membered rings
n8Ring	Number of 8-membered rings
n12Ring	Number of 12-membered rings
nG12Ring	Number of >12-membered rings
nFRing	Number of fused rings
nF6Ring	Number of 6-membered fused rings
nF7Ring	Number of 7-membered fused rings
nF8Ring	Number of 8-membered fused rings
nF9Ring	Number of 9-membered fused rings
nF10Ring	Number of 10-membered fused rings
nF11Ring	Number of 11-membered fused rings
nF12Ring	Number of 12-membered fused rings
nFG12Ring	Number of >12-membered fused rings
nTRing	Number of rings (includes counts from fused rings)
nT4Ring	Number of 4-membered rings (includes counts from fused rings)
nT5Ring	Number of 5-membered rings (includes counts from fused rings)
nT6Ring	Number of 6-membered rings (includes counts from fused rings)
nT7Ring	Number of 7-membered rings (includes counts from fused rings)

nT8Ring	Number of 8-membered rings (includes counts from fused rings)
nT9Ring	Number of 9-membered rings (includes counts from fused rings)
nT10Ring	Number of 10-membered rings (includes counts from fused rings)
nT11Ring	Number of 11-membered rings (includes counts from fused rings)
nT12Ring	Number of 12-membered rings (includes counts from fused rings)
nTG12Ring	Number of >12-membered rings (includes counts from fused rings)
nHeteroRing	Number of rings containing heteroatoms (N, O, P, S, or halogens)
n3HeteroRing	Number of 3-membered rings containing heteroatoms (N, O, P, S, or halogens)
n4HeteroRing	Number of 4-membered rings containing heteroatoms (N, O, P, S, or halogens)
n5HeteroRing	Number of 5-membered rings containing heteroatoms (N, O, P, S, or halogens)
n6HeteroRing	Number of 6-membered rings containing heteroatoms (N, O, P, S, or halogens)
n7HeteroRing	Number of 7-membered rings containing heteroatoms (N, O, P, S, or halogens)
n12HeteroRing	Number of 12-membered rings containing heteroatoms (N, O, P, S, or halogens)
nG12HeteroRing	Number of >12-membered rings containing heteroatoms (N, O, P, S, or halogens)
nF6HeteroRing	Number of fused rings containing heteroatoms (N, O, P, S, or halogens)
nF7HeteroRing	Number of 7-membered fused rings containing heteroatoms (N, O, P, S, or halogens)
nF8HeteroRing	Number of 8-membered fused rings containing heteroatoms (N, O, P, S, or halogens)
nF9HeteroRing	Number of 9-membered fused rings containing heteroatoms (N, O, P, S, or halogens)
nF10HeteroRing	Number of 10-membered fused rings containing heteroatoms (N, O, P, S, or halogens)
nF11HeteroRing	Number of 11-membered fused rings containing heteroatoms (N, O, P, S, or halogens)
nF12HeteroRing	Number of 12-membered fused rings containing heteroatoms (N, O, P, S, or halogens)
nFG12HeteroRing	Number of >12-membered fused rings containing heteroatoms (N, O, P, S, or halogens)
nT4HeteroRing	Number of 4-membered rings (includes counts from fused rings) containing heteroatoms (N, O, P, S, or halogens)
nT5HeteroRing	Number of 5-membered rings (includes counts from fused rings) containing heteroatoms (N, O, P, S, or halogens)
nT6HeteroRing	Number of 6-membered rings (includes counts from fused rings) containing heteroatoms (N, O, P, S, or halogens)
nT7HeteroRing	Number of 7-membered rings (includes counts from fused rings) containing heteroatoms (N, O, P, S, or halogens)
nT8HeteroRing	Number of 8-membered rings (includes counts from fused rings) containing heteroatoms (N, O, P, S, or halogens)
nT9HeteroRing	Number of 9-membered rings (includes counts from fused rings) containing heteroatoms (N, O, P, S, or halogens)
nT10HeteroRing	Number of 10-membered rings (includes counts from fused rings) containing heteroatoms (N, O, P, S, or halogens)
nT11HeteroRing	Number of 11-membered rings (includes counts from fused rings) containing heteroatoms (N, O, P, S, or halogens)
nT12HeteroRing	Number of 12-membered rings (includes counts from fused rings) containing heteroatoms (N, O, P, S, or halogens)
nTG12HeteroRing	Number of >12-membered rings (includes counts from fused rings) containing heteroatoms (N, O, P, S, or halogens)
pubchemcomplexity	Complexity
pubchemhbondacceptor	Number of Hydrogen Bond Acceptor

pubchemhbonddonor	Number of Hydrogen Bond Donor
pubchemrotbon	Number of Rotatable Bond
pubchemlogp	XLogP3
pubchemmass	Mass of Ligand
pubchemcharge	Charge
pubchemtsa	Total Surface Area of Ligand
pubchemdefst	Defined Atom Stereocenter Count
pubchemundefst	Undefined Atom Stereocenter Count
pubchembonddefst	Defined Bond Stereocenter Count
pubchembondundefst	Undefined Bond Stereocenter Count
pubchemisotop	Isotope Atom Count
pubchemtato	Covalently-Bonded Unit Count

Table S2.2 Features of Proteins

Features of Protein
ALA_A
Arg_R
Asn_N
Asp_D
Cys_C
Gln_Q
Glu_E
Gly_G
His_H
Ile_I
Leu_L
Lys_K
Met_M
Phe_F
Pro_P
Ser_S
Thr_T
Trp_W
Tyr_Y
Val_V
TOTAL_NUMBER_OF_RESIDUES
NUMBER_OF_CHAINS
NUMBER_OF_SS_BRIDGE
ACCESSIBLE_SURFACE_OF_PROTEIN (ANGSTROM**2)
_NUMBER_OF_HYDROGEN_BONDS_OF_TYPE_O(I)-->H-N(J)_
NUMBER_OF_HYDROGEN_BONDS_IN_PARALLEL_BRIDGES
NUMBER_OF_HYDROGEN_BONDS_IN_ANTIPARALLEL_BRIDGES
_NUMBER_OF_HYDROGEN_BONDS_OF_TYPE_O(I)-->H-N(I-5)
NUMBER_OF_HYDROGEN_BONDS_OF_TYPE_O(I)-->H-N(I-4)
NUMBER_OF_HYDROGEN_BONDS_OF_TYPE_O(I)-->H-N(I-3)
NUMBER_OF_HYDROGEN_BONDS_OF_TYPE_O(I)-->H-N(I-2)
NUMBER_OF_HYDROGEN_BONDS_OF_TYPE_O(I)-->H-N(I-1)
NUMBER_OF_HYDROGEN_BONDS_OF_TYPE_O(I)-->H-N(I+0)
NUMBER_OF_HYDROGEN_BONDS_OF_TYPE_O(I)-->H-N(I+1)
NUMBER_OF_HYDROGEN_BONDS_OF_TYPE_O(I)-->H-N(I+2)
NUMBER_OF_HYDROGEN_BONDS_OF_TYPE_O(I)-->H-N(I+3)
NUMBER_OF_HYDROGEN_BONDS_OF_TYPE_O(I)-->H-N(I+4)
NUMBER_OF_HYDROGEN_BONDS_OF_TYPE_O(I)-->H-N(I+5)