

PROTAC ligand analysis section

This section of the tool helps users analyse features of ligands present in the structure playing role as E3 ligase binding ligand and linker.

This section also includes an exclusion list that enlists all the amino acids, small, uncommon ligands, and ions that may be changed by the user.

It takes the input pdb structure or is fetched using the PDB ID from RCSB PDB and displays ligands, including ones involved in E3 ligase binding ligand and as a linker for E3 ligase binding ligand and target protein binding region.

PROTAC Ligand analysis

Enter a PDB ID or upload a .pdb file. The tool finds non-polymer ligands and enriches them via the RCSB ChemComp API.

PDB ID

We download the .pdb file from RCSB and analyze it in your browser.

Or upload a .pdb file

 No file chosen

We read only in your browser; nothing is uploaded anywhere else.

Exclusions (common non-ligands):

We ignore standard amino acids, water, and typical ions/solvents by default. You can add/remove three-letter codes below (comma-separated).

```
ALA, ARG, ASN, ASP, CYS, GLN, GLU, GLY, HIS, ILE, LEU, LYS, MET, PHE, PRO, SER, THR, TRP, TYR, VAL, SEC, PYL, HOH, WAT, DOD, NA, CL, MG, ZN, CA, SO4, PO4, HEM, NAG, MAN, BMA, PEG, MPD, GOL
```

Tip: Remove entries like NAG if you *do* want carbohydrates included.

PROTAC Ligand analysis

Enter a PDB ID or upload a .pdb file. The tool finds non-polymer ligands and enriches them via the RCSB ChemComp API.

PDB ID

8ebk

Load by ID

We download the .pdb file from RCSB and analyze it in your browser.

Or upload a .pdb file

Choose File No file chosen

Analyze Upload

We read only in your browser; nothing is uploaded anywhere else.

Exclusions (common non-ligands):

We ignore standard amino acids, water, and typical ions/solvents by default. You can add/remove three-letter codes below (comma-separated).

ALA, ARG, ASN, ASP, CYS, GLN, GLU, GLY, HIS, ILE, LEU, LYS, MET, PHE, PRO, SER, THR, TRP, TYR, VAL, SEC, PYL, HOH, WAT, DOD, NA, CL, MG, ZN, CA, SO4, PO4, HEM, NAG, MAN, BMA, PEG, MPD, GOL

Tip: Remove entries like NAG if you *do* want carbohydrates included.

Found 4 ligand type(s) in 8EBK.

Download CSV

Ligand	Chemical Name	Formula	Weight (g/mol)	Instances (chain:resid)	Number of Atoms	Details
WG0	[(6S,10P)-4-(4-chlorophenyl)-2,3,9-trimethyl-6H-thieno[3,2-f][1,2,4]triazolo[4,3-a][1,4]diazepin-6-yl]acetic acid	C19 H17 Cl N4 O2 S	400.882	B:1	26	View
3V3	1-amino-3,6,9,12-tetraoxapentadecan-15-oic acid	C11 H23 N O6	265.303	B:2	17	View
0EH	(2R)-2-amino-2-methylnonanoic acid	C10 H21 N O2	187.279	B:6	12	View
MK8	2-methyl-L-norleucine	C7 H15 N O2	145.199	B:13	9	View

Enter PDB ID or upload the PDB structure from the local system

For downloading the list of ligands in CSV format

List of all the ligands in the PDB structure, excluding ones in the 'Exclusions' list

The tool finds non-polymer ligands and enriches them via the RCSB ChemComp API.

Click on 'View' for more information

Downloaded ligand table with features

Ligand	Name	Formula	Weight_g_mol	Instances_chain:resid	TotalAtoms
WG0	[(6S,10P)-4-(4-chlorophenyl)-2,3,9-trimethyl-6H-thieno[3,2-f][1,2,4]triazolo[4,3-a][1,4]diazepin-6-yl]acetic acid	C19 H17 Cl N4 O2 S	400.882	B:1	26
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0EH	(2R)-2-amino-2-methylnonanoic acid	C10 H21 N O2	187.279	B:6	12
MK8	2-methyl-L-norleucine	C7 H15 N O2	145.199	B:13	9

After clicking the 'View' button, the window expands to list features of the specific ligand, including IUPAC name, chemical formula, molecular weight, and 2D structure.

3D structure of the ligand is displayed using PubChem, which may be extended further to see other features of the ligand by clicking the link 'Explore more on PubChem'.

Ligand	Chemical Name	Formula	Weight (g/mol)	Instances (chain:resid)	Atoms	Details
WG0	[(6S,10P)-4-(4-chlorophenyl)-2,3,9-trimethyl-6H-thieno[3,2-f][1,2,4]triazolo[4,3-a][1,4]diazepin-6-yl]acetic acid	C19 H17 Cl N4 O2 S	400.882	1:1	26	View
3V3	1-amino-3,6,9,12-tetraoxapentadecan-15-oic acid	C11 H23 N O6	265.303	1:2	17	View
0EH	(2R)-2-amino-2-methylnonanoic acid	C10 H21 N O2	187.279	1:6	12	View
MK8	2-methyl-L-norleucine	C7 H15 N O2	145.199	1:13	9	View

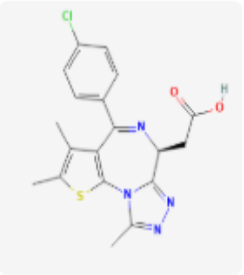
WG0

Name: [(6S,10P)-4-(4-chlorophenyl)-2,3,9-trimethyl-6H-thieno[3,2-f][1,2,4]triazolo[4,3-a][1,4]diazepin-6-yl]acetic acid

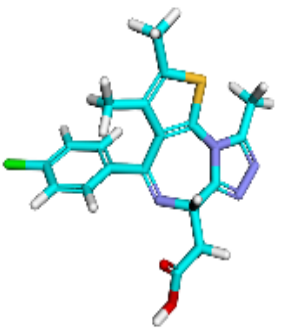
Formula: C19 H17 Cl N4 O2 S

Weight: 400.882 g/mol

2D Structure



3D Structure



[Explore more on PubChem](#)