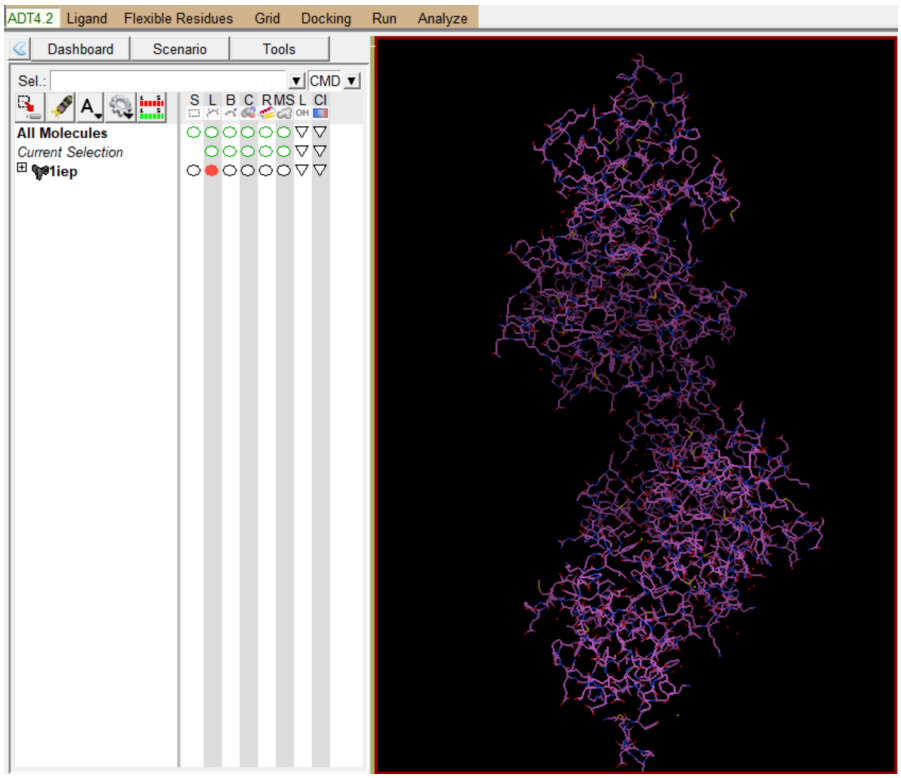
Computational Biology Lab

BE21B037 Practical 3

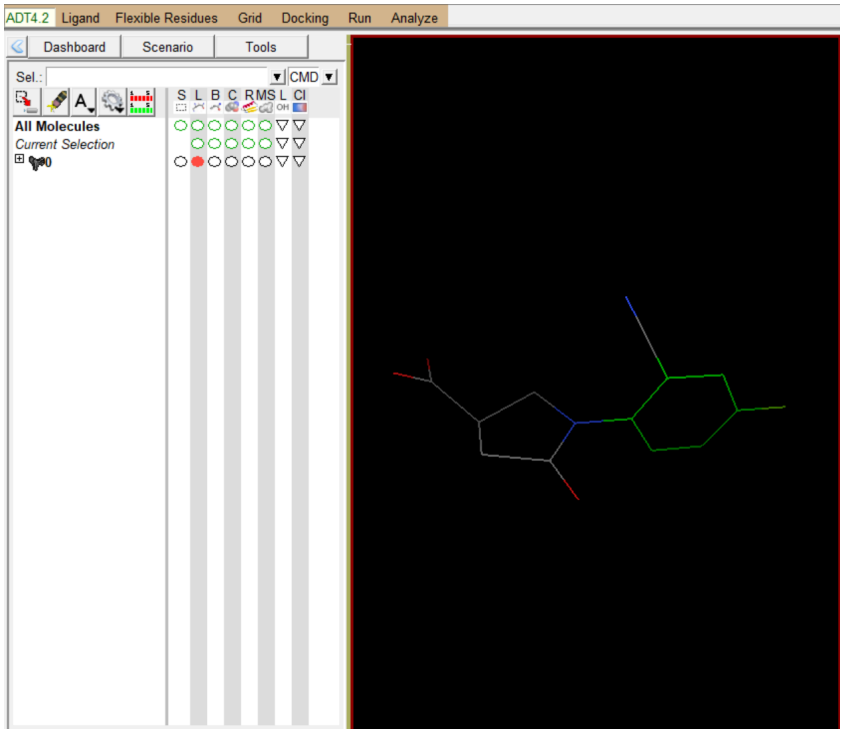
I. Rigid Docking

1. Install Autodock

2. Obtain 3D structure of the protein with PDB ID: 1IEP



3. Obtain the structure of the given ligand (ZINC ID: ZINC126204226) from Zinc database.

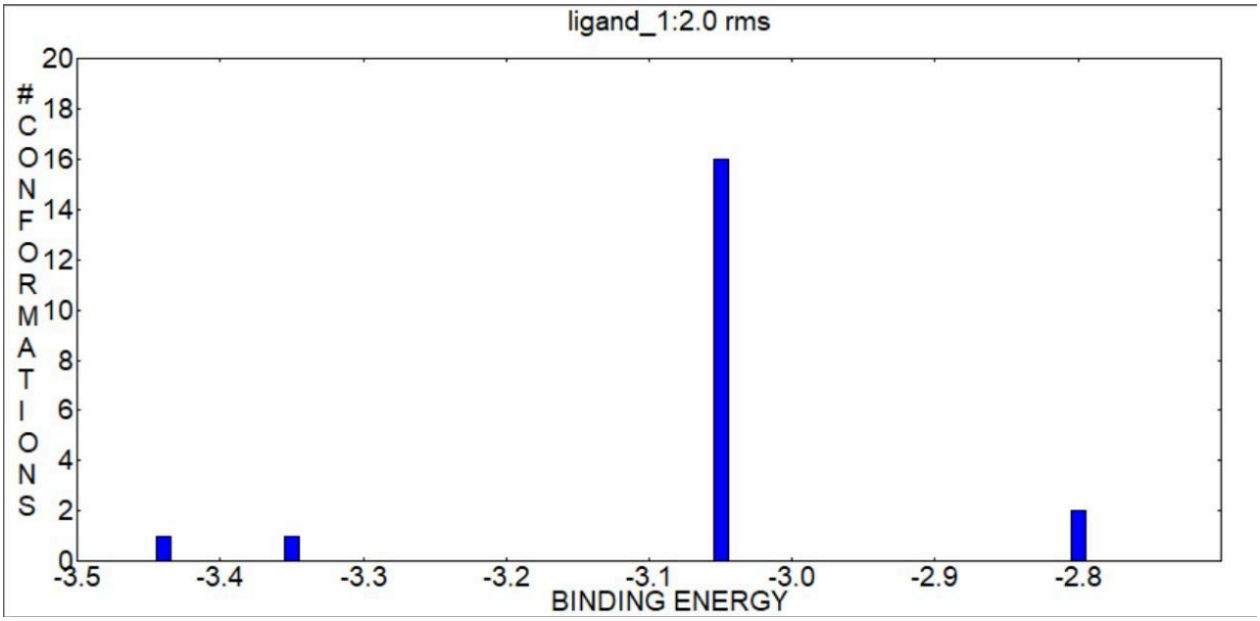


4. Get 20 different orientations of the ligand in the active site using rigid docking. (Lamarckian GA algorithm)

```
                CLUSTER ANALYSIS OF CONFORMATIONS
                _________________________________

Number of conformations = 20

RMSD cluster analysis will be performed using the ligand atoms only (18 / 18 total atoms).

Outputting structurally similar clusters, ranked in order of increasing energy.


_____________________________________________________________________________

Number of distinct conformational clusters found = 4,  out of 20 runs,
Using an rmsd-tolerance of 2.0 A


        CLUSTERING HISTOGRAM
        ____________________

_____________________________________________________________________________
     |             |     |             |     |
Clus | Lowest      | Run | Mean        | Num | Histogram
-ter | Binding     |     | Binding     | in  |
Rank | Energy      |     | Energy      | Clus|    5    10   15   20   25   30   35
_____|_____________|_____|_____________|_____|____:____|____:____|____:____|____:___
   1 |      -3.44  |  12 |      -3.44  |   1 |#
   2 |      -3.35  |  19 |      -3.35  |   1 |#
   3 |      -3.05  |  16 |      -3.02  |  16 |################
   4 |      -2.80  |  20 |      -2.79  |   2 |##
_____|_____________|_____|_____________|_____|_____________________________________


Number of multi-member conformational clusters found = 2, out of 20 runs.
```

The DLG file contains information about the clusters and their corresponding binding energies.

5. Identify the best complex using interaction energy and clustering histogram and get the interactions using LigPlot.

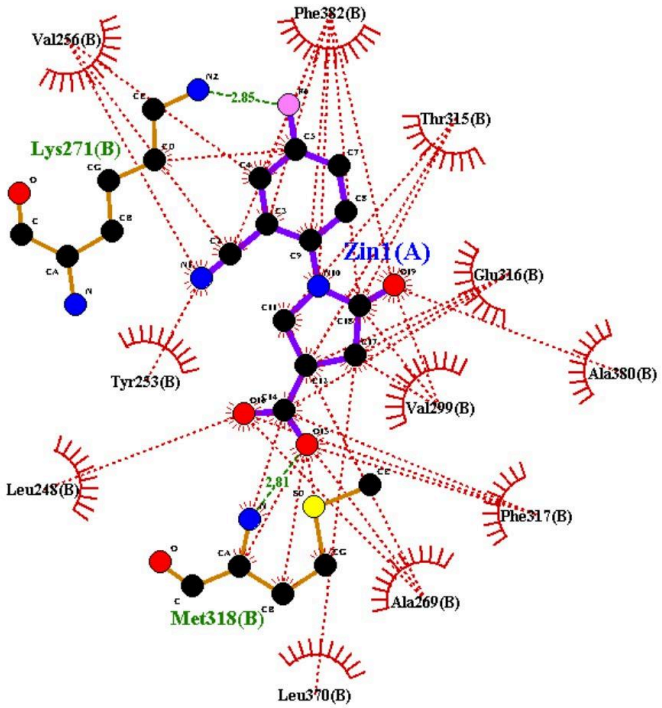


Clustering Histogram

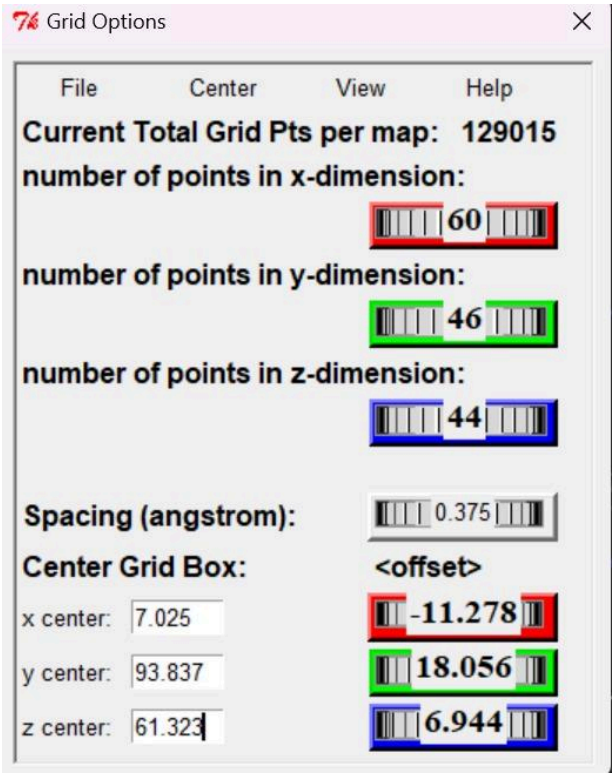
The best complex occurred on run 12 as it had the lowest binding energy, the details of run 12 are given below

```
MODEL        12
USER    Run = 12
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 1
USER
USER    RMSD from reference structure       = 112.197 A
USER
USER    Estimated Free Energy of Binding    =   -3.44 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =    3.02 mM (millimolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -4.03 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -3.69 kcal/mol
USER        Electrostatic Energy            =   -0.35 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.09 kcal/mol
USER    (3) Torsional Free Energy           =   +0.60 kcal/mol
USER    (4) Unbound System's Energy  [=(2)] =   +0.09 kcal/mol
USER
USER
USER
USER    DPF = C:/Users/shree/Desktop/ACADS/Comp_Bio_Lab/Practical_3/doc_kinase.dpf
USER    NEWDPF move     ligand_1.pdbqt
USER    NEWDPF about    2.234000 1.640000 0.158000
USER    NEWDPF tran0    13.248649 99.806271 56.204828
USER    NEWDPF axisangle0       -0.825006 0.224296 0.518706 -104.350075
USER    NEWDPF quaternion0      -0.651662 0.177168 0.409720 -0.613251
USER    NEWDPF dihe0    -27.42 -41.79
USER
USER                                  x       y       z    vdW   Elec       q     RMS
ATOM      1  N1  ZIN A   1      11.863  99.422  53.469 -0.21 -0.04    -0.390    112.197
ATOM      2  C2  ZIN A   1      11.709  99.272  54.583 -0.28 +0.03    +0.250    112.197
ATOM      3  C3  ZIN A   1      11.512  99.085  55.990 -0.30 +0.00    +0.010    112.197
ATOM      4  C4  ZIN A   1      10.280  98.642  56.474 -0.36 +0.01    +0.050    112.197
ATOM      5  C5  ZIN A   1      10.098  98.463  57.832 -0.31 +0.01    +0.100    112.197
ATOM      6  F6  ZIN A   1       8.906  98.034  58.299 -0.05 -0.06    -0.130    112.197
ATOM      7  C7  ZIN A   1      11.137  98.715  58.715 -0.32 -0.00    +0.030    112.197
ATOM      8  C8  ZIN A   1      12.358  99.159  58.249 -0.27 -0.00    +0.070    112.197
ATOM      9  C9  ZIN A   1      12.558  99.344  56.888 -0.15 +0.01    +0.190    112.197
ATOM     10  N10 ZIN A   1      13.794  99.787  56.416 +0.09 -0.04    -0.600    112.197
ATOM     11  C18 ZIN A   1      14.977  99.265  56.782 +0.05 +0.04    +0.530    112.197
ATOM     12  C17 ZIN A   1      16.106  99.992  56.086 -0.44 -0.00    +0.090    112.197
ATOM     13  O19 ZIN A   1      15.119  98.345  57.559 -0.02 -0.07    -0.530    112.197
ATOM     14  C12 ZIN A   1      15.454 101.296  55.567 -0.41 +0.02    -0.070    112.197
ATOM     15  C11 ZIN A   1      13.970 100.878  55.450 -0.13 -0.01    +0.280    112.197
ATOM     16  C14 ZIN A   1      16.011 101.679  54.221 -0.11 -0.01    +0.500    112.197
ATOM     17  O15 ZIN A   1      17.150 101.363  53.920 -0.60 -0.24    -0.680    112.197
ATOM     18  O16 ZIN A   1      15.323 102.306  53.433 +0.12 +0.00    -0.690    112.197
TER
ENDMDL
```

The ligPlot containing all hydrogen bond interactions and hydrophobic interactions is given below

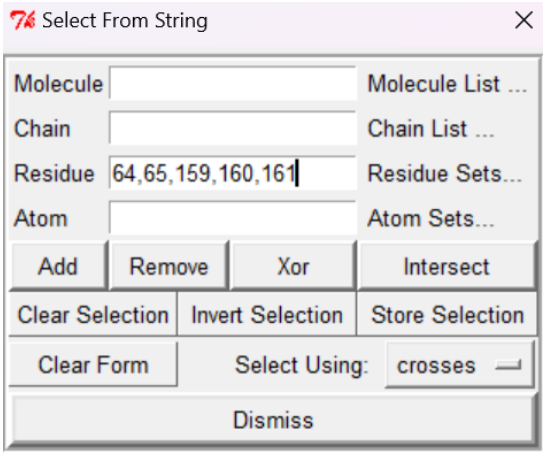


6. Use the following active site residues and grid box dimensions for center on macromolecule
Active site residues: Lys271, Thr315, Glu286
size_x = 60, size_y = 46, size_z = 44
Offset: x = -11.278, y = 18.056, z = 6.944
Spacing (angstrom) = 0.375
center_x = 7.025, center_y = 93.837, center_z = 61.323

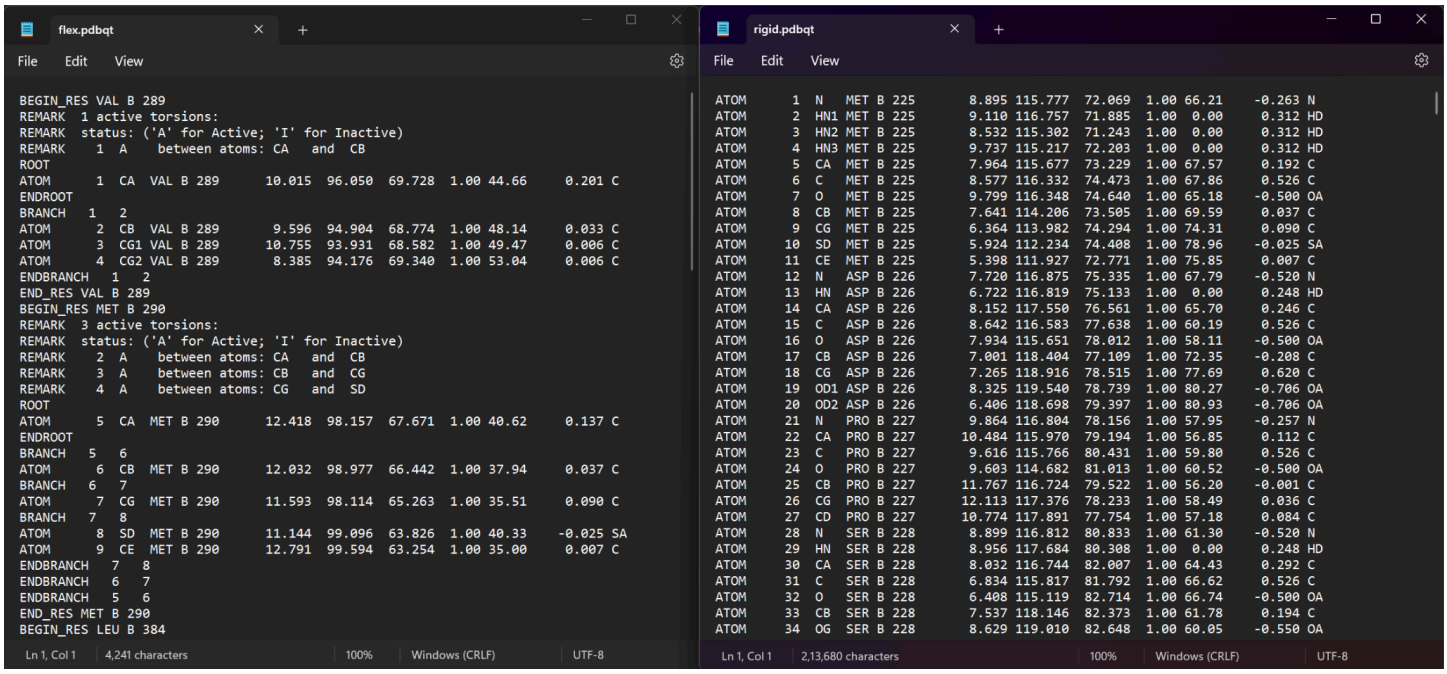


II. Flexible docking

1. Assign flexible residues using select from string option (PDB: GLU64, ALA65, ASP159, PHE160, GLY161; UniProt: GLU286, ALA287, ASP381, PHE382, GLY383)
We assign the numberings using strings as 64,65,159,160,161 in the residue section.



2. Classify the rigid and flexible residues using flexible residues option.



flex.pdbqt

```
BEGIN_RES VAL B 289
REMARK  1 active torsions:
REMARK  status: ('A' for Active; 'I' for Inactive)
REMARK    1  A    between atoms: CA   and  CB
ROOT
ATOM      1  CA  VAL B 289      10.015  96.050  69.728  1.00 44.66     0.201 C
ENDROOT
BRANCH   1   2
ATOM      2  CB  VAL B 289       9.596  94.904  68.774  1.00 48.14     0.033 C
ATOM      3  CG1 VAL B 289      10.755  93.931  68.582  1.00 49.47     0.006 C
ATOM      4  CG2 VAL B 289       8.385  94.176  69.340  1.00 53.04     0.006 C
ENDBRANCH   1   2
END_RES VAL B 289
BEGIN_RES MET B 290
REMARK  3 active torsions:
REMARK  status: ('A' for Active; 'I' for Inactive)
REMARK    2  A    between atoms: CA   and  CB
REMARK    3  A    between atoms: CB   and  CG
REMARK    4  A    between atoms: CG   and  SD
ROOT
ATOM      5  CA  MET B 290      12.418  98.157  67.671  1.00 40.62     0.137 C
ENDROOT
BRANCH   5   6
ATOM      6  CB  MET B 290      12.032  98.977  66.442  1.00 37.94     0.037 C
BRANCH   6   7
ATOM      7  CG  MET B 290      11.593  98.114  65.263  1.00 35.51     0.090 C
BRANCH   7   8
ATOM      8  SD  MET B 290      11.144  99.096  63.826  1.00 40.33    -0.025 SA
ATOM      9  CE  MET B 290      12.791  99.594  63.254  1.00 35.00     0.007 C
ENDBRANCH   7   8
ENDBRANCH   6   7
ENDBRANCH   5   6
END_RES MET B 290
BEGIN_RES LEU B 384
```

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rigid.pdbqt

```
ATOM      1  N   MET B 225       8.895 115.777  72.069  1.00 66.21    -0.263 N
ATOM      2  HN1 MET B 225       9.110 116.757  71.885  1.00  0.00     0.312 HD
ATOM      3  HN2 MET B 225       8.532 115.302  71.243  1.00  0.00     0.312 HD
ATOM      4  HN3 MET B 225       9.737 115.217  72.203  1.00  0.00     0.312 HD
ATOM      5  CA  MET B 225       7.964 115.677  73.229  1.00 67.57     0.192 C
ATOM      6  C   MET B 225       8.577 116.332  74.473  1.00 67.86     0.526 C
ATOM      7  O   MET B 225       9.799 116.348  74.640  1.00 65.18    -0.500 OA
ATOM      8  CB  MET B 225       7.641 114.206  73.505  1.00 69.59     0.037 C
ATOM      9  CG  MET B 225       6.364 113.982  74.294  1.00 74.31     0.090 C
ATOM     10  SD  MET B 225       5.924 112.234  74.408  1.00 78.96    -0.025 SA
ATOM     11  CE  MET B 225       5.398 111.927  72.771  1.00 75.85     0.007 C
ATOM     12  N   ASP B 226       7.720 116.875  75.335  1.00 67.79    -0.520 N
ATOM     13  HN  ASP B 226       6.722 116.819  75.133  1.00  0.00     0.248 HD
ATOM     14  CA  ASP B 226       8.152 117.550  76.561  1.00 65.70     0.246 C
ATOM     15  C   ASP B 226       8.642 116.583  77.638  1.00 60.19     0.526 C
ATOM     16  O   ASP B 226       7.934 115.651  78.012  1.00 58.11    -0.500 OA
ATOM     17  CB  ASP B 226       7.001 118.404  77.109  1.00 72.35    -0.208 C
ATOM     18  CG  ASP B 226       7.265 118.916  78.515  1.00 77.69     0.620 C
ATOM     19  OD1 ASP B 226       8.325 119.540  78.739  1.00 80.27    -0.706 OA
ATOM     20  OD2 ASP B 226       6.406 118.698  79.397  1.00 80.93    -0.706 OA
ATOM     21  N   PRO B 227       9.864 116.804  78.156  1.00 57.95    -0.257 N
ATOM     22  CA  PRO B 227      10.484 115.970  79.194  1.00 56.85     0.112 C
ATOM     23  C   PRO B 227       9.616 115.766  80.431  1.00 59.80     0.526 C
ATOM     24  O   PRO B 227       9.603 114.682  81.013  1.00 60.52    -0.500 OA
ATOM     25  CB  PRO B 227      11.767 116.724  79.522  1.00 56.20    -0.001 C
ATOM     26  CG  PRO B 227      12.113 117.376  78.233  1.00 58.49     0.036 C
ATOM     27  CD  PRO B 227      10.774 117.891  77.754  1.00 57.18     0.084 C
ATOM     28  N   SER B 228       8.899 116.812  80.833  1.00 61.30    -0.520 N
ATOM     29  HN  SER B 228       8.956 117.684  80.308  1.00  0.00     0.248 HD
ATOM     30  CA  SER B 228       8.032 116.744  82.007  1.00 64.43     0.292 C
ATOM     31  C   SER B 228       6.834 115.817  81.792  1.00 66.62     0.526 C
ATOM     32  O   SER B 228       6.408 115.119  82.714  1.00 66.74    -0.500 OA
ATOM     33  CB  SER B 228       7.537 118.146  82.373  1.00 61.78     0.194 C
ATOM     34  OG  SER B 228       8.629 119.010  82.648  1.00 60.05    -0.550 OA
```

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3. Get 10 different orientation of ligand (ZINC126204226) and flexible residues.

The confirmation and docking is performed for 10 different orientations

CLUSTERING HISTOGRAM

Clus-ter Rank	Lowest Binding Energy	Run	Mean Binding Energy	Num in Clus	Histogram 5 10 15 20 25 30 35
1	-3.63	2	-3.63	1	#
2	-3.60	8	-3.60	1	#
3	-2.53	10	-2.38	2	##
4	-2.39	9	-2.28	2	##
5	-2.38	5	-2.38	1	#
6	-2.20	6	-2.20	1	#
7	-2.16	7	-2.16	1	#
8	-1.29	1	-1.29	1	#

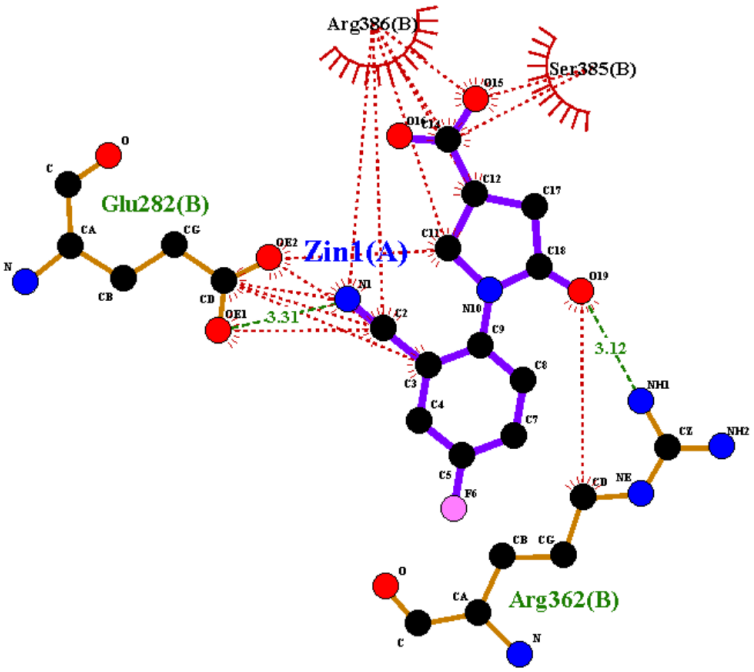
Number of multi-member conformational clusters found = 2, out of 10 runs.

The lowest binding energy of -3.63 is observed in flexible docking in run 2

The details of run 2 is given below

```
MODEL        2
USER    Run = 2
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 1
USER
USER    RMSD from reference structure       = 105.862 A
USER
USER    Estimated Free Energy of Binding    =   -3.63 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =    2.18 mM (millimolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -4.23 kcal/mol
USER        Moving Ligand-Fixed Receptor    =   +0.29 kcal/mol
USER           vdW + Hbond + desolv Energy  =   -0.06 kcal/mol
USER           Electrostatic Energy         =   +0.35 kcal/mol
USER        Moving Ligand-Moving Receptor   =   -4.52 kcal/mol
USER           vdW + Hbond + desolv Energy  =   -3.02 kcal/mol
USER           Electrostatic Energy         =   -1.50 kcal/mol
USER    (2) Final Total Internal Energy     =   -3.71 kcal/mol
USER        Internal Energy Ligand          =   +0.08 kcal/mol
USER        Internal Moving-Fixed Receptor  =   -3.95 kcal/mol
USER        Internal Moving-Moving Receptor =   +0.16 kcal/mol
USER    (3) Torsional Free Energy           =   +0.60 kcal/mol
USER    (4) Unbound System's Energy  [=(2)] =   -3.71 kcal/mol
USER
USER
USER
USER    DPF = C:/Users/shree/Desktop/ACADS/Comp_Bio_Lab/Fuckthisshit/Fuckthisnewshit/docking.dpf
USER    NEWDPF move     ligaand.pdbqt
USER    NEWDPF about    2.234000 1.640000 0.158000
USER    NEWDPF tran0    3.241214 89.035417 62.146270
USER    NEWDPF axisangle0       0.527453 -0.664788 -0.529009 133.306878
USER    NEWDPF quaternion0      0.484268 -0.610358 -0.485696 0.396292
USER    NEWDPF dihe0    -149.76 -101.56 -131.43 6.65 -0.23 -12.15 -21.73 -13.40 39.67 -40.97 114.60 30.12 126.07 90.49
USER
USER                            x       y       z     vdW   Elec       q     RMS
```

Ln 1, Col 1 | 1,80,048 characters | 100% | Windows (CRLF) | UTF-8



flexibledocking

4. What type of interactions are captured in flexible docking compared to rigid docking?

PDB code: flexibledocking

Hydrogen bonds

	<----- ATOM 1 ----->					<----- ATOM 2 ----->					
	Atom no	Atom name	Res name	Res no	Chain		Atom no	Atom name	Res name	Res no	Chain	Distance
1	48	NH1	ARG	362	B	---	17	O19	ZIN	1	A	3.117
2	1	N1	ZIN	1	A	---	37	OE1	GLU	282	B	3.312

Non-bonded contacts

	<----- ATOM 1 ----->					<----- ATOM 2 ----->					
	Atom no	Atom name	Res name	Res no	Chain		Atom no	Atom name	Res name	Res no	Chain	Distance
1	45	CD	ARG	362	B	---	17	O19	ZIN	1	A	3.673
2	25	CD	ARG	386	B	---	13	O15	ZIN	1	A	3.816
3	24	CG	ARG	386	B	---	13	O15	ZIN	1	A	2.785
4	23	CB	ARG	386	B	---	13	O15	ZIN	1	A	3.127
5	20	CA	ARG	386	B	---	13	O15	ZIN	1	A	3.569
6	52	C	SER	385	B	---	13	O15	ZIN	1	A	3.833
7	28	NH1	ARG	386	B	---	12	C14	ZIN	1	A	3.026
8	24	CG	ARG	386	B	---	12	C14	ZIN	1	A	3.529
9	55	OG	SER	385	B	---	12	C14	ZIN	1	A	3.010
10	28	NH1	ARG	386	B	---	11	C12	ZIN	1	A	3.657
11	28	NH1	ARG	386	B	---	10	C11	ZIN	1	A	3.113
12	38	OE2	GLU	282	B	---	10	C11	ZIN	1	A	3.578
13	36	CD	GLU	282	B	---	3	C3	ZIN	1	A	3.830
14	29	NH2	ARG	386	B	---	2	C2	ZIN	1	A	3.835
15	28	NH1	ARG	386	B	---	2	C2	ZIN	1	A	3.720
16	38	OE2	GLU	282	B	---	2	C2	ZIN	1	A	3.708
17	37	OE1	GLU	282	B	---	2	C2	ZIN	1	A	3.361
18	36	CD	GLU	282	B	---	2	C2	ZIN	1	A	3.575
19	27	CZ	ARG	386	B	---	1	N1	ZIN	1	A	3.471
20	36	CD	GLU	282	B	---	1	N1	ZIN	1	A	3.767

Flexible docking

PDB code: final_attempt

Hydrogen bonds

	<----- ATOM 1 ----->					<----- ATOM 2 ----->					
	Atom no	Atom name	Res name	Res no	Chain		Atom no	Atom name	Res name	Res no	Chain	Distance
1	46	NZ	LYS	271	B	---	18	F6	ZIN	1	A	2.845
2	30	N	MET	318	B	---	13	O15	ZIN	1	A	2.807

Non-bonded contacts

	<----- A T O M 1 ----->					<----- A T O M 2 ----->				
	Atom no	Atom name	Res name	Res no	Chain	Atom no	Atom name	Res name	Res no	Chain	Distance
1	29	CZ	PHE	382	B	17	O19	ZIN	1	A	3.898
2	28	CE2	PHE	382	B	17	O19	ZIN	1	A	3.091
3	125	CB	ALA	380	B	17	O19	ZIN	1	A	3.427
4	53	CG2	VAL	299	B	17	O19	ZIN	1	A	2.893
5	52	CG1	VAL	299	B	17	O19	ZIN	1	A	3.522
6	51	CB	VAL	299	B	17	O19	ZIN	1	A	3.339
7	28	CE2	PHE	382	B	16	C18	ZIN	1	A	3.271
8	95	OG1	THR	315	B	16	C18	ZIN	1	A	3.804
9	53	CG2	VAL	299	B	16	C18	ZIN	1	A	3.308
10	118	CG	LEU	370	B	15	C17	ZIN	1	A	3.865
11	99	O	GLU	316	B	15	C17	ZIN	1	A	3.713
12	53	CG2	VAL	299	B	15	C17	ZIN	1	A	3.395
13	77	CD1	PHE	317	B	14	O16	ZIN	1	A	3.593
14	70	CB	ALA	269	B	14	O16	ZIN	1	A	3.034
15	112	CD2	LEU	248	B	14	O16	ZIN	1	A	2.919
16	35	CG	MET	318	B	13	O15	ZIN	1	A	3.805
17	34	CB	MET	318	B	13	O15	ZIN	1	A	3.660
18	31	CA	MET	318	B	13	O15	ZIN	1	A	3.766
19	73	C	PHE	317	B	13	O15	ZIN	1	A	3.626
20	72	CA	PHE	317	B	13	O15	ZIN	1	A	3.525
21	30	N	MET	318	B	12	C14	ZIN	1	A	3.765
22	72	CA	PHE	317	B	12	C14	ZIN	1	A	3.754
23	99	O	GLU	316	B	12	C14	ZIN	1	A	3.410
24	70	CB	ALA	269	B	12	C14	ZIN	1	A	3.522
25	99	O	GLU	316	B	11	C12	ZIN	1	A	3.047
26	95	OG1	THR	315	B	11	C12	ZIN	1	A	3.420
27	70	CB	ALA	269	B	11	C12	ZIN	1	A	3.317
28	95	OG1	THR	315	B	10	C11	ZIN	1	A	3.656
29	70	CB	ALA	269	B	10	C11	ZIN	1	A	3.158
30	28	CE2	PHE	382	B	9	N10	ZIN	1	A	3.402
31	28	CE2	PHE	382	B	8	C9	ZIN	1	A	3.397
32	26	CD2	PHE	382	B	8	C9	ZIN	1	A	3.541
33	44	CD	LYS	271	B	5	C5	ZIN	1	A	3.668
34	26	CD2	PHE	382	B	4	C4	ZIN	1	A	3.508
35	88	CG2	VAL	256	B	4	C4	ZIN	1	A	3.820
36	28	CE2	PHE	382	B	3	C3	ZIN	1	A	3.468
37	26	CD2	PHE	382	B	3	C3	ZIN	1	A	3.196
38	28	CE2	PHE	382	B	2	C2	ZIN	1	A	3.549
39	26	CD2	PHE	382	B	2	C2	ZIN	1	A	3.428
40	87	CG1	VAL	256	B	2	C2	ZIN	1	A	3.603
41	87	CG1	VAL	256	B	1	N1	ZIN	1	A	3.443
42	61	CD2	TYR	253	B	1	N1	ZIN	1	A	3.486
43	60	CD1	TYR	253	B	1	N1	ZIN	1	A	3.777
44	59	CG	TYR	253	B	1	N1	ZIN	1	A	3.349
45	58	CB	TYR	253	B	1	N1	ZIN	1	A	3.655

Rigid Docking

Docking for flexible is more stable than the one for rigid. The rigid docking has a best binding energy of -3.44 kcal/mol but the flexible docking has its best binding energy as -3.63 kcal/mol. The interactions in both have 2 hydrogen bonds each, while flexible docking has lesser non-bonded interactions while being more stable

5. Discuss which docking strategy (rigid/flexible) yield better result. Why?
Flexible docking yields better results since it has lower binding energy with a lesser number of non-bonded interactions. Flexibility of certain residues allows for interactions that would not be possible if they were rigid, and it also more accurately mimics reality when residues are allowed to be flexible.

III. Screening- Autodock Vina

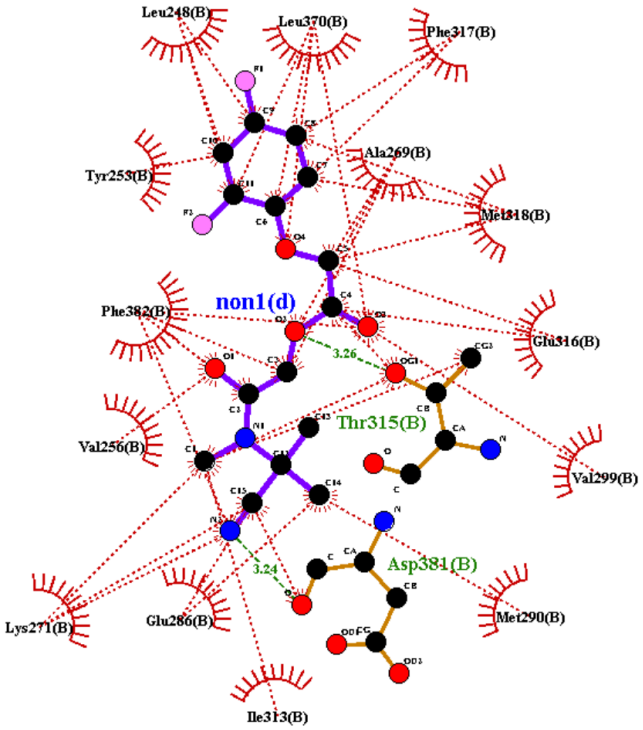
1. Obtain the structures of 6 ligands with ZINC IDs from Zinc database: ZINC1283491630, ZINC49895016, ZINC118332804, ZINC31233162, ZINC235987838, ZINC295506072
We obtain the 6 ligand structures in the zip file provided and convert each ligand to *.pdbqt format in autodock

2. Screen all of them using the protein structure, 1IEP and identify the ligands with lowest energy and score.
Screening all of the ligands using vina with exhaustiveness set to 20. The tabulated lowest energy for each of the ligands

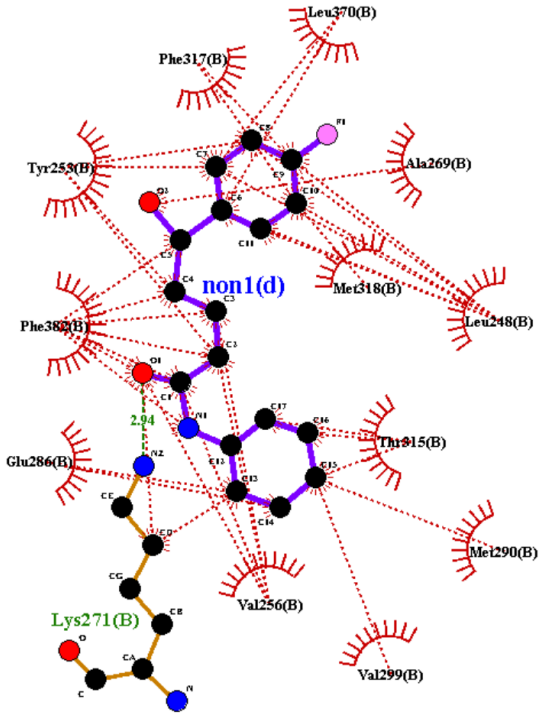
Ligand	Lowest Affinity (kcal/mol)
ZINC31233162	-8.3
ZINC49895016	-8.5
ZINC118332804	-6.3
ZINC235987838	-8.8
ZINC295506072	-6.3
ZINC1283491630	-7.1

We see that ZINC235987838 has the lowest energy of **-8.8 kcal/mol**

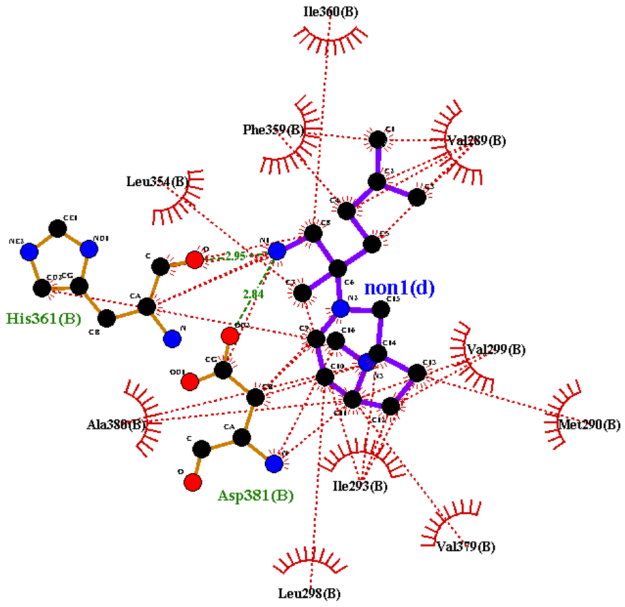
3. Tabulate the ligand interactions using ligplot/PDBSUM and discuss which ligand is binding effectively with c-Abl kinase?



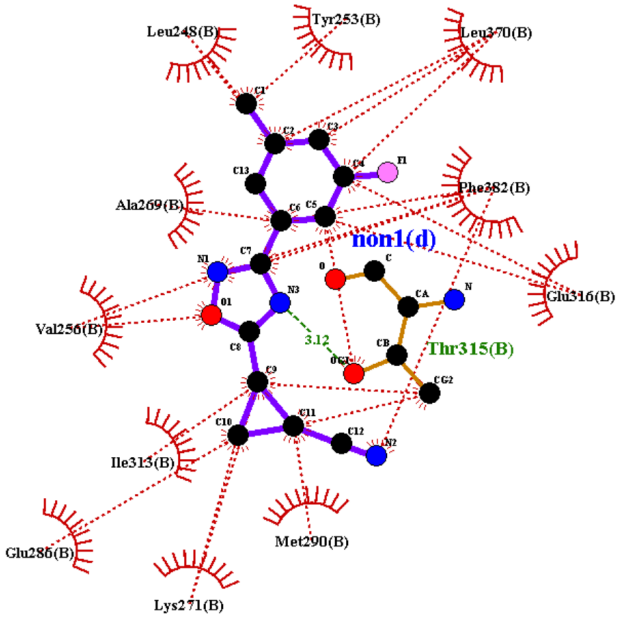
zinc_000031233162_out



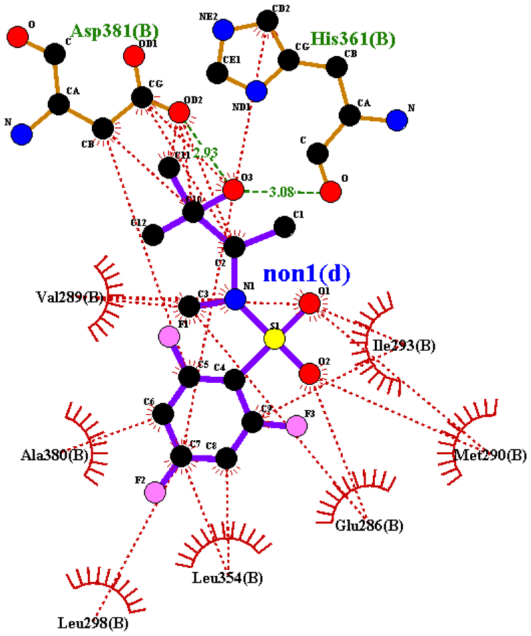
zinc_000049895016_out



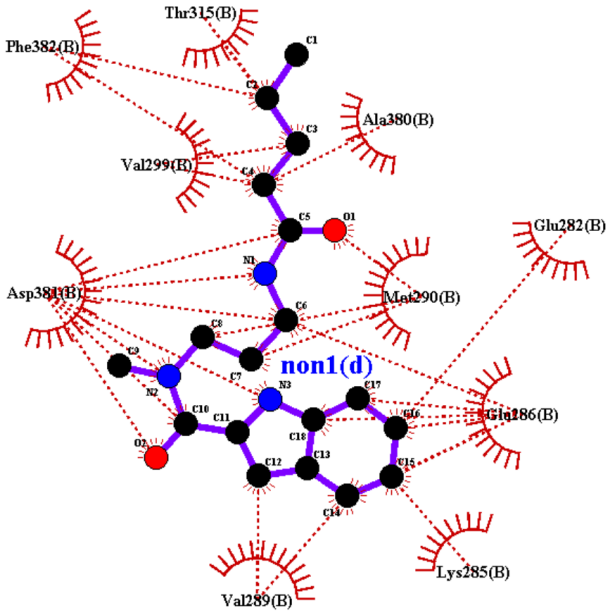
zinc_000118332804_out



zinc_000235987838_out



zinc_000295506072_out



zinc_001283491630_out

The tabulated results are given below:

The Ligand interactions show us the following

Ligand	Lowest Affinity (kcal/mol)	No. of Hydrogen Bond	No.of non-bonded contacts
ZINC31233162	-8.3	2	49
ZINC49895016	-8.5	1	52
ZINC118332804	-6.3	2	34
ZINC235987838	-8.8	1	30
ZINC295506072	-6.3	2	27
ZINC1283491630	-7.1	0	37

ZINC49895016 has the most number of interactions while ZINC118332804 has the least number of interactions. ZINC118332804 also has the highest affinity among all other ligands, hence its interaction can be considered as poor, while ZINC235987838 has the lowest affinity of -8.8 kcal/mol, while have one 1 hydrogen bonding interaction and 34 non-bonded contacts, hence we can consider this interaction the most efficient energy wise among the 6 ligands.

PDB code: zinc_000031233162_out

Hydrogen bonds

	<----- A T O M 1 ----->					<----- A T O M 2 ----->					
	Atom no	Atom name	Res name	Res no	Chain		Atom no	Atom name	Res name	Res no	Chain	Distance
1	30	OG1	THR	315	B	---	6	O2	non	1	d	3.261
2	5	N2	non	1	d	---	53	O	ASP	381	B	3.238

Non-bonded contacts

	<----- A T O M 1 ----->					<----- A T O M 2 ----->					
	Atom no	Atom name	Res name	Res no	Chain		Atom no	Atom name	Res name	Res no	Chain	Distance
1	53	O	ASP	381	B	---	21	C15	non	1	d	3.592
2	126	OE2	GLU	286	B	---	21	C15	non	1	d	3.575
3	83	CD	LYS	271	B	---	21	C15	non	1	d	3.784
4	134	CE	MET	290	B	---	20	C14	non	1	d	3.838
5	133	SD	MET	290	B	---	20	C14	non	1	d	3.892
6	126	OE2	GLU	286	B	---	20	C14	non	1	d	3.558
7	37	CD1	LEU	370	B	---	17	C11	non	1	d	3.659
8	76	CD2	LEU	248	B	---	17	C11	non	1	d	3.845
9	105	OH	TYR	253	B	---	16	C10	non	1	d	3.526
10	104	CZ	TYR	253	B	---	16	C10	non	1	d	3.538
11	102	CE1	TYR	253	B	---	16	C10	non	1	d	3.272
12	76	CD2	LEU	248	B	---	16	C10	non	1	d	3.635
13	76	CD2	LEU	248	B	---	15	C9	non	1	d	3.740
14	74	CG	LEU	248	B	---	15	C9	non	1	d	3.770
15	89	O	MET	318	B	---	14	C8	non	1	d	3.588
16	68	CZ	PHE	317	B	---	14	C8	non	1	d	3.346
17	67	CE2	PHE	317	B	---	14	C8	non	1	d	3.869
18	66	CE1	PHE	317	B	---	14	C8	non	1	d	3.424
19	89	O	MET	318	B	---	13	C7	non	1	d	3.172
20	86	N	MET	318	B	---	13	C7	non	1	d	3.541
21	66	CE1	PHE	317	B	---	13	C7	non	1	d	3.785
22	64	CD1	PHE	317	B	---	13	C7	non	1	d	3.878
23	37	CD1	LEU	370	B	---	12	C6	non	1	d	3.569
24	86	N	MET	318	B	---	11	C5	non	1	d	3.862
25	138	O	GLU	316	B	---	11	C5	non	1	d	3.258
26	110	CB	ALA	269	B	---	11	C5	non	1	d	3.755
27	37	CD1	LEU	370	B	---	10	O4	non	1	d	3.323
28	36	CG	LEU	370	B	---	10	O4	non	1	d	3.597

29	138	O	GLU	316	B	---	9	C4	non	1	d	3.742
30	30	OG1	THR	315	B	---	9	C4	non	1	d	3.766
31	48	CE2	PHE	382	B	---	8	O3	non	1	d	3.578
32	38	CD2	LEU	370	B	---	8	O3	non	1	d	3.781
33	36	CG	LEU	370	B	---	8	O3	non	1	d	3.636
34	150	CG2	VAL	299	B	---	8	O3	non	1	d	3.415
35	48	CE2	PHE	382	B	---	7	C3	non	1	d	3.866
36	110	CB	ALA	269	B	---	7	C3	non	1	d	3.804
37	110	CB	ALA	269	B	---	6	O2	non	1	d	3.439
38	41	C	PHE	382	B	---	5	N2	non	1	d	3.815
39	40	CA	PHE	382	B	---	5	N2	non	1	d	3.462
40	84	CE	LYS	271	B	---	5	N2	non	1	d	3.560
41	83	CD	LYS	271	B	---	5	N2	non	1	d	3.495
42	46	CD2	PHE	382	B	---	4	C2	non	1	d	3.887
43	46	CD2	PHE	382	B	---	3	O1	non	1	d	3.543
44	117	CG2	VAL	256	B	---	3	O1	non	1	d	3.478
45	116	CG1	VAL	256	B	---	3	O1	non	1	d	3.715
46	30	OG1	THR	315	B	---	1	C1	non	1	d	3.720
47	29	CG2	THR	315	B	---	1	C1	non	1	d	3.649
48	154	O	ILE	313	B	---	1	C1	non	1	d	3.816
49	81	CB	LYS	271	B	---	1	C1	non	1	d	3.847

ZINC49895016

PDB code: zinc_000049895016_out

Hydrogen bonds

	<----- A T O M 1 ----->					<----- A T O M 2 ----->					
	Atom no	Atom name	Res name	Res no	Chain		Atom no	Atom name	Res name	Res no	Chain	Distance
1	53	NZ	LYS	271	B	---	3	O1	non	1	d	2.938

Non-bonded contacts

	<----- A T O M 1 ----->					<----- A T O M 2 ----->					
	Atom no	Atom name	Res name	Res no	Chain		Atom no	Atom name	Res name	Res no	Chain	Distance
1	75	OG1	THR	315	B	---	20	C17	non	1	d	3.450
2	74	CG2	THR	315	B	---	20	C17	non	1	d	3.781
3	75	OG1	THR	315	B	---	19	C16	non	1	d	3.483
4	74	CG2	THR	315	B	---	19	C16	non	1	d	3.890
5	74	CG2	THR	315	B	---	18	C15	non	1	d	3.700
6	130	CG1	VAL	299	B	---	18	C15	non	1	d	3.694
7	124	CE	MET	290	B	---	18	C15	non	1	d	3.881
8	95	OE2	GLU	286	B	---	17	C14	non	1	d	3.692
9	95	OE2	GLU	286	B	---	16	C13	non	1	d	3.534
10	51	CD	LYS	271	B	---	16	C13	non	1	d	3.790
11	61	CD2	LEU	248	B	---	14	C11	non	1	d	3.856
12	99	O	MET	318	B	---	13	C10	non	1	d	3.820
13	96	N	MET	318	B	---	13	C10	non	1	d	3.471
14	84	CE1	PHE	317	B	---	13	C10	non	1	d	3.829
15	82	CD1	PHE	317	B	---	13	C10	non	1	d	3.679
16	61	CD2	LEU	248	B	---	13	C10	non	1	d	3.798
17	84	CE1	PHE	317	B	---	12	C9	non	1	d	3.858
18	61	CD2	LEU	248	B	---	12	C9	non	1	d	3.765
19	44	OH	TYR	253	B	---	11	C8	non	1	d	3.764
20	41	CE1	TYR	253	B	---	11	C8	non	1	d	3.767
21	61	CD2	LEU	248	B	---	11	C8	non	1	d	3.796
22	110	CD1	LEU	370	B	---	10	C7	non	1	d	3.861
23	44	OH	TYR	253	B	---	10	C7	non	1	d	3.752
24	43	CZ	TYR	253	B	---	10	C7	non	1	d	3.588
25	41	CE1	TYR	253	B	---	10	C7	non	1	d	3.632
26	61	CD2	LEU	248	B	---	10	C7	non	1	d	3.847
27	110	CD1	LEU	370	B	---	9	C6	non	1	d	3.851

28	61	CD2	LEU	248	B	---	9	C6	non	1	d	3.861
29	32	CZ	PHE	382	B	---	8	C5	non	1	d	3.674
30	31	CE2	PHE	382	B	---	8	C5	non	1	d	3.284
31	31	CE2	PHE	382	B	---	7	C4	non	1	d	3.582
32	40	CD2	TYR	253	B	---	7	C4	non	1	d	3.790
33	38	CG	TYR	253	B	---	7	C4	non	1	d	3.844
34	31	CE2	PHE	382	B	---	6	C3	non	1	d	3.886
35	29	CD2	PHE	382	B	---	6	C3	non	1	d	3.820
36	68	CG2	VAL	256	B	---	6	C3	non	1	d	3.790
37	67	CG1	VAL	256	B	---	6	C3	non	1	d	3.263
38	116	CB	ALA	269	B	---	5	O2	non	1	d	3.039
39	31	CE2	PHE	382	B	---	4	C2	non	1	d	3.723
40	29	CD2	PHE	382	B	---	4	C2	non	1	d	3.149
41	27	CG	PHE	382	B	---	4	C2	non	1	d	3.694
42	68	CG2	VAL	256	B	---	4	C2	non	1	d	3.446
43	40	CD2	TYR	253	B	---	4	C2	non	1	d	3.733
44	38	CG	TYR	253	B	---	4	C2	non	1	d	3.845
45	37	CB	TYR	253	B	---	4	C2	non	1	d	3.696
46	23	CA	PHE	382	B	---	3	O1	non	1	d	3.877
47	51	CD	LYS	271	B	---	3	O1	non	1	d	3.783
48	68	CG2	VAL	256	B	---	3	O1	non	1	d	3.278
49	31	CE2	PHE	382	B	---	2	N1	non	1	d	3.843
50	29	CD2	PHE	382	B	---	2	N1	non	1	d	3.263
51	29	CD2	PHE	382	B	---	1	C1	non	1	d	3.324
52	68	CG2	VAL	256	B	---	1	C1	non	1	d	3.463

PDB code: zinc_000118332804_out

Hydrogen bonds

	<----- ATOM 1 ----->					<----- ATOM 2 ----->					
	Atom no	Atom name	Res name	Res no	Chain		Atom no	Atom name	Res name	Res no	Chain	Distance
1	2	N1	non	1	d	---	27	OD2	ASP	381	B	2.839
2	2	N1	non	1	d	---	31	O	HIS	361	B	2.952

Non-bonded contacts

	<----- ATOM 1 ----->					<----- ATOM 2 ----->					
	Atom no	Atom name	Res name	Res no	Chain		Atom no	Atom name	Res name	Res no	Chain	Distance
1	20	N	ASP	381	B	---	19	C16	non	1	d	3.604
2	52	CD1	ILE	293	B	---	17	C14	non	1	d	3.296
3	52	CD1	ILE	293	B	---	16	C13	non	1	d	3.407
4	89	CG	MET	290	B	---	16	C13	non	1	d	3.523
5	63	CG1	VAL	299	B	---	15	C12	non	1	d	3.443
6	52	CD1	ILE	293	B	---	15	C12	non	1	d	3.630
7	20	N	ASP	381	B	---	14	C11	non	1	d	3.809
8	55	C	ALA	380	B	---	14	C11	non	1	d	3.701
9	54	CA	ALA	380	B	---	14	C11	non	1	d	3.370
10	111	O	VAL	379	B	---	14	C11	non	1	d	3.587
11	63	CG1	VAL	299	B	---	14	C11	non	1	d	3.738
12	99	CD2	LEU	298	B	---	13	C10	non	1	d	3.554
13	24	CB	ASP	381	B	---	12	C9	non	1	d	3.682
14	34	CD2	HIS	361	B	---	12	C9	non	1	d	3.897
15	31	O	HIS	361	B	---	11	C8	non	1	d	3.665
16	29	CA	HIS	361	B	---	11	C8	non	1	d	3.424
17	103	O	ILE	360	B	---	11	C8	non	1	d	3.476
18	72	CD2	LEU	354	B	---	10	C7	non	1	d	3.800
19	71	CD1	LEU	354	B	---	10	C7	non	1	d	3.719
20	52	CD1	ILE	293	B	---	10	C7	non	1	d	3.776
21	43	CG1	VAL	289	B	---	8	C5	non	1	d	3.797
22	80	CD2	PHE	359	B	---	7	C4	non	1	d	3.866
23	43	CG1	VAL	289	B	---	7	C4	non	1	d	3.483
24	24	CB	ASP	381	B	---	6	N3	non	1	d	3.530
25	55	C	ALA	380	B	---	6	N3	non	1	d	3.845
26	43	CG1	VAL	289	B	---	5	C3	non	1	d	3.796
27	24	CB	ASP	381	B	---	4	N2	non	1	d	3.752

28	43	CG1	VAL	289	B	---	3	C2	non	1	d	3.832
29	25	CG	ASP	381	B	---	2	N1	non	1	d	3.651
30	30	C	HIS	361	B	---	2	N1	non	1	d	3.727
31	29	CA	HIS	361	B	---	2	N1	non	1	d	3.693
32	80	CD2	PHE	359	B	---	1	C1	non	1	d	3.840
33	44	CG2	VAL	289	B	---	1	C1	non	1	d	3.892
34	43	CG1	VAL	289	B	---	1	C1	non	1	d	3.656

ZINC235987838

PDB code: zinc_000235987838_out

Hydrogen bonds

	<----- A T O M 1 ----->					<----- A T O M 2 ----->					
	Atom no	Atom name	Res name	Res no	Chain		Atom no	Atom name	Res name	Res no	Chain	Distance
1	7	N3	non	1	d	---	25	OG1	THR	315	B	3.116

Non-bonded contacts

	<----- A T O M 1 ----->					<----- A T O M 2 ----->					
	Atom no	Atom name	Res name	Res no	Chain		Atom no	Atom name	Res name	Res no	Chain	Distance
1	24	CG2	THR	315	B	---	15	C11	non	1	d	3.440
2	88	CE	MET	290	B	---	15	C11	non	1	d	3.425
3	87	SD	MET	290	B	---	15	C11	non	1	d	3.732
4	111	OE2	GLU	286	B	---	14	C10	non	1	d	3.397
5	63	CD	LYS	271	B	---	14	C10	non	1	d	3.110
6	61	CB	LYS	271	B	---	14	C10	non	1	d	3.587
7	24	CG2	THR	315	B	---	13	C9	non	1	d	3.558
8	115	O	ILE	313	B	---	13	C9	non	1	d	3.682
9	61	CB	LYS	271	B	---	13	C9	non	1	d	3.708
10	35	CE2	PHE	382	B	---	11	C7	non	1	d	3.818
11	35	CE2	PHE	382	B	---	10	C6	non	1	d	3.715
12	102	CB	ALA	269	B	---	10	C6	non	1	d	3.787
13	92	O	GLU	316	B	---	9	C5	non	1	d	3.770
14	25	OG1	THR	315	B	---	9	C5	non	1	d	3.567
15	42	CG	LEU	370	B	---	8	C4	non	1	d	3.878
16	92	O	GLU	316	B	---	8	C4	non	1	d	3.568
17	43	CD1	LEU	370	B	---	6	C3	non	1	d	3.402
18	42	CG	LEU	370	B	---	6	C3	non	1	d	3.788
19	35	CE2	PHE	382	B	---	5	N2	non	1	d	3.676
20	33	CD2	PHE	382	B	---	5	N2	non	1	d	3.573
21	43	CD1	LEU	370	B	---	4	C2	non	1	d	3.840
22	73	CD2	LEU	248	B	---	4	C2	non	1	d	3.846
23	80	CG2	VAL	256	B	---	3	O1	non	1	d	3.881
24	35	CE2	PHE	382	B	---	2	N1	non	1	d	3.766

25	33	CD2	PHE	382	B	---	2	N1	non	1	d	3.594
26	79	CG1	VAL	256	B	---	2	N1	non	1	d	3.786
27	56	OH	TYR	253	B	---	1	C1	non	1	d	3.810
28	55	CZ	TYR	253	B	---	1	C1	non	1	d	3.722
29	53	CE1	TYR	253	B	---	1	C1	non	1	d	3.661
30	73	CD2	LEU	248	B	---	1	C1	non	1	d	3.642

ZINC295506072

PDB code: zinc_000295506072_out

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Hydrogen bonds

	<----- A T O M 1 ----->						<----- A T O M 2 ----->					
	Atom no	Atom name	Res name	Res no	Chain		Atom no	Atom name	Res name	Res no	Chain	Distance
1	8	O3	non	1	d	---	28	OD2	ASP	381	B	2.930
2	8	O3	non	1	d	---	39	O	HIS	361	B	3.084

Non-bonded contacts

	<----- A T O M 1 ----->						<----- A T O M 2 ----->					
	Atom no	Atom name	Res name	Res no	Chain		Atom no	Atom name	Res name	Res no	Chain	Distance
1	28	OD2	ASP	381	B	---	16	C11	non	1	d	3.519
2	28	OD2	ASP	381	B	---	15	C10	non	1	d	3.641
3	78	CD1	ILE	293	B	---	14	C9	non	1	d	3.631
4	70	CD2	LEU	354	B	---	13	C8	non	1	d	3.468
5	69	CD1	LEU	354	B	---	13	C8	non	1	d	3.735
6	42	CD2	HIS	361	B	---	12	C7	non	1	d	3.641
7	70	CD2	LEU	354	B	---	12	C7	non	1	d	3.849
8	86	CD2	LEU	298	B	---	12	C7	non	1	d	3.693
9	89	C	ALA	380	B	---	11	C6	non	1	d	3.738
10	25	CB	ASP	381	B	---	10	C5	non	1	d	3.529
11	26	CG	ASP	381	B	---	8	O3	non	1	d	3.710
12	34	CG1	VAL	289	B	---	7	C3	non	1	d	3.718
13	33	CB	VAL	289	B	---	7	C3	non	1	d	3.730
14	51	CG	GLU	286	B	---	7	C3	non	1	d	3.608
15	47	CA	GLU	286	B	---	7	C3	non	1	d	3.858
16	60	CG	MET	290	B	---	6	O2	non	1	d	3.510
17	51	CG	GLU	286	B	---	6	O2	non	1	d	3.794
18	28	OD2	ASP	381	B	---	5	C2	non	1	d	3.575
19	26	CG	ASP	381	B	---	5	C2	non	1	d	3.604
20	25	CB	ASP	381	B	---	5	C2	non	1	d	3.771
21	78	CD1	ILE	293	B	---	3	O1	non	1	d	3.587
22	60	CG	MET	290	B	---	3	O1	non	1	d	3.198
23	56	CA	MET	290	B	---	3	O1	non	1	d	3.750
24	34	CG1	VAL	289	B	---	3	O1	non	1	d	3.136
25	33	CB	VAL	289	B	---	3	O1	non	1	d	3.686
26	31	C	VAL	289	B	---	3	O1	non	1	d	3.824
27	34	CG1	VAL	289	B	---	2	N1	non	1	d	3.782

ZINC1283491630

PDB code: zinc_001283491630_out

Non-bonded contacts

	<----- A T O M 1 ----->						<----- A T O M 2 ----->				
	Atom no	Atom name	Res name	Res no	Chain		Atom no	Atom name	Res name	Res no	Chain	Distance
1	37	CG	GLU	286	B	---	23	C18	non	1	d	3.698
2	37	CG	GLU	286	B	---	22	C17	non	1	d	3.512
3	37	CG	GLU	286	B	---	21	C16	non	1	d	3.805
4	36	CB	GLU	286	B	---	21	C16	non	1	d	3.727
5	84	O	GLU	282	B	---	21	C16	non	1	d	3.850
6	33	CA	GLU	286	B	---	20	C15	non	1	d	3.628
7	32	N	GLU	286	B	---	20	C15	non	1	d	3.661
8	95	CG	LYS	285	B	---	20	C15	non	1	d	3.801
9	80	CG2	VAL	289	B	---	19	C14	non	1	d	3.718
10	33	CA	GLU	286	B	---	19	C14	non	1	d	3.799
11	79	CG1	VAL	289	B	---	17	C12	non	1	d	3.672
12	31	OD2	ASP	381	B	---	15	C10	non	1	d	3.812
13	28	CB	ASP	381	B	---	15	C10	non	1	d	3.647
14	46	CG	MET	290	B	---	13	C8	non	1	d	3.739
15	46	CG	MET	290	B	---	12	C7	non	1	d	3.580
16	28	CB	ASP	381	B	---	11	C6	non	1	d	3.859
17	27	O	ASP	381	B	---	11	C6	non	1	d	3.548
18	40	OE2	GLU	286	B	---	11	C6	non	1	d	3.673
19	27	O	ASP	381	B	---	10	C5	non	1	d	3.579
20	72	CE2	PHE	382	B	---	9	C4	non	1	d	3.620
21	70	CD2	PHE	382	B	---	9	C4	non	1	d	3.681
22	103	CB	ALA	380	B	---	9	C4	non	1	d	3.869
23	54	CG1	VAL	299	B	---	9	C4	non	1	d	3.731
24	29	CG	ASP	381	B	---	8	N3	non	1	d	3.654
25	62	OG1	THR	315	B	---	7	C3	non	1	d	3.659
26	61	CG2	THR	315	B	---	7	C3	non	1	d	3.705
27	55	CG2	VAL	299	B	---	7	C3	non	1	d	3.815
28	54	CG1	VAL	299	B	---	7	C3	non	1	d	3.780
29	29	CG	ASP	381	B	---	6	O2	non	1	d	3.805
30	28	CB	ASP	381	B	---	6	O2	non	1	d	3.685
31	28	CB	ASP	381	B	---	5	N2	non	1	d	3.795
32	72	CE2	PHE	382	B	---	4	C2	non	1	d	3.806
33	62	OG1	THR	315	B	---	4	C2	non	1	d	3.602
34	48	CE	MET	290	B	---	3	O1	non	1	d	3.528
35	47	SD	MET	290	B	---	3	O1	non	1	d	3.586
36	26	C	ASP	381	B	---	2	N1	non	1	d	3.795
37	25	CA	ASP	381	B	---	2	N1	non	1	d	3.889

All relevant files can be found here.