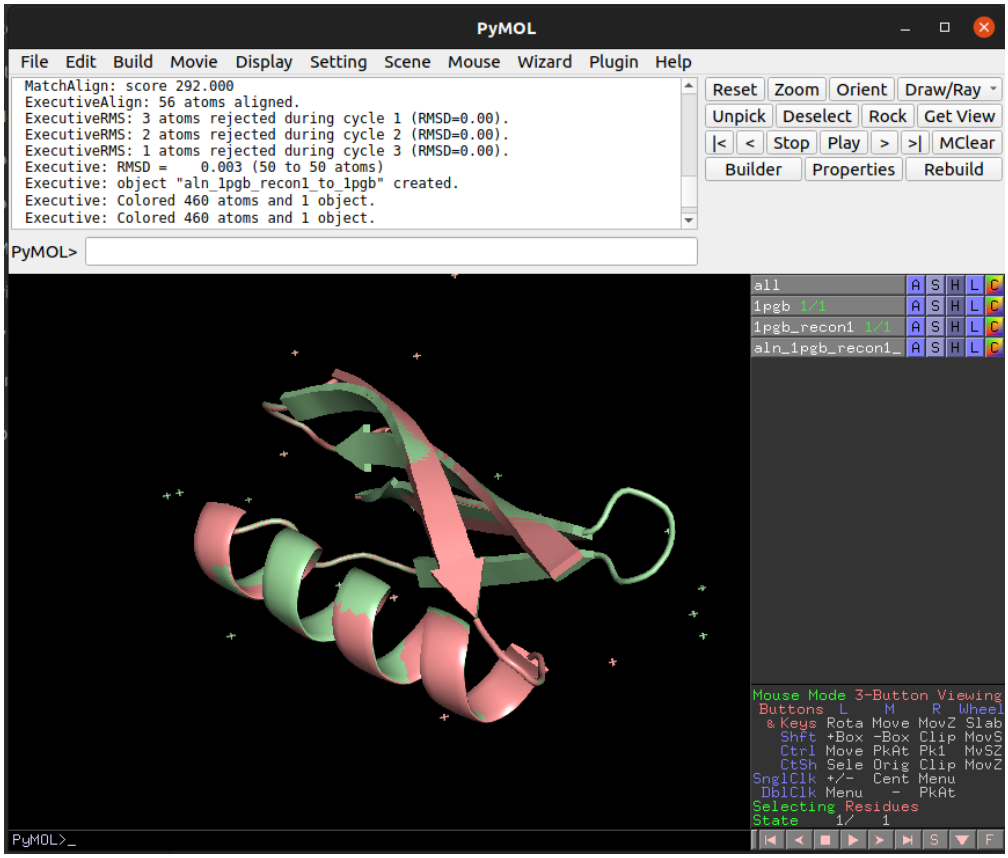
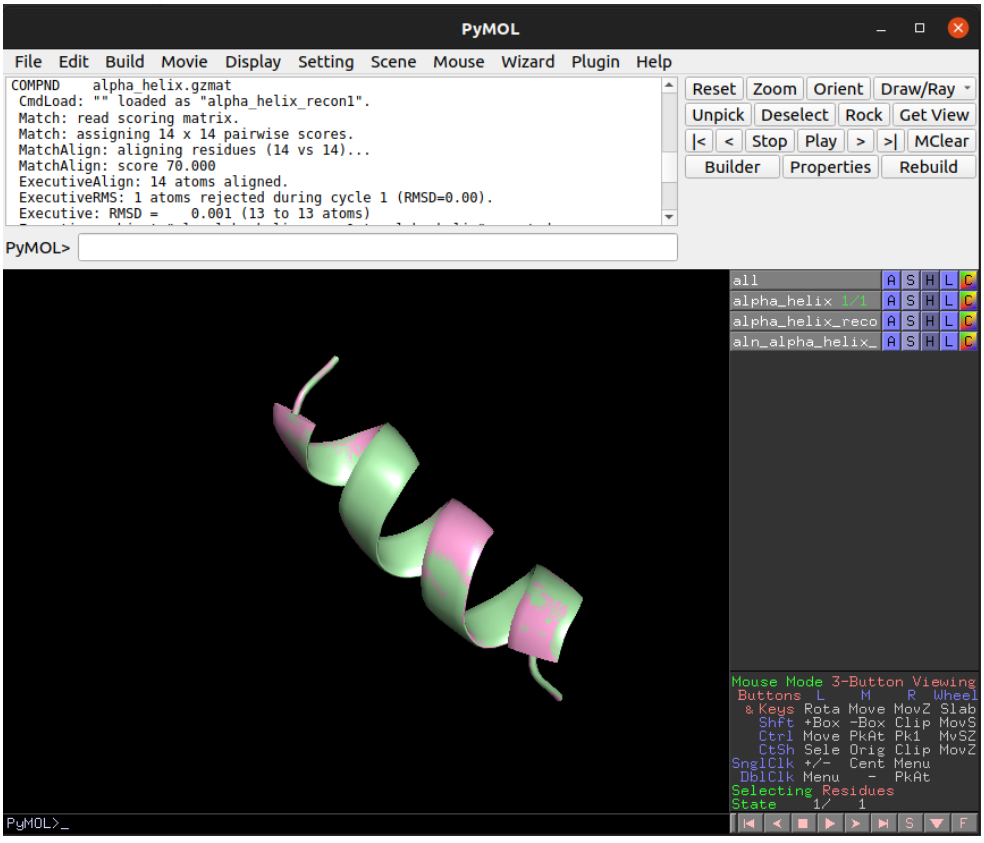
Excercise 1 :

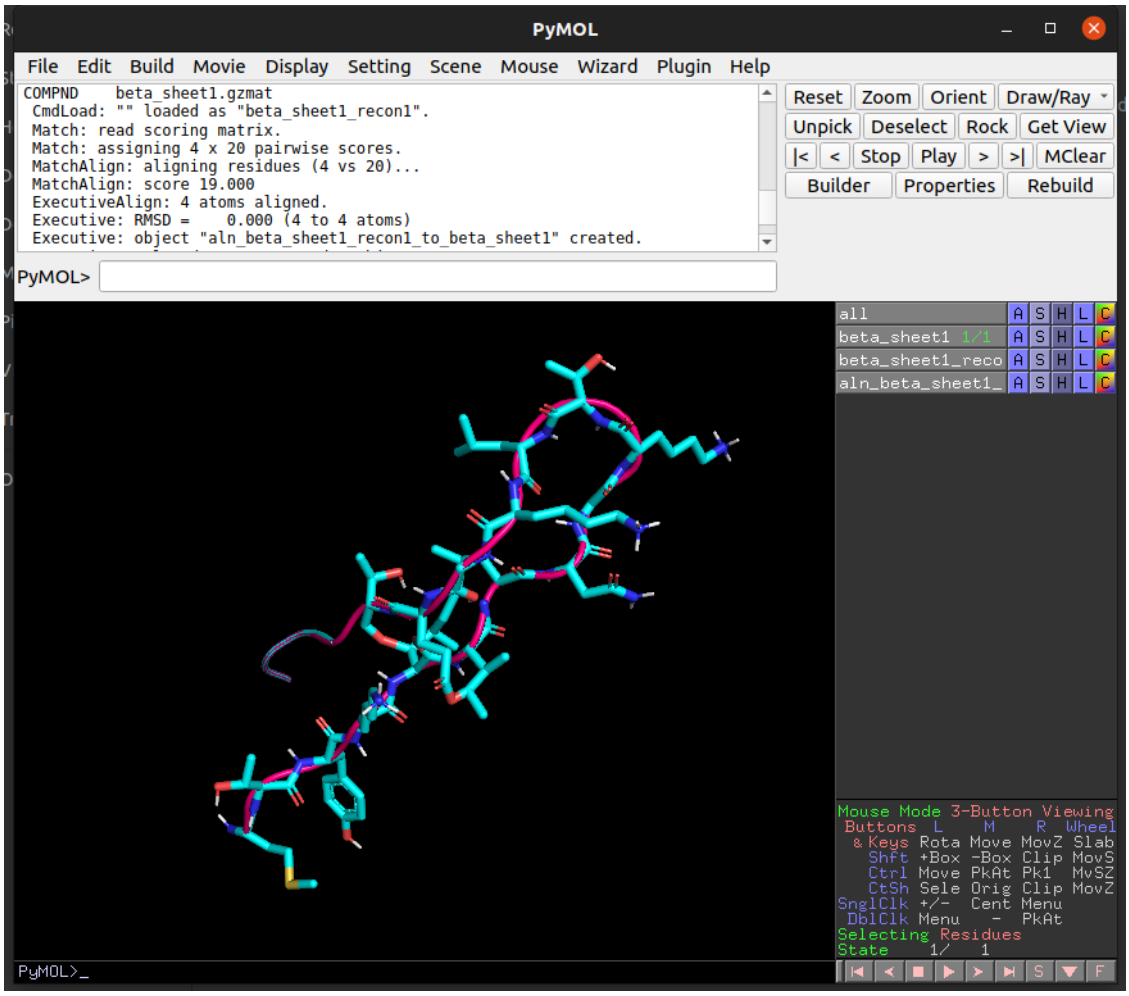
1PGB : RMSD = 0.003



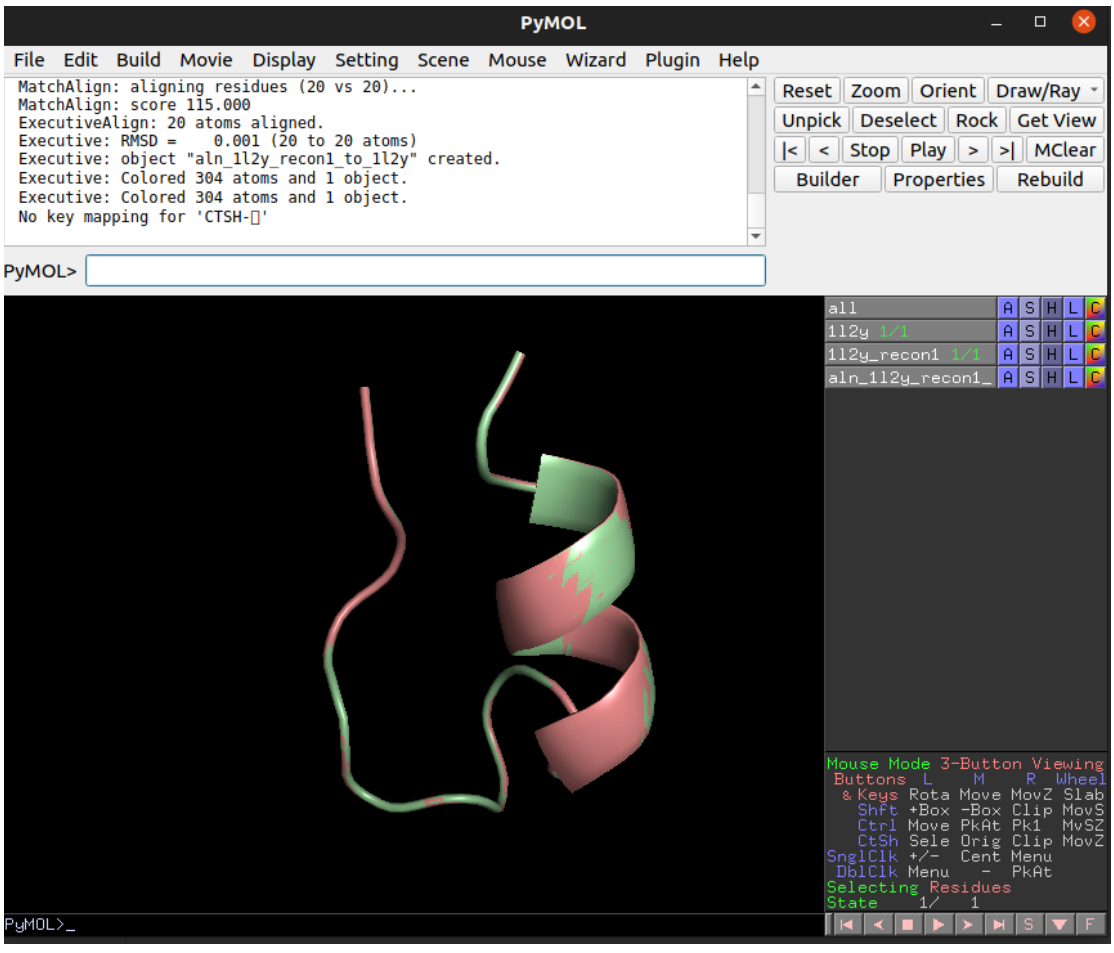
Alpha-Helix : RMSD = 0.001



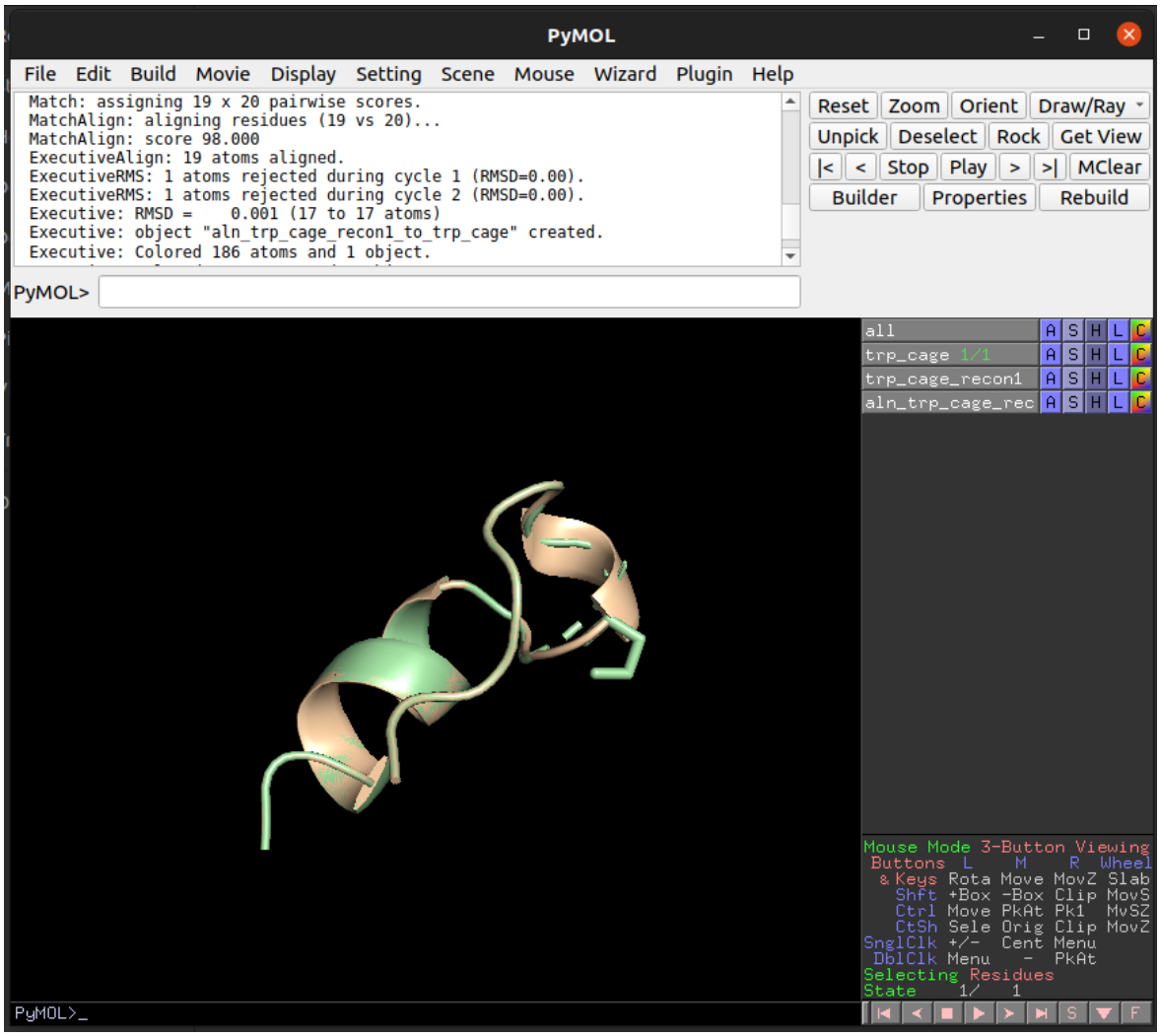
Beta-Sheet： RMSD = 0.000



1L2Y： RMSD = 0.001



TRP Cage : RMSD = 0.001



Efficacy of OpenBabel Tool :

We can observe the RMSD values of the alignment of reconstructed PDB with the original PDB. As we can see the RMSD value is very small, thus signifying that the deviation between the atoms of the two molecules is very small. Thus, we can conclude that the reconstructed molecule is very close to the original one with which we started. Thus overall we can say that efficacy of openBabel is pretty high which means that the tool is good to use.

Excercise 2 :

I used 2 other commands/features present in open babel. They are as follows --

1. *obprop* – Prints the properties of input PDB in the terminal itself.
   Attached screenshots of the output of all the molecules.

1PGB :

```
==============================
*** Open Babel Warning  in PerceiveBondOrders
  Failed to kekulize aromatic bonds in OBMol::PerceiveBondOrders

name             1pgb.pdb 1
formula          C273H471N67O119S
mol_weight       6628.1
exact_mass       6624.26
canonical_SMILES NCCCC[C@@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)NCC(=O)N[C@H](C(=O)N[C@H](C(=O)NCC(=O)N[C@H](C(=O)N[C@H](C(=O
)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)O)CCC(=O)O)[C@H](O)C)C(C)C)[C@H](O)C)Cc1ccccc1
)[C@H](O)C)CCCCN)[C@H](O)C)C)CC(=O)O)CC(=O)O)Cc1ccc(cc1)O)[C@H](O)C)CC1=CN=C2[C@@H]1C=CC=C2)CCC(=O)O)CC(=O)O)C(C)C)CC(=O)N)CC(=O)O)CC(=O)N)C)Cc1ccc(cc1)O)CCC(=O)N)CCCCN)Cc1ccccc1)C(C)C)NC(=O)[C@@H](NC(=O
)[C@@H](NC(=O)[C@H]([C@H](O)C)NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@H](C(C)C)NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@H]([C@H](O)C)NC(=O)[C@H]([C@H](O)C)NC(=O)[C@H]([C@H](O)C)NC(=O)[C@@H](NC(=O)CNC(=
O)[C@@H](NC(=O)[C@@H](NC(=O)[C@H]([C@H](O)C)NC(=O)[C@@H](NC(=O)CNC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@H]([C@H](CC)C)NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@H]([C@H](O)C)NC(=O)[C@H](CCSC)N)Cc1ccc(cc1
)O)CCCCN)CC(C)C)CC(C)C)CC(=O)N)CCCCN)CC(C)C)CCCCN)CCC(=O)O)CCC(=O)O)C)CC(=O)O)C)C)C)CCC(=O)O.O.O.O.O.O.O.O.O.O.O.O.O.O.O.O.O.O.O.O.O.O.O.O.O

==============================
*** Open Babel Warning  in InChI code
  #1 :Ambiguous stereo: center(s)
InChI            InChI=1S/C273H423N67O95S.24H2O/c1-35-129(16)210(329-254(415)173(102-124(6)7)309-235(396)162(65-47-53-96-277)303-249(410)176(106-150-70-76-154(353)77-71-150)320-266(427)213(138(25)343)332
-228(389)157(280)92-99-436-34)261(422)317-172(101-123(4)5)247(408)312-180(109-189(282)356)230(391)287-119-192(359)296-160(63-45-51-94-275)239(400)333-214(139(26)344)267(428)318-171(100-122(2)3)246(407)30
0-159(62-44-50-93-274)229(390)286-118-193(360)298-166(82-88-197(365)366)242(403)335-220(145(32)350)271(432)340-221(146(33)351)272(433)339-217(142(29)347)264(425)306-168(83-89-198(367)368)233(394)291-134(
21)225(386)326-207(126(10)11)258(419)324-185(114-203(377)378)245(406)292-130(17)222(383)290-133(20)226(387)330-211(136(23)341)262(423)295-132(19)223(384)299-169(84-90-199(369)370)237(398)301-163(66-48-54
-97-278)240(401)327-208(127(12)13)259(420)319-175(103-147-56-38-36-39-57-147)248(409)302-161(64-46-52-95-276)234(395)304-167(80-86-188(281)355)238(399)310-174(105-149-68-74-153(352)75-69-149)243(404)293-
131(18)224(385)308-182(111-191(284)358)251(412)316-186(115-204(379)380)252(413)313-181(110-190(283)357)231(392)289-121-195(362)325-206(125(8)9)257(418)323-183(112-201(373)374)232(393)288-120-194(361)297-
165(81-87-196(363)364)236(397)311-179(108-152-117-285-158-61-43-42-60-156(152)158)256(417)336-216(141(28)346)269(430)321-177(107-151-72-78-155(354)79-73-151)250(411)315-187(116-205(381)382)253(414)314-18
4(113-202(375)376)244(405)294-135(22)227(388)331-212(137(24)342)263(424)305-164(67-49-55-98-279)241(402)334-215(140(27)345)268(429)322-178(104-148-58-40-37-41-59-148)255(416)337-219(144(31)349)270(431)32
8-209(128(14)15)260(421)338-218(143(30)348)265(426)307-170(273(434)435)85-91-200(371)372;;;;;;;;;;;;;;;;;;;;;/h36-43,56-61,68-79,117,122-146,156-157,159-187,206-221,341-354H,35,44-55,62-67,80-116,118-
121,274-280H2,1-34H3,(H2,281,355)(H2,282,356)(H2,283,357)(H2,284,358)(H,286,390)(H,287,391)(H,288,393)(H,289,392)(H,290,383)(H,291,394)(H,292,406)(H,293,404)(H,294,405)(H,295,423)(H,296,359)(H,297,361)(H
,298,360)(H,299,384)(H,300,407)(H,301,398)(H,302,409)(H,303,410)(H,304,395)(H,305,424)(H,306,425)(H,307,426)(H,308,385)(H,309,396)(H,310,399)(H,311,397)(H,312,408)(H,313,413)(H,314,414)(H,315,411)(H,316,
412)(H,317,422)(H,318,428)(H,319,420)(H,320,427)(H,321,430)(H,322,429)(H,323,418)(H,324,419)(H,325,362)(H,326,386)(H,327,401)(H,328,431)(H,329,415)(H,330,387)(H,331,388)(H,332,389)(H,333,400)(H,334,402)(
H,335,403)(H,336,417)(H,337,416)(H,338,421)(H,339,433)(H,340,432)(H,363,364)(H,365,366)(H,367,368)(H,369,370)(H,371,372)(H,373,374)(H,375,376)(H,377,378)(H,379,380)(H,381,382)(H,434,435);24*1H2/t129-,130
-,131-,132-,133-,134-,135-,136+,137+,138+,139+,140+,141+,142+,143+,144+,145+,146+,156?,157-,159-,160-,161-,162-,163-,164-,165-,166-,167-,168-,169-,170-,171-,172-,173-,174-,175-,176-,177-,178-,179-,180-,1
81-,182-,183-,184-,185-,186-,187-,206-,207-,208-,209-,210-,211-,212-,213-,214-,215-,216-,217-,218-,219-,220-,221-;;;;;;;;;;;;;;;;;;;;;;;;/m0......................../s1

num_atoms        931
num_bonds        913
num_residues     80
num_rotors       262
sequence         MET-THR-TYR-LYS-LEU-ILE-LEU-ASN-GLY-LYS-THR-LEU-LYS-GLY-GLU-THR-THR-THR-GLU-ALA-VAL-ASP-ALA-ALA-THR-ALA-GLU-LYS-VAL-PHE-LYS-GLN-TYR-ALA-ASN-ASP-ASN-GLY-VAL-ASP-GLY-GLU-TRP-THR-TYR-ASP-AS
P-ALA-THR-LYS-THR-PHE-THR-VAL-THR-GLU
num_rings        7
logP             -2.2829
PSA              2907.7
MR               1608.76
$$$$
==============================
```

Alpha-Helix :

```
name             beta_sheet1.pdb 1
formula          C97H169N24O31S
mol_weight       2199.59
exact_mass       2198.21
canonical_SMILES [NH3]CCCC[C@@H](C(=O)N[C@@H]1[C@@H]2N[C@H](C(=O)N)[C@@H](C)[C@H](C)OC(=O)C[C@H](O2)[C@@H]2N[C@@H](O)CNC(=O)[C@H](CCCC[NH3])NC(=O)[C@H](CC(C)C)NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)CNC(=O)[C@@H
](NC(=O)CC[C@@H](CC[C@H]([C@@H]1O[C@@H](N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C=O)C)CCC(=O)O)[C@H](O)C)[C@H](O)C)[C@@H](NC2=O)[C@H](O)C)C)CC(=O)N)CCCC[NH3])[C@H](O)C)NC(=O)[C@@H](NC(=O)[C@H]([C@H]
(O)C)NC(=O)[C@H](CCSC)N)Cc1ccc(cc1)O

==============================
*** Open Babel Warning  in InChI code
  #1 :Accepted unusual valence(s): N(4); Ambiguous stereo: center(s)
InChI            InChI=1S/C97H169N24O31S/c1-45(2)38-63-89(143)109-59(20-14-17-34-98)84(138)104-43-70(132)114-79-66-41-72(135)150-55(12)49(6)73(82(103)136)120-97(151-66)80(119-88(142)61(22-16-19-36-100)11
0-90(144)64(39-56-26-28-57(128)29-27-56)113-92(146)74(50(7)123)115-83(137)58(101)33-37-153-13)81(152-96(78(54(11)127)118-95(79)149)121-77(53(10)126)94(148)117-76(52(9)125)91(145)111-62(30-32-71(133)134)8
6(140)106-48(5)44-122)47(4)25-23-46(3)24-31-68(130)108-65(40-67(102)129)85(139)105-42-69(131)107-60(21-15-18-35-99)87(141)116-75(51(8)124)93(147)112-63/h26-29,44-55,58-66,70,73-81,96-97,114,120-121,123-1
28,132H,14-25,30-43,101H2,1-13,98-100H3,(H2,102,129)(H2,103,136)(H,104,138)(H,105,139)(H,106,140)(H,107,131)(H,108,130)(H,109,143)(H,110,144)(H,111,145)(H,112,147)(H,113,146)(H,115,137)(H,116,141)(H,117,
148)(H,118,149)(H,119,142)(H,133,134)/t46-,47-,48+,49+,50-,51-,52-,53-,54-,55+,58+,59+,60+,61+,62+,63+,64+,65+,66+,70?,73+,74+,75+,76+,77+,78+,79+,80+,81+,96?,97?/m1/s1

num_atoms        322
num_bonds        325
num_residues     20
num_rotors       54
sequence         MET-THR-TYR-LYS-LEU-ILE-LEU-ASN-GLY-LYS-THR-LEU-LYS-GLY-GLU-THR-THR-THR-GLU-ALA
num_rings        4
logP             1.0378
PSA              860.55
MR               591.821
$$$$
==============================
```

Beta-Sheet-1 :

```
name            beta_sheet1.pdb 1
formula         C97H169N24O31S
mol_weight      2199.59
exact_mass      2198.21
canonical_SMILES [NH3]CCCC[C@@H](C(=O)N[C@@H]1[C@@H]2N[C@H](C(=O)N)[C@@H](C)[C@H](C)OC(=O)C[C@H](O2)[C@@H]2N[C@@H](O)CNC(=O)[C@H](CCCC[NH3])NC(=O)[C@H](CC(C)C)NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)CNC(=O)[C@@H](NC(=O)CC[C@@H](CC[C@H]([C@@H]1O[C@@H](N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C=O)C)CCC(=O)O)[C@H](O)C)[C@H](O)C)[C@@H](NC2=O)[C@H](O)C)C)C)CC(=O)N)CCCC[NH3])[C@H](O)C)NC(=O)[C@@H](NC(=O)[C@H]([C@H](O)C)NC(=O)[C@H](CCSC)N)Cc1ccc(cc1)O

==============================
*** Open Babel Warning  in InChI code
  #1 :Accepted unusual valence(s): N(4); Ambiguous stereo: center(s)
InChI           InChI=1S/C97H169N24O31S/c1-45(2)38-63-89(143)109-59(20-14-17-34-98)84(138)104-43-70(132)114-79-66-41-72(135)150-55(12)49(6)73(82(103)136)120-97(151-66)80(119-88(142)61(22-16-19-36-100)110-90(144)64(39-56-26-28-57(128)29-27-56)113-92(146)74(50(7)123)115-83(137)58(101)33-37-153-13)81(152-96(78(54(11)127)118-95(79)149)121-77(53(10)126)94(148)117-76(52(9)125)91(145)111-62(30-32-71(133)134)86(140)106-48(5)44-122)47(4)25-23-46(3)24-31-68(130)108-65(40-67(102)129)85(139)105-42-69(131)107-60(21-15-18-35-99)87(141)116-75(51(8)124)93(147)112-63/h26-29,44-55,58-66,70,73-81,96-97,114,120-121,123-128,132H,14-25,30-43,101H2,1-13,98-100H3,(H2,102,129)(H2,103,136)(H,104,138)(H,105,139)(H,106,140)(H,107,131)(H,108,130)(H,109,143)(H,110,144)(H,111,145)(H,112,147)(H,113,146)(H,115,137)(H,116,141)(H,117,148)(H,118,149)(H,119,142)(H,133,134)/t46-,47-,48+,49+,50-,51-,52-,53-,54-,55+,58+,59+,60+,61+,62+,63+,64+,65+,66+,70?,73+,74+,75+,76+,77+,78+,79+,80+,81+,96?,97?/m1/s1

num_atoms       322
num_bonds       325
num_residues    20
num_rotors      54
sequence        MET-THR-TYR-LYS-LEU-ILE-LEU-ASN-GLY-LYS-THR-LEU-LYS-GLY-GLU-THR-THR-THR-GLU-ALA
num_rings       4
logP            1.0378
PSA             860.55
MR              591.821
$$$$
==============================
```

Beta-Sheet-2 :

```
name            beta_sheet2.pdb 1
formula         C81H127N17O29
mol_weight      1802.97
exact_mass      1801.9
canonical_SMILES [NH3]CCCC[C@@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)NCC(=O)NC[C@]([NH]1C[C@@]([C@@H]1CCC(=O)O)(O)C(=O)N[C@@H](C[C@@H]1CN[C@@H]([C@@]2([C@@H]1C2(C)C)C)CC)C=O)(N[C@@H](CCC(=O)O)C=O)O)[C@H](O)C)Cc1ccccc1)[C@H](O)C)NC(=O)[C@H]([C@H](O)C)NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@H](Cc1ccc(cc1)O)NC(=O)C[C@H](O)C)CC(=O)O)CC(=O)O)C.N

==============================
*** Open Babel Warning  in InChI code
  #1 :Accepted unusual valence(s): N(4); Ambiguous stereo: center(s)
InChI           InChI=1S/C81H124N16O29.H3N/c1-10-56-79(9)67(78(79,7)8)47(34-83-56)31-49(37-99)87-77(124)80(125)39-97(57(80)24-26-61(109)110)81(126,96-48(36-98)21-25-60(107)108)38-85-59(106)35-84-74(121)64(42(4)101)94-73(120)53(29-45-16-12-11-13-17-45)92-76(123)66(44(6)103)95-69(116)51(18-14-15-27-82)89-75(122)65(43(5)102)93-68(115)41(3)86-70(117)54(32-62(111)112)90-72(119)55(33-63(113)114)91-71(118)52(88-58(105)28-40(2)100)30-46-19-22-50(104)23-20-46;/h11-13,16-17,19-20,22-23,36-37,40-44,47-49,51-57,64-67,83,96-97,100-104,125-126H,10,14-15,18,21,24-35,38-39H2,1-9,82H3,(H,84,121)(H,85,106)(H,86,117)(H,87,124)(H,88,105)(H,89,122)(H,90,119)(H,91,118)(H,92,123)(H,93,115)(H,94,120)(H,95,116)(H,107,108)(H,109,110)(H,111,112)(H,113,114);1H3/t40-,41+,42-,43-,44-,47?,48+,49+,51+,52+,53+,54+,55+,56-,57+,64+,65+,66+,67+,79-,80+,81-;/m1./s1

num_atoms       254
num_bonds       257
num_residues    15
num_rotors      67
sequence        GLU-TRP-THR-TYR-ASP-ASP-ALA-THR-LYS-THR-PHE-THR-VAL-THR-GLU
num_rings       5
logP            -0.7322
PSA             716.72
MR              454.176
$$$$
==============================
```

1L2Y :

```
==============================
*** Open Babel Warning  in PerceiveBondOrders
  Failed to kekulize aromatic bonds in OBMol::PerceiveBondOrders

name            1pgb.pdb 1
formula         C273H471N67O119S
mol_weight      6628.1
exact_mass      6624.26
canonical_SMILES NCCCC[C@@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)NCC(=O)N[C@H](C(=O)N[C@H](C(=O)NCC(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)O)CCC(=O)O)[C@H](O)C)C(C)C)[C@H](O)C)Cc1ccccc1)[C@H](O)C)CCCCN)[C@H](O)C)C)CC(=O)O)CC(=O)O)Cc1ccc(cc1)O)[C@H](O)C)CC1=CN=C2[C@@H]1C=CC=C2)CCC(=O)O)CC(=O)O)C(C)C)CC(=O)N)CC(=O)O)CC(=O)N)C)Cc1ccc(cc1)O)CCC(=O)N)CCCCN)Cc1ccccc1)C(C)C)NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@H]([C@H](O)C)NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@H](C(C)C)NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@H]([C@H](O)C)NC(=O)[C@H]([C@H](O)C)NC(=O)[C@H]([C@H](O)C)NC(=O)[C@@H](NC(=O)CNC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@H]([C@H](O)C)NC(=O)[C@@H](NC(=O)CNC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@H]([C@H](CC)C)NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@H]([C@H](O)C)NC(=O)[C@H](CCSC)N)Cc1ccc(cc1)O)CCCCN)CC(C)C)CC(C)C)CC(=O)N)CCCCN)CC(C)C)CCCCN)CCC(=O)O)CCC(=O)O)C)CC(=O)O)C)C)CCC(=O)O.O.O.O.O.O.O.O.O.O.O.O.O.O.O.O.O.O.O.O.O.O.O.O.O

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*** Open Babel Warning  in InChI code
  #1 :Ambiguous stereo: center(s)
InChI           InChI=1S/C273H423N67O95S.24H2O/c1-35-129(16)210(329-254(415)173(102-124(6)7)309-235(396)162(65-47-53-96-277)303-249(410)176(106-150-70-76-154(353)77-71-150)320-266(427)213(138(25)343)332-228(389)157(280)92-99-436-34)261(422)317-172(101-123(4)5)247(408)312-180(109-189(282)356)230(391)287-119-192(359)296-160(63-45-51-94-275)239(400)333-214(139(26)344)267(428)318-171(100-122(2)3)246(407)300-159(62-44-50-93-274)229(390)286-118-193(360)298-166(82-88-197(365)366)242(403)335-220(145(32)350)271(432)340-221(146(33)351)272(433)339-217(142(29)347)264(425)306-168(83-89-198(367)368)233(394)291-134(21)225(386)326-207(126(10)11)258(419)324-185(114-203(377)378)245(406)292-130(17)222(383)290-133(20)226(387)330-211(136(23)341)262(423)295-132(19)223(384)299-169(84-90-199(369)370)237(398)301-163(66-48-54-97-278)240(401)327-208(127(12)13)259(420)319-175(103-147-56-38-36-39-57-147)248(409)302-161(64-46-52-95-276)234(395)304-167(80-86-188(281)355)238(399)310-174(105-149-68-74-153(352)75-69-149)243(404)293-131(18)224(385)308-182(111-191(284)358)251(412)316-186(115-204(379)380)252(413)313-181(110-190(283)357)231(392)289-121-195(362)325-206(125(8)9)257(418)323-183(112-201(373)374)232(393)288-120-194(361)297-165(81-87-196(363)364)236(397)311-179(108-152-117-285-158-61-43-42-60-156(152)158)256(417)336-216(141(28)346)269(430)321-177(107-151-72-78-155(354)79-73-151)250(411)315-187(116-205(381)382)253(414)314-184(113-202(375)376)244(405)294-135(22)227(388)331-212(137(24)342)263(424)305-164(67-49-55-98-279)241(402)334-215(140(27)345)268(429)322-178(104-148-58-40-37-41-59-148)255(416)337-219(144(31)349)270(431)328-209(128(14)15)260(421)338-218(143(30)348)265(426)307-170(273(434)435)85-91-200(371)372;;;;;;;;;;;;;;;;;;;;;;;;/h36-43,56-61,68-79,117,122-146,156-157,159-187,206-221,341-354H,35,44-55,62-67,80-116,118-121,274-280H2,1-34H3,(H2,281,355)(H2,282,356)(H2,283,357)(H2,284,358)(H,286,390)(H,287,391)(H,288,393)(H,289,392)(H,290,383)(H,291,394)(H,292,406)(H,293,404)(H,294,405)(H,295,423)(H,296,359)(H,297,361)(H,298,360)(H,299,384)(H,300,407)(H,301,398)(H,302,409)(H,303,410)(H,304,395)(H,305,424)(H,306,425)(H,307,426)(H,308,385)(H,309,396)(H,310,399)(H,311,397)(H,312,408)(H,313,413)(H,314,414)(H,315,411)(H,316,412)(H,317,422)(H,318,428)(H,319,420)(H,320,427)(H,321,430)(H,322,429)(H,323,418)(H,324,419)(H,325,362)(H,326,386)(H,327,401)(H,328,431)(H,329,415)(H,330,387)(H,331,388)(H,332,389)(H,333,400)(H,334,402)(H,335,403)(H,336,417)(H,337,416)(H,338,421)(H,339,433)(H,340,432)(H,363,364)(H,365,366)(H,367,368)(H,369,370)(H,371,372)(H,373,374)(H,375,376)(H,377,378)(H,379,380)(H,381,382)(H,434,435);24*1H2/t129-,130-,131-,132-,133-,134-,135-,136+,137+,138+,139+,140+,141+,142+,143+,144+,145+,146+,156?,157-,159-,160-,161-,162-,163-,164-,165-,166-,167-,168-,169-,170-,171-,172-,173-,174-,175-,176-,177-,178-,179-,180-,181-,182-,183-,184-,185-,186-,187-,206-,207-,208-,209-,210-,211-,212-,213-,214-,215-,216-,217-,218-,219-,220-,221-;;;;;;;;;;;;;;;;;;;;;;;;/m0......................../s1

num_atoms       931
num_bonds       913
num_residues    80
num_rotors      262
sequence        MET-THR-TYR-LYS-LEU-ILE-LEU-ASN-GLY-LYS-THR-LEU-LYS-GLY-GLU-THR-THR-THR-GLU-ALA-VAL-ASP-ALA-ALA-THR-ALA-GLU-LYS-VAL-PHE-LYS-GLN-TYR-ALA-ASN-ASP-ASN-GLY-VAL-ASP-GLY-GLU-TRP-THR-TYR-ASP-ASP-ALA-THR-LYS-THR-PHE-THR-VAL-THR-GLU
num_rings       7
logP            -2.2829
PSA             2907.7
MR              1608.76
$$$$
==============================
```

TRP-Cage :

```
name            trp_cage.pdb 1
formula         C98H153N27O28
mol_weight      2157.43
exact_mass      2156.14
canonical_SMILES [NH3]CCCC[C@@H](C(=O)N[C@H](C(=O)NCC(=O)NCC(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)NCC(=O)N[C@H](C(=O)N1CCC[C@H]1C(=O)N1CCC[C@H]1C(=O)N1CCC[C@H]1C(=O)N[C@H](C=O)CO)CCCNC(=[NH2])N)CO)CO)CC)CC(=O)O)NC(=O)[C@@H](NC(=O)[C@H](Cc1c[nH]c2c1cccc2)NC(=O)[C@@H](NC(=O)[C@H]([C@H](CC)C)NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@H](CC(=O)N)N)CC(C)C)Cc1ccc(cc1)O)CCC(=O)N)CC(C)C

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*** Open Babel Warning  in InChI code
  #1 :Accepted unusual valence(s): N(4)
InChI           InChI=1S/C98H153N27O28/c1-8-18-61(85(141)121-71(50-129)92(148)120-70(49-128)84(140)109-46-79(135)112-64(22-14-33-105-98(103)104)95(151)124-35-16-24-73(124)97(153)125-36-17-25-74(125)96(152)123-34-15-23-72(123)93(149)110-56(47-126)48-127)111-78(134)45-107-77(133)44-108-83(139)69(42-80(136)137)119-86(142)62(21-12-13-32-99)113-88(144)66(38-52(5)6)116-90(146)68(40-55-43-106-60-20-11-10-19-58(55)60)118-87(143)63(30-31-75(101)131)114-94(150)81(53(7)9-2)122-91(147)67(39-54-26-28-57(130)29-27-54)117-89(145)65(37-51(3)4)115-82(138)59(100)41-76(102)132/h10-11,19-20,26-29,43,47,51-53,56,59,61-74,81,105-106,127-130H,8-9,12-18,21-25,30-42,44-46,48-50,100,103-104H2,1-7,99H3,(H2,101,131)(H2,102,132)(H,107,133)(H,108,139)(H,109,140)(H,110,149)(H,111,134)(H,112,135)(H,113,144)(H,114,150)(H,115,138)(H,116,146)(H,117,145)(H,118,143)(H,119,142)(H,120,148)(H,121,141)(H,122,147)(H,136,137)/t53-,56+,59-,61-,62-,63-,64-,65-,66-,67-,68-,69-,70-,71-,72-,73-,74-,81-/m0/s1

num_atoms       306
num_bonds       311
num_residues    20
num_rotors      86
sequence        ASN-LEU-TYR-ILE-GLN-TRP-LEU-LYS-ASP-GLY-GLY-PRO-SER-SER-GLY-ARG-PRO-PRO-PRO-SER
num_rings       6
logP            1.2207
PSA             857.12
MR              559.186
```

2. *obabel -ofpt* – Gives the Tanimoto coefficient between a SMILES string and all the molecules SDF Format :

Attached screenshots of the output of all the molecules.

1PDB :

```
1 molecule converted
>1pgb.pdb
>1pgb.pdb   Tanimoto from 1pgb.pdb = 1
Possible superstructure of 1pgb.pdb
2 molecules converted
```

Alpha-Helix :

```
1 molecule converted
>alpha_helix.pdb
>alpha_helix.pdb   Tanimoto from alpha_helix.pdb = 1
Possible superstructure of alpha_helix.pdb
2 molecules converted
```

Beta-Sheet-1 :

```
1 molecule converted
>beta_sheet1.pdb
>beta_sheet1.pdb   Tanimoto from beta_sheet1.pdb = 1
Possible superstructure of beta_sheet1.pdb
2 molecules converted
```

Beta-Sheet-2 :

```
1 molecule converted
>beta_sheet2.pdb
>beta_sheet2.pdb   Tanimoto from beta_sheet2.pdb = 1
Possible superstructure of beta_sheet2.pdb
2 molecules converted
```

1L2Y :

```
1 molecule converted
1 molecule converted
>1l2y.pdb
>1l2y.pdb   Tanimoto from 1l2y.pdb = 1
Possible superstructure of 1l2y.pdb
2 molecules converted
```

TRP-Cage :

```
1 molecule converted
>trp_cage.pdb
>trp_cage.pdb   Tanimoto from trp_cage.pdb = 1
Possible superstructure of trp_cage.pdb
```

We can observe from the above results that the Tanimoto Coefficient between the Original Structure and Reconstructed Structure is 1 for all the above molecules.
Thus, we can confirm that the iner-conversion efficacy of the Open Babel software is very high and it is a very powerful tool which can be used for inter-conversion of molecules.