

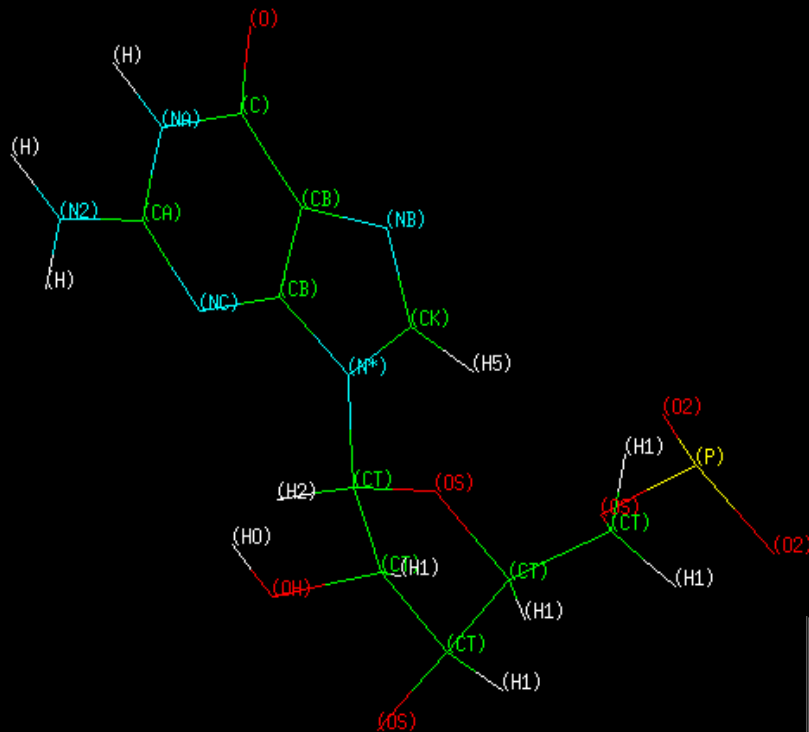
Fáze počítačových simulací

- ⇒ příprava počáteční struktury
- ⇒ ekvilibrace
- ⇒ produkční fáze
- ⇒ analýza výsledků

Program XLEaP

- ⇒ slouží k vytvoření souborů s topologií a souřadnicemi ze vstupního PDB souboru
- ⇒ umožňuje přidat ionty a box solventu
- ⇒ pracuje s knihovnou předem definovaných reziduí, kterou lze doplňovat o vlastní rezidua (např. modifikované nukleotidy)

Atomový typ

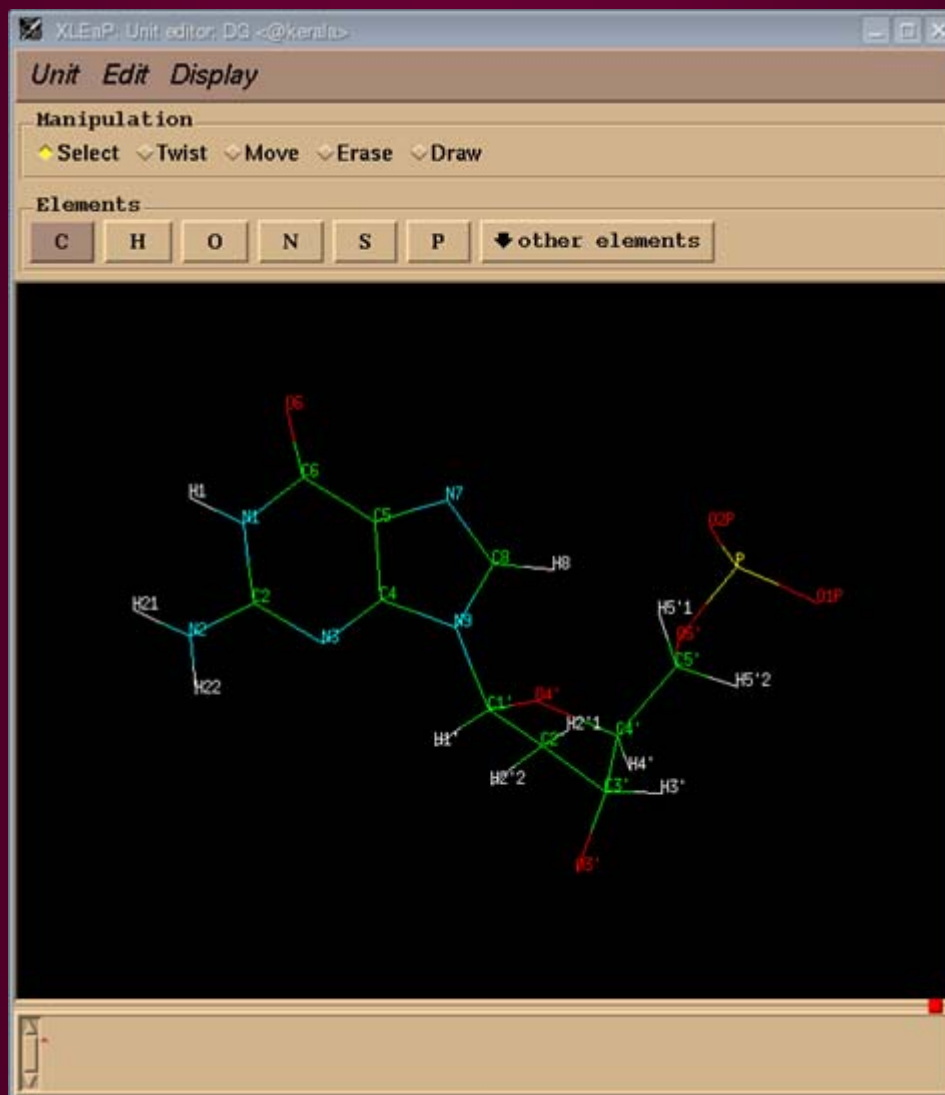


MOD4	RE	
H	0.6000 0.0157	!Ferguson base pair geom.
HO	0.0000 0.0000	OPLS Jorgensen, JACS,110,(1988),1657
HS	0.6000 0.0157	W. Cornell CH3SH --> CH3OH FEP
HC	1.4870 0.0157	OPLS
H1	1.3870 0.0157	Veenstra et al JCC,8,(1992),963
H2	1.2870 0.0157	Veenstra et al JCC,8,(1992),963
H3	1.1870 0.0157	Veenstra et al JCC,8,(1992),963
HP	1.1000 0.0157	Veenstra et al JCC,8,(1992),963
HA	1.4590 0.0150	Spellmeyer
H4	1.4090 0.0150	Spellmeyer, one electrowithdr. neighbor
H5	1.3590 0.0150	Spellmeyer, two electrowithdr. neighbor
HW	0.0000 0.0000	TIP3P water model
HZ	1.4590 0.0150	H bonded to sp C (Howard et al JCC 16)
O	1.6612 0.2100	OPLS
O2	1.6612 0.2100	OPLS
OW	1.7683 0.1520	TIP3P water model
OH	1.7210 0.2104	OPLS
OS	1.6837 0.1700	OPLS ether
C*	1.9080 0.0860	Spellmeyer
CT	1.9080 0.1094	Spellmeyer
C	1.9080 0.0860	OPLS
N	1.8240 0.1700	OPLS
N3	1.8240 0.1700	OPLS
NY	1.8240 0.1700	N in nitrile
S	2.0000 0.2500	W. Cornell CH3SH and CH3SCH3 FEP's
SH	2.0000 0.2500	W. Cornell CH3SH and CH3SCH3 FEP's
P	2.1000 0.2000	JCC,7,(1986),230;
IM	2.47 0.1	Cl- Smith & Dang, JCP 1994,100:5,3757
Li	1.1370 0.0183	Li+ Aquist JPC 1990,94,8021. (adapted)
IP	1.8680 0.00277	Na+ Aquist JPC 1990,94,8021. (adapted)

XLEaP: seznam reziduí

```
XLEaP: Universe Editor <@kerala>
File Edit Verbosity
Loading library: /opt/amber9/dat/leap/lib/all_amino94.lib
Loading library: /opt/amber9/dat/leap/lib/all_aminoc94.lib
Loading library: /opt/amber9/dat/leap/lib/all_aminont94.lib
Loading library: /opt/amber9/dat/leap/lib/ions94.lib
Loading library: /opt/amber9/dat/leap/lib/solvents.lib
> list
ACE      ALA      ARG      ASH      ASN      ASP      CALA     CARG
CASN     CASP     CCYS     CCYX     CGLN     CGLU     CGLY     CHCL3BOX
CHID     CHIE     CHIP     CHIS     CILE     CIO      CLEU     CLYS
CMET     CPHE     CPRO     CSER     CTHR     CTRP     CTYR     CVAL
CYM      CYS      CYX      C1-      Cs+      DA       DA3      DA5
DAN      DC       DC3      DC4      DC5      DCN      DG       DG3
DG5      DGN      DT       DT3      DT5      DTN      GLH      GLN
GLU      GLY      HID      HIE      HIP      HIS      HOH      IB
ILE      K+       LEU      LYN      LYS      Li+     MEOHBOX  MET
MG2      NALA     NARG     NASN     NASP     NCYS     NCYX     NGLN
NGLU     NGLY     NHE      NHID     NHIE     NHIP     NHIS     NILE
NLEU     NLYS     NMABOX   NME      NMET     NPHE     NPRO     NSER
NTHR     NTRP     NTYR     NVAL     Na+      PHE      PL3      POL3BOX
PRO      RA       RA3      RA5      RAN      RC       RC3      RC5
RCN      RG       RG3      RG5      RGN      RU       RU3      RU5
RUN      Rb+     SER      SPC      SPCBOX   SPCFWBOX  SPF      T4E
THR      TIP3PBOX TIP4PBOX TIP4PEWBOXTP3 TP4      TP5      TRP
TYR      VAL     WAT      frcmod998Bparm99
> ^
```

XLEaP: příklad stavební jednotky



Vstupní struktura

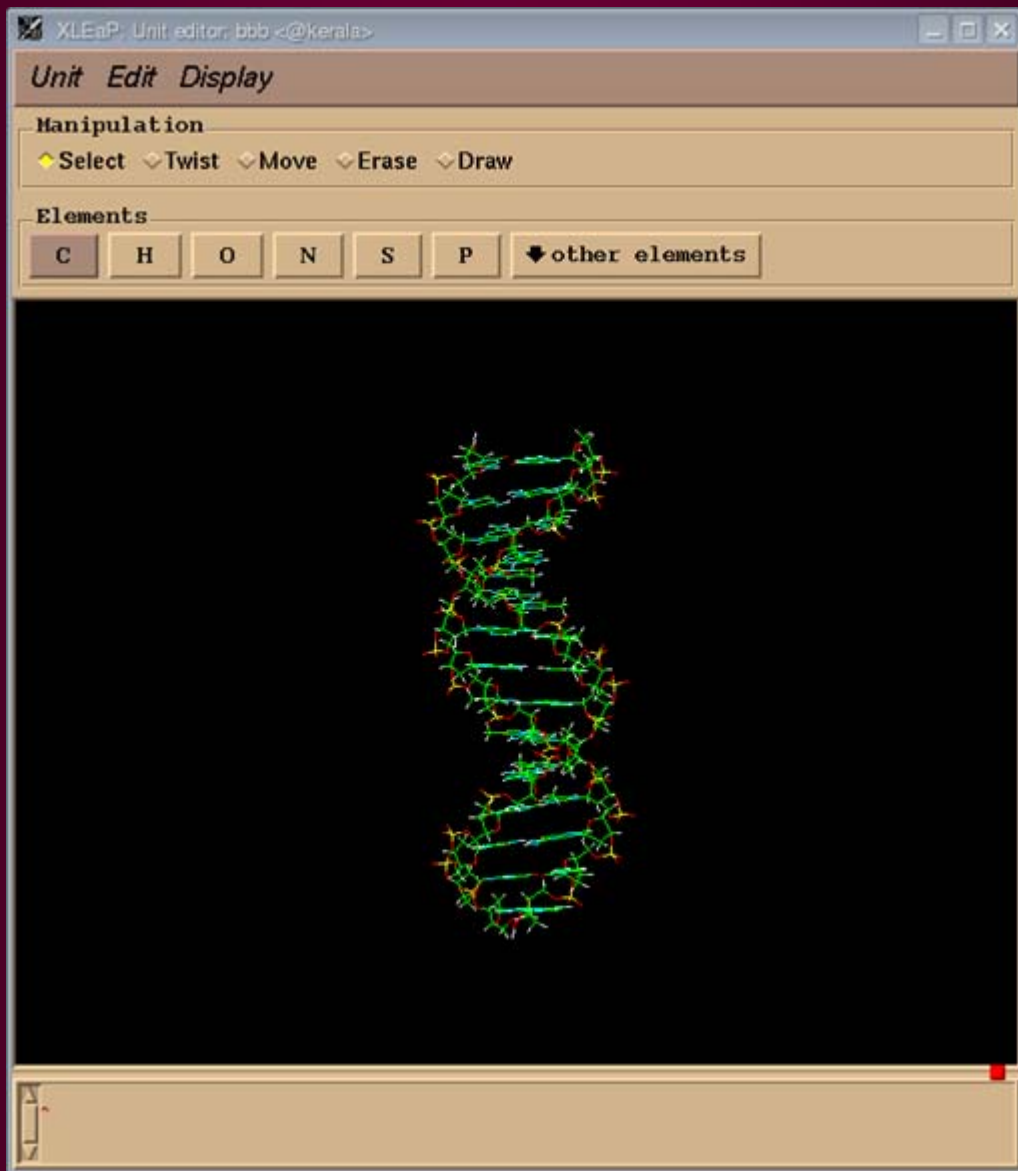
- ⇒ kanonické dvoušroubovice DNA, RNA
– pomocí programu Nucgen
- ⇒ ostatní molekuly – využití struktur z
databází NDB, PDB (struktury z RTG,
NMR)

Formát souboru PDB

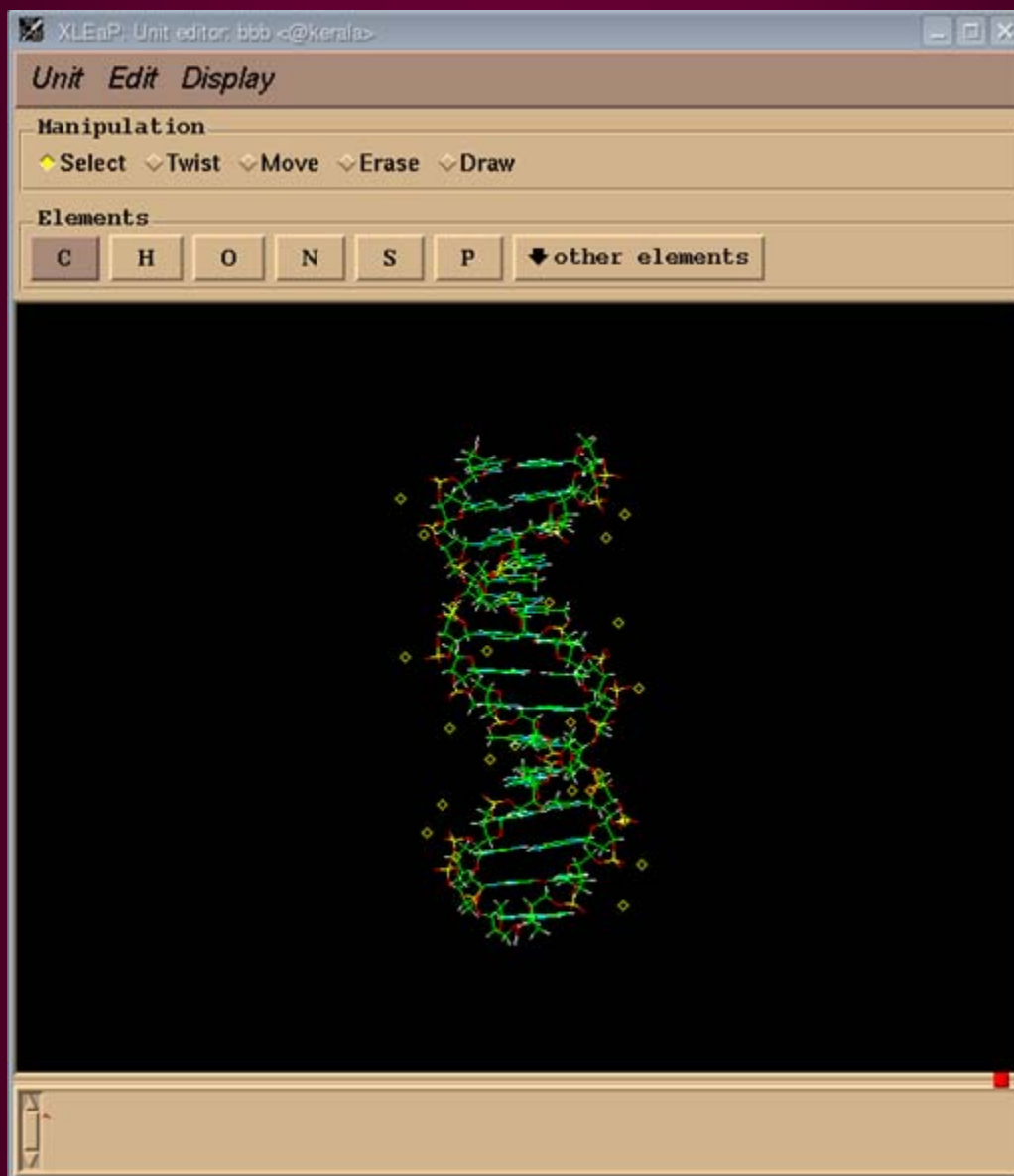
```
spackova@kerala:~/TetraLoop - ssh - Konsole
Session Edit View Bookmarks Settings Help
REMARK
ATOM      1  H5T  RCS      1      7.134  -4.763   6.451
ATOM      2  O5*  RCS      1      7.538  -3.907   6.290
ATOM      3  C5*  RCS      1      8.968  -3.825   6.160
ATOM      4  1H5* RCS      1      9.304  -4.443   5.327
ATOM      5  2H5* RCS      1      9.430  -4.176   7.083
ATOM      6  C4*  RCS      1      9.384  -2.375   5.910
ATOM      7  H4*  RCS      1     10.470  -2.299   5.860
ATOM      8  O4*  RCS      1      8.930  -1.996   4.580
ATOM      9  C1*  RCS      1      8.527  -0.626   4.580
ATOM     10  H1*  RCS      1      9.033  -0.099   3.772
ATOM     11  N1  RCS      1      7.098  -0.559   4.200
ATOM     12  C6  RCS      1      6.310  -1.679   4.190
ATOM     13  H6  RCS      1      6.733  -2.633   4.466
ATOM     14  C5  RCS      1      5.005  -1.617   3.840
ATOM     15  H5  RCS      1      4.399  -2.523   3.832
ATOM     16  C4  RCS      1      4.488  -0.322   3.480
ATOM     17  H4  RCS      1      3.224  -0.192   3.120
ATOM     18  1H4 RCS      1      2.862   0.717   2.868
ATOM     19  2H4 RCS      1      2.616  -0.999   3.100
ATOM     20  N3  RCS      1      5.264   0.768   3.490
ATOM     21  C2  RCS      1      6.575   0.679   3.850
ATOM     22  O2  RCS      1      7.323   1.664   3.870
ATOM     23  C3* RCS      1      8.758  -1.340   6.830
ATOM     24  H3* RCS      1      7.870  -1.310   7.461
ATOM     25  C2* RCS      1      8.820  -0.077   5.980
ATOM     26  1H2* RCS      1      8.183   0.585   6.566
ATOM     27  O2*  RCS      1     10.140   0.443   5.950
ATOM     28  2H0* RCS      1     10.090   1.313   5.546
ATOM     29  O3*  RCS      1      9.461  -1.229   8.060
ATOM     30  P  RG      2      8.676  -0.774   9.370
ATOM     31  O1P  RG      2      9.541  -0.969  10.560
ATOM     32  O2P  RG      2      7.357  -1.457   9.420
ATOM     33  O5*  RG      2      8.454   0.784   9.100
ATOM     34  C5*  RG      2      9.613   1.626   8.970
ATOM     35  1H5* RG      2     10.231   1.288   8.138
ATOM     36  2H5* RG      2     10.201   1.580   9.887
--More-- (11/2)
```

```
spackova@kerala:~/4Wjunctions - ssh - Konsole
Session Edit View Bookmarks Settings Help
HEADER  UD0008
ATOM      1  O5*  C A  1     -17.669   1.831  15.562   1.00  45.33   O
ATOM      2  C5*  C A  1     -19.067   1.476  15.483   1.00  47.44   C
ATOM      3  C4*  C A  1     -19.655   1.941  14.172   1.00  42.78   C
ATOM      4  O4*  C A  1     -19.421   3.354  13.956   1.00  37.44   O
ATOM      5  C3*  C A  1     -18.991   1.221  13.002   1.00  40.39   C
ATOM      6  O3*  C A  1     -20.019   0.634  12.215   1.00  45.26   O
ATOM      7  C2*  C A  1     -18.288   2.318  12.227   1.00  34.43   C
ATOM      8  C1*  C A  1     -19.092   3.530  12.605   1.00  27.74   C
ATOM      9  N1  C A  1     -18.374   4.788  12.482   1.00  21.56   N
ATOM     10  C2  C A  1     -18.185   5.256  11.238   1.00  19.05   C
ATOM     11  O2  C A  1     -18.493   4.573  10.317   1.00  27.89   O
ATOM     12  N3  C A  1     -17.632   6.427  11.031   1.00  24.18   N
ATOM     13  C4  C A  1     -17.180   7.115  12.043   1.00  23.92   C
ATOM     14  H4  C A  1     -16.570   8.258  11.726   1.00  33.27   H
ATOM     15  C5  C A  1     -17.388   6.650  13.304   1.00  20.64   C
ATOM     16  C6  C A  1     -17.919   5.481  13.559   1.00  17.41   C
ATOM     17  P  C A  2     -20.282  -0.940  12.287   1.00  52.27   P
ATOM     18  O1P  C A  2     -21.478  -1.301  11.604   1.00  52.18   O
ATOM     19  O2P  C A  2     -20.022  -1.223  13.762   1.00  56.93   O
ATOM     20  O5*  C A  2     -18.930  -1.549  11.513   1.00  50.12   O
ATOM     21  C5*  C A  2     -18.890  -1.641  10.044   1.00  42.44   C
ATOM     22  C4*  C A  2     -17.470  -1.617   9.518   1.00  32.05   C
ATOM     23  O4*  C A  2     -16.892  -0.313   9.738   1.00  32.09   O
ATOM     24  C3*  C A  2     -16.502  -2.628  10.144   1.00  30.80   C
ATOM     25  O3*  C A  2     -15.696  -3.247   9.121   1.00  42.73   O
ATOM     26  C2*  C A  2     -15.600  -1.772  11.016   1.00  28.15   C
ATOM     27  C1*  C A  2     -15.588  -0.463  10.267   1.00  23.96   C
ATOM     28  N1  C A  2     -15.272   0.727  11.050   1.00  17.87   N
ATOM     29  C2  C A  2     -15.040   1.900  10.384   1.00  21.95   C
ATOM     30  O2  C A  2     -15.056   1.906   9.136   1.00  24.64   O
ATOM     31  N3  C A  2     -14.794   3.013  11.074   1.00  18.20   N
ATOM     32  C4  C A  2     -14.758   2.987  12.401   1.00  21.02   C
ATOM     33  H4  C A  2     -14.548   4.134  13.042   1.00  16.58   H
ATOM     34  C5  C A  2     -14.949   1.789  13.127   1.00  21.79   C
ATOM     35  C6  C A  2     -15.210   0.681  12.410   1.00  23.54   C
ATOM     36  P  G A  3     -16.272  -4.511   8.261   1.00  45.64   P
--More-- (4/2)
```

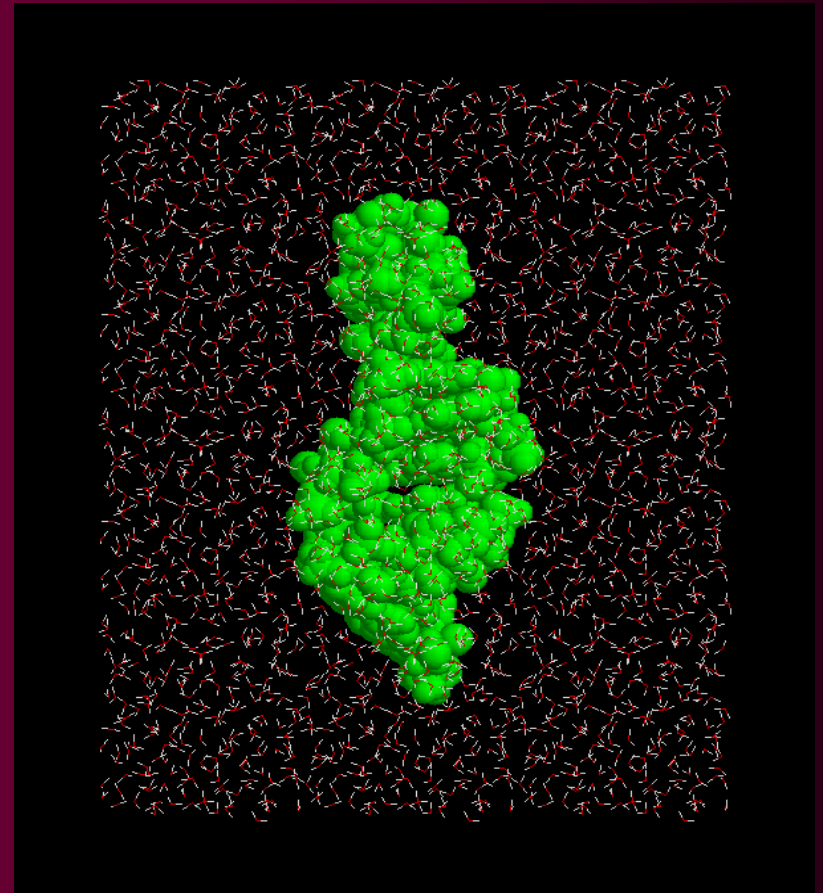
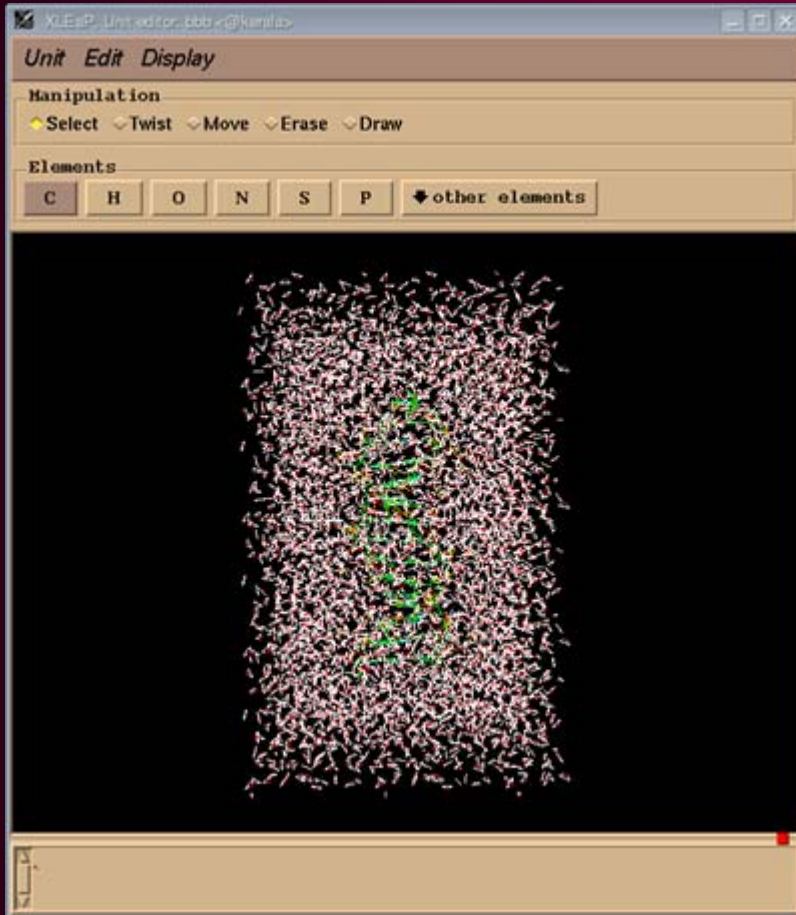
XLEaP: zobrazení načtené molekuly



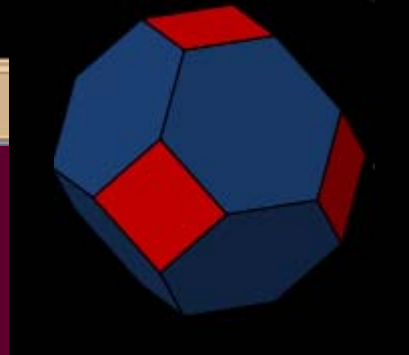
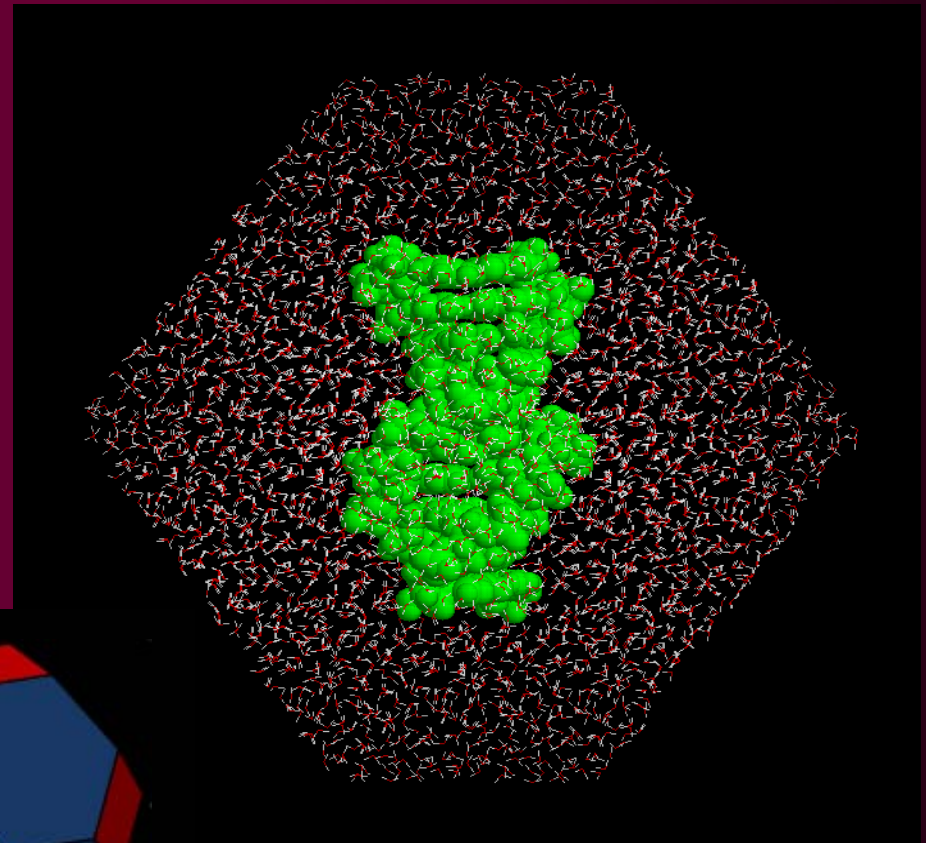
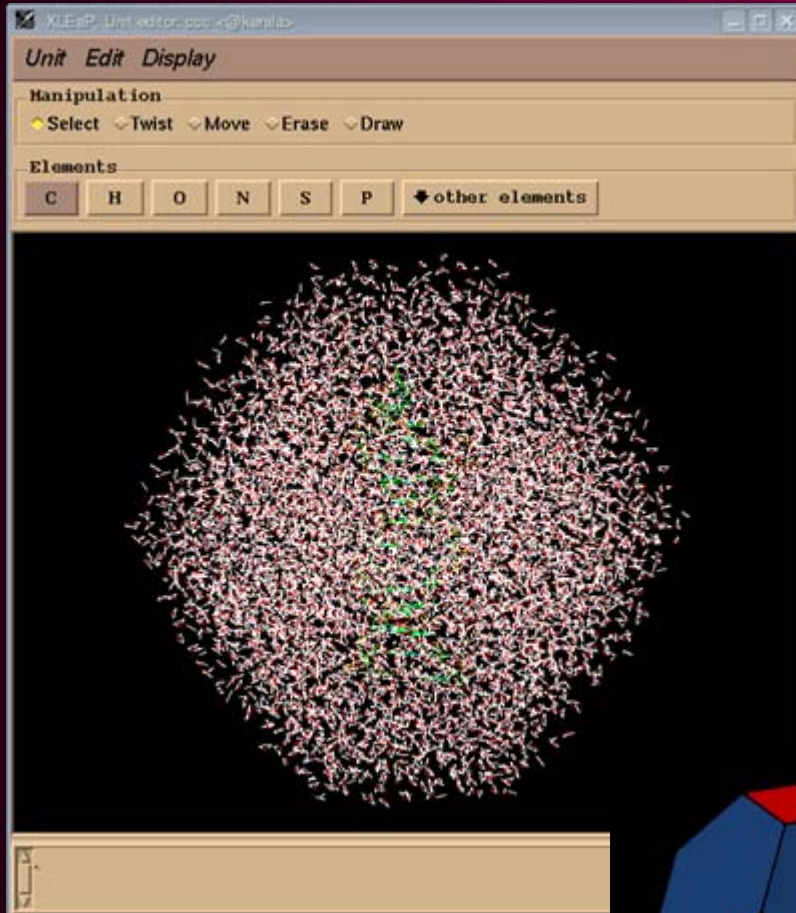
XLEaP: přidání iontů



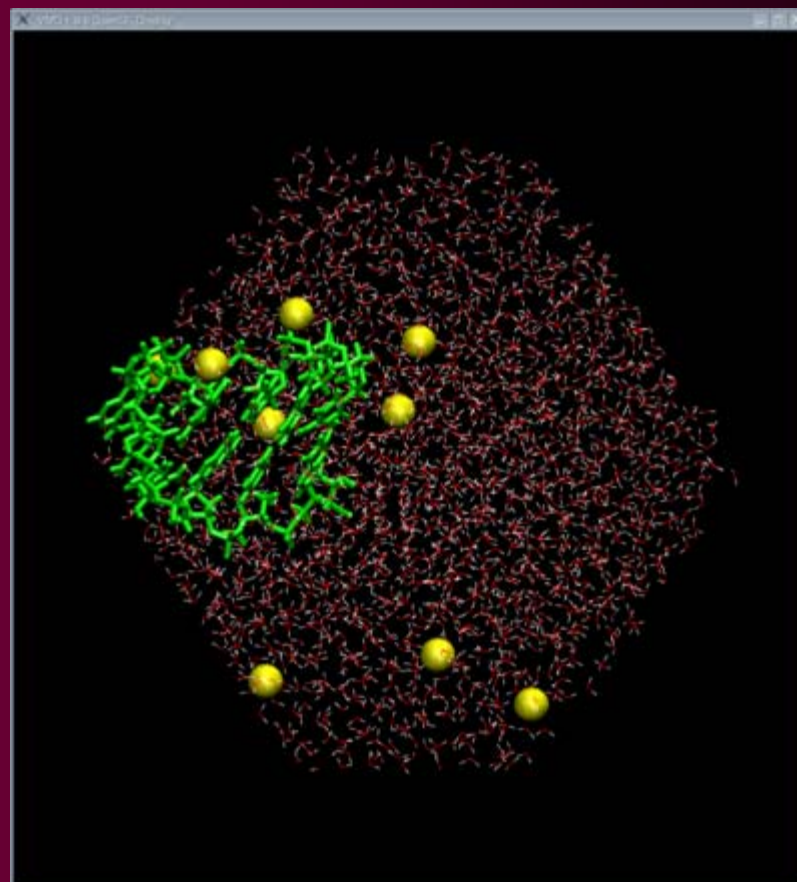
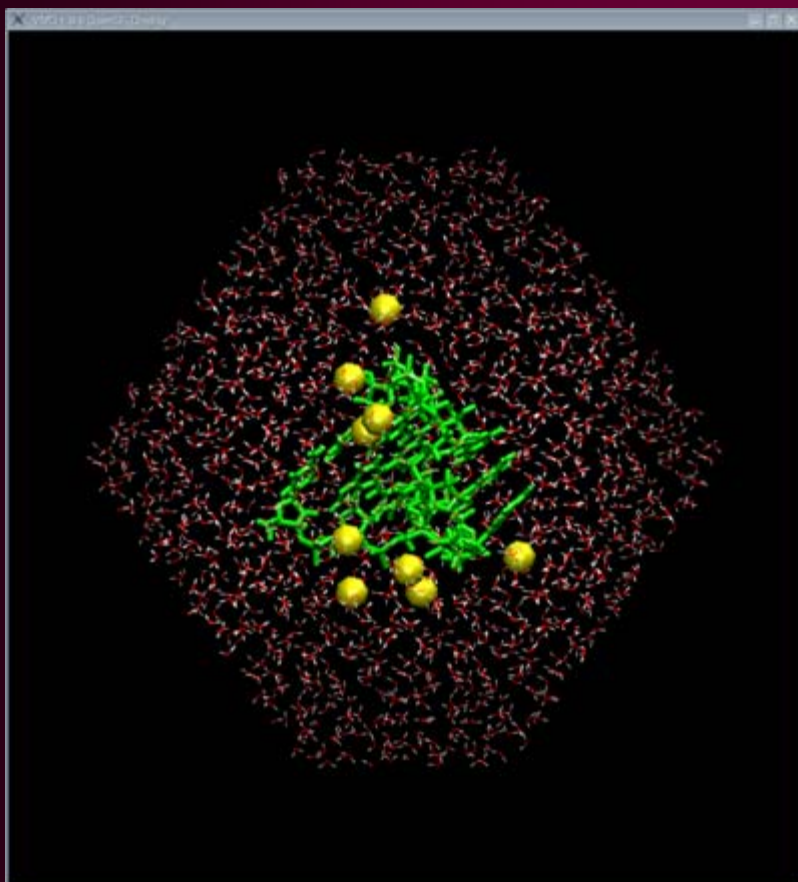
XLEaP: přidání boxu vody



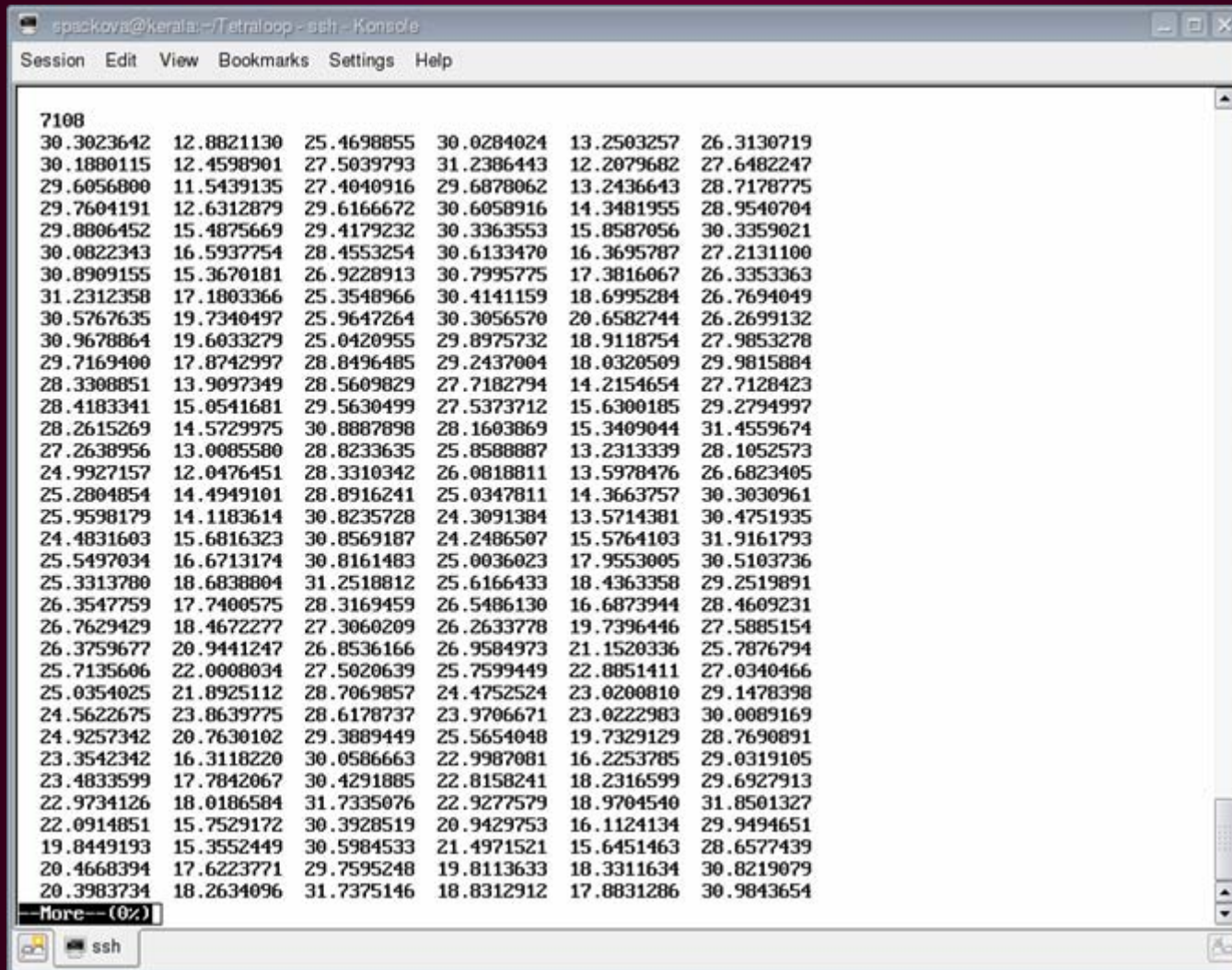
Oktahedrální typ boxu



Pohyb molekuly v boxu



Formát souboru *.crd



The screenshot shows a terminal window titled "spackova@kerala:~/TetraLoop - ssh - Konsole". The window contains a list of 60 numbers arranged in a 10x6 grid. The numbers are integers ranging from 7108 to 30.9843654. At the bottom of the terminal, there is a status bar that says "More--(0%)".

```
7108
30.3023642 12.8821130 25.4698855 30.0284024 13.2503257 26.3130719
30.1880115 12.4598901 27.5039793 31.2386443 12.2079682 27.6482247
29.6056800 11.5439135 27.4040916 29.6878062 13.2436643 28.7178775
29.7604191 12.6312879 29.6166672 30.6058916 14.3481955 28.9540704
29.8806452 15.4875669 29.4179232 30.3363553 15.8587056 30.3359021
30.0822343 16.5937754 28.4553254 30.6133470 16.3695787 27.2131100
30.8909155 15.3670181 26.9228913 30.7995775 17.3816067 26.3353363
31.2312358 17.1803366 25.3548966 30.4141159 18.6995284 26.7694049
30.5767635 19.7340497 25.9647264 30.3056570 20.6582744 26.2699132
30.9678864 19.6033279 25.0420955 29.8975732 18.9118754 27.9853278
29.7169400 17.8742997 28.8496485 29.2437004 18.0320509 29.9815884
28.3308851 13.9097349 28.5609829 27.7182794 14.2154654 27.7128423
28.4183341 15.0541681 29.5630499 27.5373712 15.6300185 29.2794997
28.2615269 14.5729975 30.8887898 28.1603869 15.3409044 31.4559674
27.2638956 13.0085580 28.8233635 25.8588887 13.2313339 28.1052573
24.9927157 12.0476451 28.3310342 26.0818811 13.5978476 26.6823405
25.2804854 14.4949101 28.8916241 25.0347811 14.3663757 30.3030961
25.9598179 14.1183614 30.8235728 24.3091384 13.5714381 30.4751935
24.4831603 15.6816323 30.8569187 24.2486507 15.5764103 31.9161793
25.5497034 16.6713174 30.8161483 25.0036023 17.9553005 30.5103736
25.3313780 18.6838804 31.2518812 25.6166433 18.4363358 29.2519891
26.3547759 17.7400575 28.3169459 26.5486130 16.6873944 28.4609231
26.7629429 18.4672277 27.3060209 26.2633778 19.7396446 27.5885154
26.3759677 20.9441247 26.8536166 26.9584973 21.1520336 25.7876794
25.7135606 22.0008034 27.5020639 25.7599449 22.8851411 27.0340466
25.0354025 21.8925112 28.7069857 24.4752524 23.0200810 29.1478398
24.5622675 23.8639775 28.6178737 23.9706671 23.0222983 30.0089169
24.9257342 20.7630102 29.3889449 25.5654048 19.7329129 28.7690891
23.3542342 16.3118220 30.0586663 22.9987081 16.2253785 29.0319105
23.4833599 17.7842067 30.4291885 22.8158241 18.2316599 29.6927913
22.9734126 18.0186584 31.7335076 22.9277579 18.9704540 31.8501327
22.0914851 15.7529172 30.3928519 20.9429753 16.1124134 29.9494651
19.8449193 15.3552449 30.5984533 21.4971521 15.6451463 28.6577439
20.4668394 17.6223771 29.7595248 19.8113633 18.3311634 30.8219079
20.3983734 18.2634096 31.7375146 18.8312912 17.8831286 30.9843654
```

More--(0%)

Formát souboru *.top

```
spackova@kerala:~/TetraLoop - ssh - Konsole
Session Edit View Bookmarks Settings Help

%VERSION VERSION_STAMP = U0001.000 DATE = 08/21/07 16:47:28
%FLAG TITLE
%FORMAT(20a4)

%FLAG POINTERS
%FORMAT(10I8)
  7108      17    6883    242    252    377    531    706      0      0
 10859    2276    242    377    706    40    76    44    28    1
   0        0      0      0      0      0      0      2    35    0
  0

%FLAG ATOM_NAME
%FORMAT(20a4)
H5T O5' C5' H5' 1H5' 2C4' H4' O4' C1' H1' N1 C6 H6 C5 H5 C4 N4 H41 H42 N3
C3' H3' C2' H2' 1O2' H0' 2O3' H3T Na+ Na+ Na+ Na+ Na+ Na+ Na+ Na+ 0 H1 H2
O H1 H2 0 H1 H2 0 H1 H2 0 H1 H2 0 H1 H2 0 H1 H2 0 H1 H2 0 H1
H2 0 H1 H2 0 H1 H2 0 H1 H2 0 H1 H2 0 H1 H2 0 H1 H2 0

%FLAG CHARGE
%FORMAT(5E16.8)
  7.82647785E+00 -1.13397373E+01  1.01680434E+00  1.23729417E+00  1.23729417E+00
  1.94067495E+00  2.13929802E+00 -6.46527204E+00  1.20267180E-01  3.69730467E+00

%FLAG MASS
%FORMAT(5E16.8)
  1.00800000E+00  1.60000000E+01  1.20010000E+01  1.00800000E+00  1.00800000E+00
  1.20100000E+01  1.00800000E+00  1.60000000E+01  1.20100000E+01  1.00800000E+00

%FLAG ATOM_TYPE_INDEX
%FORMAT(10I8)
   1      2      3      4      4      3      4      5      3      6
   7      8      9      8     10      8      7     11     11      7

%FLAG NUMBER_EXCLUDED_ATOMS
%FORMAT(10I8)
   5      7     10      5      4     12      6     11     15      7
  12      9      4      7      3      6      4      2      1      2

%FLAG NONBONDED_PARM_INDEX
%FORMAT(10I8)
   1      2      4      7     11     16     22     29     37     46
  56     67     79     92    106    121    137      2      3      5

%FLAG RESIDUE_LABEL
```

17,1 Top

Nestandardní rezidua

⇒ geometrie:

úprava standardních reziduí v xLeapu
použití souřadnic odjinud (QM)

⇒ náboje

⇒ atomové typy

již existující – někdy třeba dodefinovat
chybějící parametry

nové – nutno vždy dodefinovat chybějící
parametry

Nové atomové typy

