

- YASARA - Yet Another Scientific Artificial Reality Application

File Edit Simulation Analyze 3DM View Effects Options Window Help

SCENE CONTENT

Obj	Name	Vis	Act	Atom
1	TPS3	Yes	Yes	1
2		No	No	
3		No	No	
4		No	No	
5		No	No	
6		No	No	
7		No	No	
8		No	No	
9		No	No	
10		No	No	

Number: 1394
Name: CA
Element: Carbon [C]
Occupancy: 100% Bfactor: -9.70
Residue: VAL 97 A
Object: 1 (TPS3)

Position: X = -00002.46300 Å
Y = 00012.45600 Å
Z = 00015.94300 Å

Speed: X = 00000.0000 m/s
Y = 00000.0000 m/s
Z = 00000.0000 m/s
Total = 00000.0000 m/s

Active X = 0000000000 FN
Forces: X = 0000000000 FN
Y = 0000000000 FN
Z = 0000000000 FN
Total = 0000000000 FN

Bonds: 4
1) Type = to N (VAL 97)
Length = 1.461 Å (VAL 97)
2) Type = to O6 (VAL 97)
Length = 1.400 Å (VAL 97)
3) Type = to C (VAL 97)
Length = 1.532 Å (VAL 97)
4) Type = to CB (VAL 97)
Length = 1.532 Å

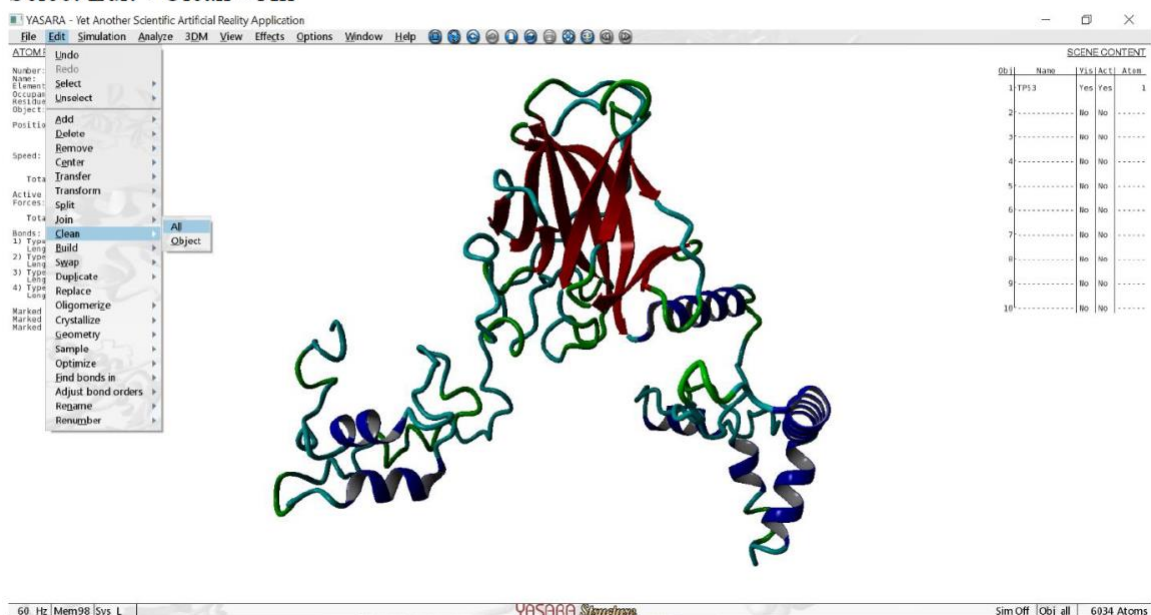
Marked Distance: ----- Å
Marked Angle: ----- °
Marked Dihedral: ----- °

60 Hz | Mem98 | Svs L | 6035 Atoms

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- The screenshot displays the YASARA software interface. At the top, the menu bar includes File, Edit, Simulation, Analyze, 3DM, View, Effects, Options, Window, and Help. Below the menu bar is a toolbar with various icons. The main window shows a 3D ribbon model of a protein structure. A dialog box titled "Select new amino acid or nucleotide" is open in the center. The dialog has two tabs: "Residue" and "Special residue names". The "Residue" tab is active, showing a list of amino acids with "Val" (Valine) selected. The "Special residue names" tab lists various special residues like Ash, Cys, Glu, His, etc. The bottom status bar shows the current selection as "Val" and the simulation status as "Sim Off".
- YASARA - Yet Another Scientific Realistic Application**
- File Edit Simulation Analyze 3DM View Effects Options Window Help**
- ATOM PROPERTIES**
- Number: 1294
Name: CA
Element: Carbon (C)
Occupancy: 100% BFactor: -9.78
Residue: VAL 97 A
Object: 1 (TPS3)
- Position: X = -00003.46380 Å
Y = -00014.05400 Å
Z = 00015.94380 Å
- Speed: X = 00000.0000 n/s
Y = 00000.0000 n/s
Z = 00000.0000 n/s
Total = 00000.0000 n/s
- Active X = 0000000000 FN
Forces: Y = 0000000000 FN
Z = 0000000000 FN
Total = 0000000000 FN
- Bonds: 4
1) Type: to N (VAL 97)
Length: 1.401 Å
2) Type: to HA (VAL 97)
Length: 1.095 Å
3) Type: to C (VAL 97)
Length: 1.396 Å
4) Type: to CB (VAL 97)
Length: 1.952 Å
- Marked Distance: Å
Marked Angle: °
Marked Dihedral: °
- SCENE CONTENT**
- | Obj | Name | Vis | Act | Atom |
|-----|------|-----|-----|------|
| 1 | TPS3 | Yes | Yes | 1 |
| 2 | | No | No | |
| 3 | | No | No | |
| 4 | | No | No | |
| 5 | | No | No | |
| 6 | | No | No | |
| 7 | | No | No | |
| 8 | | No | No | |
| 9 | | No | No | |
| 10 | | No | No | |
- Select new amino acid or nucleotide**
- Residue:**
- > Arg
 - > Asp
 - > His
 - > Ile
 - > Leu
 - > Lys
 - > Met
 - > Phe
 - > Pro
 - > Ser
 - > Thr
 - > Trp
- Special residue names:**
- Ash: Neutral Asp with H on OD2
 - Cys: Negatively charged Cys
 - Cys: Cysteine in disulfide bridge
 - Glu: Neutral Glu with H on OE2
 - His: Neutral His with H on ND1
 - His: Neutral His with H on NE2
 - His: Positively charged His
- ☒ L-amino acid
☐ D-amino acid
- D K**
- PRO ALA ALA ALA PRO ALA PRO SER TRP PRO LEU SER SER VAL PRO SER GLN LYS THR TYR GLN GLY SER TYR GLY PHE ARG LEU**
- 12 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100 101 102 103 104 105 106 107 108 109 110 111**
- Obj: 1 Mol A C E C T T T T C C E E**
- 60 Hz Mem 98 Sys L**
- YASARA Version**
- Sim Off Obj all 6035 Atom**

3) Clean the scene to repair bonds

a) Select Edit->Clean->All



4) Perform an Energy Minimization

a) Select Options->Choose Experiment->Energy Minimization

