**nature** | **methods**

# Visualization of macromolecular structures

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Supplementary figures and text:

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|---|---|
| **Supplementary Figure 1** | Relibase comparison of human estrogen receptor structures |
| **Supplementary Table 1** | Tools for visualizing RNA secondary structure |

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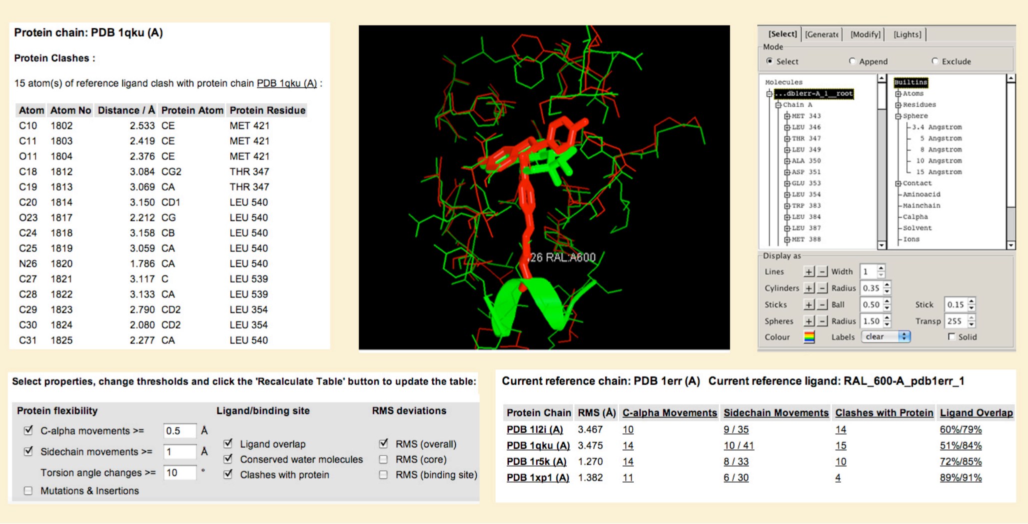

**Protein chain: PDB 1qku (A)**

**Protein Clashes :**

15 atom(s) of reference ligand clash with protein chain PDB 1qku (A) :

| Atom | Atom No | Distance / Å | Protein Atom | Protein Residue |
|---|---|---|---|---|
| C10 | 1802 | 2.533 | CE | MET 421 |
| C11 | 1803 | 2.419 | CE | MET 421 |
| O11 | 1804 | 2.376 | CE | MET 421 |
| C18 | 1812 | 3.084 | CG2 | THR 347 |
| C19 | 1813 | 3.069 | CA | THR 347 |
| C20 | 1814 | 3.150 | CD1 | LEU 540 |
| O23 | 1817 | 2.212 | CG | LEU 540 |
| C24 | 1818 | 3.158 | CB | LEU 540 |
| C25 | 1819 | 3.059 | CA | LEU 540 |
| N26 | 1820 | 1.786 | CA | LEU 540 |
| C27 | 1821 | 3.117 | C | LEU 539 |
| C28 | 1822 | 3.133 | CA | LEU 539 |
| C29 | 1823 | 2.790 | CD2 | LEU 354 |
| C30 | 1824 | 2.080 | CD2 | LEU 354 |
| C31 | 1825 | 2.277 | CA | LEU 540 |

Mode: ● Select ○ Append ○ Exclude

Width 1
Radius 0.35
Ball 0.50 Stick 0.15
Radius 1.50 Transp 255
Labels clear ☐ Solid

**Select properties, change thresholds and click the 'Recalculate Table' button to update the table:**

**Protein flexibility**
☑ C-alpha movements >= 0.5 Å
☑ Sidechain movements >= 1 Å
Torsion angle changes >= 10 °
☐ Mutations & Insertions

**Ligand/binding site**
☑ Ligand overlap
☑ Conserved water molecules
☑ Clashes with protein

**RMS deviations**
☑ RMS (overall)
☐ RMS (core)
☐ RMS (binding site)

**Current reference chain: PDB 1err (A) Current reference ligand: RAL_600-A_pdb1err_1**

| Protein Chain | RMS (Å) | C-alpha Movements | Sidechain Movements | Clashes with Protein | Ligand Overlap |
|---|---|---|---|---|---|
| **PDB 1l2i (A)** | 3.467 | 10 | 9 / 35 | 14 | 60%/79% |
| **PDB 1qku (A)** | 3.475 | 14 | 10 / 41 | 15 | 51%/84% |
| **PDB 1r5k (A)** | 1.270 | 14 | 8 / 33 | 10 | 72%/85% |
| **PDB 1xp1 (A)** | 1.382 | 11 | 6 / 30 | 4 | 89%/91% |

**Supplementary Figure 1 |** Relibase comparison of human estrogen receptor structures. The superimposition is calculated based on minimal RMSD to the C$\alpha$ binding site atoms of the reference structure (PDB 1ERR-A). In the top left corner is OpenAstexViewer[1] showing the human estrogen complexed with the antagonist raloxifene (PDB 1ERR, red) and with the agonist estrogen (PDB 1qku, green). Below the embedded viewer is the table calculated by Relibase+ highlighting differences in protein structure. Clicking on a link in the table creates a pop-up window (bottom right) giving details about the protein movement. The C$\alpha$ movements are caused by the differences in volume of the agonist and antagonist (shown in stick representation), where the antagonist prevents Helix 12 (green) from closing the binding site and from building an interface to the co-activator. The view has been assembled with the help of the hierarchical selection menu (top right) that is part of the Astex viewer.

## **Supplementary Table 1 |** Tools for visualizing RNA secondary structure

| **Name** | **OS** | **Input formats** | **2D layout** | **Features and strengths**[b] | **Limitations** | **URL** |
|---|---|---|---|---|---|---|
| jViz.Rna[2] | Win, Mac, Linux | Bracket notation<br>BPSEQ<br>CT | Circular<br>Dot plot<br>Linear<br>Squiggle | 2D manipulation, pseudoknots. Can compare different structures with the same sequence. | Has a confusing squiggle layout | http://jviz.cs.sfu.ca |
| NAVRNA[3] | Linux only | PDB | Squiggle | 2D editing & manipulation, interactive 2D & 3D display, pseudoknots. Uses novel approach to interact with structural data. | Requires hardware not available to many users | http://tinyurl.com/NAVRNA |
| PseudoViewer[4] | Win only | Bracket notation<br>BPSEQ<br>CT<br>Custom format | Squiggle | 2D manipulation. Can easily recover RNA secondary structures with any kind of pseudoknots. | | http://tinyurl.com/pseudoview |
| RNAFamily | Win, Mac, Linux | CT | Linear | Can render several secondary structures in the same display. | Linear layout only | http://tinyurl.com/rnafmly |
| RNAMovies[5] | Win, Mac, Linux | Custom format<br>DCSE<br>RNAStructML | Squiggle | Pseudoknots. Currently the only tool that can make movies. | No other functionality | http://tinyurl.com/rnamovies |
| Rnaviz[6] | Win, Mac, Linux | DCSE<br>CT<br>RNAML | Squiggle | 2D manipulation, annotation, pseudoknots. Use of skeleton files makes it easily produce and save RNA layout. | No recent update | http://rnaviz.sourceforge.net |
| S2S Assemble*[7] | Win, Mac, Linux | BPSEQ<br>Bracket notation<br>CT<br>FASTA<br>PDB<br>RNAML<br>Stockholm | Squiggle | 2D editing & manipulation, non-canonical interactions, pseudoknots, interactive 2D & 3D display, interactive 3D modeling, secondary structure prediction. Has very rich set of features. | Steep learning curve | http://bioinformatics.org/s2s<br>http://bioinformatics.org/assemble |
| StructureLab[8] | Linux only | Various formats are supported depending on linked algorithm | Dot plot<br>Stem trace<br>Squiggle | 2D manipulation, annotations, pseudoknots. interactive 2D & 3D display, interactive 3D modeling, secondary structure prediction. | Steep learning curve due to rich feature set | http://tinyurl.com/structureLab |
| VARNA*[9] | Win, Mac, Linux | BPSEQ<br>Bracket notation<br>CT<br>RNAML | Circular<br>Linear<br>Squiggle | 2D manipulation, 2D editing, annotations, non-canonical interactions, pseudoknots. Can be embedded in webpages. | | http://varna.lri.fr |
| XRNA | Win, Mac, Linux | Custom format (XRNA) | Squiggle | 2D manipulation, annotations. | Constrains on 2D editing | http://rna.ucsc.edu/rnacenter/xrna |

* means our recommendations. All tools listed are free for academic use; [b]Tools with '2D editing' can modify the secondary structure definition; tools with 'Non-canonical' can handle non-canonical interactions. Tools with interactive 2D & 3D display allow simultaneous visualization, and interaction between, both secondary structure and tertiary structure in a 3D viewer, e.g., PyMOL.

## References

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   **Simple, easy-to-use, and feature-rich tool for searching, display and manipulation of RNA secondary structures. Can be embedded in webpages.**