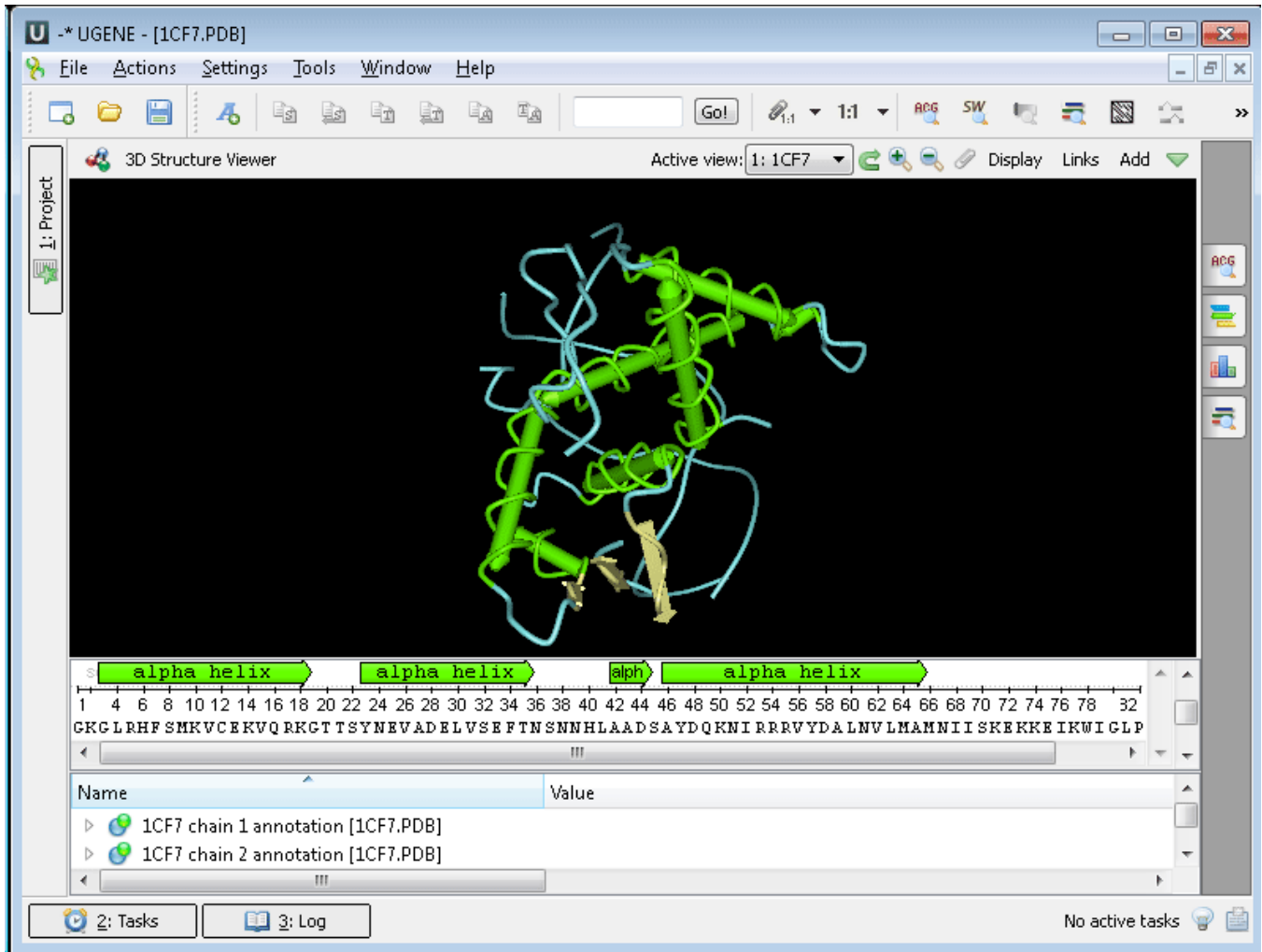


3D structures and surface algorithms

3D structures (3D Structure Viewer). The *3D Structure Viewer* is intended for visualization of 3D structures of biological molecules. Using the *3D Structure Viewer* you can work with data from the Protein Data Bank (PDB) - a repository for the 3D structural data of large biological molecules, such as proteins and nucleic acids, maintained by the Worldwide Protein Data Bank (wwPDB). You can work as well with data from the NCBI Molecular Modeling DataBase (MMDB), also known as "Entrez Structure", a database of experimentally determined structures obtained from the RCSB Protein Data Bank.

The *3D Structure Viewer* is opened automatically when you open a PDB or MMDB file. For example, open `$ugene/data/samples/PDB/1CF7.PDB`. The *3D Structure Viewer* adds a view to the upper part of the *Sequence View*.



Using the *3D Structure Viewer* you can:

- Changing 3D Structure Appearance;
- Moving, zooming and spinning 3D structure;
- Highlighting sequence region;
- Selecting models to display;
- Exporting 3D structures image;
- Working with several 3D structure views.

Example 5: Calculating Molecular Surface. To calculate the molecular surface of a molecule select the *Molecular Surface* item in the *3D Structure Viewer* context menu or in the Display menu on the toolbar and check one of the following items:

- SAS (solvent-accessible surface)
- SES (solvent-excluded surface)
- vdWS (van der Waals surface)

To remove the molecular surface that has already been calculated select the O item. You can also select the Molecular Surface Render Style to modify the calculated molecular surface appearance:

- Convex Map
- Dots

U -* UGENE - [1CF7.PDB]

File Actions Settings Tools Window Help

3D Structure Viewer Active view: 1: 1CF7

1: Project

ACG SW Display Links Add

alpha helix alpha helix alpha alpha helix

1 4 6 8 10 12 14 16 18 20 22 24 26 28 30 32 34 36 38 40 42 44 46 48 50 52 54 56 58 60 62 64 66 68 70 72 74 76 78 80

GKGLRHF SMKVCERVQ RKGTTSYNEVADELVSEFTNSNNHLAADSA YDQKNI RRRVYDALNVLMAMNII SREKRE IKWIGLP

Name	Value
1CF7 chain 1 annotation [1CF7.PDB]	
1CF7 chain 2 annotation [1CF7.PDB]	

2: Tasks 3: Log No active tasks

vdWS (van der Waals surface)