

# DawnDock

## User Manual & Tutorial

Molecular docking on Windows, from protein to pose.

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# Contents

**Before you start** 3
System requirements 3
Installing 4
File formats you can use 4
**Part 1. Quick Run** 5
Step 1. Open DawnDock and load the protein 5
Step 2. Check what was loaded 6
Step 3. Find the pocket from the bound molecule 6
Step 4. Prepare the receptor 7
Step 5. Add the ligand 8
Step 6. Check the search box 9
Step 7. Choose the engine 10
Step 8. Run it 10
Step 9. Read the result 11
Step 10. Save your work 12
**Part 2. Detailed Guide** 14
How the window is arranged 14
Step 1. Receptor 15
Step 2. Ligands 18
Step 3. Binding site 21
Step 4. Dock 23
Step 5. Batch results 26
Step 6. Analysis 27
The results inspector 29
The menus 31
**Troubleshooting** 32
Messages about the order of work 32
Problems preparing a structure 32
Problems with an engine 33
When the answer looks wrong 33
If you need to report a problem 33
**How to cite DawnDock** 34
**Support** 34

# Before you start

DawnDock is a Windows program for **molecular docking**. Docking predicts how a small molecule sits inside a protein, and gives a score for how well it fits. You load a protein, choose a pocket, add one molecule or a whole library, run a docking engine, and look at the result in 3D.

Everything happens in one window. There is no command line to learn and nothing to install separately.

### A few words you will meet

| | |
|---|---|
| **Receptor** | The protein you dock into. Usually a PDB file from an experiment. |
| **Ligand** | The small molecule you dock. A drug, an inhibitor, a natural product. |
| **Binding site** | The place on the protein where the ligand should go. Also called the pocket. |
| **Search box** | The 3D box that tells the engine where to look. The engine only searches inside it. |
| **Pose** | One predicted way the ligand can sit in the pocket. An engine returns several. |
| **Affinity** | The score, in kcal/mol. More negative means a better predicted fit. |
| **Docking engine** | The program that does the search. DawnDock ships with five. |

## System requirements

| | |
|---|---|
| **Operating system** | Windows 10 or 11, 64-bit |
| **Disk space** | About 1 GB. The installer is 312 MB and unpacks to roughly 740 MB. |
| **Memory** | 4 GB is enough for a single run. 8 GB or more if you screen a library. |
| **Processor** | Any modern 64-bit CPU. Docking uses the CPU, so more cores finish sooner. |
| **Administrator rights** | Not needed. |
| **Internet** | Not needed to install or to dock. Only to download the installer, to fetch a PDB entry by its ID, to check for updates, or to add the optional Linux engines. |

No Python, no compiler and no separate toolkit. Everything the program needs is inside the installer.

## Installing

Run `DawnDock-Setup-1.0.1.exe`. It installs for you alone, into `%LOCALAPPDATA%\Programs\DawnDock`, so Windows never asks for an administrator password. It adds a Start menu entry, offers a desktop shortcut, and registers an uninstaller, so you can remove it later from Settings, Apps, like any other program.

> **If Windows warns you about the publisher**
>
> The first time you run the installer, Windows may show **"Windows protected your PC"** or **"unknown publisher"**. Choose More info, then Run anyway. This appears because DawnDock is not yet signed with a paid code-signing certificate. It does not mean anything is wrong with the file. You can check the download against the published SHA-256 checksum if you wish.

The first launch shows a loading screen while the 3D view and the chemistry libraries start, so you can see that the program is opening.

## File formats you can use

| For | Formats |
|---|---|
| Receptor | PDB ( `.pdb` , `.ent` ) and mmCIF ( `.cif` , `.mmcif` ). You can also type a 4-letter PDB ID and let DawnDock download it. |
| Ligand | SDF ( `.sdf` , `.sd` ), MOL ( `.mol` ), MOL2 ( `.mol2` ), PDB ( `.pdb` ), SMILES ( `.smi` , `.smiles` , `.txt` ) and CSV ( `.csv` with a `smiles` column). You can also paste a SMILES string straight into the window. |

> **The example used in this manual**
>
> Every picture in this manual comes from one worked example: the protein **1IEP**, which is the Abl kinase, and the drug **imatinib**, which is the molecule bound inside it. The file `1IEP.pdb` is installed with DawnDock in its `examples` folder, so you can follow along exactly.

# Part 1. Quick Run

This part takes you through one complete docking run, from opening the program to saving the result. Follow the steps in order. Each step is one action, and the picture shows you where to click.

The example docks **imatinib** back into **Abl kinase**. The whole run takes a few minutes on a normal laptop.

## Step 1. Open DawnDock and load the protein

Start DawnDock from the Start menu. The window opens on the `Receptor` step. Click `Open structure file` and choose your PDB file. For this tutorial, use `examples\1IEP.pdb`.

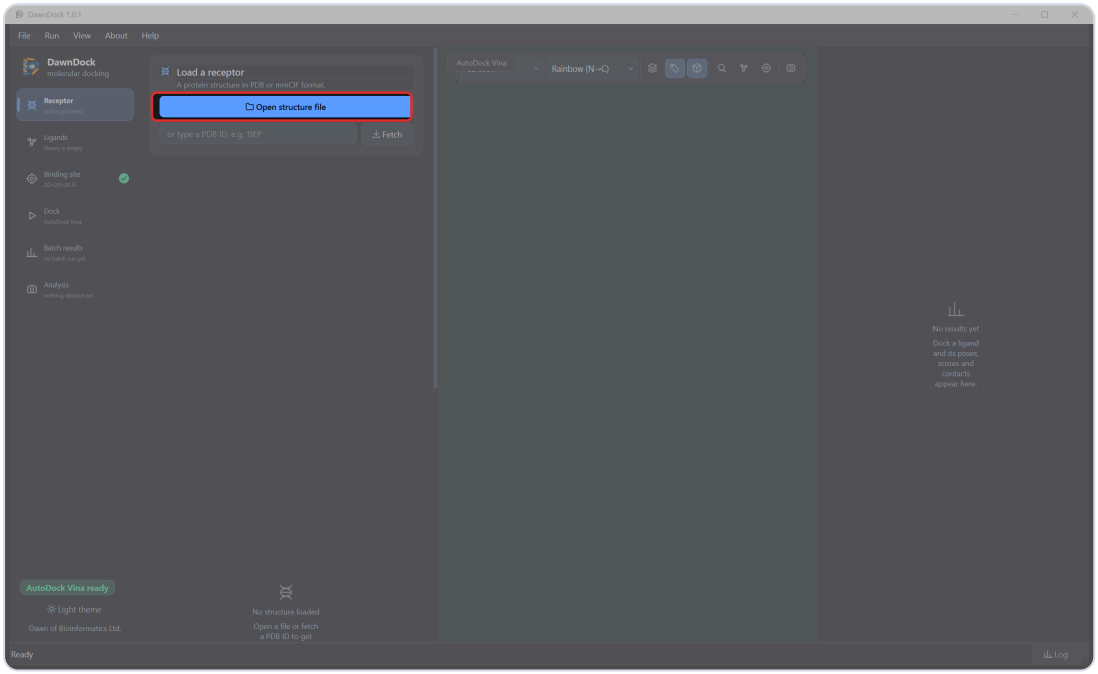



**Figure 1.** The window as it opens. The six steps run down the left side. Click **Open structure file** to begin.

> You can also type a PDB ID such as `1IEP` in the box below the button and press `Fetch` to download it.

## Step 2. Check what was loaded

The Structure card fills in as soon as the file is read. Check the number of chains and residues looks right for your protein.

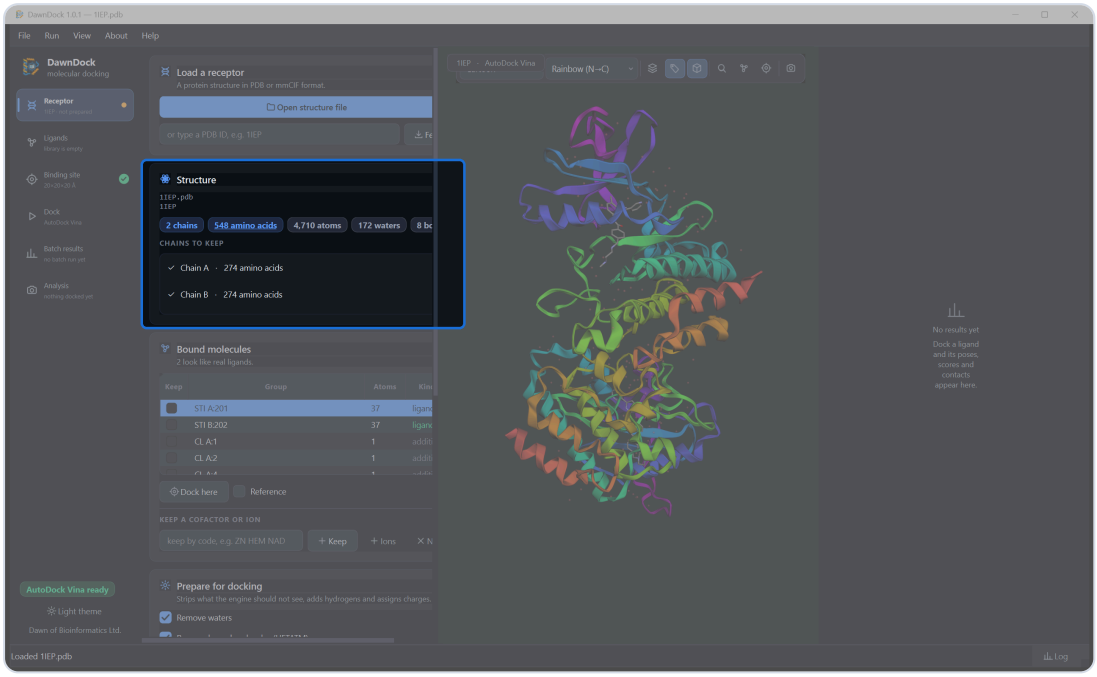



**Figure 2.** The protein appears in the 3D view, and the Structure card reports what is in the file. For 1IEP that is 2 chains, 548 amino acids and 4,710 atoms.

## Step 3. Find the pocket from the bound molecule

Scroll down to Bound molecules. DawnDock lists every non-protein group in the file and marks the ones that look like real ligands. Select **STI A:201**, which is imatinib, then click Dock here. This puts the search box around that molecule.

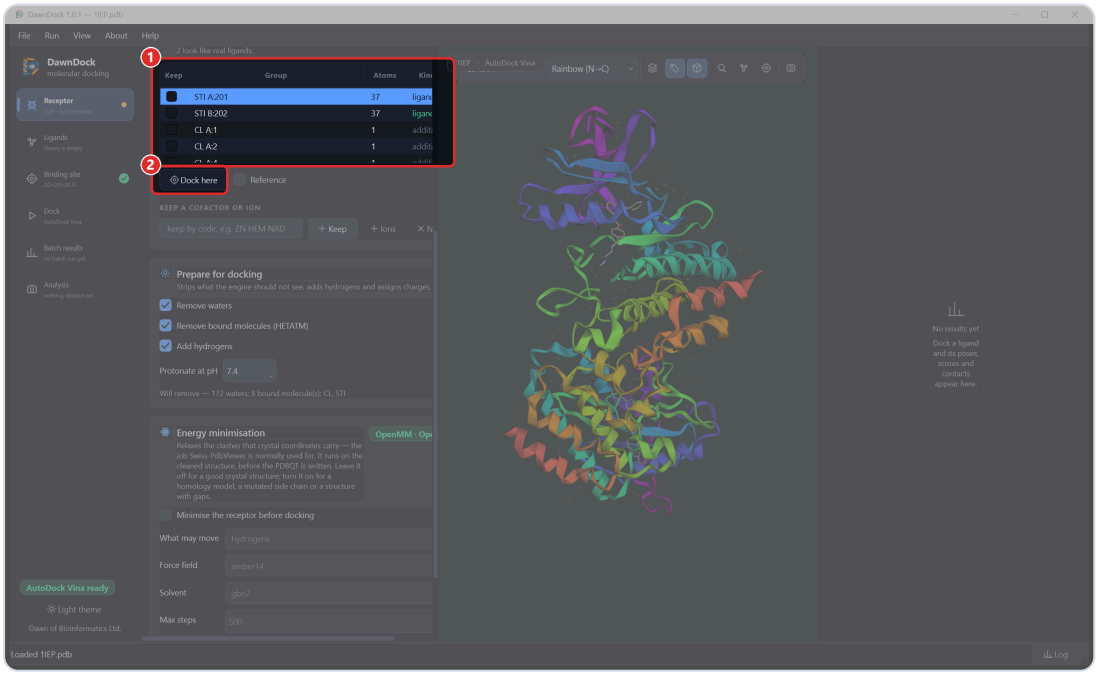



**Figure 3.** Select the bound molecule (1), then click **Dock here** (2) to put the search box around it.

**No bound molecule in your file?**

Go to the Binding site step and use Find the pockets for me. DawnDock will search the surface and offer the best pockets it finds.

## Step 4. Prepare the receptor

Scroll to Prepare for docking and click Prepare receptor. This removes the water and the bound molecules, adds hydrogens, and assigns the charges the engine needs.

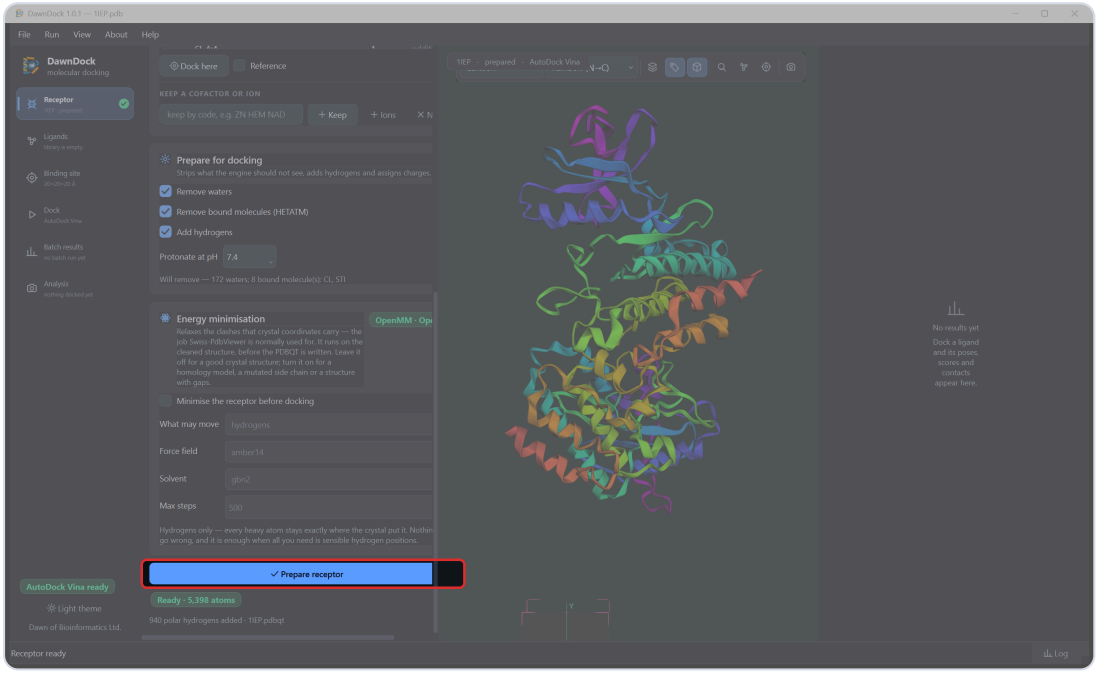



**Figure 4.** Click **Prepare receptor**. When it finishes, the Receptor step shows a green tick and the badge reads "prepared".

You must prepare the receptor before you can dock. The tick on the Receptor step tells you it is done.

## Step 5. Add the ligand

Click Ligands in the left rail. Paste this SMILES string into the box and give it the name `imatinib`, then click Add:

```
CC1=C(C=C(C=C1)NC(=O)C2=CC=C(C=C2)CN3CCN(CC3)C)NC4=NC=CC(=N4)C5=CN=CC=C5
```

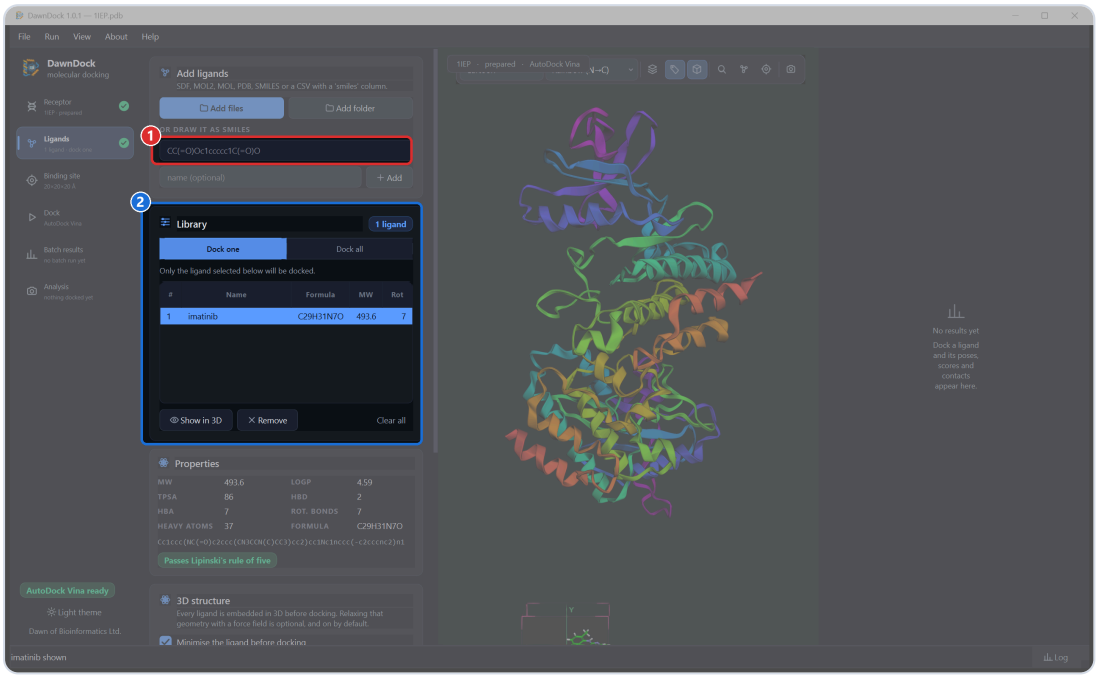



**Figure 5.** Paste the SMILES and click Add (1). The molecule is built in 3D and appears in the library (2).

You can also click Add files to load an SDF, MOL2 or PDB file, or Add folder to load a whole library at once.

## Step 6. Check the search box

Click **Binding site**. The box you set in Step 3 is shown, with its centre and its size in angstroms. The pink cage in the 3D view is the volume the engine will search.

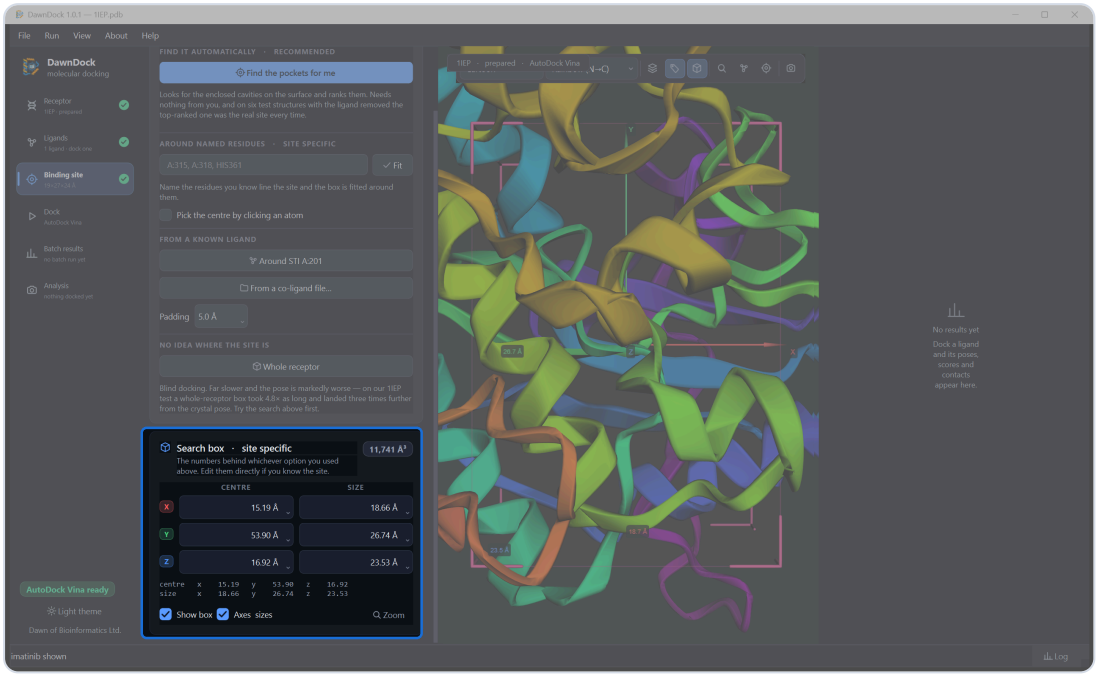



**Figure 6.** The search box, set from the bound ligand. For this example it comes out about 19 x 27 x 24 angstroms.

> **The box matters more than anything else**
>
> If the box is in the wrong place, the engine searches empty space and the scores are meaningless. Always look at the pink cage in the 3D view and check it sits on the pocket before you run.

## Step 7. Choose the engine

Click Dock. The engines are listed best first, by how often each one reproduced a known crystal pose in our own tests. AutoDock Vina is a good first choice: it is fast, well established, and the one most papers cite.

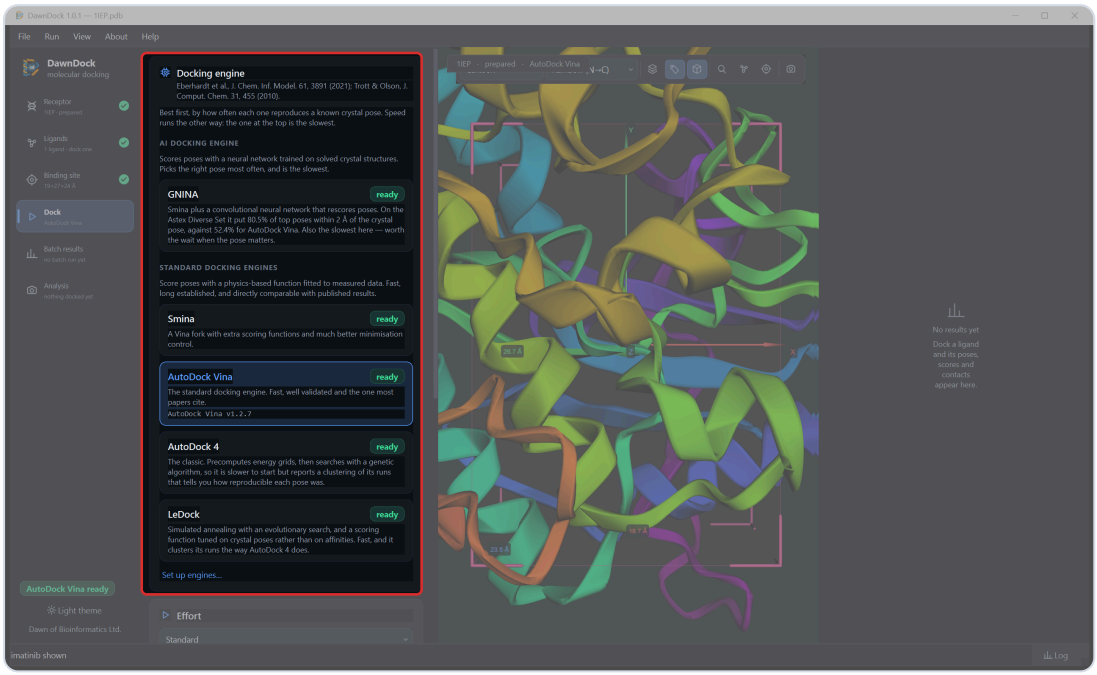



**Figure 7.** Pick an engine from the cards. Leave Effort on "Standard" for your first run.

## Step 8. Run it

Scroll down and press the start button. It is named after the molecule you selected, so for this tutorial it reads Dock imatinib. If no ligand is selected it reads Start docking.

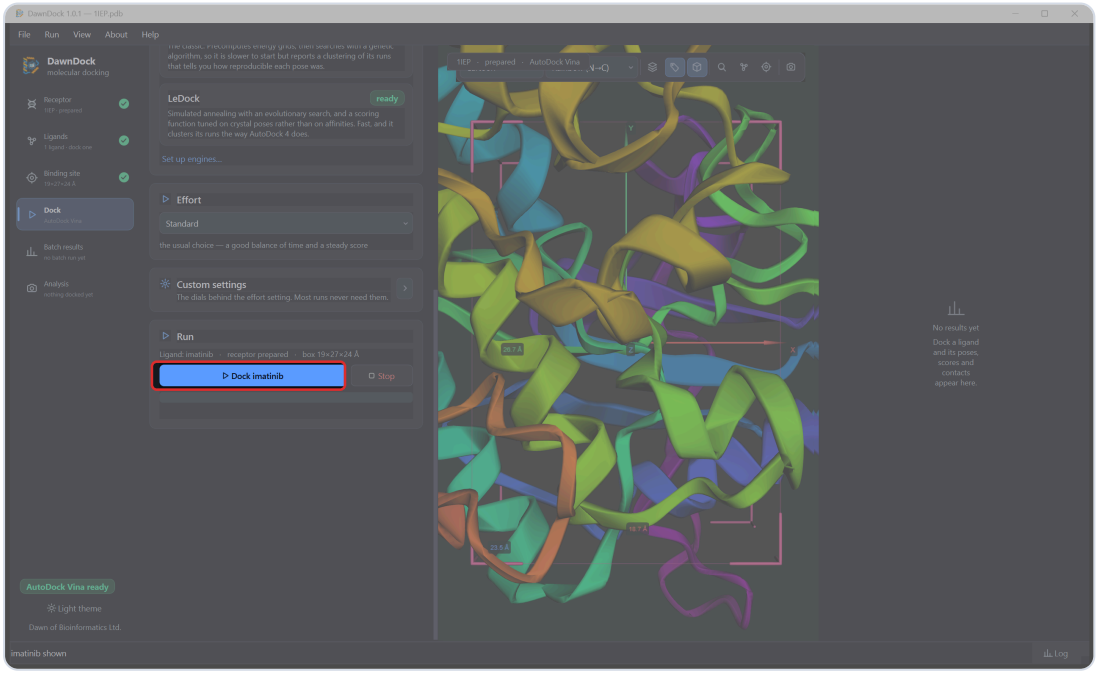



**Figure 8.** Press **Dock imatinib** to start.

The log at the bottom shows what the engine is doing. A single ligand with AutoDock Vina takes about ten to twenty seconds.

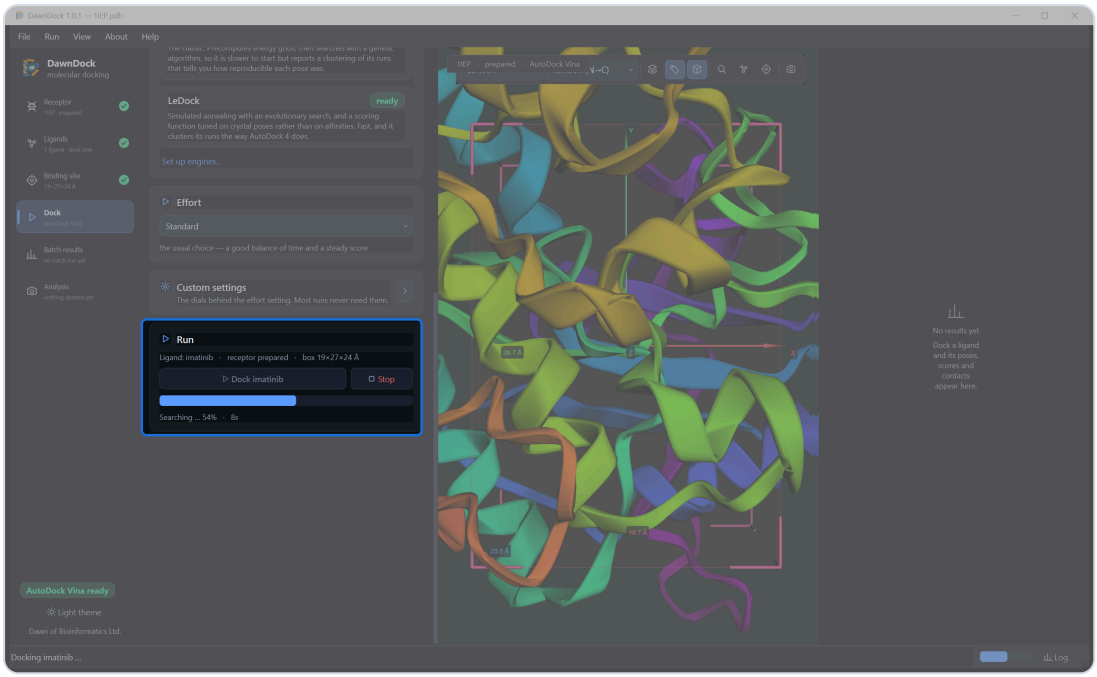



**Figure 9.** While the run is going, the Dock step shows its progress. You can stop it at any time.

## Step 9. Read the result

When the run finishes, the panel on the right fills in. The big number is the **affinity** of the best pose, in kcal/mol. More negative means a better predicted fit.

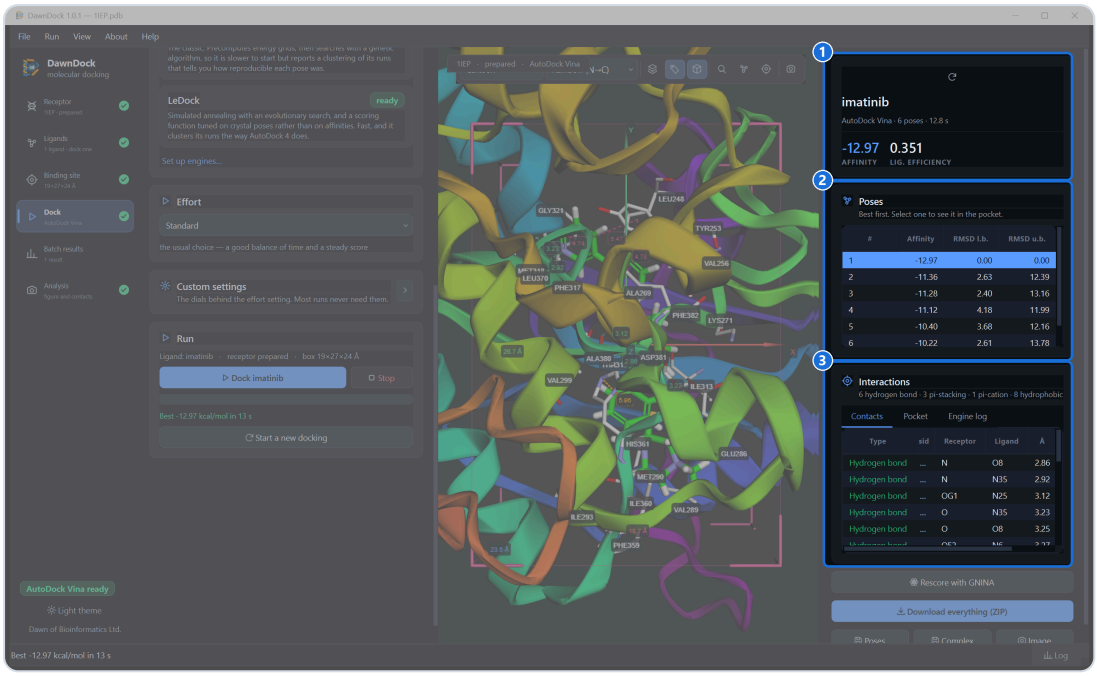



**Figure 10.** The result. The score and ligand efficiency (1), every pose the engine returned (2), and the contacts the best pose makes with the protein (3).

1. **Affinity and ligand efficiency.** For this example the best pose scores about **-12.97 kcal/mol**.
2. **Poses.** Best first. Click any row to see that pose in the 3D view.
3. **Interactions.** The hydrogen bonds, pi-stacking and other contacts the pose makes. For imatinib you should see contacts with THR315, MET318 and ASP381, which are the residues it is known to bind.

## Step 10. Save your work

Click Download everything (ZIP) on the right to save the poses, the prepared receptor, the scores and the log in one archive. The Analysis step has the controls for making a figure.

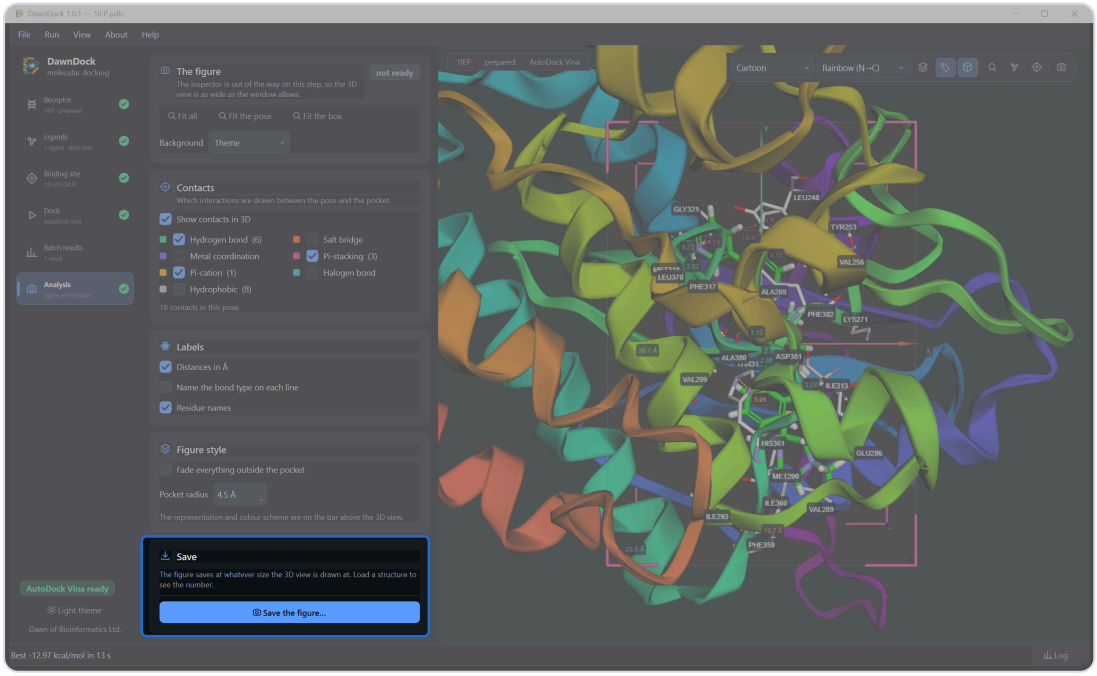



**Figure 11.** The Analysis step gives the 3D view the whole window, and holds everything that decides what a saved figure shows.

### What you should see

If you followed every step, you should now have:

- a green tick on the Receptor, Ligands, Binding site and Dock steps;
- a best affinity of roughly **-12 to -13 kcal/mol**;
- six to nine poses in the table;
- hydrogen bonds listed in the Interactions panel.

Your numbers will not match the ones here exactly. Docking engines search at random, so the same run twice can differ a little. A difference of a few tenths of a kcal/mol is normal.

# Part 2. Detailed Guide

This part goes through the window section by section, in the order the steps appear. Use it to look things up. You do not need to read it from start to finish.

## How the window is arranged

The window has four parts:

- **The step rail**, down the left. Six steps in the order the work happens. Each one shows a short status and a tick when it is done.
- **The settings panel**, in the middle. Its contents change with the step you are on.
- **The 3D view**, in the centre, with its controls floating on top of it.
- **The results inspector**, on the right, where scores, poses and contacts appear.

At the bottom left a badge tells you which engines are ready to use. The status bar at the bottom shows the last thing that happened, and `Log` opens the full engine log.

## Step 1. Receptor

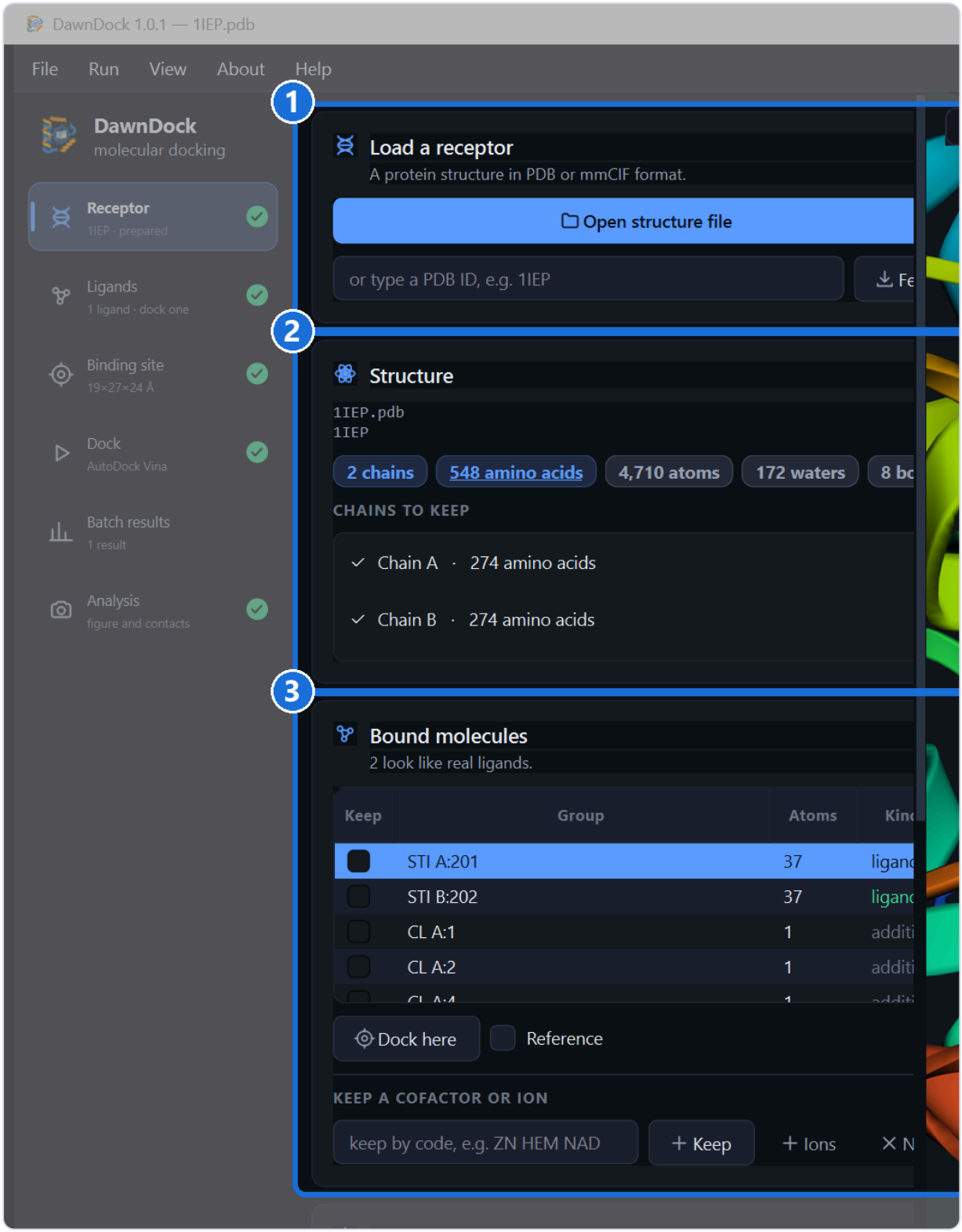



**Figure 12.** The Receptor step.

1. **Load a receptor.** Open a PDB or mmCIF file, or type a 4-letter PDB ID and press Fetch to download it from the RCSB PDB.
2. **Structure.** What is in the file: chains, amino acids, atoms and waters. Tick the chains you want to keep. For a protein that crystallised as a dimer you often only need one chain.
3. **Bound molecules.** Every non-protein group in the file. Use Dock here to put the search box around one, or Reference to keep it on screen in pink so you can compare your poses with it. Use Keep to hold on to a cofactor or metal ion the protein needs.

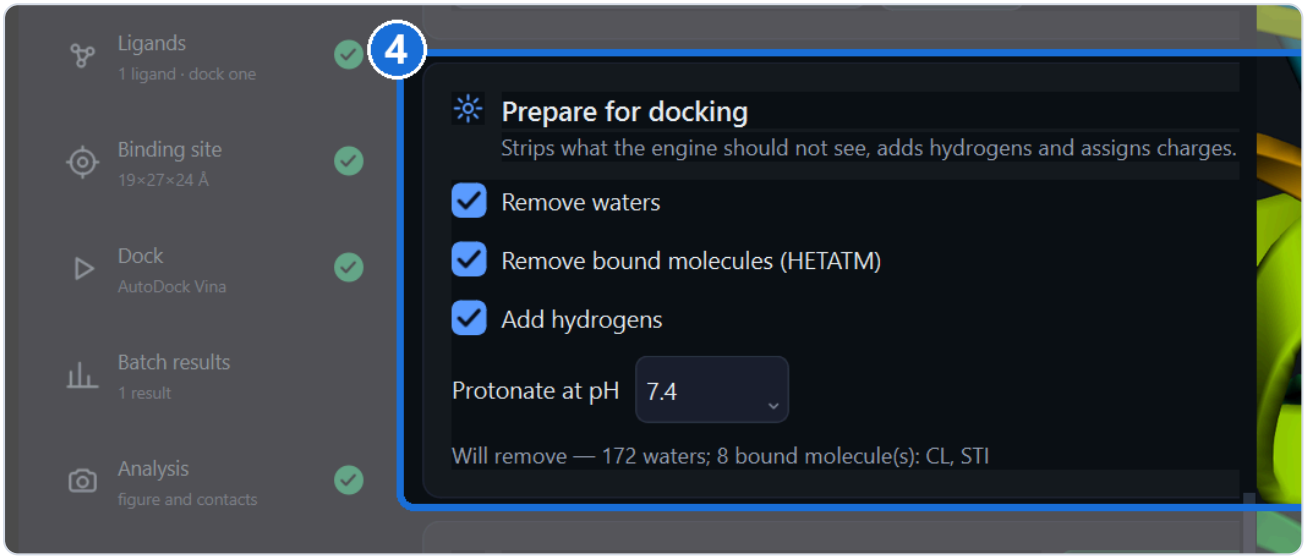



**Figure 13.** Lower down the same panel: **Prepare for docking** (4). This strips what the engine should not see, adds hydrogens and assigns charges. You must do this before docking.

## What the preparation options do

| Option | What it does | Recommended |
|---|---|---|
| **Remove waters** | Deletes crystal water. Most docking is done without water. | On |
| **Remove bound molecules** | Deletes the ligands and additives from the crystal, so the pocket is empty for your own molecule. | On |
| **Add hydrogens** | X-ray structures rarely have hydrogens. The engine needs them. | On |
| **Prepare and minimise** | Also relaxes the structure with a force field. Slower, and useful when the structure has strained geometry or added atoms. | Off for a first run |

## Step 2. Ligands

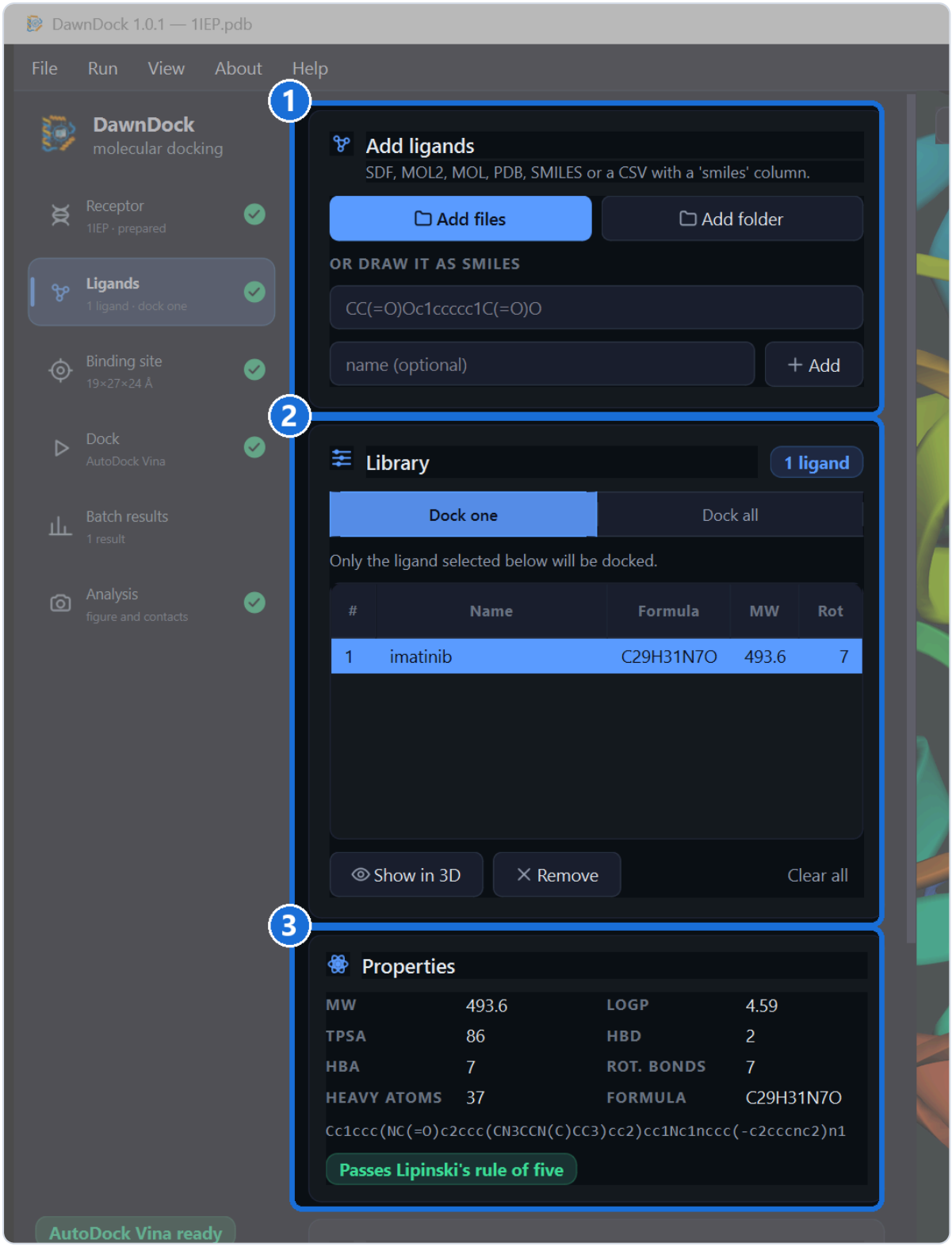



**Figure 14.** The Ligands step.

1. **Add.** Add files for SDF, MOL, MOL2 or PDB; Add folder for a whole library at once; or paste a SMILES string and give it a name.
2. **Library.** Everything you have added. Choose Dock one to dock the selected molecule, or Dock all to run the whole library as a batch.
3. **Properties.** Molecular weight, logP and the other numbers used in rule-of-five filtering, for the molecule you have selected.

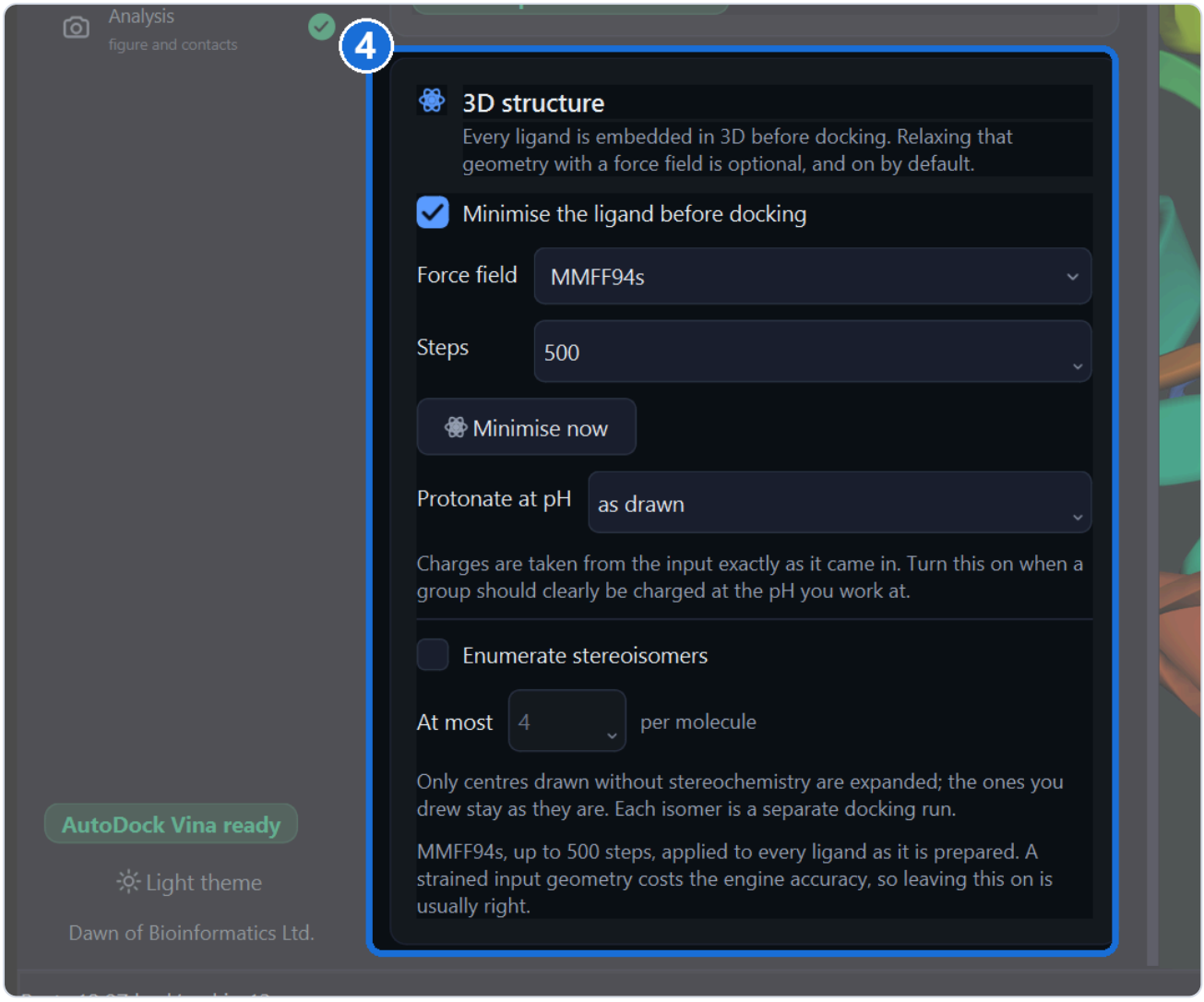



**Figure 15.** Lower down the same panel: **3D structure** (4), which decides how each ligand is built in 3D before docking.

## Ligand preparation settings

| Setting | What it does | Default |
|---|---|---|
| **Force field** | Which field relaxes the 3D shape. MMFF94s is the usual choice for drug-like molecules. UFF covers unusual elements and metals. | MMFF94s |
| **Minimisation steps** | How long to relax the shape. More steps give a cleaner starting geometry and cost a little time. | 200 |
| **pH** | Sets which groups are charged, which matters for salt bridges. 7.4 is body pH. | 7.4 |
| **Stereoisomers** | When a SMILES does not say which way a centre points, DawnDock can build several forms and dock each. | Off |

## Step 3. Binding site

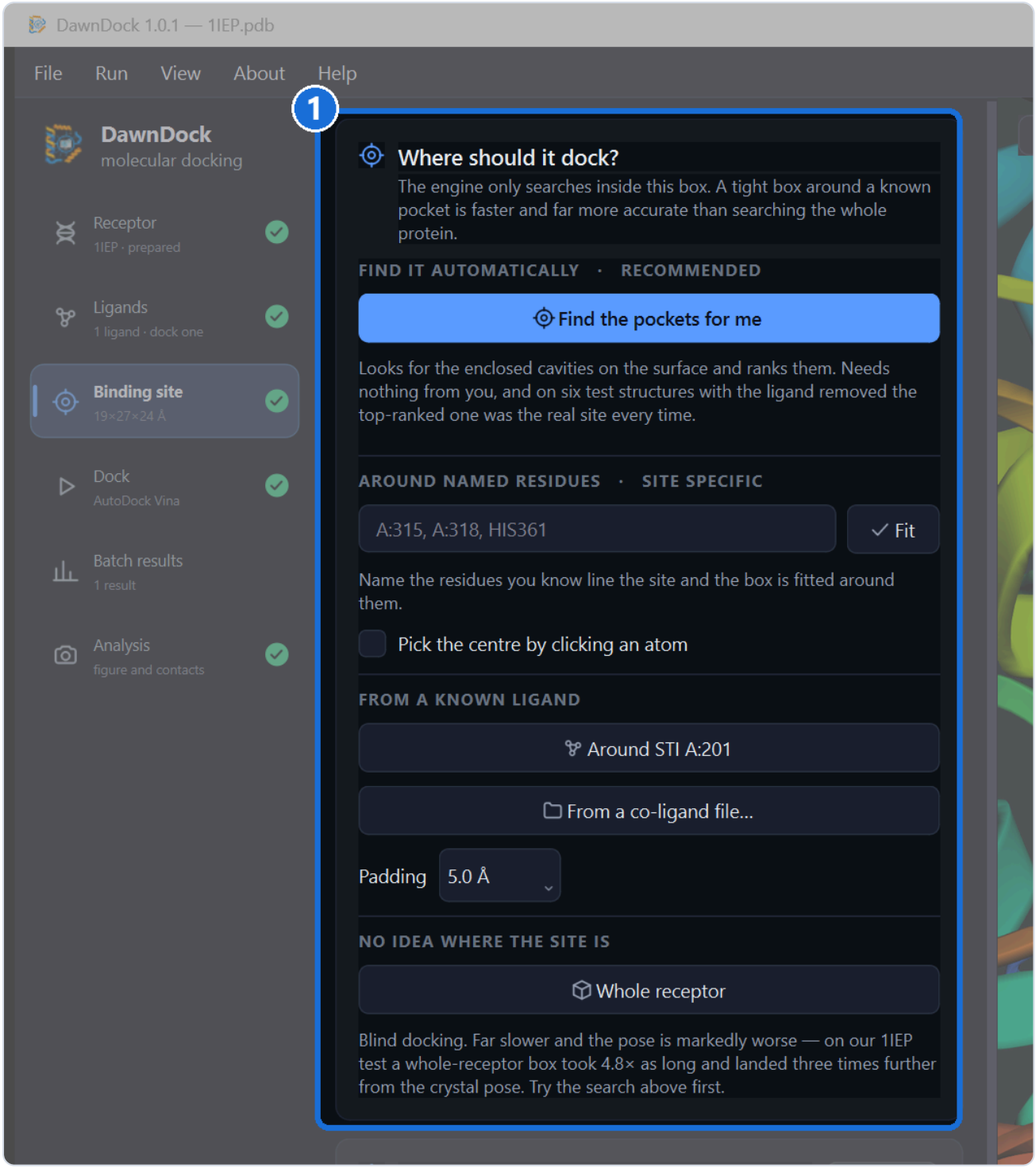



**Figure 16.** The Binding site step.

1 **Where should it dock?** Every way of setting the box: from a pocket DawnDock finds for you, from named residues, from a bound molecule, from a separate reference file, or around the whole protein.

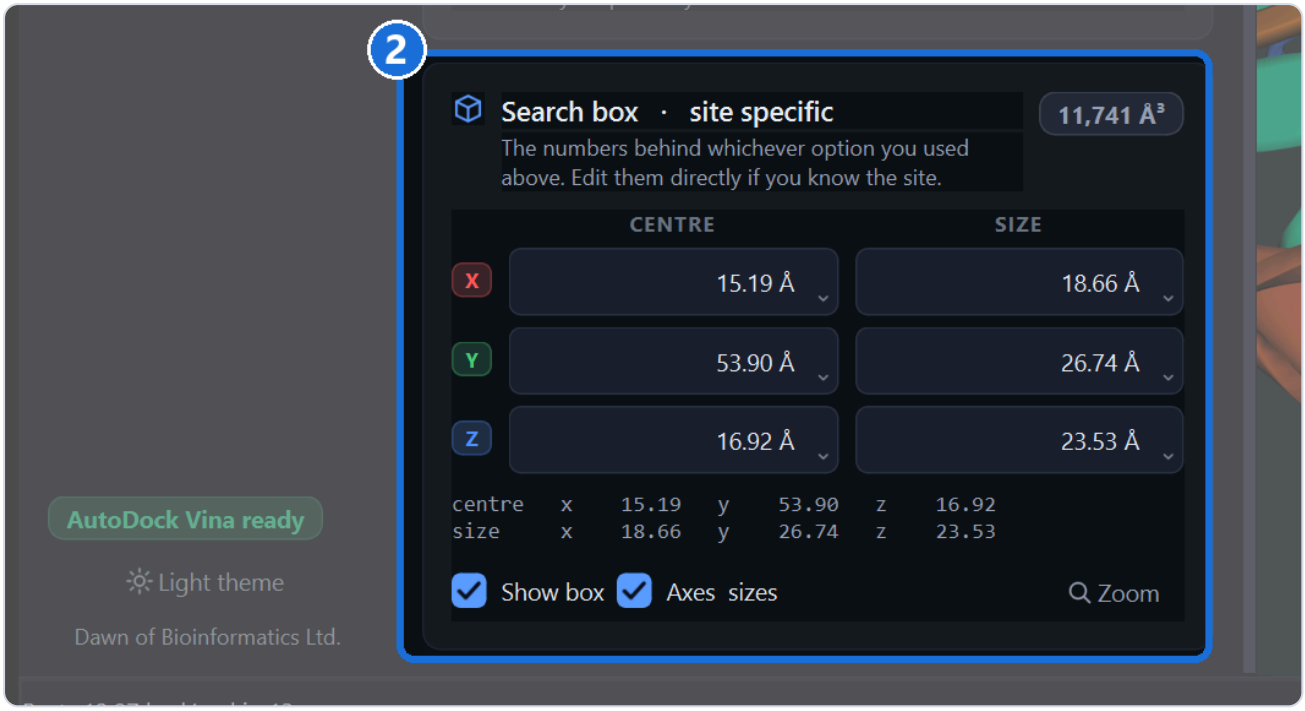



**Figure 17.** Lower down the same panel: **the box itself** (2), with its centre, its size in angstroms and the padding added around whatever you fit it to. A box of about 20 to 25 angstroms a side suits most drug-like molecules.

## Choosing a binding site

- **If the structure has a bound ligand**, use it. This is the most reliable way, and the one this manual's example uses.
- **If it does not**, press `Find the pockets for me`. DawnDock scans the surface and ranks the pockets it finds by size and how enclosed they are.
- **If you know the residues**, type them in, for example `A:315 A:318 A:381`.

> **Keep the box tight**
> A bigger box is not safer. The engine has to search every corner of it, so a large box takes longer and is more likely to put the ligand somewhere wrong. Fit the box to the pocket, not to the protein.

## Step 4. Dock

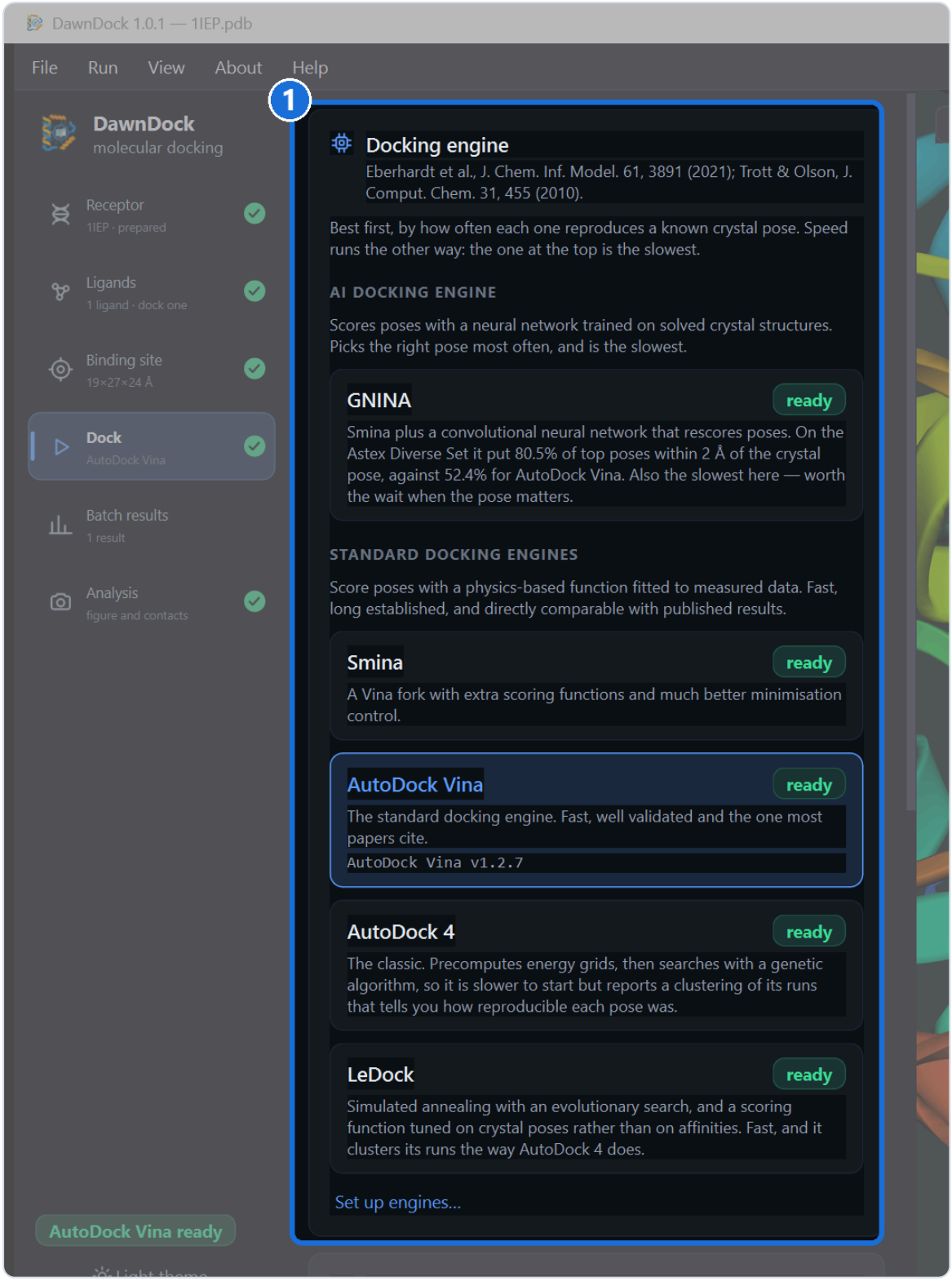



**Figure 18.** The Dock step.

1 **Docking engine.** The five engines, listed best first by measured accuracy. Each card says what the engine is good at, and a green `ready` badge means it is installed and working.

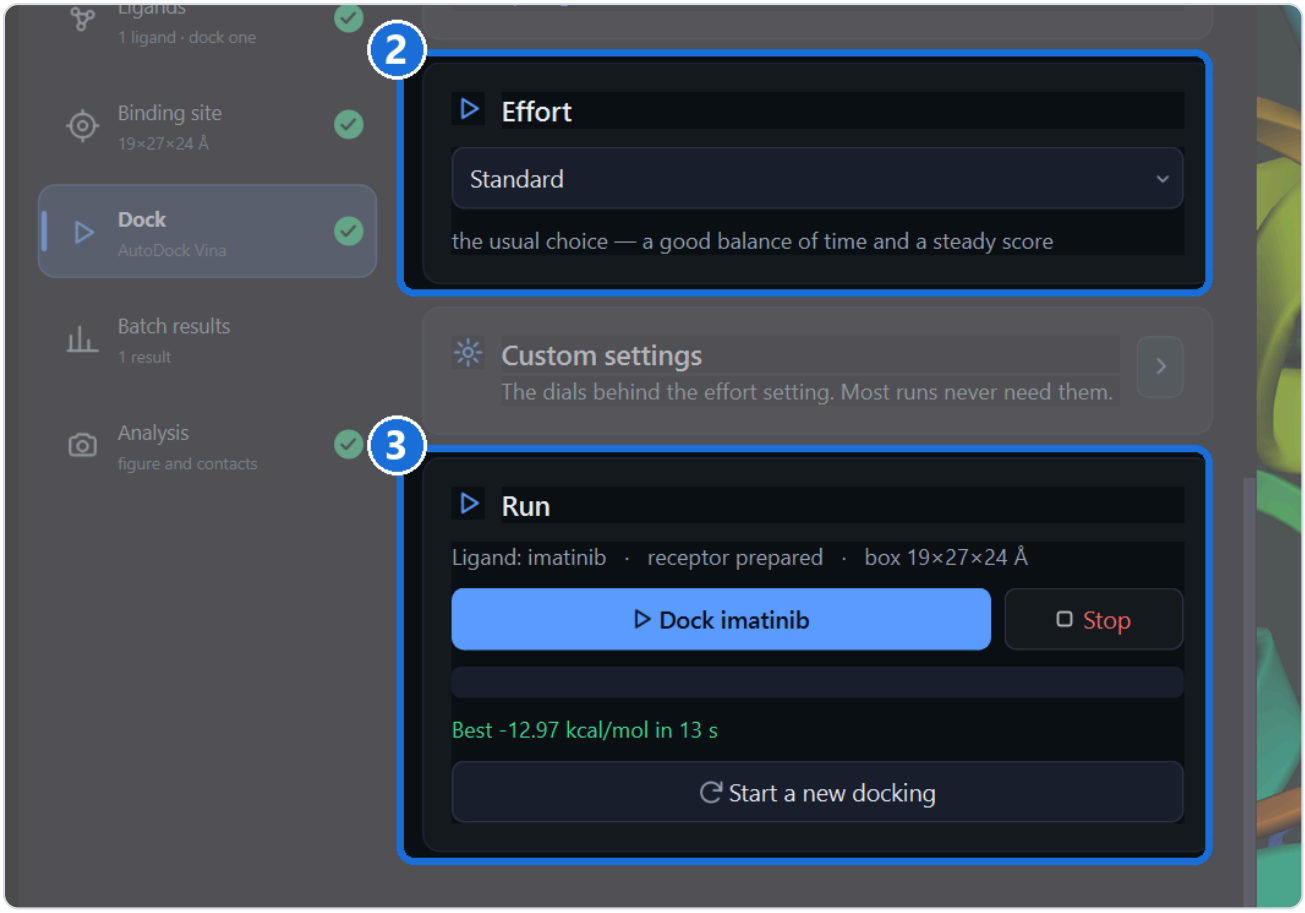



**Figure 19.** Lower down the same panel: **Effort** (2), how hard the engine searches, and **Run** (3), which starts the docking and stops it again.

## The five engines

| Engine | What it is | When to use it |
|---|---|---|
| **GNINA** | An AI engine. It docks like Smina, then rescores the poses with a neural network trained on solved crystal structures. | When the pose matters most. It picks the right pose most often, and is the slowest. |
| **Smina** | A fork of Vina with extra scoring functions and better control over minimisation. | A good middle choice. Its Vinardo function often poses better than stock Vina. |
| **AutoDock Vina** | The standard docking engine, fast and well validated. | Your first run, and anything you want to compare with published work. |
| **AutoDock 4** | The classic. Precomputes energy grids, then searches with a genetic algorithm. | When you want its clustering, which tells you how reproducible a pose was. |
| **LeDock** | Simulated annealing with an evolutionary search, scored against crystal poses. | A useful second opinion, because it works differently from the others. |

> **Two kinds of engine**
> An **AI docking engine** learns what a correct pose looks like from thousands of solved structures. A **standard docking engine** adds up physical terms such as sterics and hydrogen bonds. Running one of each and comparing is worth more than trusting either alone.

## Effort

| | |
|---|---|
| **Quick** | For a first look or a large library, when you mainly want a ranking. |
| **Standard** | The usual choice, and a good balance of time and a steady score. Start here. |
| **Thorough** | For a final answer on a molecule that matters, or a pocket that is large or flexible. |

## Step 5. Batch results

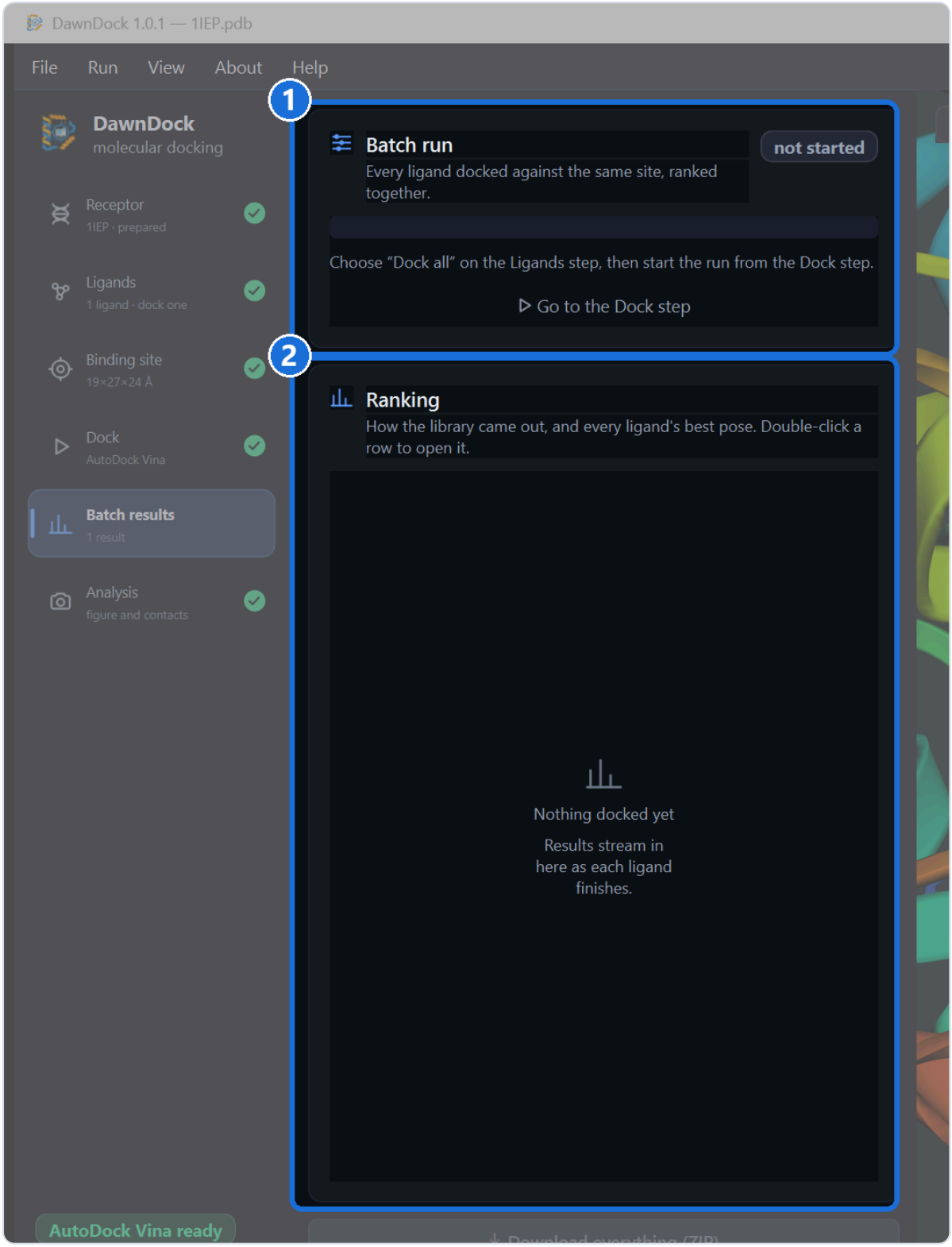



**Figure 20.** The Batch results step, for when you dock a whole library.

1. **The run.** Starts a batch over every ligand in your library, and shows how far it has got.
2. **The ranking.** Every ligand with its best score, best first. Click a row to load that result into the inspector and the 3D view.

A batch is the normal way to screen a set of compounds. Add a folder of molecules on the Ligands step, set the mode to `Dock all`, and run.

## Step 6. Analysis

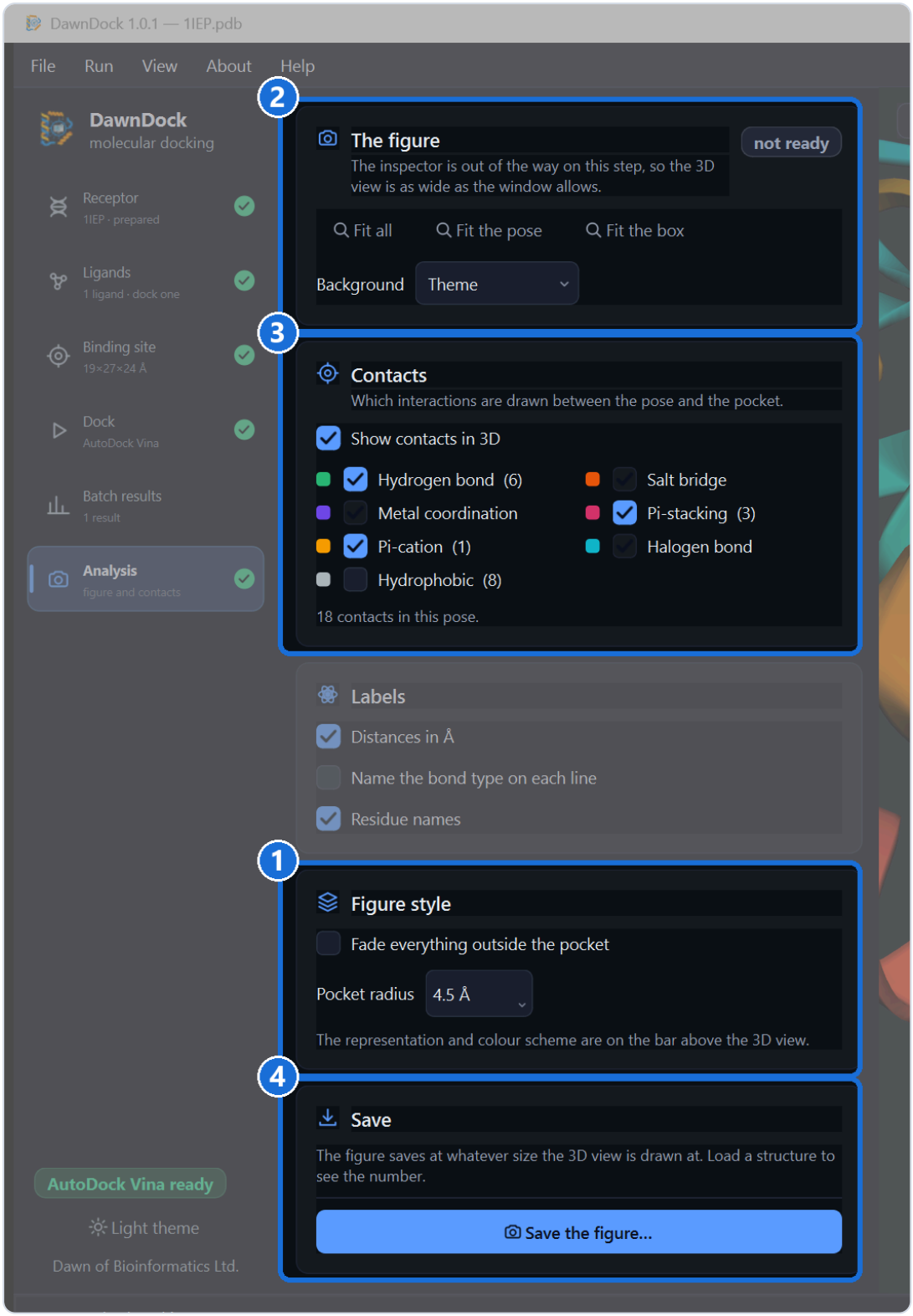



**Figure 21.** The Analysis step. The inspector steps aside so the 3D view gets the rest of the window.

1. **Style.** How the protein is drawn, what the colours mean, and whether a surface is shown.
2. **View.** What is visible: the whole protein or just the pocket, the search box, the reference molecule, the background colour.
3. **Contacts.** Which interaction types are drawn as dashed lines, and whether their distances are labelled.
4. **Save.** Writes the figure as a PNG at the size shown.

# The results inspector




**Figure 22.** The inspector on the right, after a run.

1. **The headline.** The ligand name, the engine, how many poses and how long it took, then the best **affinity** in kcal/mol and the **ligand efficiency**, which is the affinity divided by the number of heavy atoms. Ligand efficiency lets you compare a small molecule fairly with a large one.
2. **Poses.** Every pose, best first, with its affinity and its RMSD from the best pose. RMSD is a distance in angstroms: a small value means the pose is close to the top one, a large value means it is a genuinely different arrangement.
3. **Interactions.** The contacts the selected pose makes. The `Pocket` tab lists the residues lining the site, and `Engine log` shows exactly what the engine printed.
4. **Saving.** `Download everything (ZIP)` writes the poses, the prepared receptor, the scores and the log in one archive. The separate buttons save just the poses, the complex, or the picture.

### Rescoring

`Rescore with GNINA` takes poses you already have and scores them again with the neural network. It is the cheapest way to improve a ranking, because the slow search has already been done.

## The menus

| | |
|---|---|
| **File** | Open a receptor, add ligands, save and open a session, set up the docking engines, and quit. |
| **Run** | Start and stop a docking run, and clear the current results to set up another. |
| **View** | Jump straight to any of the six steps, and switch between the light and dark themes. |
| **About** | The version, the author, and buttons that open the licence and the third-party notices in a window you can read and copy from. |
| **Help** | `Getting started` (F1), `Check for updates`, and `Copy diagnostics`, which puts everything worth pasting into a bug report on the clipboard. |

# Troubleshooting

These are the messages DawnDock actually shows, and what to do about each.

## Messages about the order of work

| Message | What to do |
|---|---|
| **Load a receptor first.** | Nothing is loaded yet. Go to the Receptor step and open a structure file. |
| **Prepare the receptor first (Receptor step, Prepare receptor).** | The structure is loaded but not prepared. Click Prepare receptor. |
| **Select a ligand on the Ligands step.** | No molecule is selected. Add one, then click it in the library. |
| **Add at least one ligand on the Ligands step.** | The library is empty. Add a file, a folder, or a SMILES string. |
| **Tick at least one chain to keep.** | You have unticked every chain in the Structure card. Tick at least one. |
| **A docking run is already going.** | Wait for it, or stop it from the Dock step. |
| **Dock something first. / Run a docking first.** | You asked for a result that does not exist yet. Run a docking. |

## Problems preparing a structure

| Message | What it means and what to do |
|---|---|
| **This structure has no polymer residues.** | The file holds no protein chain, only small molecules. Check you opened the right file. |
| **The prepared receptor came out empty.** | Everything was stripped away. This usually means every chain was unticked, or the file holds only water and additives. |
| **Meeko could not prepare the ligand.** | The molecule has something the preparation cannot handle, often an unusual valence or a broken bond block. Try the molecule as a clean SDF, or build it from SMILES instead. |
| **The receptor PDBQT carries no partial charges.** | Preparation finished but produced no charges, so the score would be meaningless. Prepare again, and if it persists try the structure without the modified residue. |
| **Could not read [file].** | The file is not in a format DawnDock reads, or it is damaged. Check the format list in File formats you can use. |
| **Invalid SMILES.** | The string could not be parsed. Check for a missing bracket or a stray character. |

## Problems with an engine

| Message | What it means and what to do |
|---|---|
| **Could not start [engine].** | The engine is not installed or cannot run. Open File, Docking engines and install it from there. |
| **No neural-network engine is installed.** | Rescoring needs GNINA. Install it from the engine setup window. |
| **AutoDock 4 produced no docked poses.** | Almost always the search box. Check the box sits on the pocket and is big enough for the molecule. |
| **LeDock produced no docked poses.** | The same check. LeDock also needs a ligand with real 3D coordinates, so build it from SMILES or load a 3D SDF. |
| **LeDock looks frozen.** | It is not. LeDock prints nothing while it works. Give it time. |
| **No OpenMM platform on this machine could run the minimisation.** | Minimisation could not start. Prepare the receptor without minimising. |

## When the answer looks wrong

| What you see | What it usually means |
|---|---|
| **Every affinity is 0.00** | The engine searched empty space. The search box is not on the pocket. Go back to the Binding site step and set it again. |
| **No contacts are listed** | The pose is not touching the protein, which again points at the box. |
| **The ligand sits outside the protein** | The same cause. Look at the pink cage in the 3D view. |
| **The score changes between runs** | Normal. Docking searches at random. A few tenths of a kcal/mol is expected. Raise the Effort for a steadier number. |
| **The pose is upside down but scores well** | This happens in symmetric pockets. Compare with a reference molecule if you have one. |

## If you need to report a problem

Open Help, then Copy diagnostics. This copies the version, your results folder, every engine it found with its version, and the OpenMM build, which answers most of the first questions anyone would ask. If the program closed unexpectedly, there may also be a log at:

`%APPDATA%\DawnDock\crash.log`

Send that text, and say what you were doing when it happened.

# How to cite DawnDock

If DawnDock helped with work you publish, please cite it:

> Ahmed, S. F. (2026). *DawnDock: a multi-engine GUI application for molecular docking with deep learning scoring* (Version 1.0.1) [Computer software]. Dawn of Bioinformatics Ltd. https://doi.org/10.5281/zenodo.24198678

That is the form APA gives for software, and it is the same citation the program shows under **Help**, then **About**, where it can be copied straight out. Every version has its own DOI and a published one is never repointed, so a paper points at the exact version its results came from.

Please also cite the engine you actually used. DawnDock runs these programs, it does not replace them, and their authors deserve the credit:

| | |
|---|---|
| **AutoDock Vina** | Eberhardt, J. et al. (2021) *J. Chem. Inf. Model.* **61**, 3891. Trott, O. & Olson, A. J. (2010) *J. Comput. Chem.* **31**, 455. |
| **AutoDock 4** | Morris, G. M. et al. (2009) *J. Comput. Chem.* **30**, 2785. |
| **Smina** | Koes, D. R., Baumgartner, M. P. & Camacho, C. J. (2013) *J. Chem. Inf. Model.* **53**, 1893. |
| **GNINA** | McNutt, A. T. et al. (2021) *J. Cheminform.* **13**, 43. |
| **LeDock** | Zhao, H. & Caflisch, A. (2013) *Bioorg. Med. Chem. Lett.* **23**, 5721. |

# Support

Questions, problems and licence enquiries:

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### A word on what docking can tell you

A docking score is an estimate from a scoring function. It is not a measured binding free energy, and it does not reliably predict how potent a compound will be. Poses, scores and rankings are predictions, and they can be wrong. Treat a docking result as a hypothesis to test in the laboratory, not as an answer.

DawnDock is a research tool. It is not a medical device and must not be used for diagnosis, treatment or any clinical decision.

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