LigPrep Command Options

The syntax of the `ligprep` command is as follows.

`$SCHRODINGER/ligprep` [*options*|*meta-options*] {`-imae`|`-isd`|`-ismi`|`-icsv`} *infile* {`-omae`|`-osd`} *outfile*

The options are listed in Table 1, grouped by stage. The meta-options are listed in Table 2, and the action of the meta-options is explained in Table 3. The `ligprep` command also supports the standard Job Control options, which are described in Section 2.3 of the *Job Control Guide*. Other job options, including options for distribution over multiple processors, are listed in Table 4.

Table 1. Options for the ligprep command

Option	Definition
General	
`-a`	Append structures to the output file. Default is to overwrite the output file if it already exists.
`-inp` *filename*	Use input file to obtain values for options. Values given on the command line supersede values given in the input file.
`-kp` | `-keep_props`	Transmit properties from input to output at each stage, and retain properties in the output structure file. The `ionizer` and `bmin` delete properties by default.
`-ma` *number*	Skip over structures containing more than this number of atoms in some steps. Sets the `-ma` option for those steps. Default: 200.
`-n` *structs*	Specify a comma-delimited series of colon-separated ranges and single values to convert. For example: `1:10,14` Structures 1 through 10, and 14 `2:` Structures 2 through end of file `:5,13:18` Structures 1 through 5, and 13 through 18 Default: `1:` (convert all structures)
`-nc`	Do not remove intermediate files. Default is to remove intermediate files.
`-np`	Remove files containing problematic structures. Default is to keep problematic structure files.
`-nz`	Do not create tar archive of intermediate files. Default is to create a tar archive.

`-R {b|c|d|e|f|h|i|n|p|r|s|t}`	Run only the stage of ligand preparation specified by the letter code:
	`b` `bmin` minimization — `i` `ionizer`
	`c` `sdconvert` — `n` `neutralizer`
	`d` `desalter` — `p` `premin`
	`e` `epik` — `r` `ring_conf`
	`f` filter (`ligfilter`) — `s` `stereoizer`
	`h` `applyhtreat` — `t` `tautomerizer`
	Structure file conversion is done automatically with any `-R` option; `c` is retained for backward compatibility.

`-readinp` *filename*	Read the command options from the specified LigPrep input file, print them out, and then stop. Not valid with `-writeinp`.
`-runinp`	Run the LigPrep job when writing out the LigPrep input file. Only valid in conjunction with `-writeinp`.
`-run_from {b|cf|d|e|f|h|i|n|p|r|s|t}`	Run the ligand preparation job, starting from the stage specified by the letter code. The letter codes are the same as for `-R`.
`-sif_docs`	Display documentation for the LigPrep (simplified) input file, and exit.
`-verb`	Report on the progress of the ligand preparation.

Table 1. Options for the ligprep command (Continued)

Option	Definition

`-W` *string*	Options for various stages of ligand preparation. *string* consists of comma-separated designators. The first designator specifies the program that options are to be passed to and must be one of:
	`ci` `sdconvert` on input structures
	`co` `sdconvert` on output structures
	`e` `epik`
	`f` filter (`ligfilter` or `ligparse`)
	`i` `ionizer`
	`r` `ring_conf`
	`s` `stereoizer`
	The remaining designators are passed to the program in the order specified with the commas removed. For example: `r,-l,1,-n,16` passes the arguments `-l 1 -n 16` to `ring_conf`. Multiple `-W` options are permitted, but only the last one pertaining to a particular program is used. For `ring_conf` and `stereoizer`, these options are used in addition to the default options and override redundant specifications.
	When `ligparse` is in use, it is passed the following arguments by default: `-any -j 5` (filter by rejecting structures if any criteria listed in the filter file are matched). If the `-W` option is used to pass arguments to `ligparse`, the default set of arguments is not used by `ligparse`.

`-writeinp` *filename*	Write the command options to the specified LigPrep input file.
Desalting	
`-nd`	Do not use the `desalter`. Default is to use the `desalter`.
Ionization	
`-emb`	Use the Epik metal binding option for ionization and tautomerization of ligands bound to protein metals. An alternative form of this option is `-epik_metal_binding`.
`-epik`	Use Epik for the ionization and tautomerization stages.
`-es` *filename*	Use the specified nonstandard Epik pK_a file.
`-etl` *time*	Epik time limit per input structure, in seconds. Default: 60.
`-i` *number*	Ionization treatment `0` Do not neutralize or ionize. `1` Neutralize only. `2` Neutralize and ionize. Default: 1. Ionization is performed by default with the `ionizer`. If `-epik` is used, this option only controls neutralization.
`-is` *filename*	Use non-standard `ionizer` specification file, named *filename*.
`-mbs` *filename*	Use the specified nonstandard Epik metal binding file.
`-mg` *number*	Instruct `ionizer` to skip structures that have more than this number of ionizable groups. Default: 10
`-ph` *value*	Set the target (effective) pH to the specified value.
`–pht` *value*	Set the pH tolerance for generated structures to the specified value. The minimum probability for generated states is determined from $-\log_{10}(p) =$ *value*. When tautomerization is disallowed, this is equivalent to keeping structures whose pK_a value lies within *value* units of the target pH value.
Tautomerization	
`-emb`	Use Epik metal binding option for ionization and tautomerization of ligands bound to protein metals. An alternative form of this option is `-epik_metal_binding`.
`-epik`	Use Epik for the ionization and tautomerization stages.
`-mbs` *filename*	Use the specified nonstandard Epik metal binding file.

Table 1. Options for the ligprep command (Continued)

Option	Definition
`-nt`	Do not generate tautomers. Default is to generate tautomers.
`-t` *number*	Generate up to *number* tautomers per input structure. Default: 8
`-ts` *filename*	Specify a custom tautomer database.
`-tp` *number*	Set the minimum tautomerization probability to *number*, where 0 < *number* < 1.0. Structures with net tautomerization probabilities lower than this value are not retained. Default: 0.01
Stereoisomers	
`-ac`	Do not respect existing chirality properties or use chiralities from the input geometry. Generate stereoisomers for all chiral centers up to the number permitted (specified using the `-s` option).
`-g`	Respect chiralities from input geometry when generating stereoisomers. For chiral centers whose chirality cannot be determined from the input geometry, stereoisomers will be generated.
`-ns`	Do not generate stereoisomers. Chiral properties in the input file are still enforced. You should not normally need to use this option. If you use this option, you should also use `-nr` to suppress ring conformations. Default is to generate stereoisomers.
`-s` *number*	Generate up to *number* stereoisomers per input structure. Default: 32
Ring conformations	
`-l` *number*	Control how `ring_conf` handles atoms that are not in flexible rings. `1` Use input geometries. `2` Use idealized geometries even for rigid rings. `3` Use idealized geometries for non-ring portions and input geometries for rigid rings. Default: 3
`-nr`	Do not generate ring conformations. You should not normally need to use this option. Default is to generate ring conformations.
`-r` *number*	Generate up to *number* ring conformations per input structure. Default: 1
`-re` *number*	Generate ring conformations with energies lower than *number* (kJ/mol) relative to the lowest energy conformer. This number sets the maximum number of ring conformers to 8 unless a different number is provided using the `-r` option.
Filtering	
`-f` *filename*	Filter structures using filtering criteria from *filename*. Default: do not filter.
`-fc` *filename*	Use custom composite descriptors for `ligparse` from *filename*. Only valid when used with `-f` and `-use_ligparse`. Default: use composite descriptors from `composite.types` file in the installation.
`-fs` *filename*	Use custom SMARTS patterns (descriptors) for `ligparse` from *filename*. Only valid when used with `-f` and `-use_ligparse`. Default: use composite descriptors from `str_keys.types` file in the installation.
`-lab`	Add an internal tracking label that can be used for filtering.
`-lab_filter` *options*	Filter the output based on the tracking labels introduced with `-lab`, which is turned on by this option. The filtering process is controlled by the options. Only one option is supported: `ionizer:`*n*—select at most *n* output structures for each ionizer input structure such that the formal charge on each ionizable group is minimized.
`-lp`	Include calculated `ligfilter` properties in the output structure file. Not valid with `-use_ligparse`, which includes properties by default.
`-use_ligparse`	Use `ligparse` for filtering. Default: use `ligfilter`.
Final optimization	
`-bff` *number*	Instruct `bmin` to use the force field specified. Only 10 (MMFFs), 11 (OPLS_2001), and 14 (OPLS_2005, default) are supported.

Table 1. Options for the ligprep command (Continued)

Option	Definition
`-bvac`	Perform `bmin` minimization in a vacuum. By default `bmin` minimizations are carried out using a distance-dependent dielectric.
`-br`	Instruct `bmin` to discard structures with incorrect chiralities.
`-bns`	Instruct `bmin` to perform minimizations only. By default, `bmin` performs short conformational searches on distorted structures.
`-btc` *number*	Torsional constraints to use in `bmin`. `-1` Do not use torsional constraints. `0`, `1` Torsional constraints for C=C, carboxylic acids, esters and amides. `2` Torsional constraints for C=C.
`-bts` *number*	Torsional sampling level to use in `bmin`. Overrides the `-btc` option and sets it to 1. 0 Restricted 1 Intermediate 2 Enhanced 3 Extended For a definition of the levels, see page 80 of the *MacroModel User Manual*

Table 2. Meta-options for the `ligprep` *command. Suffix values are given for each meta-option that requires a suffix.*

Option	Description
`-adjust_`*suffix*	Adjust to a suitable state. Any combination of `c` (chirality), `i` (ionization states) or `t` (tautomers) can be used for *suffix*.
`-expand_`*suffix*	Aggressively expand states. Any combination of `c` (chirality), `i` (ionization states) or `t` (tautomers) can be used for *suffix*.
`-pcp`	Run CombiGlide protocore preparation.
`-retain_`*suffix*	Retain the original state in the output. Any combination of `c` (chirality), `i` (ionization states) or `t` (tautomers) can be used for *suffix*. Suffix values determine which state is kept. If *suffix* is `i`, both the original ionization state and the original tautomer are retained. If no suffix value is given (i.e. just `-retain` is specified), input structures are not retained, but chemically redundant structures resulting from the same input structure are eliminated.
`-unt`	Run `stereoizer`, `premin` and `bmin` to untangle structures. Used by CombiGlide.
`-vary_`*suffix*	Generate a small number of states. Any combination of `c` (chirality), `i` (ionization states) or `t` (tautomers) can be used for *suffix*.
`-vcs` *functional-group*	Run CombiGlide reagent preparation.

Table 3. Action performed by meta-options.

Suffix	Action of `adjust`	Action of `vary`	Action of `expand`
`c`	Produce only one stereoisomer	Produce at most 2 stereoisomers	Produce at most 32 stereoisomers
`i`	Produce the ionization state with the lowest overall penalty	Set pH tolerance to 1.0	Set pH tolerance to 2.0
`t`	Produce only the most probable tautomer	Produce at most the 2 most probable tautomers	Produce at most the 8 most probable tautomers

Table 4. Other job options specifically supported by the ligprep command.

Option	Description
`-first` *firstlig*	First ligand to include. Default 1.
`-HOSTFILE` *filename*	The name of the hosts file to use for this run. The default hosts file is the installed version of `schrodinger.hosts`.
`-j` *subjobs*	Only run the specified subjobs. The subjobs list can be a comma-separated list of subjob numbers or ranges in the format *n*`:`*m*. If spaces are included, the list must be quoted. Example: `1:5,14,18`. Default: run all subjobs.
`-JOBCTS` *number*	Maximum number of structures (CTs) in any subjob. Default: 10000.
`-last` *lastlig*	Last ligand to include. Default: last ligand in the file.
`-LOCAL`	Do not use a temporary directory for intermediate files. Keep files in the current working directory.
`-MAX_RETRIES` *number*	Maximum number of times a subjob is retried before it is regarded as failed.
`-NJOBS` *jobs*	Divide the job into at least the specified number of subjobs. The specified number is increased if the limit on the number of structures per subjob is exceeded. The number of subjobs can be greater than the number of processors used. For efficient load balancing the number of subjobs should be several times the number of processors. Default: 1.
`-NO_JOBCONTROL`	Do not use Job Control to run the job, and print LigPrep messages to *jobname*`.log`. The job runs locally, and you are responsible for all file handling. This option is mainly useful in scripts.
`-NOJOBID`	Do not use Job Control to run the job, and print LigPrep log file contents to the screen. The job runs locally, and you are responsible for all file handling. This option is mainly useful in scripts.
`-nx`	Do not run jobs, but create specified subjob directories and input structure files locally.
`-OUTPUT_ORG` *option*	Produce more than one output structure file. If *option* is `BY_SUBJOB` then produce one output file for each subjob. Otherwise, create a new directory called *option* and create separate output files for each input ligand within this new directory.
`-RESTART`	Restart the previously failed parent job, running only the subjobs that did not finish. This facility works only for local jobs (i.e. jobs started with `-LOCAL` and `-nc`).
`-STRICT_END`	Terminate the job if any of the subjobs fails.
`-SUBHOST` *host-list*	Specify the hosts for the subjobs. *host-list* is a list of one or more hosts. The list must be quoted if multiple hosts are specified: for example, `"hostname1:nprocs1 hostname2:nprocs2..."` Default: `localhost:1`