# SimSite3D gen_points reference sheet

**Purpose:** The intended use of gen_points is to generate query sitemaps or a small number of sitemaps. If you wish to generate a large number of sitemaps, please consult the documentation for auto_gen_sitemaps.py.

Note: `<text>` : denotes a required argument supplied by a user
`[text]` : denotes an optional argument supplied by a user

## Getting help on screen

- Short help:
  **gen_points** `[--usage]`
- Longer help:
  **gen_points --help**
- Getting the version of gen_points:
  **gen_points --version**

## Building sitemaps with gen_points – Note: a protein flag with pdb file and either a ligand flag with mol2 file or a sphere is required

- Building a sitemap from ligand volume with an optional output filename:
  **gen_points -p** `<XXXXXX_p>`**.pdb** `-l <XXXXXX_l>`**.mol2** `[path_to_store_sitemap]`
- Building a sitemap using a sphere with an optional output filename:
  **gen_points -p** `<XXXXXX_p>`**.pdb --sphere** `"Cx Cy Cz r" [path_to_store_sitemap]`
  `(where C = (Cx,Cy,Cz) is the center of the sphere and r is the radius)`
- Specifying a temporary directory (disk space used by gen_points for temporary files while building sitemaps):
  **gen_points --scratch_dir <path/to/temporary/directory>**
- Building a sitemap without computing the normalization stats (Note: this option is not recommended if you intend to use the sitemap as a query since the normalization will only be delayed till search time)
  **gen_points --no_normalization**
- Specifying a directory other than your current directory to save the sitemap
  **gen_points --proj_output** `<saved/sitemap/directory>`

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## gen_points <u>expert</u> options

- Including all metals in the binding site (and in the protein PDB file) as part of the protein:

  **`gen_points --include_metals`**
- Including listed waters in the binding site as part of the protein:

  **`gen_points --waters`** `<"H2O residues">`

NOTE: waters in PDB files must be specified exactly with respect to their chain id, residue number, and insertion code. As an example, the using the flag `--waters "55W 101 A64W"`, the residues will be interpreted as:

- `"101"`: as residue 101 with blank insertion code and blank chain identifier
- `"55W"`: as residue 55 with insertion code W and blank chain identifier
- `"A64W"`: as residue 64 with insertion code W and from chain A

Specified residues that do not exist in the PDB file will be ignored and will generate a warning message.