



twwistPDB Overview

TWWISTPDB

[Overview](#)

[twwistPDB Help Output](#)

[twwistPDB Tutorial](#)

twwistPDB Overview

twwistPDB transforms the coordinates of one PDB file to the reference frame of another pdb file. The transformed first PDB file is output as a new PDB file. The coordinate transformation is specified as 3 specific atoms from the first PDB file to be respectively mapped to 3 specific atoms of the second reference PDB file.

twistPDB Help Output ("twistPDB -h" output)

NAME

twistPDB (version 1.3.0) -- maps pdb file1 to pdb file2

SYNOPSIS

twistPDB [options] pdb1_fn pdb1_pt1 pdb1_pt2 pdb1_pt3 pdb2_fn pdb2_pt1 pdb2_pt2 pdb2_pt3

required (in order!):

pdb1_fn pdb filename for first set of 3 points
 pdb1_pt1 number of first atom in first set
 pdb1_pt2 number of second atom in first set
 pdb1_pt3 number of third atom in first set
 pdb2_fn pdb filename for second set of 3 points
 pdb2_pt1 number of first atom in second set
 pdb2_pt2 number of second atom in second set
 pdb2_pt3 number of third atom in second set

CHARACTER OPTION	KEYWORD OPTION	DESCRIPTION	DEFAULT
-a <model#> --model1=<model#>	... MODEL number of pdb1ptX in pdb1_fn	... first model
-b <model#> --model2=<model#>	... MODEL number of pdb2ptX in pdb2_fn	... first model
-d --list list point values no list
-e --exact process points in exact order reorder
-m --minimize average new pdb1 to pdb2 distances	... no average
-o <filename>	.. --output=<filename>	. output filename for modified pdb1_fn	. stdout
-x --extend extend pdb1_point3 and pdb2_point3	... constrict
-h --help prints help (Enter 'twistPDB -h' for help.)	
<NO OPTIONS> shorter option synopsis (Enter 'twistPDB'.)	
	--license prints license terms for twistPDB.	

DESCRIPTION

twistPDB maps pdb1_fn atom coordinates to pdb2_fn coordinates.
3 points must be specified, by ATOM # or HETATM #, for both pdb files.
For ambiguous ATOM # or HETATM #, one or more MODEL # must be provided.
Option '--model1=' ('-a') specifies the MODEL number of the specified pdb1_fn atoms.
Option '--model2=' ('-b') specifies the MODEL number of the specified pdb1_fn atoms.

By default, the first set of points is mapped onto the second set of points.
By using the option '--extend' ('-x'), pdb1_pt3 and pdb2_pt3 atoms will be extended away from each other.

twistPDB translates the coordinates of pdb1_fn to align the first points and then rotates the coordinates of pdb1_fn to align the second and third points. By default, twistPDB reorders points to minimize alignment error, such that the distance from point1 to point2 is the longest distance, and the distance from point1 to point3 is the shortest distance. Using option '--exact' ('-e') overrides this default behavior, causing the points to be processed in the exact order listed.

Option '--minimize' ('-m') averages the distances between the new pdb1 points and the existing pdb2 points.

Option '--output=' ('-o') specifies the output filename. If option '--output=' ('-o') is not present, output will be written to stdout.

New "REMARK 250" lines will be added to the output PDB specifying execution details.

Errors and warnings go to stderr.

EXAMPLE

The twistPDB command, below, maps the Streptococcus pneumoniae R6 (3H72) neuraminidase atoms numbered 207, 1957, and 2569 to the influenza A (1W1X) N6 neuraminidase atoms numbered 3302, 4122, and 4520, respectively, resulting in a new pdb file, STRontoN6.pdb. This new output file consists of the original Streptococcus (3H72) coordinates transformed to be in the same orientation as the N6 neuraminidase (1W1X) coordinates; no relative position within the 3H72 structure was changed.

With keyword options:

```
twistPDB --output=STRontoN6.pdb 3H72.pdb 207 1957 2569 1W1X.pdb 3302 4122 4520
```

With character options:

```
twistPDB -o STRontoN6.pdb 3H72.pdb 207 1957 2569 1W1X.pdb 3302 4122 4520
```

LICENSE INFORMATION

twistPDB is a software program from Arthur Weininger (www.weiningerworks.com).
twistPDB is subject to a license; use the keyword option '--license' in order to view the license terms. Your use of this software constitutes an agreement to the license terms. Do not use this software if you do not agree to the license terms.

twistPDB Tutorial

twistPDB Tutorial Page gives examples of using **twistPDB**.

The **Picornavirus Monograph Superposition Shell Script** gives examples of using **twistPDB**.

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