

SymD Manual and Examples

SymD (Symmetry Detection)

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Manual and Examples

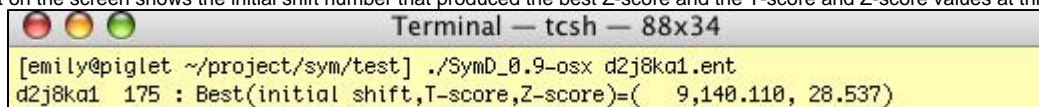
Input:

The input to SymD is a protein structure in PDB format. File extension should be **.ent** or **.pdb**.

The input to mAxesD is the -info.txt output from SymD. File extension should be **-info.txt**.

Output Options:

The default output on the screen shows the initial shift number that produced the best Z-score and the T-score and Z-score values at this initial shift.

A terminal window titled "Terminal — tcsh — 88x34" showing the execution of SymD. The command is `./SymD_0.9-osx d2j8ka1.ent`. The output is `d2j8ka1 175 : Best(initial shift,T-score,Z-score)=(9,140.110, 28.537)`.

```
Terminal — tcsh — 88x34
[emily@piglet ~/project/sym/test] ./SymD_0.9-osx d2j8ka1.ent
d2j8ka1 175 : Best(initial shift,T-score,Z-score)=( 9,140.110, 28.537)
```

In addition, two files are generated: **-info.txt** and **-trfm.pdb**.

The format of "info" file (information file): The first 2 rows give the input PDB file name and the number of residues in the structure. The next 8 rows give information for the sequence alignment/structure superposition that gave the best Z-score. Disregard the last 2 items ('Derived unit angle' and 'Derived unit pitch'), as these were derived from an old algorithm, which was found to be unreliable. These lines are followed by a line of column headers and then by a set of lines that give 7 columns of numbers. The 7 columns are described below. The number of lines after the column header is 3 less than the protein length, one line for each initial shift.

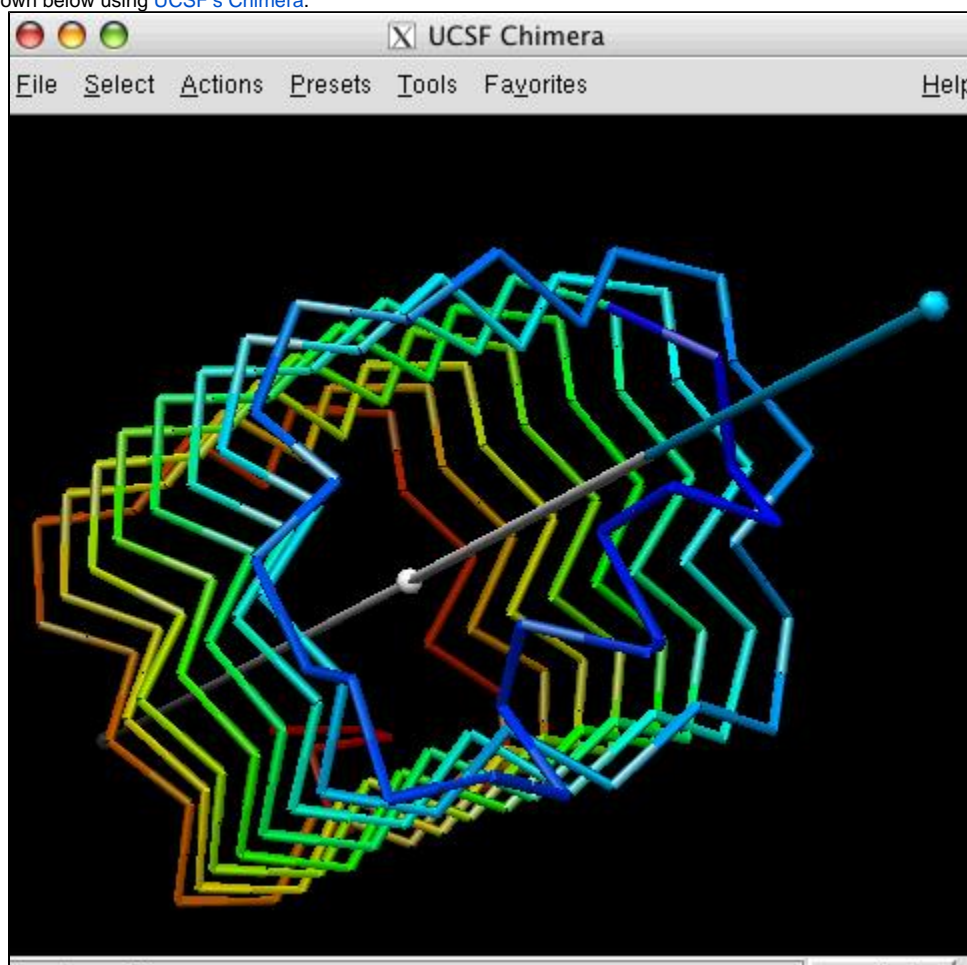
Column Descriptions

- 1) IS: Initial Shift = The number of residues shifted initially for circular permutation and initial alignment.
- 2) Len: The number of aligned residues in the RSE-refined alignments.
- 3) Angle: Rotation angle for the structure superposition according to the RSE-refined alignment.
- 4) Pitch: Translation along the rotation axis for the structure superposition according to the RSE-refined alignment.
- 5) Z-score: Z-score for the RSE-refined alignment.
- 6) T-score: Alignment score ($=\sum(1/(1+(dij/do)^2))$). Do = 2.0 Å for version 0.9.

7) Candidate = 1, if the rotation axis of the given alignment aligns with the rotation axis of the alignment with the best T-score within $\arccos(0.95) \sim 18.2^\circ$, and 0 otherwise.

Terminal — more — 88x34						
! Protein Name: d2j8ka1						
! Protein Size: 175						
! Best IS: 9						
! Best T-score: 140.110						
! Best RMSD: 0.589						
! Best Z-score: 28.537						
! Highest-scoring angle: 179.10						
! Highest-scoring pitch: 2.45						
! Derived unit angle: 87.90						
! Derived unit pitch: 1.20						
!						
IS	Len	Angle	Pitch	Z-score	T-score	Candidate
1	174	0.00	0.000	-1.363	0.000	0
2	170	32.68	0.439	-1.363	0.000	1
3	158	54.25	0.780	-1.363	0.000	1
4	165	88.60	1.291	28.268	138.850	1
5	165	88.60	1.291	28.268	138.850	1
6	165	88.60	1.291	28.268	138.850	1
7	156	123.88	1.880	9.296	49.949	1
8	163	142.14	2.172	9.421	50.537	1
9	148	179.10	2.451	28.537	140.110	1
10	148	179.10	2.451	28.537	140.110	1
11	148	179.10	2.451	28.537	140.110	1
12	148	213.93	2.989	8.839	47.809	1
13	152	232.18	3.399	9.064	48.859	1
14	143	268.61	3.661	27.421	134.881	1
15	143	268.61	3.661	27.421	134.881	1
16	143	268.61	3.661	27.421	134.881	1
17	143	303.43	4.196	8.461	46.036	1
18	147	321.52	4.595	8.725	47.275	1
19	152	1.93	4.421	25.857	127.555	1

The "trfm" pdb file contains two chains. The first chain is the input structure transformed according to the alignment that gave the best Z-score. The second chain is made of three atoms that define the rotation axis. The three atoms (N, Ca and C) are placed at the beginning, middle and at the end of the rotation axis. The direction of the axis is such that a positive rotation angle advances a right-handed screw along the positive direction of the axis. A sample structure is shown below using [UCSF's Chimera](#).



Other options are:

-**fasta** to generate fasta alignment file for each shift.

-**structure** to generate permuted structure pdb file of each shift.

-**complete** to obtain detailed information on each shift.

First 12 lines:

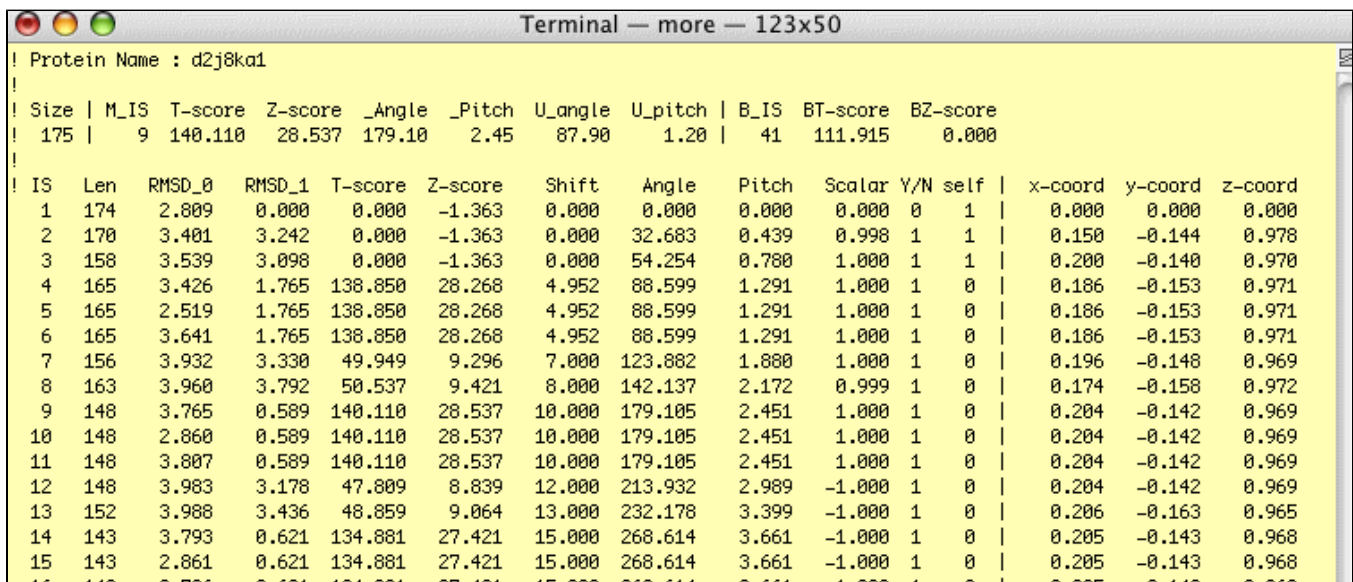
- 1) Protein Name: pdb file name
- 2) Protein Size: Number of amino acid residues
- 3) M_IS: The IS corresponding to the best T-score
- 4) T-score: The best T-score among the RSE-refined alignments for all initial shifts.
- 5) Z-score: Z-score of the best T-score.
- 6) _Angle: The rotation angle for the alignment with Tmax
- 7) _Pitch: The translation along the rotation axis for the alignment with Tmax
- 8) U_angle*: This was supposed to be the angle for one unit rotation.
- 9) U_pitch*: This was supposed to be the pitch for one unit rotation.
- 10) B_IS: The IS of the best noise alignment. An alignment is a noise alignment if the cosine of the angle between its rotation axis and that of the best alignment is less than 0.95.
- 11) BT-score: The best T-score among the noise alignments.

12) BZ-score: Z-score for the BT-score

*Disregard. These values were computed using an old algorithm, which was found to be unreliable.

Column Descriptions

- 1) IS: The number of residues shifted initially for circular permutation and initial alignment.
- 2) Len: The number of aligned residues in the RSE-refined alignments.
- 3) RMSD_0: The rmsd for the initial superposition.
- 4) RMSD_1: The rmsd for the refined superposition.
- 5) T-score: The highest alignment score among the RSE-refined alignments for all initial shifts.
- 6) Z-score: Z-score of the corresponding T-score.
- 7) Shift: Average shift (average difference in the serial numbers of the aligned residue pairs).
- 8) Angle: The translation along the rotation axis from the transformation matrix of the alignment.
- 9) Pitch: The pitch from the transformation matrix of the alignment.
- 10) Scalar: Scalar product between the axes of the alignments with Tmax and the given alignment.
- 11) Y/N: 1 if Scalar product is greater than or equal to 0.95; otherwise, 0.
- 12) self: 1 for the alignment wherein all aligned residue pairs are self-aligned ($|i-j| \leq 3$).
- 13) x-,y-,z- coord: The components for the rotation axis vector.



! Protein Name : d2j8ka1																									
!																									
! Size M_IS T-score Z-score _Angle _Pitch U_angle U_pitch B_IS BT-score BZ-score																									
! 175 9 140.110 28.537 179.10 2.45 87.90 1.20 41 111.915 0.000																									
!																									
IS	Len	RMSD_0	RMSD_1	T-score	Z-score	Shift	Angle	Pitch	Scalar	Y/N	self	x-coord	y-coord	z-coord											
1	174	2.809	0.000	0.000	-1.363	0.000	0.000	0.000	0.000	0	1	0.000	0.000	0.000											
2	170	3.401	3.242	0.000	-1.363	0.000	32.683	0.439	0.998	1	1	0.150	-0.144	0.978											
3	158	3.539	3.098	0.000	-1.363	0.000	54.254	0.780	1.000	1	1	0.200	-0.140	0.970											
4	165	3.426	1.765	138.850	28.268	4.952	88.599	1.291	1.000	1	0	0.186	-0.153	0.971											
5	165	2.519	1.765	138.850	28.268	4.952	88.599	1.291	1.000	1	0	0.186	-0.153	0.971											
6	165	3.641	1.765	138.850	28.268	4.952	88.599	1.291	1.000	1	0	0.186	-0.153	0.971											
7	156	3.932	3.330	49.949	9.296	7.000	123.882	1.880	1.000	1	0	0.196	-0.148	0.969											
8	163	3.960	3.792	50.537	9.421	8.000	142.137	2.172	0.999	1	0	0.174	-0.158	0.972											
9	148	3.765	0.589	140.110	28.537	10.000	179.105	2.451	1.000	1	0	0.204	-0.142	0.969											
10	148	2.860	0.589	140.110	28.537	10.000	179.105	2.451	1.000	1	0	0.204	-0.142	0.969											
11	148	3.807	0.589	140.110	28.537	10.000	179.105	2.451	1.000	1	0	0.204	-0.142	0.969											
12	148	3.983	3.178	47.809	8.839	12.000	213.932	2.989	-1.000	1	0	0.204	-0.142	0.969											
13	152	3.988	3.436	48.859	9.064	13.000	232.178	3.399	-1.000	1	0	0.206	-0.163	0.965											
14	143	3.793	0.621	134.881	27.421	15.000	268.614	3.661	-1.000	1	0	0.205	-0.143	0.968											
15	143	2.861	0.621	134.881	27.421	15.000	268.614	3.661	-1.000	1	0	0.205	-0.143	0.968											

The example output of mAxesD is

The columns in the output for mAxesD are:

1. axis id
2. the input info file name
3. the initial shift
4. the TM-score
5. the Z score
6. the rotation angle

mAxesD example output

Terminal — tcsh — 96x5				
[emily@Roo ~/project/sym/altaxis/test] ./mAxesD d1o5ua_-info.txt				
0. d1o5ua_-info.txt	60	0.50540	8.55000	180.00000
1. d1o5ua_-info.txt	-36	0.48030	6.57000	178.70000
2. d1o5ua_-info.txt	10	0.43200	6.33000	160.60001