

SE Manual and Example

SE (Seed Extension)

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Manual and Example

Input:

The input to the SE is two superimposed structure files, in either PDB format, ASTRAL domain ent format or SHEBA env format. If the structure contains non-standard residues, these are translated to standard ones according to the translation table on the ASTRAL Web site at <http://astral.berkeley.edu/raf.html>.

Output Options:

The default output is the sequence alignment on the screen. Aligned residues are in Upper case while unaligned ones are in lower case. The secondary structure information of the sequences is shown in different colors: **red** for alpha-helix, **green** for beta-sheet and **blue** for turns. It also gives statistics of the alignment including:

- the number of residues in the structure,
- the number of aligned residues,
- m score: the number of aligned residues / the average number of residues in the two input superimposed structures.
- ma: the number of aligned residues / the number of residues in the first structure
- mb: the number of aligned residues / the number of residues in the second structure
- identical: the number of identical residues among aligned ones.

-fasta to show the statistics and the alignment in FASTA format on screen as well as in a file PDB1-PDB2.fasta.

Example:

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[piglet:se/se2.02/test] emily% ./se
SE (Seed Extension, Version 2.02)
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se [.pdb or .ent or .env] [.pdb or .ent or .env]: default sequence alignment on
the screen
se -fasta [.pdb or .ent or .env] [.pdb or .ent or .env]: sequence alignment out
put in FASTA format
The two input structures should be superimposed first.
[.pdb] pdb file
[.ent] ASTRAL domain file
[.env] environment file
[piglet:se/se2.02/test] emily%
[piglet:se/se2.02/test] emily% ./se cd03493-2fbw.pdb cd03493-1l0v.pdb

cd03493-2fbw( 75) cd03493-1l0v(100)  aligned: 73  m score:83  ma:97  mb:73
identical: 5

      10      20      30      40      50
      ....*.....|....*.....|....*.....|....*.....|....*.....|
cd03493-2fbw: 11 TSERAVSALLLGLLPAAAYLYP-----GPAVDYSL 39
cd03493-1l0v: 26 MLREGTAVPAVWFSIELIFGLfalkngpeawagfvdf lqnpvIVIINLIT 75
      10      20      30      40      50
      ....*.....|....*.....|....*.....|....*.....|....*.....|
cd03493-2fbw: 40 AAALTLHGHWGLGQVITDYvh----GDTPIKVANTGLYVLSAITFTGLCY 85
cd03493-1l0v: 76 LAAALLHTKTWFELAPKAAniivkdEKMGPETIIKSLWAVTVVATIVILF 125
      10      20      30      40      50
      ....*.....|....*.....|....*.....|....*.....|....*.....|
cd03493-2fbw:  0 85
cd03493-1l0v:  0 125
[piglet:se/se2.02/test] emily%
[piglet:se/se2.02/test] emily% ./se -fasta cd03493-2fbw.pdb cd03493-1l0v.pdb

cd03493-2fbw( 75) cd03493-1l0v(100)  aligned: 73  m score:83  ma:97  mb:73
identical: 5

The fasta format output is in cd03493-2fbw-cd03493-1l0v.fasta.
[piglet:se/se2.02/test] emily%
[piglet:se/se2.02/test] emily% cat cd03493-2fbw-cd03493-1l0v.fasta
>cd03493-2fbw
TSERAVSALLLGLLPAAAYLYP-----GPAVDYSL
AAALTLHGHWGLGQVITDYvh----GDTPIKVANTGLYVLSAITFTGLCY

>cd03493-1l0v
MLREGTAVPAVWFSIELIFGLfalkngpeawagfvdf lqnpvIVIINLIT
LAAALLHTKTWFELAPKAAniivkdEKMGPETIIKSLWAVTVVATIVILF

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