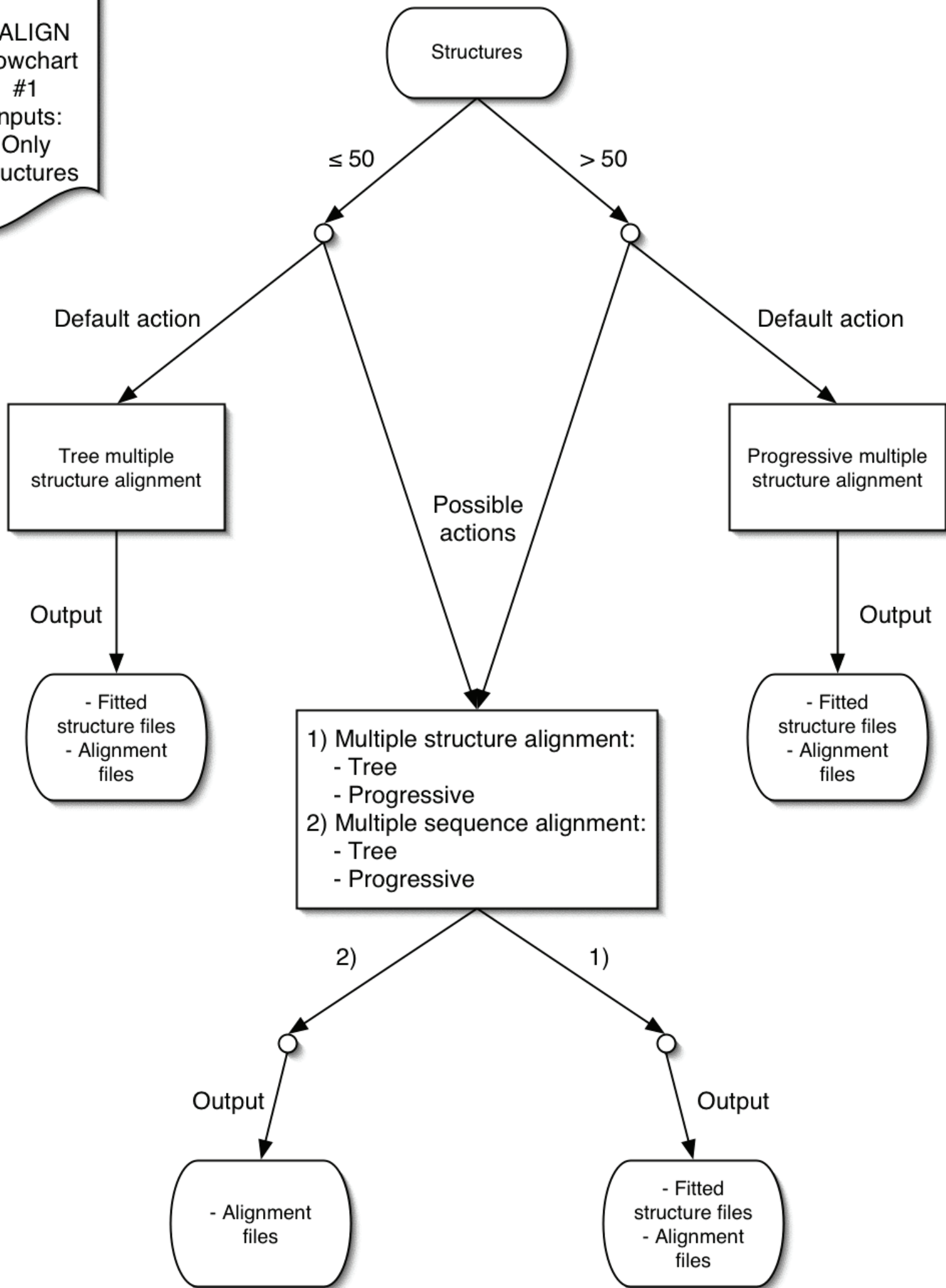
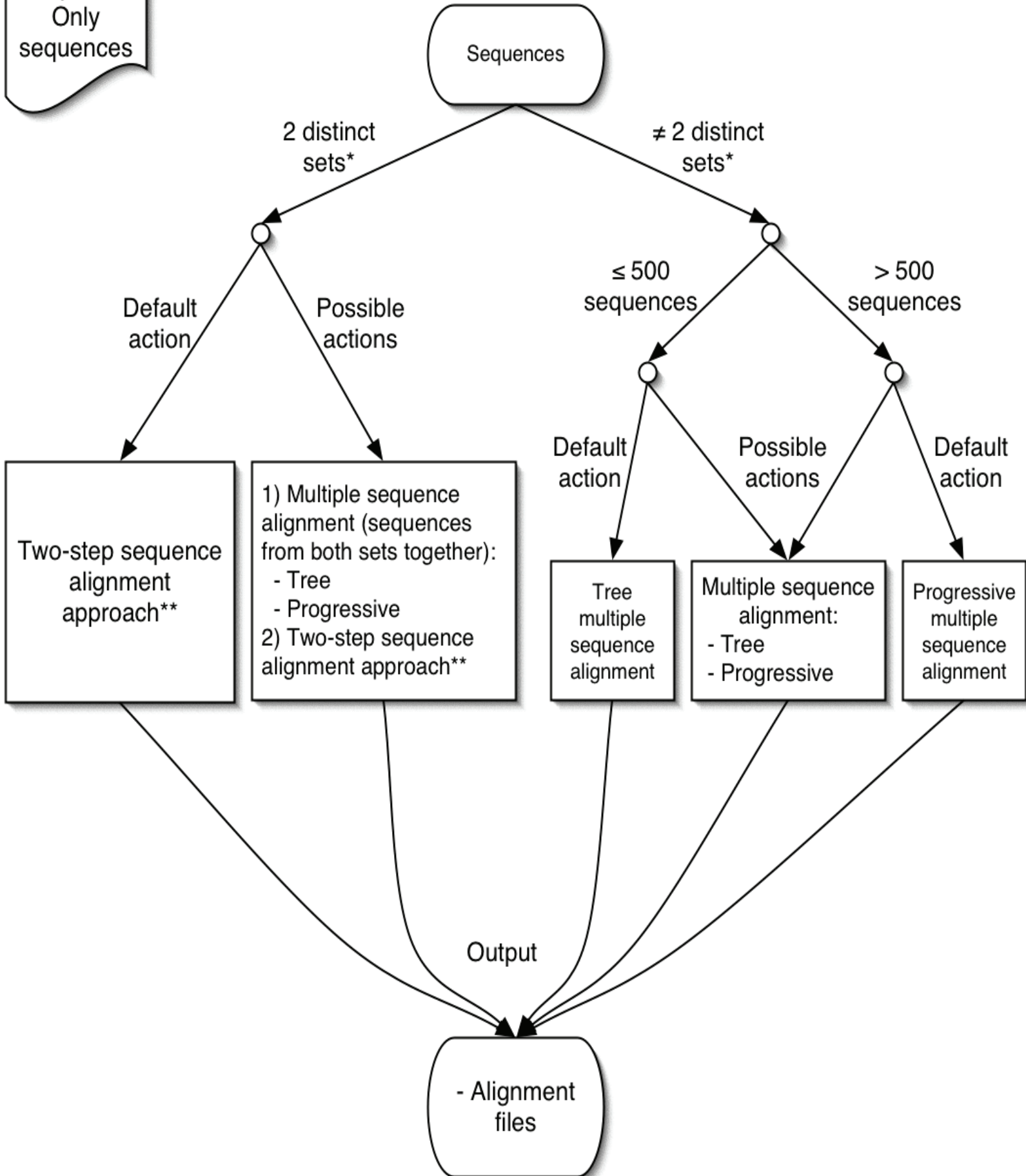


SALIGN
Flowchart
#1
Inputs:
Only
structures



SALIGN
Flowchart
#2
Inputs:
Only
sequences



SALIGN
Flowchart
#3
Inputs:
Structures
and
sequences

Structures
and
sequences

2 distinct
sets*

≠ 2 distinct
sets*

One set has
only structures

Sequences
present in
both sets

Default
action

Default
action

Default
action

Possible
actions

Structure-
sequence
alignment
approach^

Two-step
sequence
alignment
approach**

Structure-
sequence
alignment
approach^

1) Structure-sequence
alignment approach^
2) Multiple sequence
alignment (sequences
from both sets together):
- Tree
- Progressive

1) Two-step sequence
alignment approach**
2) Structure-sequence
alignment approach^
3) Multiple sequence
alignment (sequences
from both sets together):
- Tree
- Progressive

1) Structure-sequence
alignment approach^
2) Multiple sequence
alignment (all sequences
together):
- Tree
- Progressive

1),3)

2)

2)

2)

1)

1)

- Alignment
files

Output

- Fitted
structure files
- Alignment
files

This page contains descriptions of terms introduced in the flowcharts, as well as information about additional output files.

*

Set of sequences/structures:

Any number of sequences/structures that have been uploaded "together". Each uploaded alignment file is considered one set, and all pasted sequences are grouped together as one set.

**

Two-step sequence alignment approach:

Step 1: The two sets are multiply aligned (sequence-sequence) independently. Sets consisting of more than 500 entries are not aligned in step 1 and should thus be prealigned.

Step 2: The resulting alignments from step 1 are aligned to each other by matching their profiles.

Even when applied to structures, this approach does only utilize sequence information.

^

Structure-sequence alignment approach:

Step 1: Independent multiple alignments of structures (structure-structure) and sequences (sequence-sequence) are performed, regardless of the distributions in the uploaded files.

Step 2: The resulting alignments from step 1 are aligned to each other by a structure-sequence alignment if neither set contains > 50 entries. For larger sets a profile-profile alignment is performed.

In addition to the output files in the flowcharts, all output packages include MODELLER log files, which give details pertaining to the alignment process, and MODELLER input files, which can be used with any stand-alone version of MODELLER, version 8 and higher. If a tree alignment has been performed, a dendrogram file is also provided.