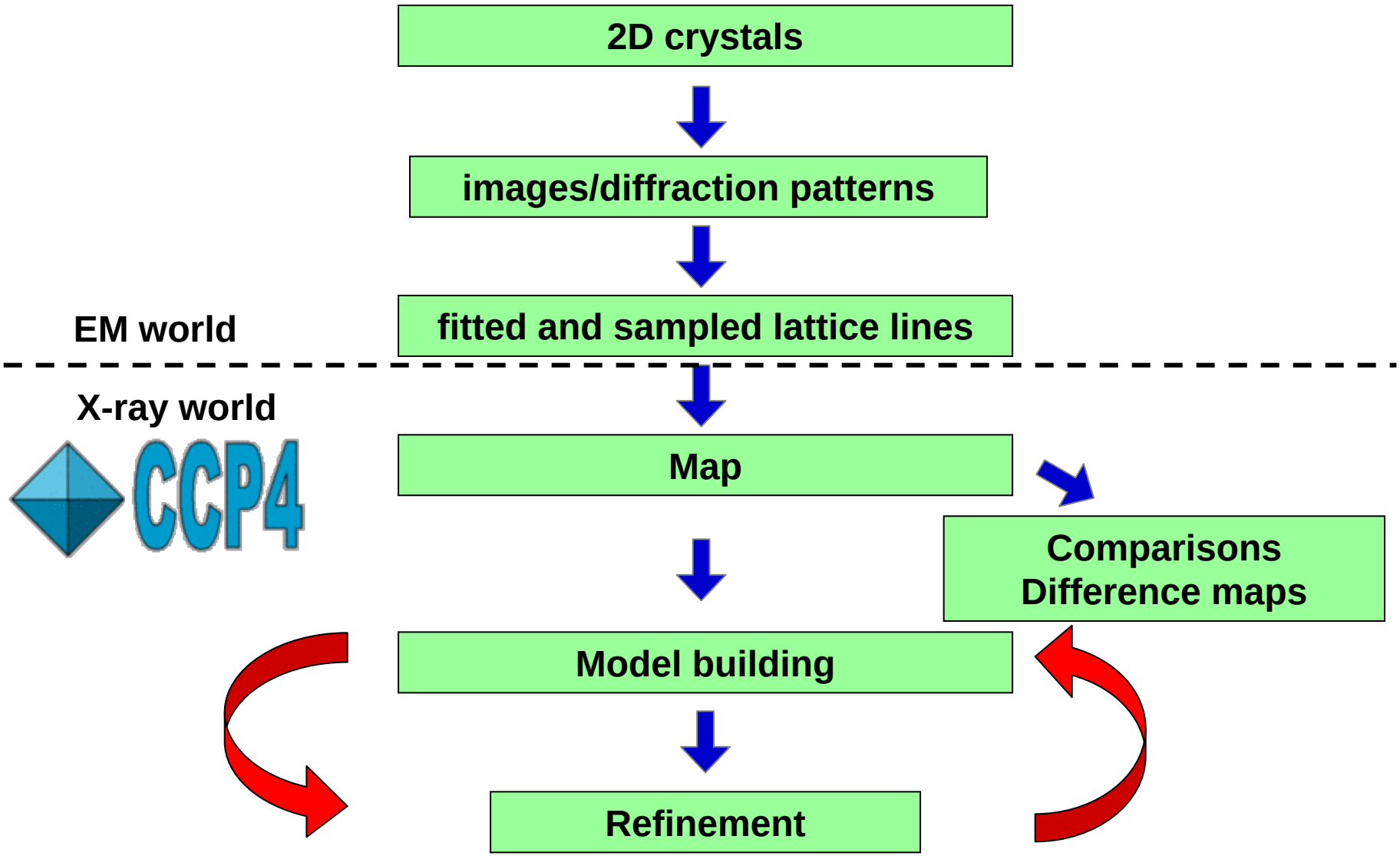
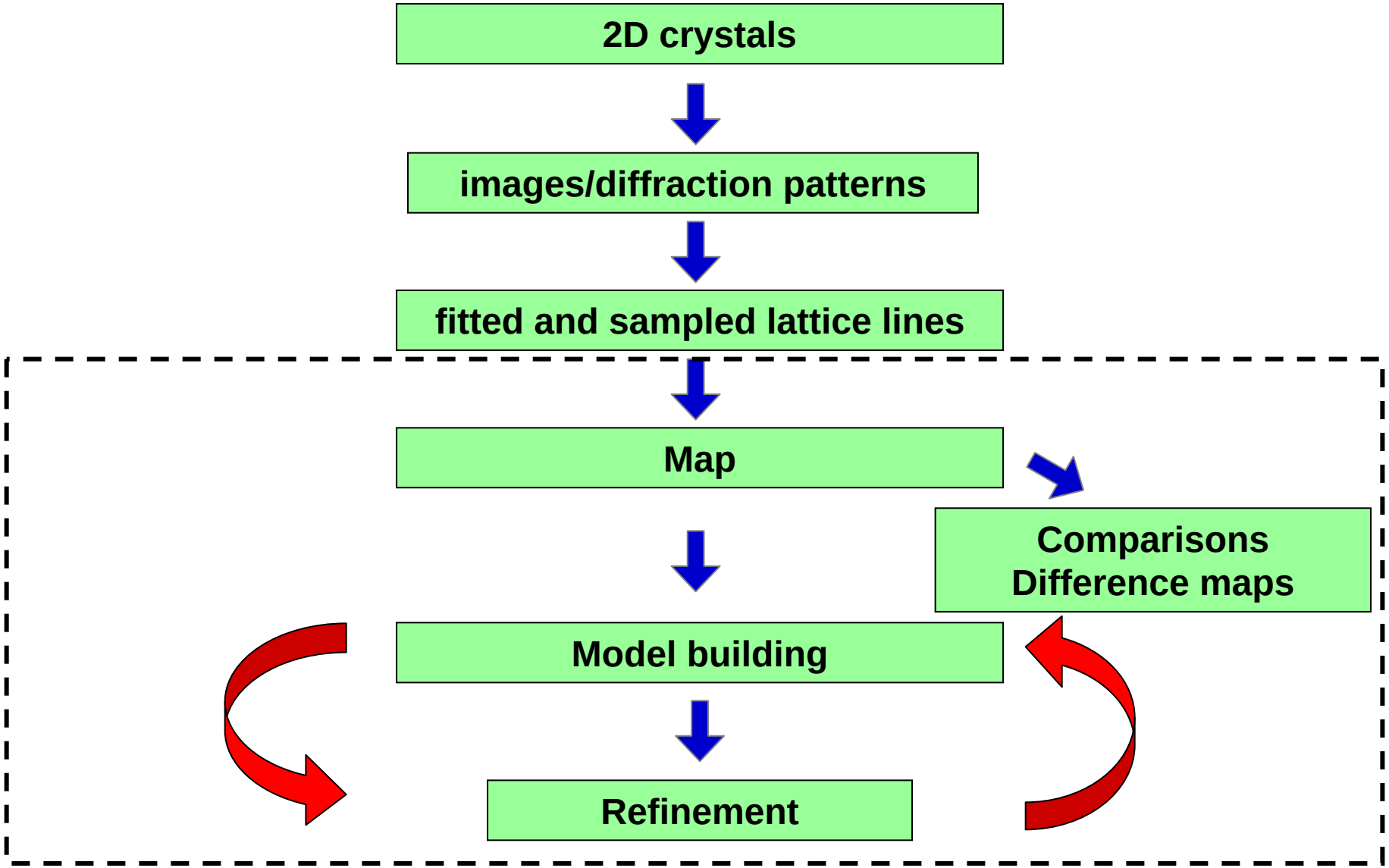
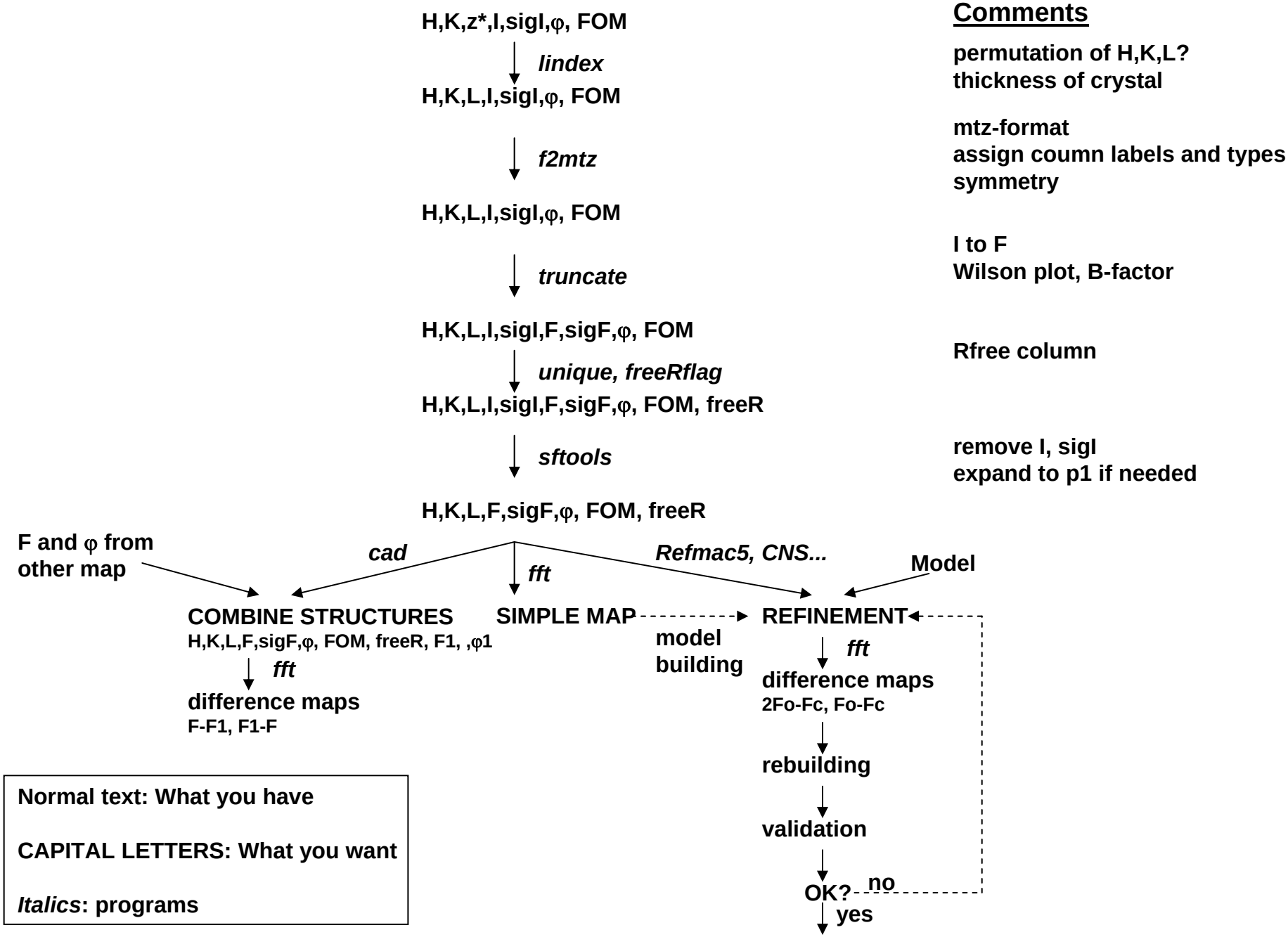
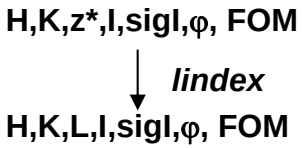
2D crystal structure determination



2D crystal structure determination

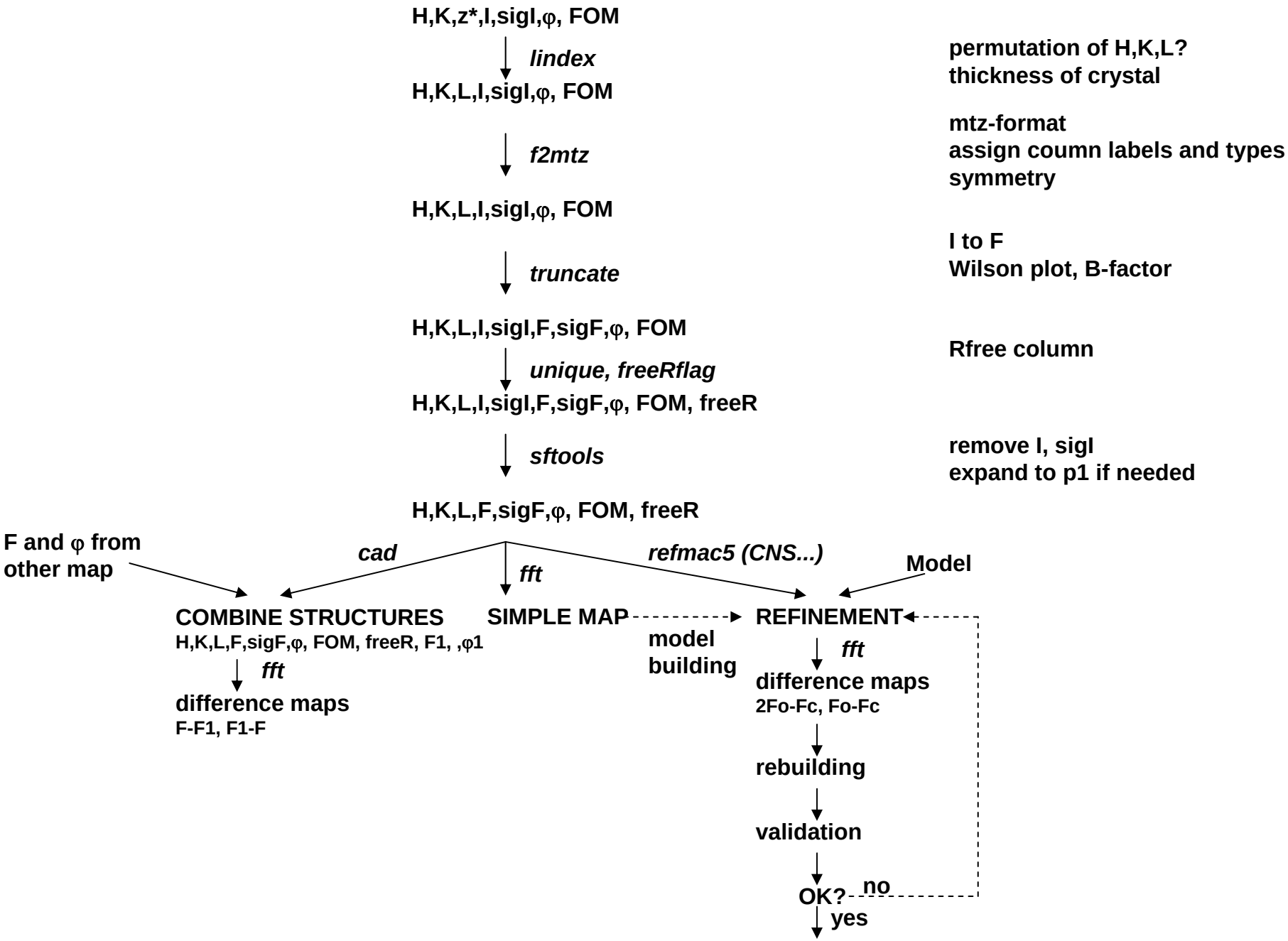


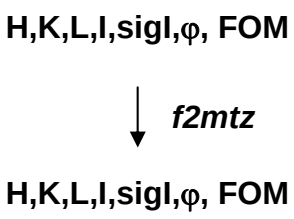

H,K,z*,I,sigI,φ, FOM
lindex
H,K,L,I,sigI,φ, FOM
f2mtz
H,K,L,I,sigI,φ, FOM
truncate
H,K,L,I,sigI,F,sigF,φ, FOM
unique, freeRflag
H,K,L,I,sigI,F,sigF,φ, FOM, freeR
sftools
H,K,L,F,sigF,φ, FOM, freeR
F and φ from other map
cad
fft
Refmac5, CNS...
Model
COMBINE STRUCTURES
H,K,L,F,sigF,φ, FOM, freeR, F1, ,φ1
fft
difference maps
F-F1, F1-F
SIMPLE MAP
model building
REFINEMENT
fft
difference maps
2Fo-Fc, Fo-Fc
rebuilding
validation
OK?
no
yes
Comments
permutation of H,K,L?
thickness of crystal
mtz-format
assign coumn labels and types
symmetry
I to F
Wilson plot, B-factor
Rfree column
remove I, sigI
expand to p1 if needed
Normal text: What you have
CAPITAL LETTERS: What you want
Italics: programs



AXIS <fast> <medium> <slow>

- <fast> <medium> <slow> are the letters X, Y and Z in the appropriate order. Note that many of the FFT space-group specific routines have FIXED axis orders. In general these are Y,X,Z for those which have rotation axes along c, and are best output with z-sections (all space-groups with space-group number greater than 18 (P21212)).
- For P1, the monoclinic space-groups, and space-groups 16 (P 2 2 2), 17 (P 2 2 21) and 18 (P 21 21 2), the required axis order is Z,X,Y, which gives y-sections.


H,K,z*,I,sigI,φ, FOM
lindex
H,K,L,I,sigI,φ, FOM
permutation of H,K,L?
thickness of crystal
f2mtz
mtz-format
assign coumn labels and types
symmetry
H,K,L,I,sigI,φ, FOM
truncate
I to F
Wilson plot, B-factor
H,K,L,I,sigI,F,sigF,φ, FOM
unique, freeRflag
Rfree column
H,K,L,I,sigI,F,sigF,φ, FOM, freeR
sftools
remove I, sigI
expand to p1 if needed
H,K,L,F,sigF,φ, FOM, freeR
F and φ from other map
cad
fft
refmac5 (CNS...)
Model
COMBINE STRUCTURES
H,K,L,F,sigF,φ, FOM, freeR, F1, ,φ1
fft
difference maps
F-F1, F1-F
SIMPLE MAP
model building
REFINEMENT
fft
difference maps
2Fo-Fc, Fo-Fc
rebuilding
validation
OK?
no
yes



text file

binary file

f2mtz - Convert a formatted reflection file to MTZ format

LABOUT

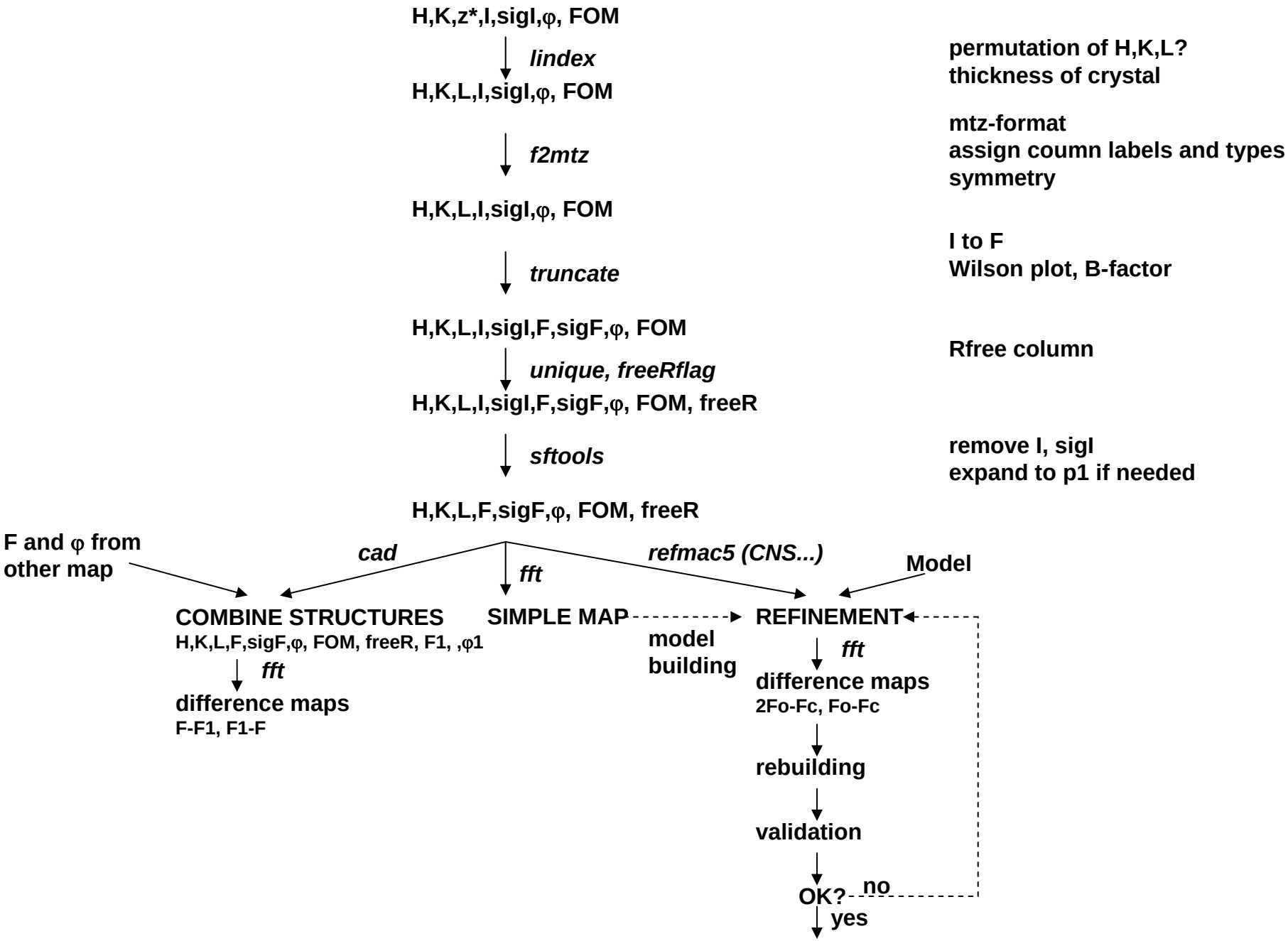
In the specification of the MTZ format, each data column has an associated label and type. The LABOUT command allows you to specify the column labels.

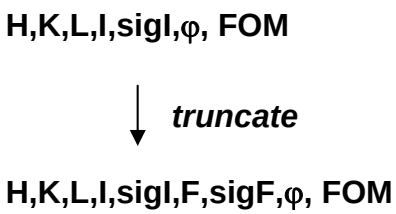
The standard label names used are as follows:

The standard label names used

Name	Item
H, K, L	**Miller indices.**
S	(4 sin**2 theta / lambda**2).
IC	Centric flag.
M/ISYM	Partial flag and symmetry number.
BATCH	Batch number.
I	**Intensity**.
I'	Selected mean intensity.
SIGI	**sigma(I).**
SIGI'	sigma(I').
FRACTIONCALC	Calculated partial fraction.
IMEAN	**mean intensity.**
SIGIMEAN	**sigma(IMEAN).**
RATDELSD	Agreement factor between films in a pack.
FP	**Native `F' value.**
FC	**Calculated `F'.**
FPHn	` F' value for derivative `n'.

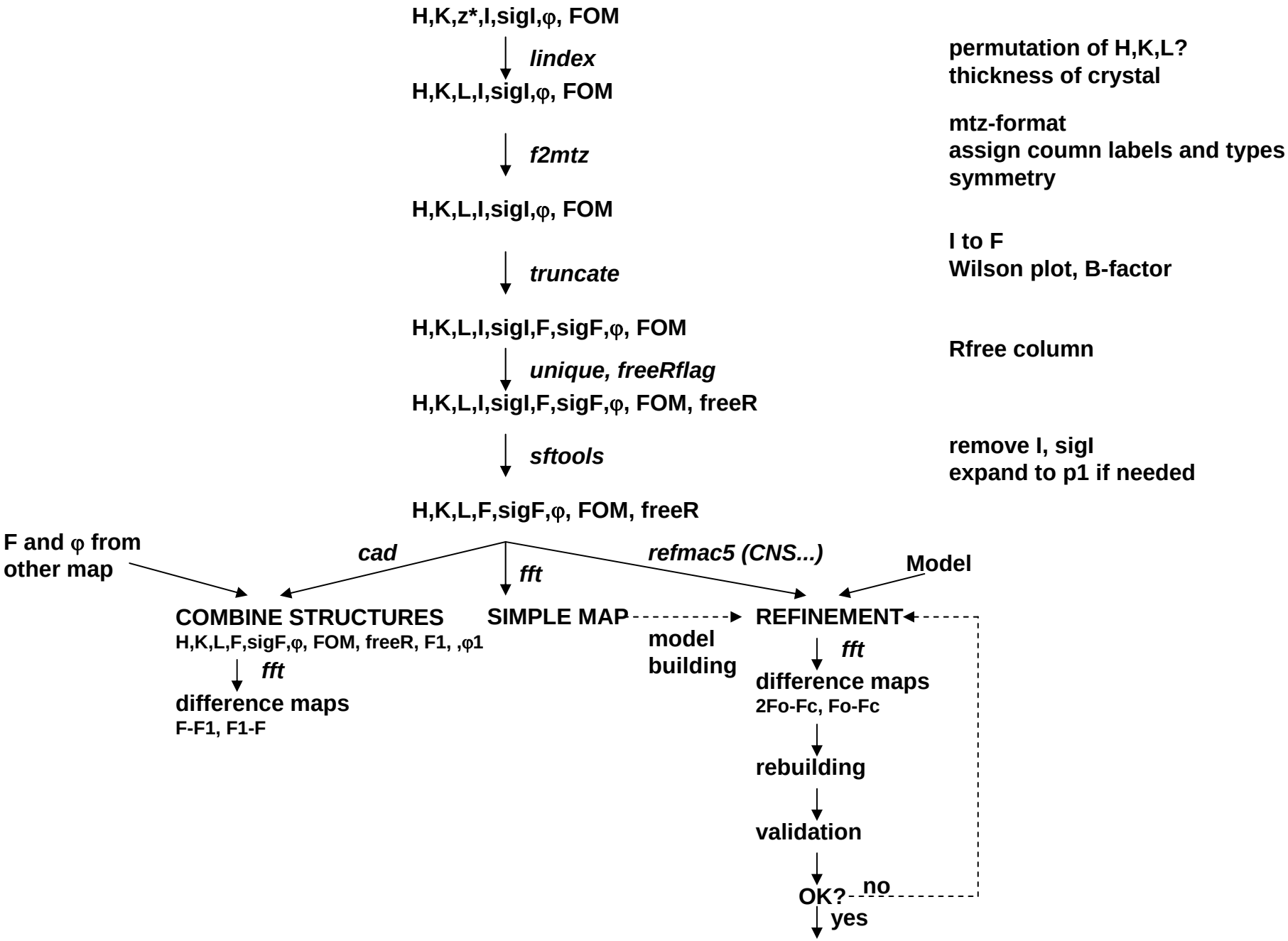
Name	Item
DP	Anomalous difference for native data.
DPHn	Anomalous difference for derivative `n'.
SIGFP	**sigma(FP).**
SIGDP	sigma(DP).
SIGFPHn	sigma(Fn).
SIGDPHn	sigma(DELn).
PHIC	**Calc Phase.**
PHIM	Most prob phase.
PHIB	**Phase.**
FOM	**figure of merit.**
WT	weight
HLA	ABCD H/L coeffs
HLB	
HLC	
HLD	

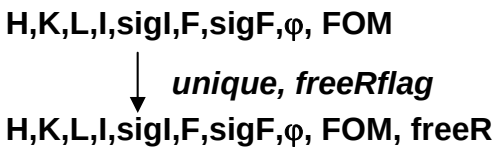

H,K,z*,I,sigI,φ, FOM
lindex
H,K,L,I,sigI,φ, FOM
permutation of H,K,L?
thickness of crystal
f2mtz
mtz-format
assign coumn labels and types
symmetry
H,K,L,I,sigI,φ, FOM
truncate
I to F
Wilson plot, B-factor
H,K,L,I,sigI,F,sigF,φ, FOM
unique, freeRflag
Rfree column
H,K,L,I,sigI,F,sigF,φ, FOM, freeR
sftools
remove I, sigI
expand to p1 if needed
H,K,L,F,sigF,φ, FOM, freeR
F and φ from other map
cad
fft
refmac5 (CNS...)
Model
COMBINE STRUCTURES
H,K,L,F,sigF,φ, FOM, freeR, F1, ,φ1
fft
difference maps
F-F1, F1-F
SIMPLE MAP
model building
REFINEMENT
fft
difference maps
2Fo-Fc, Fo-Fc
rebuilding
validation
OK?
no
yes



truncate - obtain structure factor amplitudes using truncate procedure and/or generate useful intensity statistics

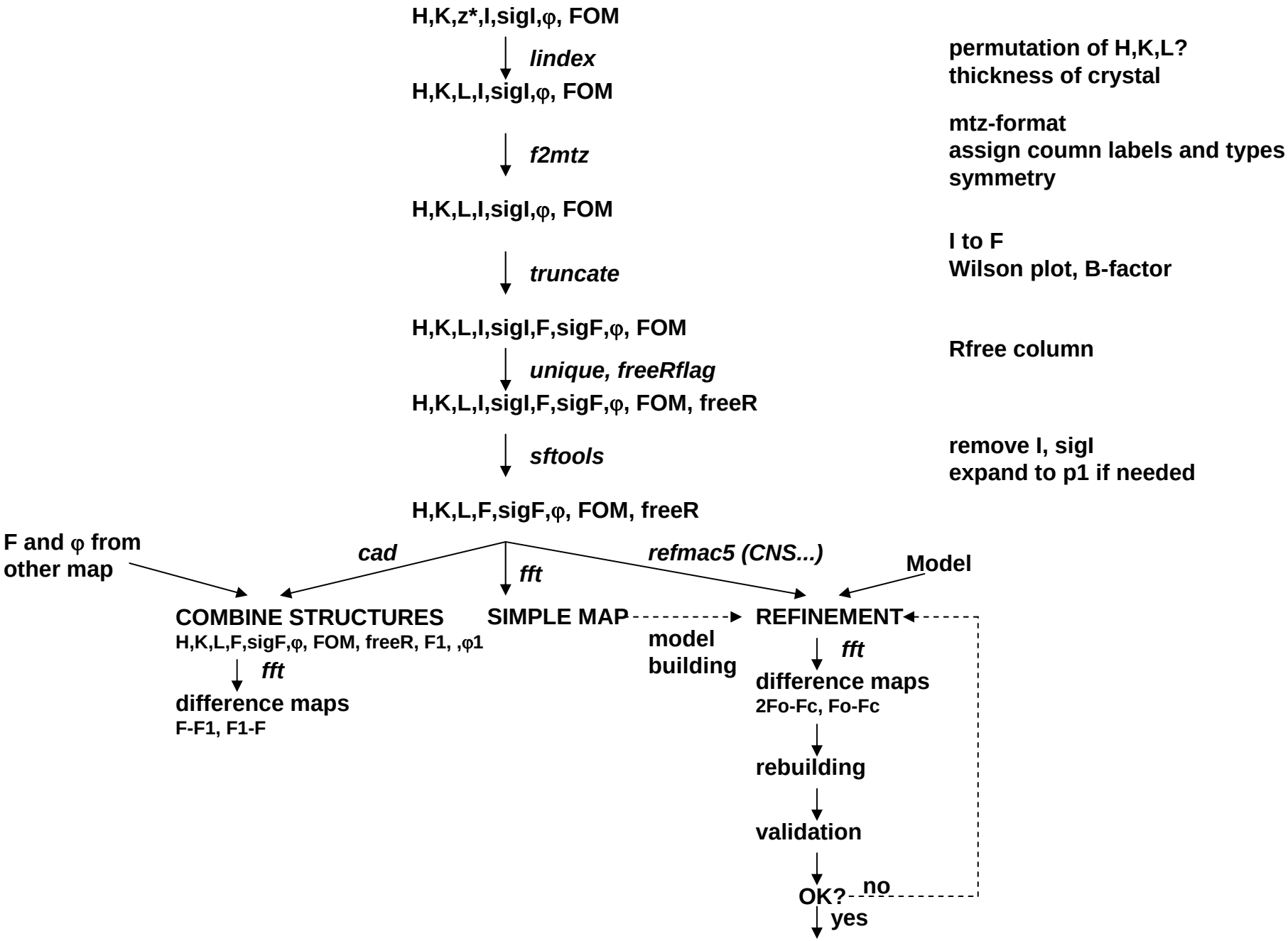
I ➔ F, Wilson plot, overall B-factor

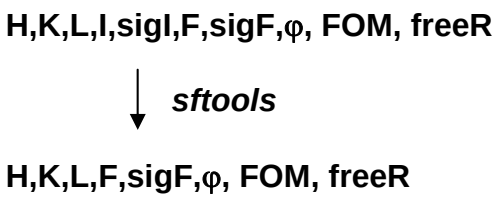

H,K,z*,I,sigI,φ, FOM
lindex
H,K,L,I,sigI,φ, FOM
permutation of H,K,L?
thickness of crystal
f2mtz
mtz-format
assign coumn labels and types
symmetry
H,K,L,I,sigI,φ, FOM
truncate
I to F
Wilson plot, B-factor
H,K,L,I,sigI,F,sigF,φ, FOM
unique, freeRflag
Rfree column
H,K,L,I,sigI,F,sigF,φ, FOM, freeR
sftools
remove I, sigI
expand to p1 if needed
H,K,L,F,sigF,φ, FOM, freeR
F and φ from other map
cad
fft
refmac5 (CNS...)
Model
COMBINE STRUCTURES
H,K,L,F,sigF,φ, FOM, freeR, F1, ,φ1
fft
difference maps
F-F1, F1-F
SIMPLE MAP
model building
REFINEMENT
fft
difference maps
2Fo-Fc, Fo-Fc
rebuilding
validation
OK?
no
yes



unique - Generate a unique list of reflections
freerflag - tags each reflection in an MTZ file with a flag for cross-validation

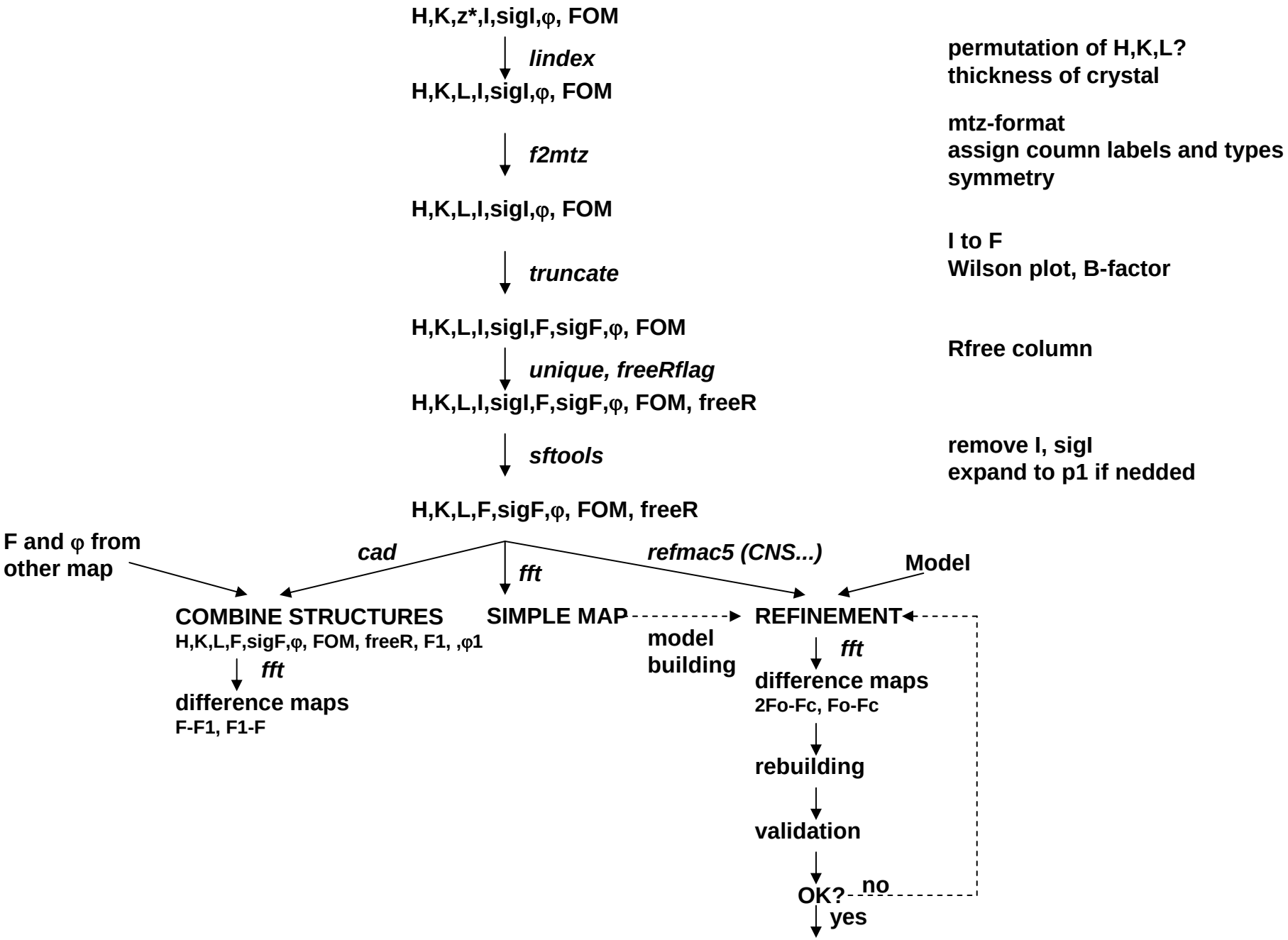
Rfree column added


H,K,z*,I,sigI,φ, FOM
lindex
H,K,L,I,sigI,φ, FOM
permutation of H,K,L?
thickness of crystal
f2mtz
mtz-format
assign coumn labels and types
symmetry
H,K,L,I,sigI,φ, FOM
truncate
I to F
Wilson plot, B-factor
H,K,L,I,sigI,F,sigF,φ, FOM
unique, freeRflag
Rfree column
H,K,L,I,sigI,F,sigF,φ, FOM, freeR
sftools
remove I, sigI
expand to p1 if needed
H,K,L,F,sigF,φ, FOM, freeR
F and φ from other map
cad
fft
refmac5 (CNS...)
Model
COMBINE STRUCTURES
H,K,L,F,sigF,φ, FOM, freeR, F1, ,φ1
fft
difference maps
F-F1, F1-F
SIMPLE MAP
model building
REFINEMENT
fft
difference maps
2Fo-Fc, Fo-Fc
rebuilding
validation
OK?
no
yes



sftools - reflection data file utility program

remove I, sigI
expand to p1 if needed


H,K,z*,I,sigI,φ, FOM
lindex
H,K,L,I,sigI,φ, FOM
permutation of H,K,L?
thickness of crystal
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H,K,L,I,sigI,F,sigF,φ, FOM
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H,K,L,I,sigI,F,sigF,φ, FOM, freeR
sftools
remove I, sigI
expand to p1 if nedded
H,K,L,F,sigF,φ, FOM, freeR
F and φ from other map
cad
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refmac5 (CNS...)
Model
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H,K,L,F,sigF,φ, FOM, freeR, F1, ,φ1
SIMPLE MAP
model building
REFINEMENT
fft
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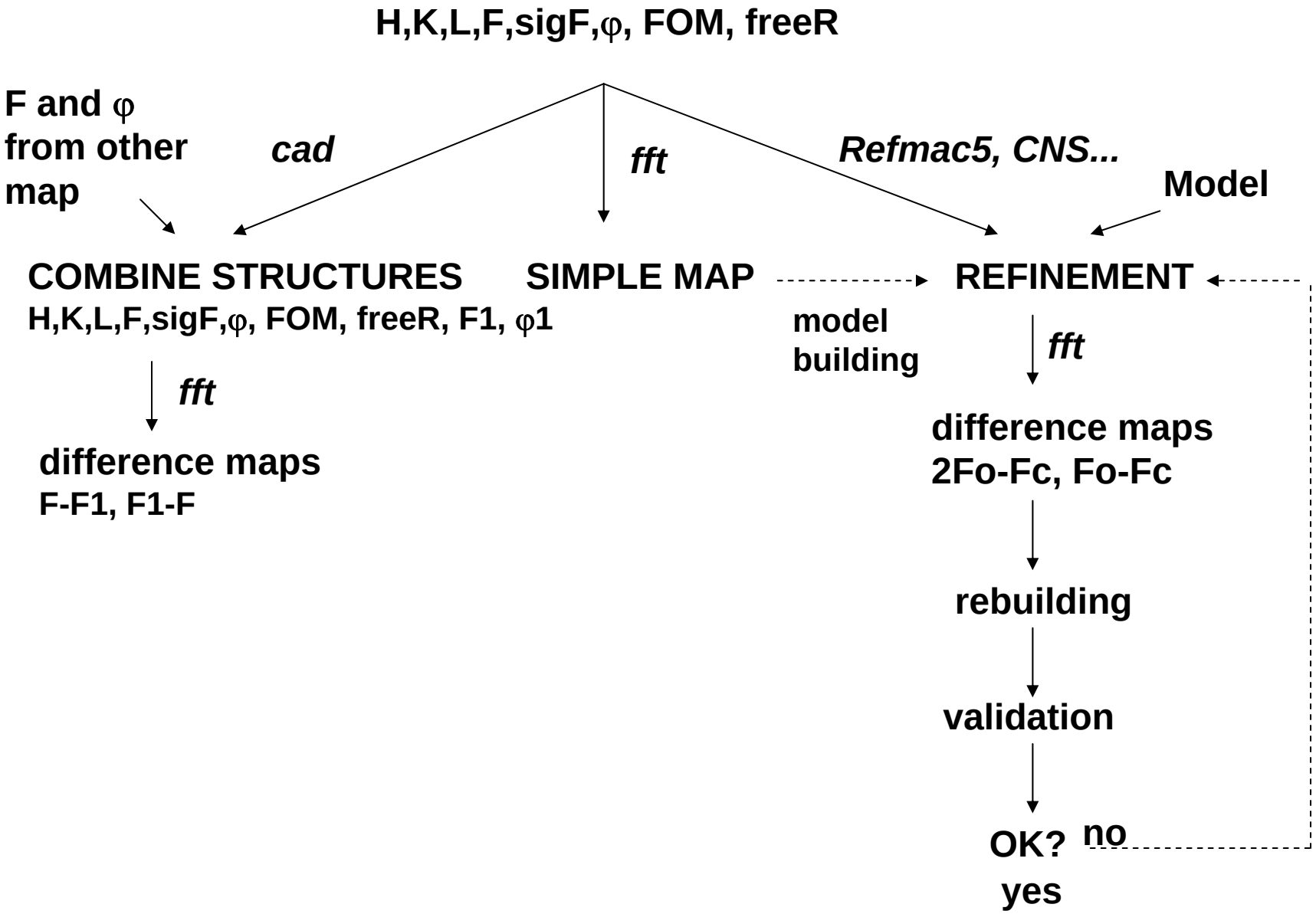
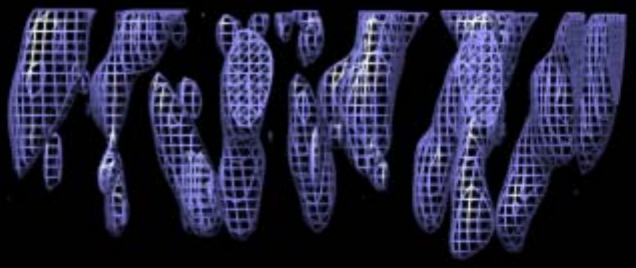
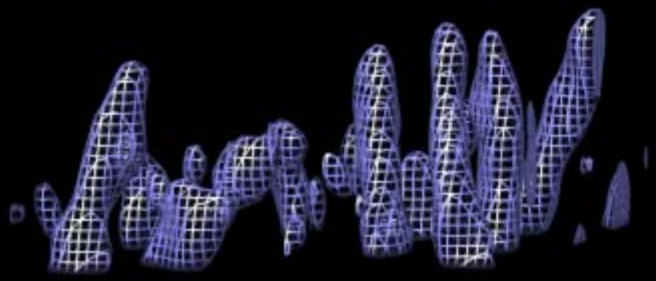
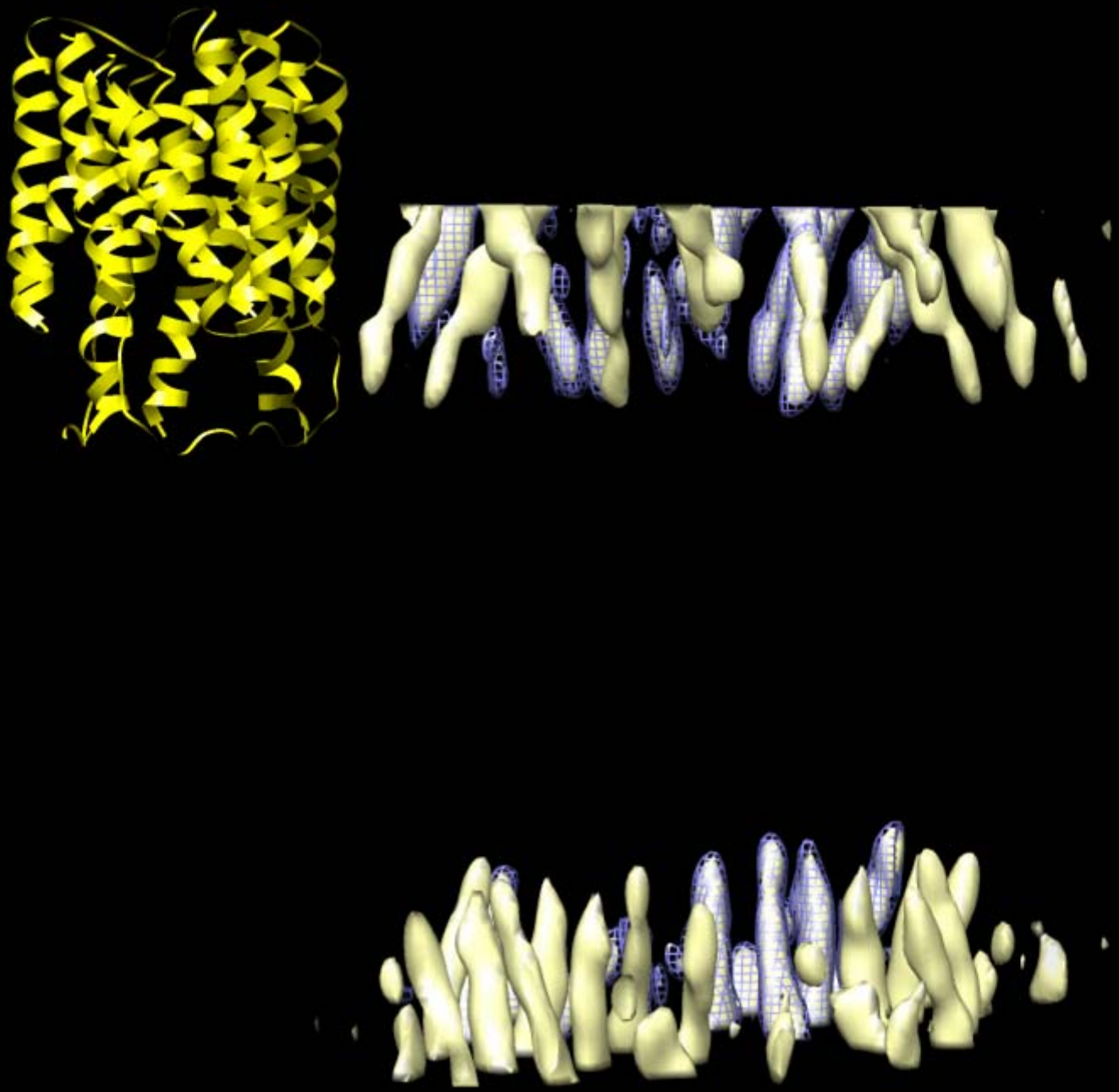
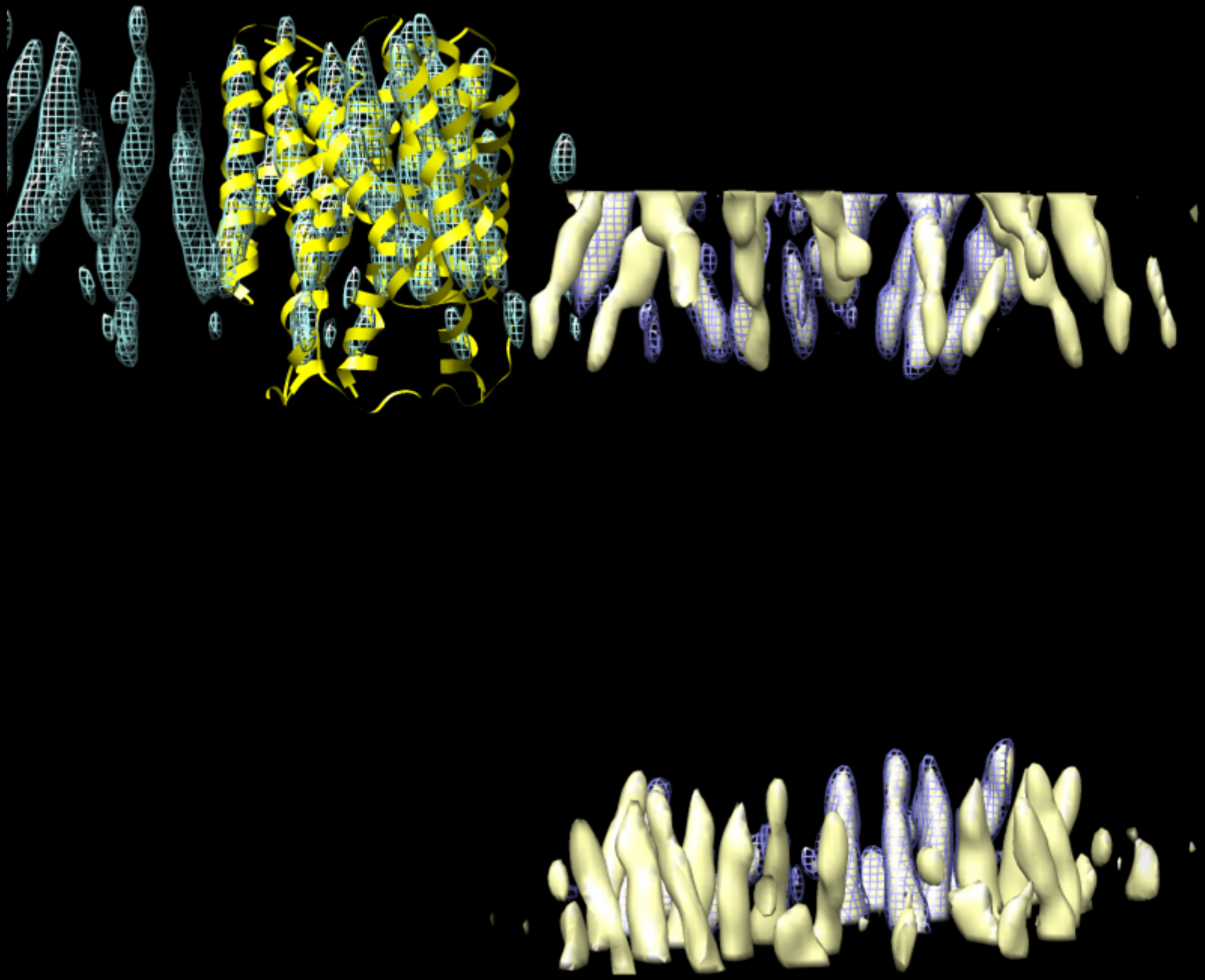
F-F1, F1-F
fft
difference maps
2Fo-Fc, Fo-Fc
rebuilding
validation
OK?
no
yes

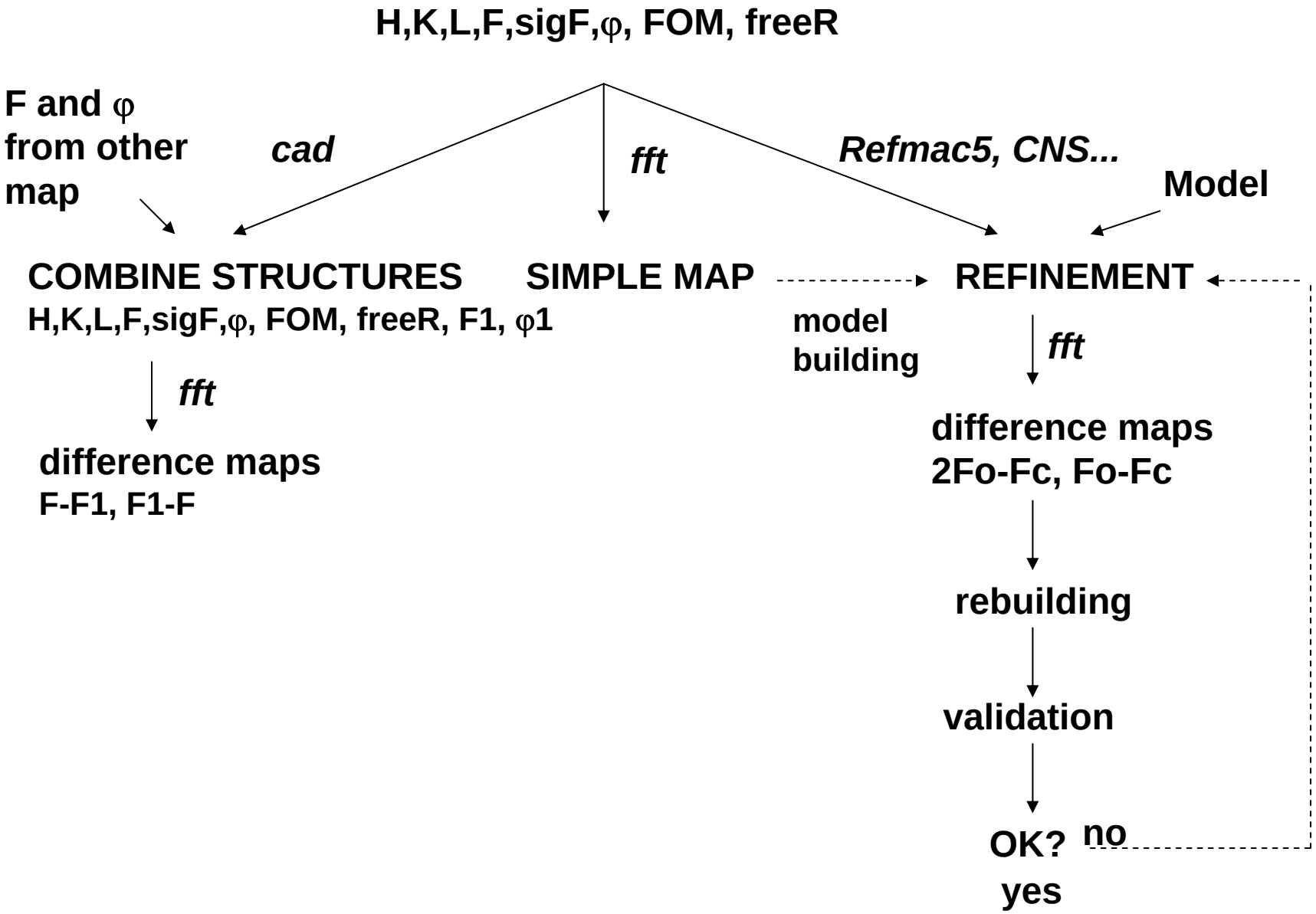

H,K,L,F,sigF,φ, FOM, freeR
F and φ from other map
cad
fft
Refmac5, CNS...
Model
COMBINE STRUCTURES
H,K,L,F,sigF,φ, FOM, freeR, F1, φ1
SIMPLE MAP
model building
REFINEMENT
fft
fft
difference maps
F-F1, F1-F
difference maps
2Fo-Fc, Fo-Fc
rebuilding
validation
OK?
no
yes










H,K,L,F,sigF,φ, FOM, freeR
F and φ from other map
cad
fft
Refmac5, CNS...
Model
COMBINE STRUCTURES
H,K,L,F,sigF,φ, FOM, freeR, F1, φ1
SIMPLE MAP
model building
REFINEMENT
fft
fft
difference maps
F-F1, F1-F
difference maps
2Fo-Fc, Fo-Fc
rebuilding
validation
OK?
no
yes

Map to model/map to map comparisons