

## Supplementary material

**Table S1** List of refinement program combinations that were found in PDB entries and our decision on which one most likely was used last.

PDB File	Interpretation	PDB File	Interpretation
CNS + ARP	CNS	REFMAC + X-PLOR	REFMAC
CNS + NUCLSQ	CNS	RESTRAIN + ATOM	RESTRAIN
CNS + REFMAC	REFMAC	SHELXL + CNS	SHELXL
CNS + X-PLOR	CNS	SHELXL + NUCLSQ	SHELXL
EREF + PROLSQ	PROLSQ	SHELXL + X-PLOR	SHELXL
NUCLIN + NUCLSQ	NUCLSQ	TNT + NUCLSQ	TNT
PROFFT + NUCLSQ	NUCLSQ	TNT + PROLSQ	TNT
PROLSQ + AMORE	PROLSQ	TNT + X-PLOR	TNT
PROLSQ + ATOM	PROLSQ	X-PLOR + AMORE	X-PLOR
PROLSQ + EREF	PROLSQ	X-PLOR + ARP	X-PLOR
PROLSQ + X-PLOR	X-PLOR	X-PLOR + FRODO	X-PLOR
PROTIN + NUCLSQ	NUCLSQ	X-PLOR + NCS	CNS
REFMAC + AMORE	REFMAC	X-PLOR + NUCLSQ	X-PLOR
REFMAC + ARP	REFMAC	X-PLOR + QUANTA	X-PLOR
REFMAC + NCS	REFMAC	X-PLOR + RESTRAIN	X-PLOR
REFMAC + NUCLSQ	REFMAC		

## Other supplementary material

Additional material can be found at <http://swift.cmbi.ru.nl/gv/whatcheck/HTML/TAU/>.