Table 1. Rotation angles and corresponding rotations. Matrices $R_X(\xi)$, $R_Y(\xi)$, $R_Z(\xi)$ for the primitive rotations are defined in the text. Most distributed molecular replacement program packages are indicated which use the corresponding rotation system. PROTEIN rotation matrices are inverted X-PLOR ones.

System	Limits for the triclinic group	Alternative solution	Rotation matrix as a product of matrices for elementary rotations	Program packages
Polar Rossmann,1962	$0\le\phi<2\pi$ $0\le\psi\le\pi$ $0\le\kappa<2\pi$	$\phi=\phi+\pi$ $\psi=-\psi+\pi$ $\kappa=-\kappa$	$R_Y(\phi)\cdot R_Z(-\psi)\cdot R_Y(-\kappa)\cdot R_Z(\psi)\cdot R_Y(-\phi)$	X-PLOR
Polar Dodson et al.,1966 Crowther,1972	$0\le\phi<2\pi$ $0\le\psi\le\pi$ or $0\le\omega\le\pi$ $0\le\kappa<2\pi$	$\phi=\phi+\pi$ $\psi=-\psi+\pi$ $\kappa=-\kappa$	$R_Z(\phi)\cdot R_Y(\psi)\cdot R_Z(-\kappa)\cdot R_Y(-\psi)\cdot R_Z(-\phi)$ $R_Z(\phi)\cdot R_Y(\omega)\cdot R_Z(-\kappa)\cdot R_Y(-\omega)\cdot R_Z(-\phi)$	ALMN AMoRe
Direction cosines	$0\le\kappa<2\pi$ $-1\le\cos x\le1$ $-1\le\cos y\le1$ $-1\le\cos z\le1$ $\cos x^2+\cos y^2+$ $+\cos z^2=1$	$\kappa=-\kappa$ $\cos x=-\cos x$ $\cos y=-\cos y$ $\cos z=-\cos z$	can be written through recalculated angles	AMoRe
Eulerian Rossmann,1962	$0\le\theta_1<2\pi$ $0\le\theta_2<2\pi$ $0\le\theta_3<2\pi$	$\theta_1=\theta_1+\pi$ $\theta_2=-\theta_2$ $\theta_3=\theta_3+\pi$	$R_Z(-\theta_3)\cdot R_X(-\theta_2)\cdot R_Z(-\theta_1)$	X-PLOR
Eulerian Lattman,1966	$0\le\theta_+<4\pi$ $0\le\theta_2<2\pi$ $-2\pi\le\theta_-<2\pi$	$\theta_1=\theta_1+2\pi$ $\theta_2=-\theta_2$ $\theta_3=\theta_3$	$R_Z[-(\theta_+-\theta_-)/2]\cdot R_X(-\theta_2)\cdot R_Z[-(\theta_++\theta_-)/2]$	X-PLOR
Eulerian Crowther,1972	$0\le\alpha<2\pi$ $0\le\beta<2\pi$ $0\le\gamma<2\pi$	$\alpha=\alpha+\pi$ $\beta=-\beta$ $\gamma=\gamma+\pi$	$R_Z(-\gamma)\cdot R_Y(-\beta)\cdot R_Z(-\alpha)$	ALMN MERLOT
Eulerian Nordman,1966	$0\le\phi<2\pi$ $0\le\theta<2\pi$ $0\le\psi<2\pi$	$\phi=\phi+\pi$ $\theta=-\theta$ $\psi=\psi+\pi$	$R_X(-\phi)\cdot R_Y(-\theta)\cdot R_X(-\psi)$	
Eulerian Huber,1969	$0\le\psi<2\pi$ $0\le\theta<2\pi$ $0\le\phi<2\pi$	$\phi=\phi+\pi$ $\theta=-\theta$ $\psi=\psi+\pi$	$R_Z(\psi)\cdot R_X(\theta)\cdot R_Y(\phi)$	PROTEIN
Eulerian Navaza,1994	$0\le\alpha<2\pi$ $0\le\beta<2\pi$ $0\le\gamma<2\pi$	$\alpha=\alpha+\pi$ $\beta=-\beta$ $\gamma=\gamma+\pi$	$R_Z(\alpha)\cdot R_Y(\beta)\cdot R_Z(\gamma)$	AMoRe