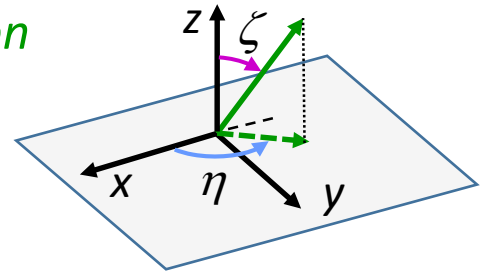
Polar : zenith axis Z , azimuth axis X

Matrix product :

$$R = R_z(\eta)\, R_y(\zeta)\, R_z(\kappa)\, R_y(-\zeta)\, R_z(-\eta)$$

Rotation axis



Rotation matrix

$$\begin{pmatrix} r_{11} & r_{12} & r_{13} \\ r_{21} & r_{22} & r_{23} \\ r_{31} & r_{32} & r_{33} \end{pmatrix} = \begin{pmatrix} \sin^2\zeta\cos^2\eta\,(1-\cos\kappa) + \cos\kappa & \sin^2\zeta\sin\eta\cos\eta\,(1-\cos\kappa) - \cos\zeta\sin\kappa & \sin\zeta\cos\zeta\cos\eta\,(1-\cos\kappa) + \sin\zeta\sin\eta\sin\kappa \\ \sin^2\zeta\sin\eta\cos\eta\,(1-\cos\kappa) + \cos\zeta\sin\kappa & \sin^2\zeta\sin^2\eta\,(1-\cos\kappa) + \cos\kappa & \sin\zeta\cos\zeta\sin\eta\,(1-\cos\kappa) - \sin\zeta\cos\eta\sin\kappa \\ \sin\zeta\cos\zeta\cos\eta\,(1-\cos\kappa) - \sin\zeta\sin\eta\sin\kappa & \sin\zeta\cos\zeta\sin\eta\,(1-\cos\kappa) + \sin\zeta\cos\eta\sin\kappa & \cos^2\zeta\,(1-\cos\kappa) + \cos\kappa \end{pmatrix}$$

Getting angles from the rotation matrix

$$0 \le \kappa \le \pi$$
$$0 \le \zeta \le \pi$$
$$0 \le \eta < 2\pi$$

Equivalent angles :

$\kappa' = 2\pi - \kappa$; $\zeta' = \pi - \zeta$; $\eta' = \eta + \pi$

$\kappa = \arccos(r_{11}+r_{22}+r_{33}-1)/2$

if $\kappa = 0$:
- $\zeta = 0$
- $\eta = 0$

If $0 < \kappa < \pi$: $\zeta = \arccos(\frac{1}{2}(r_{21}-r_{12})/\sin\kappa)$
- *if* $\zeta = 0$: $\eta = 0$
- *if* $0 < \zeta < \pi$: $\eta = \text{atan2}(r_{13}-r_{31}, r_{32}-r_{23})$
- *if* $\zeta = \pi$: $\eta = 0$

If $\kappa = \pi$: $\zeta = \frac{1}{2}\arccos(r_{33})$
- *if* $\zeta = 0$: $\eta = 0$
- *if* $0 < \zeta < \pi/2$: $\eta = \text{atan2}(r_{23}+r_{32}, r_{13}+r_{31})$
- *if* $\zeta = \pi/2$: $\eta = \frac{1}{2}\,\text{atan2}(r_{12}+r_{21}, 2r_{11})$

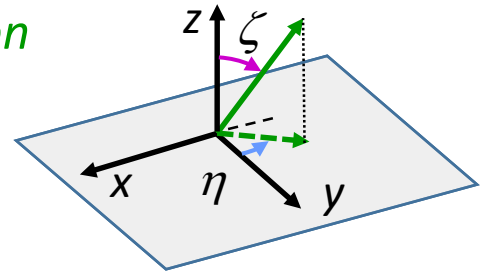
Relevant programs : CCP4, phenix

Polar : *zenith axis Z , azimuth axis Y*

Matrix product :

$$R = R_z(\eta+\pi/2)\, R_y(\zeta)\, R_z(\kappa)\, R_y(-\zeta)\, R_z(-\eta-\pi/2)$$

Rotation axis



Rotation matrix

$$\begin{pmatrix} r_{11} & r_{12} & r_{13} \\ r_{21} & r_{22} & r_{23} \\ r_{31} & r_{32} & r_{33} \end{pmatrix} =$$

The same as for (zenith axis Z , azimuth axis X) substituting everywhere in the matrix 'η ' by 'η+π/2' , e.g. making

$$r_{11} = \sin^2\zeta \cos^2(\eta+\pi/2)\,(1-\cos\kappa) + \cos\kappa$$

Getting angles from the rotation matrix

The same as for (zenith axis Z , azimuth axis X) substituting everywhere 'η ' by 'η-π/2' , e.g. making

If $0 < \kappa < \pi$: $\zeta = \arccos(\tfrac{1}{2}(r_{21}-r_{12})/\sin\kappa)$

if $\sin\zeta = 0$, $\eta = -\pi/2$

if $\sin\zeta > 0$, $\eta = \mathrm{atan2}(r_{13}-r_{31}, r_{32}-r_{23}) - \pi/2$

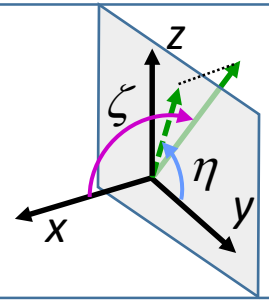
Relevant programs : n/a

Polar : zenith axis X , azimuth axis Y

Matrix product :

$$R = R_x(\eta)\, R_z(\zeta)\, R_x(\kappa)\, R_z(-\zeta)\, R_x(-\eta)$$

Rotation axis



Rotation matrix

$$\begin{pmatrix} r_{11} & r_{12} & r_{13} \\ r_{21} & r_{22} & r_{23} \\ r_{31} & r_{32} & r_{33} \end{pmatrix} =$$

$$\begin{pmatrix} \cos^2\zeta(1-\cos\kappa)+\cos\kappa & \sin\zeta\cos\zeta\cos\eta(1-\cos\kappa)-\sin\zeta\sin\eta\sin\kappa & \sin\zeta\cos\zeta\sin\eta(1-\cos\kappa)+\sin\zeta\cos\eta\sin\kappa \\ \sin\zeta\cos\zeta\cos\eta(1-\cos\kappa)+\sin\zeta\sin\eta\sin\kappa & \sin^2\zeta\cos^2\eta(1-\cos\kappa)+\cos\kappa & \sin^2\zeta\sin\eta\cos\eta(1-\cos\kappa)-\cos\zeta\sin\kappa \\ \sin\zeta\cos\zeta\sin\eta(1-\cos\kappa)-\sin\zeta\cos\eta\sin\kappa & \sin^2\zeta\sin\eta\cos\eta(1-\cos\kappa)+\cos\zeta\sin\kappa & \sin^2\zeta\sin^2\eta(1-\cos\kappa)+\cos\kappa \end{pmatrix}$$

Getting angles from the rotation matrix

$$0 \le \kappa \le \pi$$
$$0 \le \zeta \le \pi$$
$$0 \le \eta < 2\pi$$

Equivalent angles :

$\kappa' = 2\pi - \kappa$; $\zeta' = \pi - \zeta$; $\alpha' = \eta + \pi$

$\kappa = \arccos(r_{11}+r_{22}+r_{33}-1)/2$

if $\kappa = 0$:
- $\zeta = 0$
- $\eta = 0$

If $0 < \kappa < \pi$: $\zeta = \arccos(\frac{1}{2}(r_{32}-r_{23})/\sin\kappa)$
- *if* $\zeta = 0$: $\eta = 0$
- *if* $0 < \zeta < \pi$: $\eta = \text{atan2}(r_{21}-r_{12},\, r_{13}-r_{31})$
- *if* $\zeta = \pi$: $\eta = 0$

If $\kappa = \pi$: $\zeta = \frac{1}{2}\arccos(r_{11})$
- *if* $\zeta = 0$: $\eta = 0$
- *if* $0 < \zeta < \pi/2$: $\eta = \text{atan2}(r_{31}+r_{13},\, r_{21}+r_{12})$
- *if* $\zeta = \pi/2$: $\eta = \frac{1}{2}\,\text{atan2}(r_{23}+r_{32},\, 2r_{22})$

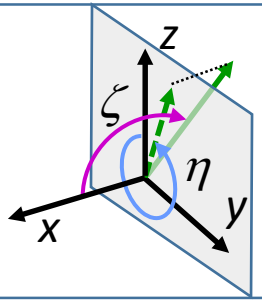
Relevant programs : n/a

Polar : zenith axis X , azimuth axis Z

Matrix product :

$$R = R_x(\eta+\pi/2)\, R_z(\zeta)\, R_x(\kappa)\, R_z(-\zeta)\, R_x(-\eta-\pi/2)$$

Rotation axis



Rotation matrix

$$\begin{pmatrix} r_{11} & r_{12} & r_{13} \\ r_{21} & r_{22} & r_{23} \\ r_{31} & r_{32} & r_{33} \end{pmatrix} =$$

The same as for (zenith axis X , azimuth axis Y) substituting everywhere in the matrix 'η ' by 'η+π/2' , e.g. making

$$r_{22} = \sin^2\zeta \cos^2(\eta+\pi/2)\,(1-\cos\kappa) + \cos\kappa$$

Getting angles from the rotation matrix

The same as for (zenith axis X , azimuth axis Y) substituting everywhere 'η ' by 'η-π/2' , e.g. making

If $0 < \kappa < \pi$: $\zeta = \arccos(\tfrac{1}{2}(r_{32}-r_{23})/\sin\kappa)$

if $\sin\zeta = 0$, $\eta = -\pi/2$

if $\sin\zeta > 0$, $\eta = \mathrm{atan2}(r_{21}-r_{13},\, r_{13}-r_{31}) - \pi/2$

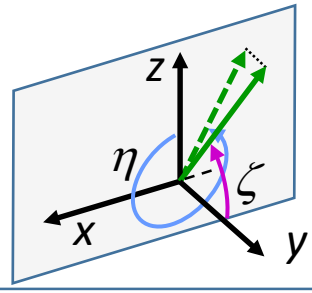
Relevant programs : n/a

Polar : zenith axis Y , azimuth axis Z

Matrix product :

$$R = R_y(\eta)\, R_x(\zeta)\, R_y(\kappa)\, R_x(-\zeta)\, R_y(-\eta)$$

Rotation axis



Rotation matrix

$$\begin{pmatrix} r_{11} & r_{12} & r_{13} \\ r_{21} & r_{22} & r_{23} \\ r_{31} & r_{32} & r_{33} \end{pmatrix} = \begin{pmatrix} \sin^2\zeta \sin^2\eta\,(1-\cos\kappa) + \cos\kappa & \sin\zeta\cos\zeta\sin\eta\,(1-\cos\kappa) - \sin\zeta\cos\eta\sin\kappa & \sin^2\zeta\sin\eta\cos\eta\,(1-\cos\kappa) + \cos\zeta\sin\kappa \\ \sin\zeta\cos\zeta\sin\eta\,(1-\cos\kappa) + \sin\zeta\cos\eta\sin\kappa & \cos^2\zeta\,(1-\cos\kappa) + \cos\kappa & \sin\zeta\cos\zeta\cos\eta\,(1-\cos\kappa) - \sin\zeta\sin\eta\sin\kappa \\ \sin^2\zeta\sin\eta\cos\eta\,(1-\cos\kappa) - \cos\zeta\sin\kappa & \sin\zeta\cos\zeta\cos\eta\,(1-\cos\kappa) + \sin\zeta\sin\eta\sin\kappa & \sin^2\zeta\cos^2\eta\,(1-\cos\kappa) + \cos\kappa \end{pmatrix}$$

Getting angles from the rotation matrix

$$0 \le \kappa \le \pi$$
$$0 \le \zeta \le \pi$$
$$0 \le \eta < 2\pi$$

Equivalent angles :

$\kappa' = 2\pi - \kappa$; $\zeta' = \pi - \zeta$; $\eta' = \eta + \pi$

$\kappa = \arccos(r_{11}+r_{22}+r_{33}-1)/2$

if $\kappa = 0$:
- $\zeta = 0$
- $\eta = 0$

If $0 < \kappa < \pi$: $\zeta = \arccos(\tfrac{1}{2}(r_{13}-r_{31})/\sin\kappa)$
- *if* $\zeta = 0$: $\eta = 0$
- *if* $0 < \zeta < \pi$: $\eta = \text{atan2}(r_{32}-r_{23},\, r_{21}-r_{12})$
- *if* $\zeta = \pi$: $\eta = 0$

If $\kappa = \pi$: $\zeta = \tfrac{1}{2}\arccos(r_{22})$
- *if* $\zeta = 0$: $\eta = 0$
- *if* $0 < \zeta < \pi/2$: $\eta = \text{atan2}(r_{12}+r_{21},\, r_{32}+r_{23})$
- *if* $\zeta = \pi/2$: $\eta = \tfrac{1}{2}\,\text{atan2}(r_{31}+r_{13},\, 2r_{33})$

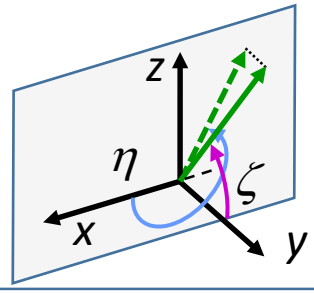
Relevant programs : n/a

Polar : *zenith axis Y , azimuth axis X*

Matrix product :

$$R = R_y(\eta+\pi/2)\, R_x(\zeta)\, R_y(\kappa)\, R_x(-\zeta)\, R_y(-\eta-\pi/2)$$

Rotation axis



Rotation matrix

$$\begin{pmatrix} r_{11} & r_{12} & r_{13} \\ r_{21} & r_{22} & r_{23} \\ r_{31} & r_{32} & r_{33} \end{pmatrix} =$$

The same as for (zenith axis Y , azimuth axis Z) substituting everywhere in the matrix 'η' by 'η+π/2', e.g. making

$$r_{33} = \sin^2\zeta \cos^2(\eta+\pi/2)(1-\cos\kappa) + \cos\kappa$$

Getting angles from the rotation matrix

The same as for (zenith axis Y , azimuth axis Z) substituting everywhere 'η' by 'η-π/2', e.g. making

If $0 < \kappa < \pi$: $\zeta = \arccos(\tfrac{1}{2}(r_{13}-r_{31})/\sin\kappa)$

if $\sin\zeta = 0$, $\eta = -\pi/2$

if $\sin\zeta > 0$, $\eta = \mathrm{atan2}(r_{32}-r_{23}, r_{21}-r_{12}) - \pi/2$

Relevant programs : n/a