SUPPORTING INFORMATION

X-ray induced reduction of heme metal centers is protein-independent - kinetics of photo-reduction and active site perturbations

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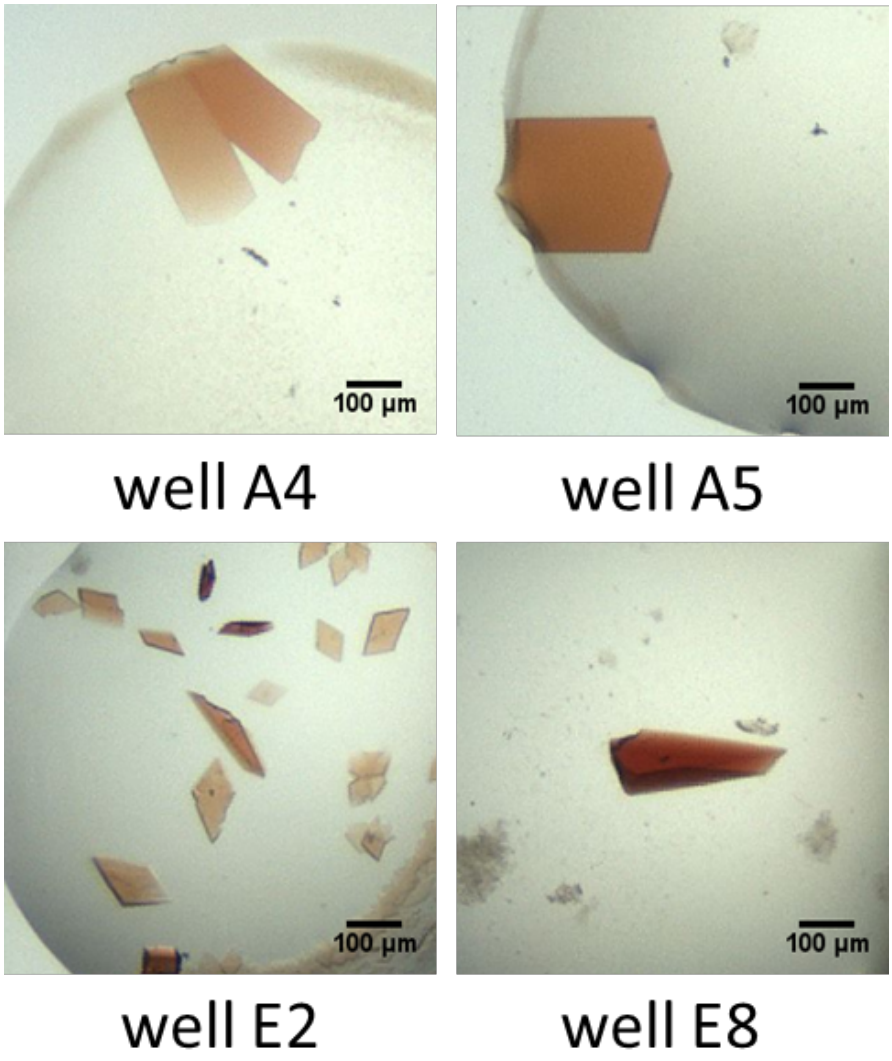

Figure S1. Representative crystal forms and sizes of NdCld obtained by the PACT screen (Molecular Dimensions).

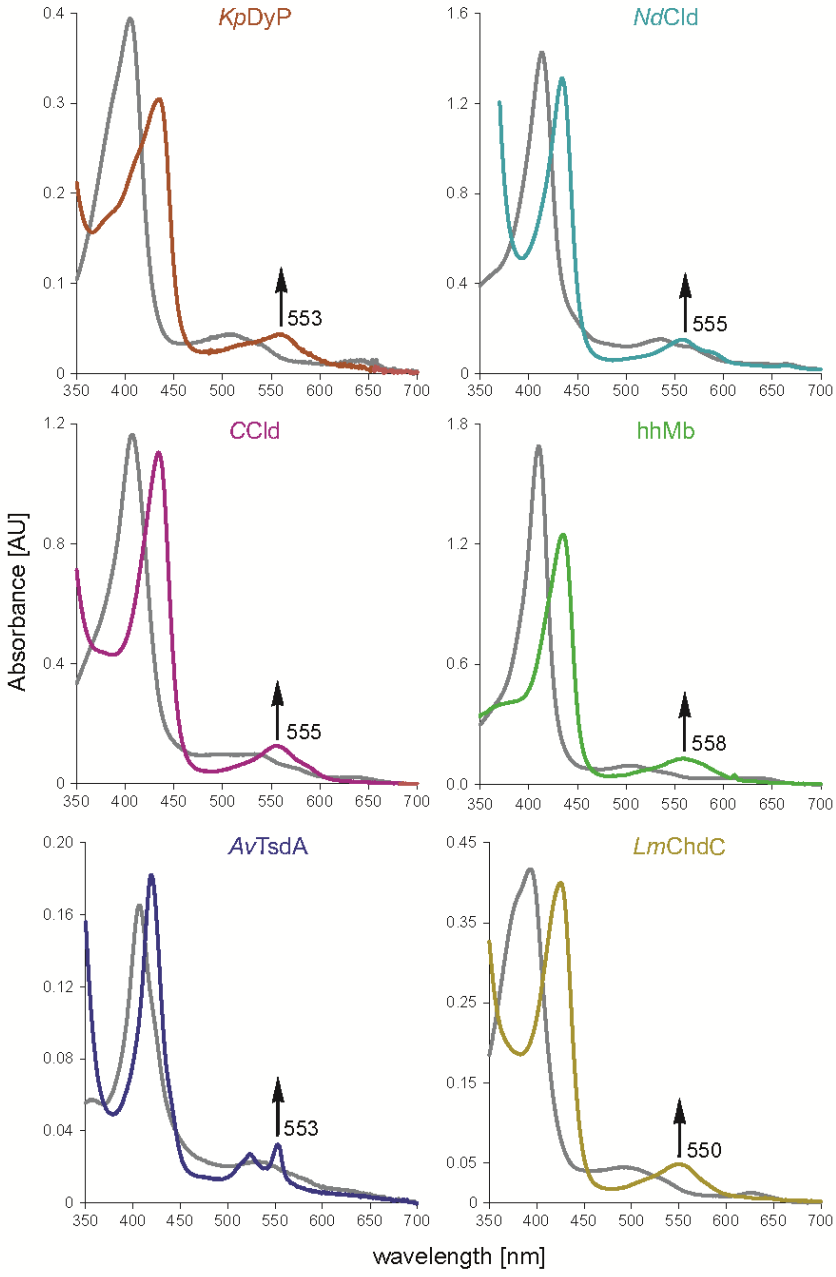

Figure S2. In solution spectra of ferric and ferrous forms of all six investigated proteins, reduced by sodium dithionite in 50 mM phosphate buffer, pH 7.0.

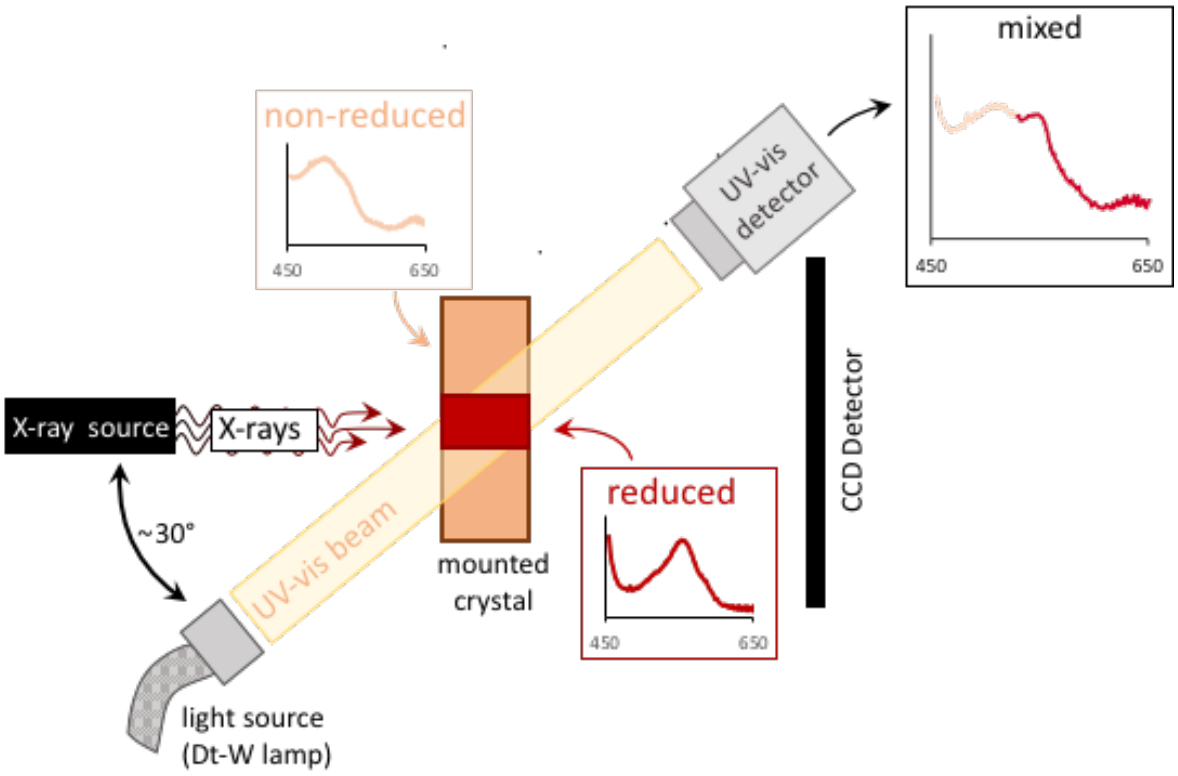

Figure S3. Schematic representation of the experimental setup at beamline I24 at Diamond Lightsource, Didcot, UK. The light path of the online UV-vis instrumentation was approximately 30° tilted relative to the X-ray axis. Representative spectra of the visible region of *Kp*DyP at different reduction states are given in this scheme. The ferric (non-reduced) part and the corresponding UV-vis spectrum of the representative crystal is depicted in salmon, the ferrous (fully reduced) part of the crystal and its corresponding spectrum in red. Due to the off-axis set-up of the instrumentation a mixed spectrum is expected to be observed by the UV-vis detector (represented in both colours). Nevertheless, the part irradiated by X-rays is fully reduced and this can reliably be confirmed by the plateau (at the selected maximum; 550-570 nm) of the dose trace of each sample, regardless of the final observed spectrum.

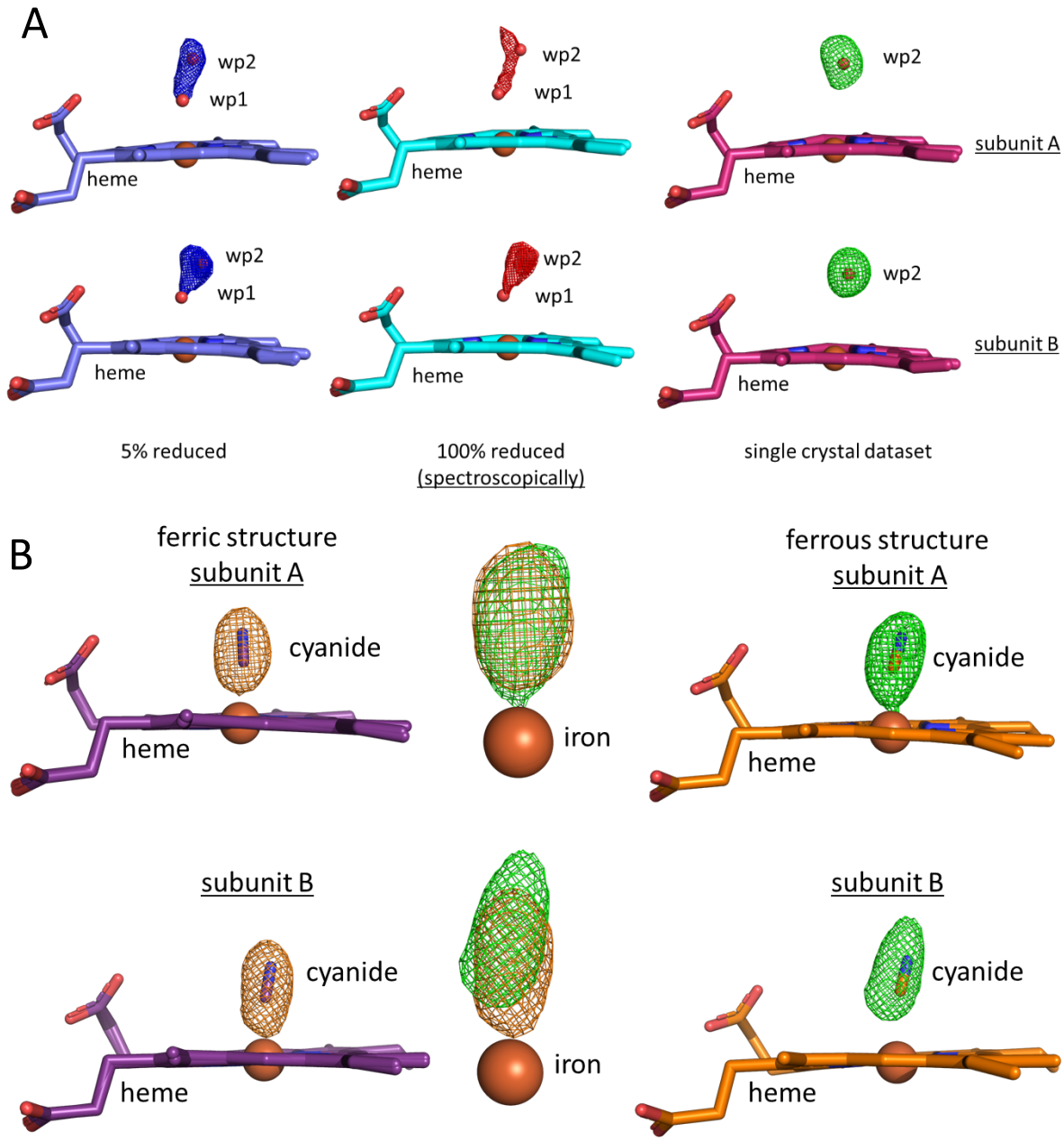

Figure S4. Presentation of omit maps of cyanide- and water ligated *Kp*DyP. (A) Active site of *Kp*DyP with water on the distal side of the heme. (Fo-Fc) omit maps (σ = 3) are shown in blue for the 5% reduced structure, in red for the 100% reduced structure of the multi-crystal data-set according to UV-vis spectroscopy and in green for the fully reduced single-crystal data set. (B) Active site of *Kp*DyP with cyanide on the distal side of the heme. (Fo-Fc) omit maps (σ = 3) are shown in orange for the ferric structure (5% reduced) and in green for the ferrous structure (fully reduced, single-crystal data set).

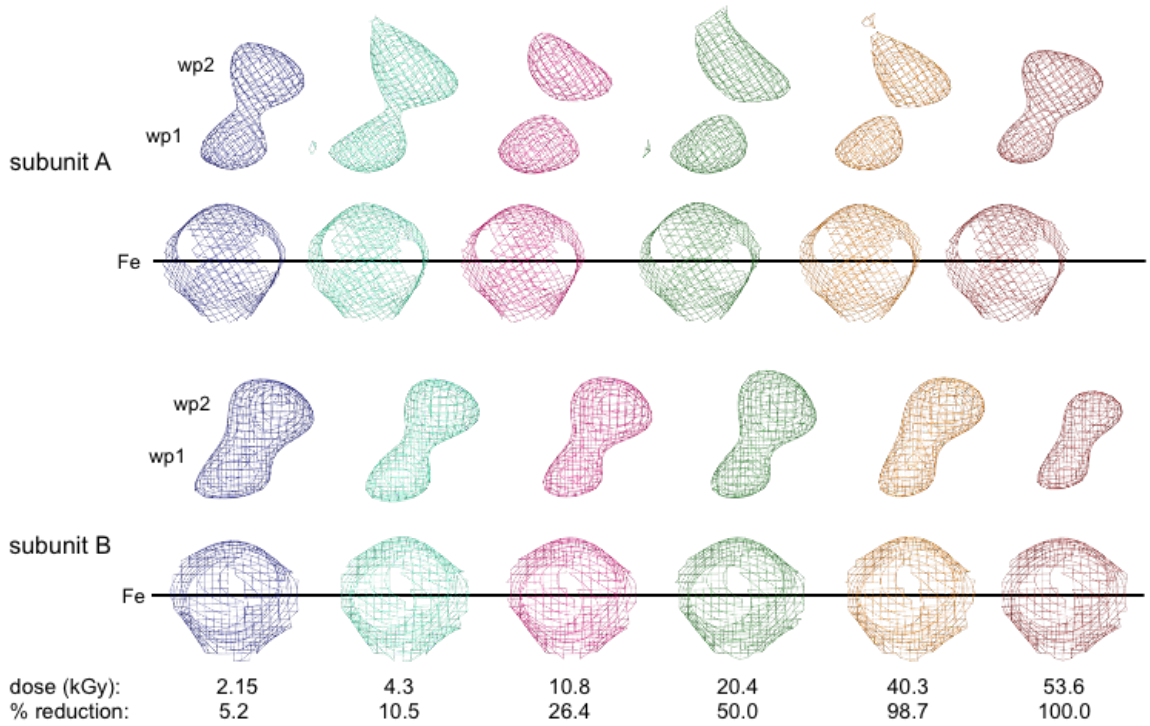

Figure S5. Representation of distal active site water molecules and the heme iron (sphere) are represented from KpDyP subunit A (top) and B (bottom) for the 5% reduced (blue, 6RQY), 10% reduced (turquoise, 6RR1), 26% reduced (pink, 6RR4), 50 % reduced (green, 6RR5), 99% reduced (orange, 6RR6), and the 100% reduced (red, 6RR8) structure, based on UV-vis spectroscopy, from the multi-crystal approach. 2mFo-DFc (contoured at 1 σ) electron density maps are displayed.

Dose calculation D1. Input parameters for *Av*TsdA crystals

```
##############################################################################
#                          Crystal Block                                     #
##############################################################################

Crystal
                # AvTsdA 4wq7
Type Cuboid
    # Crystal shape can be Cuboid or Spherical

Dimensions 20 20 5
    # Dimensions of the crystal in X,Y,Z in µm.
    # Z is the beam axis, Y the rotation axis and
    # X completes the right handed set
    #   (vertical if starting face-on).

PixelsPerMicron 0.5
    # This defines the coarseness of the simulation
    # (i.e. how many voxels the crystal is divided into.)
    # Preferably set as high as possible, however for a higher
    # value the simulation will take longer to complete.
    # Recommended to try increasing between 0.5 and 5 and ensure
    # the reported dose value converges as PixelsPerMicron increases.
    # As a rule of thumb, this needs to be at least 10x the beam
    # FWHM for a Gaussian beam.
    # e.g. 20µm FWHM beam -> 2µm voxels -> 0.5 voxels/µm

# NOTE: Use AngleP/AngleL if your crystal is not face-on to the beam.
# See RD3D user guide for more details

# Also need to specify the crystal composition below (Example case for insulin given):
AbsCoefCalc  RD3D
    # Absorption Coefficients calculated
    # using RADDOSE-3D (Zeldin et al. 2013).

UnitCell   80  70  58
    # unit cell size: a, b, c with alpha, beta and gamma angles default to 90°

NumMonomers  1
    # number of monomers in unit cell

NumResidues  252
    # number of residues per monomer

ProteinHeavyAtoms Fe 2 S 10
    # heavy atoms added to protein part of the
    # monomer, i.e. S, coordinated metals, Se in Se-Met

SolventHeavyConc P 50 S 100 I 50 Na 50
    # concentration of elements in the solvent
    # in mmol/l. Oxygen and lighter elements
    # should not be specified

SolventFraction 0.43
    # fraction of the unit cell occupied by solvent

##############################################################################
#                          Beam Block                                        #
##############################################################################

Beam

Type Gaussian
    # beam profile can be Gaussian or TopHat
Flux 4.2e12
    # in photons per second (2e12 = 2 * 10^12)
FWHM 20 20
    # in µm, horizontal by vertical for a Gaussian beam
Energy 12.1
    # photon energy in keV

Collimation Rectangular 100 100
    # Horizontal/Vertical collimation of the beam
    # For 'uncollimated' Gaussians, 3xFWHM recommended


##############################################################################
#                          Wedge Block                                       #
##############################################################################

Wedge 0 10
    # Start and End rotational angle of the crystal with Start < End

ExposureTime 1
    # Total time for entire angular range

# AngularResolution 0.1
    # Only change from the defaults when using very
    # small wedges, e.g 5°.

# NOTE: To define more complex geometries (helical, de-centred, or offset),
# see the StartOffset, TranslatePerDegree, and RotAxBeamOffset keywords
# in the User Guide
```

Dose calculation D2. Input parameters for *C*Cld crystals

```
##############################################################################
#                          Crystal Block                                     #
##############################################################################

Crystal
                # CCld 5mau
Type Cuboid
    # Crystal shape can be Cuboid or Spherical

Dimensions 20 20 20
    # Dimensions of the crystal in X,Y,Z in µm.
    # Z is the beam axis, Y the rotation axis and
    # X completes the right handed set
    #   (vertical if starting face-on).

PixelsPerMicron 0.5
    # This defines the coarseness of the simulation
    # (i.e. how many voxels the crystal is divided into.)
    # Preferably set as high as possible, however for a higher
    # value the simulation will take longer to complete.
    # Recommended to try increasing between 0.5 and 5 and ensure
    # the reported dose value converges as PixelsPerMicron increases.
    # As a rule of thumb, this needs to be at least 10x the beam
    # FWHM for a Gaussian beam.
    # e.g. 20µm FWHM beam -> 2µm voxels -> 0.5 voxels/µm

# NOTE: Use AngleP/AngleL if your crystal is not face-on to the beam.
# See RD3D user guide for more details

# Also need to specify the crystal composition below (Example case for insulin given):
AbsCoefCalc  RD3D
    # Absorption Coefficients calculated
    # using RADDOSE-3D (Zeldin et al. 2013).

UnitCell   51  53  55
    # unit cell size: a, b, c with alpha, beta and gamma angles default to 90°

NumMonomers  2
    # number of monomers in unit cell

NumResidues  182
    # number of residues per monomer

ProteinHeavyAtoms Fe 1 S 4
    # heavy atoms added to protein part of the
    # monomer, i.e. S, coordinated metals, Se in Se-Met

SolventHeavyConc P 50 Mg 75 S 125
    # concentration of elements in the solvent
    # in mmol/l. Oxygen and lighter elements
    # should not be specified

SolventFraction 0.59
    # fraction of the unit cell occupied by solvent

##############################################################################
#                          Beam Block                                        #
##############################################################################

Beam

Type Gaussian
    # beam profile can be Gaussian or TopHat
Flux 4.2e12
    # in photons per second (2e12 = 2 * 10^12)
FWHM 20 20
    # in µm, horizontal by vertical for a Gaussian beam
Energy 12.1
    # photon energy in keV

Collimation Rectangular 100 100
    # Horizontal/Vertical collimation of the beam
    # For 'uncollimated' Gaussians, 3xFWHM recommended


##############################################################################
#                          Wedge Block                                       #
##############################################################################

Wedge 0 10
    # Start and End rotational angle of the crystal with Start < End

ExposureTime 1
    # Total time for entire angular range

# AngularResolution 0.1
    # Only change from the defaults when using very
    # small wedges, e.g 5°.

# NOTE: To define more complex geometries (helical, de-centred, or offset),
# see the StartOffset, TranslatePerDegree, and RotAxBeamOffset keywords
# in the User Guide
```

Dose calculation D3. Input parameters for *Nd*Cld crystals from PACT condition E2

```
##############################################################################
#                          Crystal Block                                     #
##############################################################################

Crystal
                # NdCld 3nn1 PACT E2
Type Cuboid
     # Crystal shape can be Cuboid or Spherical

Dimensions 20 20 10
     # Dimensions of the crystal in X,Y,Z in µm.
     # Z is the beam axis, Y the rotation axis and
     # X completes the right handed set
     #   (vertical if starting face-on).

PixelsPerMicron 0.5
     # This defines the coarseness of the simulation
     # (i.e. how many voxels the crystal is divided into.)
     # Preferably set as high as possible, however for a higher
     # value the simulation will take longer to complete.
     # Recommended to try increasing between 0.5 and 5 and ensure
     # the reported dose value converges as PixelsPerMicron increases.
     # As a rule of thumb, this needs to be at least 10x the beam
     # FWHM for a Gaussian beam.
     # e.g. 20µm FWHM beam -> 2µm voxels -> 0.5 voxels/µm

# NOTE: Use AngleP/AngleL if your crystal is not face-on to the beam.
# See RD3D user guide for more details

# Also need to specify the crystal composition below (Example case for insulin given):
AbsCoefCalc  RD3D
     # Absorption Coefficients calculated
     # using RADDOSE-3D (Zeldin et al. 2013).

UnitCell   146  146  136
     # unit cell size: a, b, c with alpha, beta and gamma angles default to 90°

NumMonomers  5
     # number of monomers in unit cell

NumResidues  238
     # number of residues per monomer

ProteinHeavyAtoms Fe 1 S 7
     # heavy atoms added to protein part of the
     # monomer, i.e. S, coordinated metals, Se in Se-Met

SolventHeavyConc P 50 Na 100 Br 100
     # concentration of elements in the solvent
     # in mmol/l. Oxygen and lighter elements
     # should not be specified

SolventFraction 0.56
     # fraction of the unit cell occupied by solvent

##############################################################################
#                          Beam Block                                        #
##############################################################################

Beam

Type Gaussian
     # beam profile can be Gaussian or TopHat
Flux 4.2e12
     # in photons per second (2e12 = 2 * 10^12)
FWHM 20 20
     # in µm, horizontal by vertical for a Gaussian beam
Energy 12.1
     # photon energy in keV

Collimation Rectangular 100 100
     # Horizontal/Vertical collimation of the beam
     # For 'uncollimated' Gaussians, 3xFWHM recommended


##############################################################################
#                          Wedge Block                                       #
##############################################################################

Wedge 0 10
     # Start and End rotational angle of the crystal with Start < End

ExposureTime 1
     # Total time for entire angular range

# AngularResolution 0.1
     # Only change from the defaults when using very
     # small wedges, e.g 5°.

# NOTE: To define more complex geometries (helical, de-centred, or offset),
# see the StartOffset, TranslatePerDegree, and RotAxBeamOffset keywords
# in the User Guide
```

Dose calculation D4. Input parameters for *Nd*Cld crystals from PACT condition E8

```
############################################################################
#                          Crystal Block                                   #
############################################################################

Crystal
                # NdCld 3nn1 PACT E8
Type Cuboid
     # Crystal shape can be Cuboid or Spherical

Dimensions 20 20 10
     # Dimensions of the crystal in X,Y,Z in µm.
     # Z is the beam axis, Y the rotation axis and
     # X completes the right handed set
     #   (vertical if starting face-on).

PixelsPerMicron 0.5
     # This defines the coarseness of the simulation
     # (i.e. how many voxels the crystal is divided into.)
     # Preferably set as high as possible, however for a higher
     # value the simulation will take longer to complete.
     # Recommended to try increasing between 0.5 and 5 and ensure
     # the reported dose value converges as PixelsPerMicron increases.
     # As a rule of thumb, this needs to be at least 10x the beam
     # FWHM for a Gaussian beam.
     # e.g. 20µm FWHM beam -> 2µm voxels -> 0.5 voxels/µm

# NOTE: Use AngleP/AngleL if your crystal is not face-on to the beam.
# See RD3D user guide for more details

# Also need to specify the crystal composition below (Example case for insulin given):
AbsCoefCalc  RD3D
     # Absorption Coefficients calculated
     # using RADDOSE-3D (Zeldin et al. 2013).

UnitCell   146  146  136
     # unit cell size: a, b, c with alpha, beta and gamma angles default to 90°

NumMonomers  5
     # number of monomers in unit cell

NumResidues  238
     # number of residues per monomer

ProteinHeavyAtoms Fe 1 S 7
     # heavy atoms added to protein part of the
     # monomer, i.e. S, coordinated metals, Se in Se-Met

SolventHeavyConc P 50 Na 100 S 100
     # concentration of elements in the solvent
     # in mmol/l. Oxygen and lighter elements
     # should not be specified

SolventFraction 0.56
     # fraction of the unit cell occupied by solvent

############################################################################
#                          Beam Block                                      #
############################################################################

Beam

Type Gaussian
     # beam profile can be Gaussian or TopHat
Flux 4.2e12
     # in photons per second (2e12 = 2 * 10^12)
FWHM 20 20
     # in µm, horizontal by vertical for a Gaussian beam
Energy 12.1
     # photon energy in keV

Collimation Rectangular 100 100
     # Horizontal/Vertical collimation of the beam
     # For 'uncollimated' Gaussians, 3xFWHM recommended


############################################################################
#                          Wedge Block                                     #
############################################################################

Wedge 0 10
     # Start and End rotational angle of the crystal with Start < End

ExposureTime 1
     # Total time for entire angular range

# AngularResolution 0.1
     # Only change from the defaults when using very
     # small wedges, e.g 5°.

# NOTE: To define more complex geometries (helical, de-centred, or offset),
# see the StartOffset, TranslatePerDegree, and RotAxBeamOffset keywords
# in the User Guide
```

Dose calculation D5. Input parameters for *Nd*Cld crystals from PACT condition A4 and A5

```
############################################################################
#                          Crystal Block                                   #
############################################################################

Crystal
                # NdCld 3nn1 PACT A4 A5
Type Cuboid
    # Crystal shape can be Cuboid or Spherical

Dimensions 20 20 10
    # Dimensions of the crystal in X,Y,Z in µm.
    # Z is the beam axis, Y the rotation axis and
    # X completes the right handed set
    #   (vertical if starting face-on).

PixelsPerMicron 0.5
    # This defines the coarseness of the simulation
    # (i.e. how many voxels the crystal is divided into.)
    # Preferably set as high as possible, however for a higher
    # value the simulation will take longer to complete.
    # Recommended to try increasing between 0.5 and 5 and ensure
    # the reported dose value converges as PixelsPerMicron increases.
    # As a rule of thumb, this needs to be at least 10x the beam
    # FWHM for a Gaussian beam.
    # e.g. 20µm FWHM beam -> 2µm voxels -> 0.5 voxels/µm

# NOTE: Use AngleP/AngleL if your crystal is not face-on to the beam.
# See RD3D user guide for more details

# Also need to specify the crystal composition below (Example case for insulin given):
AbsCoefCalc  RD3D
    # Absorption Coefficients calculated
    # using RADDOSE-3D (Zeldin et al. 2013).

UnitCell   146  146  136
    # unit cell size: a, b, c with alpha, beta and gamma angles default to 90°

NumMonomers  5
    # number of monomers in unit cell

NumResidues  238
    # number of residues per monomer

ProteinHeavyAtoms Fe 1 S 7
    # heavy atoms added to protein part of the
    # monomer, i.e. S, coordinated metals, Se in Se-Met

SolventHeavyConc P 50 Na 50
    # concentration of elements in the solvent
    # in mmol/l. Oxygen and lighter elements
    # should not be specified

SolventFraction 0.56
    # fraction of the unit cell occupied by solvent

############################################################################
#                          Beam Block                                      #
############################################################################

Beam

Type Gaussian
    # beam profile can be Gaussian or TopHat
Flux 4.2e12
    # in photons per second (2e12 = 2 * 10^12)
FWHM 20 20
    # in µm, horizontal by vertical for a Gaussian beam
Energy 12.1
    # photon energy in keV

Collimation Rectangular 100 100
    # Horizontal/Vertical collimation of the beam
    # For 'uncollimated' Gaussians, 3xFWHM recommended


############################################################################
#                          Wedge Block                                     #
############################################################################

Wedge 0 10
    # Start and End rotational angle of the crystal with Start < End

ExposureTime 1
    # Total time for entire angular range

# AngularResolution 0.1
    # Only change from the defaults when using very
    # small wedges, e.g 5°.

# NOTE: To define more complex geometries (helical, de-centred, or offset),
# see the StartOffset, TranslatePerDegree, and RotAxBeamOffset keywords
# in the User Guide
```

Dose calculation D6. Input parameters for hhMb crystals

```
##############################################################################
#                          Crystal Block                                     #
##############################################################################

Crystal
                # hhMb 1wla
Type Cuboid
     # Crystal shape can be Cuboid or Spherical

Dimensions 20 20 5
     # Dimensions of the crystal in X,Y,Z in µm.
     # Z is the beam axis, Y the rotation axis and
     # X completes the right handed set
     #   (vertical if starting face-on).

PixelsPerMicron 0.5
     # This defines the coarseness of the simulation
     # (i.e. how many voxels the crystal is divided into.)
     # Preferably set as high as possible, however for a higher
     # value the simulation will take longer to complete.
     # Recommended to try increasing between 0.5 and 5 and ensure
     # the reported dose value converges as PixelsPerMicron increases.
     # As a rule of thumb, this needs to be at least 10x the beam
     # FWHM for a Gaussian beam.
     # e.g. 20µm FWHM beam -> 2µm voxels -> 0.5 voxels/µm

# NOTE: Use AngleP/AngleL if your crystal is not face-on to the beam.
# See RD3D user guide for more details

# Also need to specify the crystal composition below (Example case for insulin given):
AbsCoefCalc  RD3D
     # Absorption Coefficients calculated
     # using RADDOSE-3D (Zeldin et al. 2013).

UnitCell   64  29  36
     # unit cell size: a, b, c with alpha, beta and gamma angles default to 90°

NumMonomers  1
     # number of monomers in unit cell

NumResidues  154
     # number of residues per monomer

ProteinHeavyAtoms Fe 1 S 2
     # heavy atoms added to protein part of the
     # monomer, i.e. S, coordinated metals, Se in Se-Met

SolventHeavyConc P 50 S 1800
     # concentration of elements in the solvent
     # in mmol/l. Oxygen and lighter elements
     # should not be specified

SolventFraction 0.34
     # fraction of the unit cell occupied by solvent

##############################################################################
#                          Beam Block                                        #
##############################################################################

Beam

Type Gaussian
     # beam profile can be Gaussian or TopHat
Flux 4.2e12
     # in photons per second (2e12 = 2 * 10^12)
FWHM 20 20
     # in µm, horizontal by vertical for a Gaussian beam
Energy 12.1
     # photon energy in keV

Collimation Rectangular 100 100
     # Horizontal/Vertical collimation of the beam
     # For 'uncollimated' Gaussians, 3xFWHM recommended


##############################################################################
#                          Wedge Block                                       #
##############################################################################

Wedge 0 10
     # Start and End rotational angle of the crystal with Start < End

ExposureTime 1
     # Total time for entire angular range

# AngularResolution 0.1
     # Only change from the defaults when using very
     # small wedges, e.g 5°.

# NOTE: To define more complex geometries (helical, de-centred, or offset),
# see the StartOffset, TranslatePerDegree, and RotAxBeamOffset keywords
# in the User Guide.
```

Dose calculation D7. Input parameters for *Kp*DyP crystals

```
##############################################################################
#                          Crystal Block                                     #
##############################################################################

Crystal
                # KpDyP 6fks
Type Cuboid
     # Crystal shape can be Cuboid or Spherical

Dimensions 20 20 15
     # Dimensions of the crystal in X,Y,Z in µm.
     # Z is the beam axis, Y the rotation axis and
     # X completes the right handed set
     #   (vertical if starting face-on).

PixelsPerMicron 0.5
     # This defines the coarseness of the simulation
     # (i.e. how many voxels the crystal is divided into.)
     # Preferably set as high as possible, however for a higher
     # value the simulation will take longer to complete.
     # Recommended to try increasing between 0.5 and 5 and ensure
     # the reported dose value converges as PixelsPerMicron increases.
     # As a rule of thumb, this needs to be at least 10x the beam
     # FWHM for a Gaussian beam.
     # e.g. 20µm FWHM beam -> 2µm voxels -> 0.5 voxels/µm

# NOTE: Use AngleP/AngleL if your crystal is not face-on to the beam.
# See RD3D user guide for more details

# Also need to specify the crystal composition below (Example case for insulin given):
AbsCoefCalc  RD3D
     # Absorption Coefficients calculated
     # using RADDOSE-3D (Zeldin et al. 2013).

UnitCell   51  76  76
     # unit cell size: a, b, c with alpha, beta and gamma angles default to 90°

NumMonomers  2
     # number of monomers in unit cell

NumResidues  299
     # number of residues per monomer

ProteinHeavyAtoms Fe 1 S 9
     # heavy atoms added to protein part of the
     # monomer, i.e. S, coordinated metals, Se in Se-Met

SolventHeavyConc P 50 Mg 50 Cl 50
     # concentration of elements in the solvent
     # in mmol/l. Oxygen and lighter elements
     # should not be specified

SolventFraction 0.41
     # fraction of the unit cell occupied by solvent

##############################################################################
#                          Beam Block                                        #
##############################################################################

Beam

Type Gaussian
     # beam profile can be Gaussian or TopHat
Flux 4.2e12
     # in photons per second (2e12 = 2 * 10^12)
FWHM 20 20
     # in µm, horizontal by vertical for a Gaussian beam
Energy 12.1
     # photon energy in keV

Collimation Rectangular 100 100
     # Horizontal/Vertical collimation of the beam
     # For 'uncollimated' Gaussians, 3xFWHM recommended


##############################################################################
#                          Wedge Block                                       #
##############################################################################

Wedge 0 10
     # Start and End rotational angle of the crystal with Start < End

ExposureTime 1
     # Total time for entire angular range

# AngularResolution 0.1
     # Only change from the defaults when using very
     # small wedges, e.g 5°.

# NOTE: To define more complex geometries (helical, de-centred, or offset),
# see the StartOffset, TranslatePerDegree, and RotAxBeamOffset keywords
# in the User Guide
```

Dose calculation D8. Input parameters for *Lm*ChdC crystals

```
##############################################################################
#                          Crystal Block                                     #
##############################################################################

Crystal
                # LmChdC 6fxj
Type Cuboid
     # Crystal shape can be Cuboid or Spherical

Dimensions 20 20 10
     # Dimensions of the crystal in X,Y,Z in µm.
     # Z is the beam axis, Y the rotation axis and
     # X completes the right handed set
     #   (vertical if starting face-on).

PixelsPerMicron 0.5
     # This defines the coarseness of the simulation
     # (i.e. how many voxels the crystal is divided into.)
     # Preferably set as high as possible, however for a higher
     # value the simulation will take longer to complete.
     # Recommended to try increasing between 0.5 and 5 and ensure
     # the reported dose value converges as PixelsPerMicron increases.
     # As a rule of thumb, this needs to be at least 10x the beam
     # FWHM for a Gaussian beam.
     # e.g. 20µm FWHM beam -> 2µm voxels -> 0.5 voxels/µm

# NOTE: Use AngleP/AngleL if your crystal is not face-on to the beam.
# See RD3D user guide for more details

# Also need to specify the crystal composition below (Example case for insulin given):
AbsCoefCalc  RD3D
     # Absorption Coefficients calculated
     # using RADDOSE-3D (Zeldin et al. 2013).

UnitCell   78  129  78
     # unit cell size: a, b, c with alpha, beta and gamma angles default to 90°

NumMonomers  5
     # number of monomers in unit cell

NumResidues  251
     # number of residues per monomer

ProteinHeavyAtoms Fe 1 S 10
     # heavy atoms added to protein part of the
     # monomer, i.e. S, coordinated metals, Se in Se-Met

SolventHeavyConc P 50
     # concentration of elements in the solvent
     # in mmol/l. Oxygen and lighter elements
     # should not be specified

SolventFraction 0.53
     # fraction of the unit cell occupied by solvent

##############################################################################
#                          Beam Block                                        #
##############################################################################

Beam

Type Gaussian
     # beam profile can be Gaussian or TopHat
Flux 4.2e12
     # in photons per second (2e12 = 2 * 10^12)
FWHM 20 20
     # in µm, horizontal by vertical for a Gaussian beam
Energy 12.1
     # photon energy in keV

Collimation Rectangular 100 100
     # Horizontal/Vertical collimation of the beam
     # For 'uncollimated' Gaussians, 3xFWHM recommended


##############################################################################
#                          Wedge Block                                       #
##############################################################################

Wedge 0 10
     # Start and End rotational angle of the crystal with Start < End

ExposureTime 1
     # Total time for entire angular range

# AngularResolution 0.1
     # Only change from the defaults when using very
     # small wedges, e.g 5°.

# NOTE: To define more complex geometries (helical, de-centred, or offset),
# see the StartOffset, TranslatePerDegree, and RotAxBeamOffset keywords
# in the User Guide
```

Dose calculation D9. Input parameters for generic crystal (2 monomers)

```
##############################################################################
#                          Crystal Block                                     #
##############################################################################

Crystal
                # generic crystal 2 monomers
Type Cuboid
     # Crystal shape can be Cuboid or Spherical

Dimensions 20 20 20
     # Dimensions of the crystal in X,Y,Z in µm.
     # Z is the beam axis, Y the rotation axis and
     # X completes the right handed set
     #   (vertical if starting face-on).

PixelsPerMicron 0.5
     # This defines the coarseness of the simulation
     # (i.e. how many voxels the crystal is divided into.)
     # Preferably set as high as possible, however for a higher
     # value the simulation will take longer to complete.
     # Recommended to try increasing between 0.5 and 5 and ensure
     # the reported dose value converges as PixelsPerMicron increases.
     # As a rule of thumb, this needs to be at least 10x the beam
     # FWHM for a Gaussian beam.
     # e.g. 20µm FWHM beam -> 2µm voxels -> 0.5 voxels/µm

# NOTE: Use AngleP/AngleL if your crystal is not face-on to the beam.
# See RD3D user guide for more details

# Also need to specify the crystal composition below (Example case for insulin given):
AbsCoefCalc  RD3D
     # Absorption Coefficients calculated
     # using RADDOSE-3D (Zeldin et al. 2013).

UnitCell   80  95  120
     # unit cell size: a, b, c with alpha, beta and gamma angles default to 90°

NumMonomers  2
     # number of monomers in unit cell

NumResidues  350
     # number of residues per monomer

ProteinHeavyAtoms Fe 1 S 13
     # heavy atoms added to protein part of the
     # monomer, i.e. S, coordinated metals, Se in Se-Met

SolventHeavyConc P 100
     # concentration of elements in the solvent
     # in mmol/l. Oxygen and lighter elements
     # should not be specified

SolventFraction 0.43
     # fraction of the unit cell occupied by solvent

##############################################################################
#                          Beam Block                                        #
##############################################################################

Beam

Type Gaussian
     # beam profile can be Gaussian or TopHat
Flux 4.2e12
     # in photons per second (2e12 = 2 * 10^12)
FWHM 20 20
     # in µm, horizontal by vertical for a Gaussian beam
Energy 12.1
     # photon energy in keV

Collimation Rectangular 100 100
     # Horizontal/Vertical collimation of the beam
     # For 'uncollimated' Gaussians, 3xFWHM recommended


##############################################################################
#                          Wedge Block                                       #
##############################################################################

Wedge 0 10
     # Start and End rotational angle of the crystal with Start < End

ExposureTime 1
     # Total time for entire angular range

# AngularResolution 0.1
     # Only change from the defaults when using very
     # small wedges, e.g 5°.

# NOTE: To define more complex geometries (helical, de-centred, or offset),
# see the StartOffset, TranslatePerDegree, and RotAxBeamOffset keywords
# in the User Guide
```

Dose calculation D10. Input parameters for generic crystal (3 monomers)

```
##############################################################################
#                          Crystal Block                                     #
##############################################################################

Crystal
                # generic crystal 3 monomers
Type Cuboid
     # Crystal shape can be Cuboid or Spherical

Dimensions 20 20 20
     # Dimensions of the crystal in X,Y,Z in µm.
     # Z is the beam axis, Y the rotation axis and
     # X completes the right handed set
     #   (vertical if starting face-on).

PixelsPerMicron 0.5
     # This defines the coarseness of the simulation
     # (i.e. how many voxels the crystal is divided into.)
     # Preferably set as high as possible, however for a higher
     # value the simulation will take longer to complete.
     # Recommended to try increasing between 0.5 and 5 and ensure
     # the reported dose value converges as PixelsPerMicron increases.
     # As a rule of thumb, this needs to be at least 10x the beam
     # FWHM for a Gaussian beam.
     # e.g. 20µm FWHM beam -> 2µm voxels -> 0.5 voxels/µm

# NOTE: Use AngleP/AngleL if your crystal is not face-on to the beam.
# See RD3D user guide for more details

# Also need to specify the crystal composition below (Example case for insulin given):
AbsCoefCalc  RD3D
     # Absorption Coefficients calculated
     # using RADDOSE-3D (Zeldin et al. 2013).

UnitCell   80  95  120
     # unit cell size: a, b, c with alpha, beta and gamma angles default to 90°

NumMonomers  3
     # number of monomers in unit cell

NumResidues  350
     # number of residues per monomer

ProteinHeavyAtoms Fe 1 S 13
     # heavy atoms added to protein part of the
     # monomer, i.e. S, coordinated metals, Se in Se-Met

SolventHeavyConc P 100
     # concentration of elements in the solvent
     # in mmol/l. Oxygen and lighter elements
     # should not be specified

SolventFraction 0.43
     # fraction of the unit cell occupied by solvent

##############################################################################
#                          Beam Block                                        #
##############################################################################

Beam

Type Gaussian
     # beam profile can be Gaussian or TopHat
Flux 4.2e12
     # in photons per second (2e12 = 2 * 10^12)
FWHM 20 20
     # in µm, horizontal by vertical for a Gaussian beam
Energy 12.1
     # photon energy in keV

Collimation Rectangular 100 100
     # Horizontal/Vertical collimation of the beam
     # For 'uncollimated' Gaussians, 3xFWHM recommended


##############################################################################
#                          Wedge Block                                       #
##############################################################################

Wedge 0 10
     # Start and End rotational angle of the crystal with Start < End

ExposureTime 1
     # Total time for entire angular range

# AngularResolution 0.1
     # Only change from the defaults when using very
     # small wedges, e.g 5°.

# NOTE: To define more complex geometries (helical, de-centred, or offset),
# see the StartOffset, TranslatePerDegree, and RotAxBeamOffset keywords
# in the User Guide
```