

Appendix 1 : EDNA characterisation output :

Summary of characterisation:

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Diffraction plan:

BEST complexity : min  
Aimed I/sigma at highest resolution : 3.0  
Max exposure time per data collection : 100000.0 [s]  
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Indexing : Summary of indexing:

Indexing : -----

Indexing : MOSFLM : Version 7.0.1 for Image plate and CCD data 20th August 2007  
Indexing : MOSFLM : Execution of MOSFLM indexing successful.  
Indexing : MOSFLM : Image directory : /mntdirect/\_data\_id14eh2\_inhouse/mxih1/20090209/Ana\_Maria/AA374/edna\_p10  
Indexing : MOSFLM : Image template : p10\_1\_###.img  
Indexing : MOSFLM : Images used in indexing : 1 2  
Indexing : MOSFLM :  
Indexing : MOSFLM : List of possible solutions (index, penalty, lattice and cell):  
Indexing : MOSFLM : 11 174 oC 79.81 276.37 119.13 89.92 90.04 106.70  
Indexing : MOSFLM : 10 92 oC 177.97 178.17 79.81 90.03 90.09 83.98  
Indexing : MOSFLM : 9 92 tP 119.13 132.35 79.81 90.08 90.04 90.06  
Indexing : MOSFLM : 8 92 mC 177.97 178.17 79.81 89.97 90.09 96.02  
Indexing : MOSFLM : 7 91 mC 177.97 178.17 79.81 90.03 90.09 83.98  
Indexing : MOSFLM : 6 1 mP 79.81 119.13 132.35 90.06 90.08 90.04  
Indexing : MOSFLM : 5 1 mP 119.13 79.81 132.35 90.08 90.06 90.04  
Indexing : MOSFLM : 4 1 oP 79.81 119.13 132.35 90.06 90.08 90.04  
Indexing : MOSFLM : 3 1 mP 79.81 132.35 119.13 90.06 90.04 90.08  
Indexing : MOSFLM : 2 0 aP 79.81 119.13 132.35 89.94 89.92 90.04  
Indexing : MOSFLM : 1 0 aP 79.81 119.13 132.35 90.06 90.08 90.04  
Indexing : MOSFLM :  
Indexing : MOSFLM : Chosen solution number : 4  
Indexing : MOSFLM : Selected space group : P222  
Indexing : MOSFLM : Refined cell : 79.82 119.13 132.35 90.0 90.0 90.0  
Indexing : MOSFLM : Number of spots used : 262  
Indexing : MOSFLM : Number of spots total : 272  
Indexing : MOSFLM : Spot deviation positional : 0.08 [mm]  
Indexing : MOSFLM : Spot deviation angular : 0.36 [degrees]  
Indexing : MOSFLM : Beam shift (X, Y) : -0.396, -0.126 [mm]  
Indexing : MOSFLM : Estimated mosaicity : 0.48 [degrees]  
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Indexing : Prediction : Summary of generation of image(s) with prediction:

Indexing : Prediction : Path to prediction image number 2 :

/mntdirect/\_data\_id14eh2\_inhouse/mxih1/20090209/Ana\_Maria/AA374/edna\_p10/20090209-160254\_EDApplication-v0.1/EDPluginControlCCP4iv01/Characterisation/Indexing/EDPluginControlGeneratePredictionv01/EDPluginMOSFLMv01GeneratePrediction-02/EDPluginMOSFLMv01GeneratePrediction-02\_image.jpg

Indexing : Prediction : Path to prediction image number 1 :

/mntdirect/\_data\_id14eh2\_inhouse/mxih1/20090209/Ana\_Maria/AA374/edna\_p10/20090209-160254\_EDApplication-v0.1/EDPluginControlCCP4iv01/Characterisation/Indexing/EDPluginControlGeneratePredictionv01/EDPluginMOSFLMv01GeneratePrediction-01/EDPluginMOSFLMv01GeneratePrediction-01\_image.jpg  
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Integration : Summary of integration:

Integration : -----

Integration : MOSFLM : Version 7.0.1 for Image plate and CCD data 20th August 2007  
Integration : MOSFLM : Execution of MOSFLM integration successful.  
Integration : MOSFLM : Image directory : /mntdirect/\_data\_id14eh2\_inhouse/mxih1/20090209/Ana\_Maria/AA374/edna\_p10  
Integration : MOSFLM : Image template : p10\_1\_###.img  
Integration : MOSFLM : Image start : 1  
Integration : MOSFLM : Image end : 1  
Integration : MOSFLM : Rotation axis start : 0.0 [degrees]  
Integration : MOSFLM : Rotation axis end : 1.0 [degrees]  
Integration : MOSFLM :  
Integration : MOSFLM : Number of fully recorded reflections : 532  
Integration : MOSFLM : Number of partials : 2869  
Integration : MOSFLM : Number of overlapped reflections : 0  
Integration : MOSFLM : Number of reflections with negative intensity : 1044  
Integration : MOSFLM : Number of bad reflections : 4  
Integration : MOSFLM :  
Integration : MOSFLM : RMS spot deviation : 0.035 [mm]  
Integration : MOSFLM : Average I/sigma overall : 5.9  
Integration : MOSFLM : Average I/sigma at highest resolution : 1.7  
Integration : MOSFLM :  
Integration : MOSFLM : Analysis as a function of resolution:  
Integration : MOSFLM : Res (Ang) 5.67 4.01 3.27 2.83 2.53 2.31 2.14 2.00 Overall  
Integration : MOSFLM : Profile fitted fully recorded:  
Integration : MOSFLM : Number 46 88 115 133 86 43 15 3 529  
Integration : MOSFLM : <I> 11836 4981 1004 193 98 25 -34 196 2143  
Integration : MOSFLM : <I/sigma> 26.0 14.8 3.8 1.0 0.6 0.2 -0.3 1.7 5.9

Integration : MOSFLM : Profile fitted partials:  
Integration : MOSFLM : Number 221 427 568 621 540 306 147 28 2858  
Integration : MOSFLM : <l> 10318 4177 1103 255 78 36 22 -90 1715  
Integration : MOSFLM : <l/sigma> 17.1 9.7 3.2 0.8 0.3 0.2 0.1 -0.5 3.7  
Integration : MOSFLM :  
Integration : MOSFLM : Path to MTZ file :  
/mntdirect/\_data\_id14eh2\_inhouse/mxih1/20090209/Ana\_Maria/AA374/edna\_p10/20090209-160254\_EDApplication-  
v0.1/EDPluginControlCCP4iv01/Characterisation/Integration/EDPluginMOSFLMv01Integration-01/EDPluginMOSFLMv01Integration-  
01\_process\_1\_1.mtz

Integration : -----  
Integration : MOSFLM : Version 7.0.1 for Image plate and CCD data 20th August 2007  
Integration : MOSFLM : Execution of MOSFLM integration successful.  
Integration : MOSFLM : Image directory : /mntdirect/\_data\_id14eh2\_inhouse/mxih1/20090209/Ana\_Maria/AA374/edna\_p10  
Integration : MOSFLM : Image template : p10\_1\_###.img  
Integration : MOSFLM : Image start : 2  
Integration : MOSFLM : Image end : 2  
Integration : MOSFLM : Rotation axis start : 90.0 [degrees]  
Integration : MOSFLM : Rotation axis end : 91.0 [degrees]  
Integration : MOSFLM :  
Integration : MOSFLM : Number of fully recorded reflections : 549  
Integration : MOSFLM : Number of partials : 2855  
Integration : MOSFLM : Number of overlapped reflections : 0  
Integration : MOSFLM : Number of reflections with negative intensity : 1049  
Integration : MOSFLM : Number of bad reflections : 2  
Integration : MOSFLM :  
Integration : MOSFLM : RMS spot deviation : 0.025 [mm]  
Integration : MOSFLM : Average l/sigma overall : 6.8  
Integration : MOSFLM : Average l/sigma at highest resolution : 0.8  
Integration : MOSFLM :  
Integration : MOSFLM : Analysis as a function of resolution:  
Integration : MOSFLM : Res (Ang) 5.67 4.01 3.27 2.83 2.53 2.31 2.14 2.00 Overall  
Integration : MOSFLM : Profile fitted fully recorded:  
Integration : MOSFLM : Number 46 83 112 148 89 40 21 6 545  
Integration : MOSFLM : <l> 10082 4305 1165 381 167 36 -86 339 1880  
Integration : MOSFLM : <l/sigma> 26.6 17.3 5.5 2.2 1.2 0.3 -0.7 0.8 6.8  
Integration : MOSFLM : Profile fitted partials:  
Integration : MOSFLM : Number 230 454 576 597 523 298 146 26 2850  
Integration : MOSFLM : <l> 8065 3849 1378 296 112 50 30 77 1633  
Integration : MOSFLM : <l/sigma> 12.9 8.3 3.7 1.1 0.5 0.2 0.1 0.4 3.5  
Integration : MOSFLM :  
Integration : MOSFLM : Path to MTZ file :  
/mntdirect/\_data\_id14eh2\_inhouse/mxih1/20090209/Ana\_Maria/AA374/edna\_p10/20090209-160254\_EDApplication-  
v0.1/EDPluginControlCCP4iv01/Characterisation/Integration/EDPluginMOSFLMv01Integration-02/EDPluginMOSFLMv01Integration-  
02\_process\_2\_2.mtz

Strategy : Summary of Strategy:  
Strategy : -----  
Strategy : Raddose : version 4.2 // 2007/07/05  
Strategy : Raddose : Execution of radiation dose estimation successful.  
Strategy : Raddose :  
Strategy : Raddose : Flux : 1.2e+11 [photons/s]  
Strategy : Raddose : Crystal size : 0.100 x 0.100 x 0.100 [mm]  
Strategy : Raddose : Beam size : 0.150 x 0.150 [mm]  
Strategy : Raddose : Solvent : 52.90 [%]  
Strategy : Raddose : Dose rate : 1.9e+03 [Grays/s]  
Strategy : Raddose : Time to reach Henderson limit : 1.1e+04 [s]  
Strategy :  
Strategy : Calculations assuming polymer crystal with:  
Strategy : -----  
Strategy :  
Strategy : Number of structure copies in asymmetric unit: 4.00  
Strategy :  
Strategy : Chains:  
Strategy : Type : protein  
Strategy : Number of residues : 267.00  
Strategy : Number of heavy atoms : S=10 ca=1  
Strategy : Number of copies in structure : 1.00  
Strategy :  
Strategy : -----  
Strategy : Best : Version 3.1.0.d // 16.07.2007  
Strategy : Best :  
Strategy : Best : Plan for data collection:  
Strategy : Best : N | Phi\_start | N.of.images | Rot.width | Exposure | Distance | Overlap |  
Strategy : Best : 1 | 54.00 | 267 | 0.30 | 14.10 | 278.9 | No |  
Strategy : Best : 2 | 134.10 | 83 | 0.30 | 40.52 | 278.9 | No |  
Strategy : Best : 3 | 159.00 | 17 | 0.30 | 85.06 | 278.9 | No |  
Strategy : Best :  
Strategy : Best : Attenuation : 1.0

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Strategy : Best : Total rotation range      : 110.1 [degrees]
Strategy : Best : Total number of images   : 367
Strategy : Best : Total exposure time     : 8573.9 [s]
Strategy : Best : Total data collection time  : 9491.4 [s]
Strategy : Best : Resolution                       : 2.9 [Å]
Strategy : Best : Resolution reasoning              : Resolution limit is set by the radiation damage
Strategy : Best : Ranking resolution                 : 2.91 [Å]
Strategy : Best :
Strategy : Best : Predicted statistics:
Strategy : Best : Completeness                       : 98.9 [%]
Strategy : Best : I/sigma at highest resolution      : 2.8
Strategy : Best : Multiplicity                         : 4.6
Strategy : Best :
Strategy : Best : Statistics according to the plan:
Strategy : Best : Resolution Compl. Average I/Sigma I/Sigma Chi**2 R-fact Overload
Strategy : Best : Lower Upper % Intensity Sigma /Chi % %
Strategy : Best : -----
Strategy : Best : 12.00 9.08 95.0 27311.6 411.8 66.3 60.6 1.20 2.3 0.00
Strategy : Best : 9.08 7.60 96.0 18607.0 285.5 65.2 56.5 1.33 2.6 0.00
Strategy : Best : 7.60 6.67 97.0 11793.6 196.6 60.0 50.7 1.40 2.9 0.00
Strategy : Best : 6.67 6.01 98.0 8305.5 154.1 53.9 44.7 1.45 3.4 0.00
Strategy : Best : 6.01 5.52 98.0 7643.9 151.0 50.6 40.8 1.54 3.7 0.00
Strategy : Best : 5.52 5.13 98.0 8436.9 166.3 50.7 39.4 1.66 3.9 0.00
Strategy : Best : 5.13 4.81 98.0 9316.0 183.9 50.7 37.8 1.80 4.0 0.00
Strategy : Best : 4.81 4.54 98.0 9686.2 196.2 49.4 35.9 1.89 4.2 0.00
Strategy : Best : 4.54 4.32 98.0 8999.4 201.6 44.6 32.3 1.91 4.7 0.00
Strategy : Best : 4.32 4.12 99.0 7668.9 190.2 40.3 29.5 1.87 5.1 0.00
Strategy : Best : 4.12 3.95 99.0 6316.0 182.1 34.7 26.0 1.77 5.8 0.00
Strategy : Best : 3.95 3.80 99.0 5175.8 181.7 28.5 22.4 1.62 6.8 0.00
Strategy : Best : 3.80 3.67 99.0 4247.3 188.7 22.5 18.6 1.46 8.1 0.00
Strategy : Best : 3.67 3.55 99.0 3438.7 189.5 18.1 15.7 1.34 9.7 0.00
Strategy : Best : 3.55 3.44 99.0 2762.4 186.1 14.8 13.2 1.27 11.5 0.00
Strategy : Best : 3.44 3.34 100.0 2187.3 186.0 11.8 10.8 1.19 14.0 0.00
Strategy : Best : 3.34 3.24 100.0 1701.1 184.7 9.2 8.7 1.13 17.5 0.00
Strategy : Best : 3.24 3.16 100.0 1310.7 187.4 7.0 6.7 1.09 22.3 0.00
Strategy : Best : 3.16 3.08 100.0 1026.3 186.7 5.5 5.3 1.06 28.0 0.00
Strategy : Best : 3.08 3.01 100.0 812.2 186.6 4.4 4.3 1.04 34.9 0.00
Strategy : Best : 3.01 2.94 100.0 641.9 187.7 3.4 3.4 1.03 43.7 0.00
Strategy : Best : 2.94 2.91 100.0 534.5 188.4 2.8 2.8 1.02 0.5 0.00
Strategy : Best : 12.00 2.91 99.0 5194.7 189.7 27.4 23.3 1.38 6.5 0.00
Strategy :
EDApplication-v0.1::Runtime: 32.5743911266 [s]

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