

Day 1 - Saturday, January 30

19h00 – 20h00 Registration and Welcome Reception at Hotel Riviera
Free evening

Day 2 – Sunday, January 31

08h30 – Bus departs from Hotel Riviera

09h00 – Bus arrives at ITQB

09h00 – 09h45 Registration and Welcome Coffee

Session 1

(Chair: Pedro Matias)

09h45 – 10h00 *Introduction* (Pedro Matias)

10h00 – 11h00 *Overview of the use of ensembles and multiple models in crystallography* (Paul Adams)

11h00 – 11h45 *TLS and multicopy models for diffuse scattering* (Alexandre Urzhumtsev)

12h00 – 13h30 Lunch

Session 2

(Chair: Manfred Weiss)

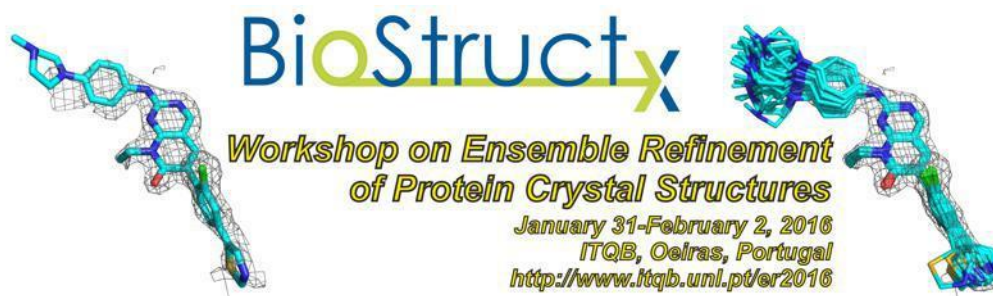
13h30 – 16h00 *Tutorial session 1*

16h00 – 16h30 Tea break

16h30 – 17h30 *Ensemble refinement of protein crystal structures in PHENIX* (Tom Burnley)

17h30 – 18h15 *Tutorial session 2*

18h30 – Bus departs to Hotel Riviera
Free evening



Day 3 - Monday, February 1

08h30 – Bus departs from Hotel Riviera

09h00 – Bus arrives at ITQB

Session 3

(Chair: Manfred Weiss)

09h00 – 10h30 *Tutorial session 3*

10h30 - 11h00 **Coffee break**

11h00 – 11h45 *Multicopy models: phasing and ML refinement and validation* (Alexandre Urzhumtsev)

11h45 – 12h30 *Combining crystallography, SAXS and NMR to describe the structural ensemble of proteins* (Remy Loris)

12h30 - 14h00 **Lunch**

Session 4

(Chair: Pedro Matias)

14h00 – 14h45 *Modelling dynamics in HSP90 crystal structures by ensemble refinement* (Marta Amaral)

14h45 – 15h30 *Macromolecular refinement underestimates the heterogeneity in crystals* (Raj Pannu)

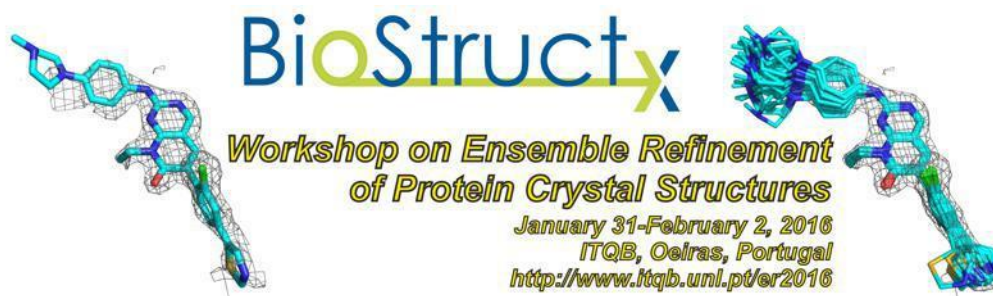
15h30 – 16h00 *General Discussion 1*

16h00 – 16h30 **Tea break**

16h30 - 18h30 *Tutorial Session 4*

18h45 – Bus departs to Hotel Riviera

19h45 – Workshop Dinner at Hotel Riviera



Day 4 - Tuesday, February 2

09h00 – Bus departs from Hotel Riviera

09h30 – Bus arrives at ITQB

Session 5

(Chair: Manfred Weiss)

09h30 – 10h00 *Visualizing results with PyMOL* (Pedro Matias)

10h00 – 10h30 *Visualizing results with COOT* (Bernhard Lohkamp)

10h30 – 11h00 *Tutorial wrap-up*

11h00 – 11h30 Coffee break

11h30 – 12h00 *General Discussion 2*

12h00 – 12h30 *Conclusions, end of meeting*