MS07 P01

Autodep 4.1 : A web-based deposition and archival system S. Sen, G.Van Ginkel, A.Kapopoulou, G. Sahni, G.J. Swaminathan, R.H.Newman, S.Velankar, K.Henrick
Macromolecular Structural Database, European Bioinformatics Institure, Hinxton, Cambridge CB10 1SD. United Kingdom. Email: ssen@ebi.ac.uk

Keywords: protein database, computer software, structural biology

The Macromolecular Structure Database (MSD) (http://www.ebi.ac.uk/msd/) [1] group is one of the four partners in the worldwide Protein Data Bank (wwPDB) [2], the consortium entrusted with the collation, maintenance and distribution of the global repository of macromolecular structure data. Structures can be deposited at the MSD using the AutoDep [3] deposition tool or with the other wwPDB partners using the ADIT system. The AutoDep 4.1 is an extension of the previously developed software AutoDep 4.0 [4], [5] which was a complete rewrite of the original AutoDep system. The AutoDep system allows value-added information to be returned in a safe and secure manner into the password-protected deposition session only accessible to the depositor, following annotation of the structure by curation staff, within 2 days of deposition. AutoDep 4.1 is also available for download and installation in-house, where a deposition can be completed and validated before uploading the whole deposition session to the MSD site, where submission to the wwPDB can be completed in minutes. The extended version of AutoDep (4.1) provides detailed information regarding the ligand binding sites, Uniprot sequence mapping and taxonomy information, applets for viewing the files, in addition to structure factor validation statistics, quaternary structure assessments, and new ligand dictionaries. With structures being determined at an ever increasing rate, it is imperative that deposition tools keep pace with this exponential growth of data. We believe that the latest release of AutoDep has significantly automated the deposition process, reduced the time taken to deposit a structure, and at the same time harnessed services offered by the MSD group in returning useful information to the depositor.

[1] H.Boutselakis et al., *Nucleic acid Res*., 2003, 31, D458.
[2] H.Berman et al., *Nature Struct. Biol*., 2003, 10, 980.
[3] D. Lin et al., *Acta Crystallogr*., 2000, D56, 828.
[4] M.Tagari et al., *Nuclei Acids Res*., 2006, 34, D287.
[5] G.J.Swaminathan et al., *Acta Crystallogr.* 2006, A62, S15.

MS07 P02

High resolution X-ray structure of Triclinic Hen Egg-White Lysozyme at 0.83Å Akifumi Higashiura[a], Hiroaki Tanaka[b], Koji Inaka[d], Masaru Sato[c], Shigeru Sugiyama[d], Sachiko Takahashi[b], Mari Yamanaka[b], Moritoshi Motohara[c], Satoshi Sano[c], Tomoyuki Kobayashi[c], Mamoru Suzuki[a], Tetsuo Tanaka[c] and Atsushi Nakagawa[a], [a]*Institute for Protein Research, Osaka University, Osaka, Japan,* [b]*Confocal Science Inc., Tokyo, Japan,* [c]*Japan Aerospace Exploration Agency, Ibaraki, Japan,* [d]*Maruwa Food and Biosciences, Inc., Nara, Japan.*
E-mail: hgsur-a@protein.osaka-u.ac.jp

Keywords: high resolution X-ray crystallography, data treatment, refinement method

Recent progress on using high brilliance and small divergence synchrotron beamlines, X-ray data collection at low temperature and technical advances in crystallographic analysis have significantly improved the resolution on X-ray crystallography. In this study hen egg-white lysozyme was used as a model protein for high resolution X-ray crystallography. High resolution crystals were obtained from highly purified hen egg-white Lysozyme. Data collections were performed using synchrotron radiation from SPring-8 beamline BL44XU and Photon Factory beamline BL5A. Two crystals were used to increase completeness and two data sets were collected for high and low resolution data to avoid the saturation of high intensity diffraction for each crystals. The high resolution diffraction data were observed up to 0.75Å. The data were integrated, scaled and merged using the *DENZO* and SCALEPACK programs. At the merging process low resolution dataset were carefully truncated. Hen egg-white lysozyme crystals belong to space group *P*1 with the cell dimensions a=26.7, b=31.0, c=33.7Å, α=89.2, β=72.5 and γ=67.7 degree. The overall R_{merge} based on intensities for all data was 5.4% with its completeness of 92.0% against data to 0.76Å. Refinement was carried out by *SHELX* programs. The refinement were proceeding against data to 0.83Å. An *R*-factor and *free-R*-factor was 11.0% and 12.6%, respectively. Hydrogen atoms were added to the model at predicted positions, lowering the *R*-factor and *free-R*-factor by approximately 1.0%. The final model consists of 1,305 atoms (without hydrogen atoms) and 163 water molecules. 24 side chains and 1 main chain were modeled in two conformations. *B* factors were 7.4, 10.1 and 19.6Å for main chain, side chain and water molecules. At the refinement process using loose restraints gave different distribution of bond length and angles. These results implied the necessity to improve refinement method of high resolution X-ray crystallography.

MS07 P03

The crystal structures of sphericase at 0.80Å resolution - insights into the catalysis mechanism of subtilisins Orna Almog[a], Marina de Leeuw[a] Ana González[b]
[a]*Department of Clinical Biochemistry, Faculty of Health Sciences, Ben-Gurion University, Beer Sheva, 84105 , Israel.* [b]*Stanford Synchrotron Radiation Laboratory, 2575 Sand Hill Road, MS 99, Menlo Park, CA 94025 , USA.* E-mail: almogo@bgu.ac.il

Keywords: serine protease, psychrophilic, calcium binding

We previously determined the crystal structure of Sph, a mesophilic subtilisin, at 0.93 Å resolution using the Eu/MAD method. The final model included all 310 amino acids, one disulfide bond, 679 water molecules and five calcium ions. None of the calcium binding sites correlated with the well-known high affinity calcium-binding site (site I; also known also as Site A) of the subtilisin family. In this study, we determine the crystal structure of Sph at a higher resolution and in a different crystal form using the molecular replacement method and the above-mentioned Sph structure as the starting model. Compared to the 0.93 Å model of Sph, there was further improvement in the details of the electron density map, which enabled us to locate a hydrogen atom in the catalytic site and a borate anion bound to the active site residue Ser250. Structural analysis indicated a structure identical to S41, a