



	Experiment title: Structure analysis of ribosomal protein <i>S7</i> .	Experiment number: LS847
Beamline: BM14	Date of Experiment: from: 08.DEC.97 to: 09.DEC.97	Date of Report: 08-SEP-98
Shifts: 3 shifts	Local contact(s): Dr. V. Stojanoff	<i>Received at ESRF :</i> 14 SEP. 1998

Names and affiliations of applicants (*indicates experimentalists):

Dr. Isao Tanaka, Graduate School of Science, Hokkaido univ., Sapporo, Japan

Dr. Atsushi Nakagawa, Graduate School of Science, Hokkaido univ., Sapporo, Japan

Ms. Harumi Hosaka, Graduate School of Science, Hokkaido univ., Sapporo, **Japan**

*Dr. Yao Min, ESRF, Grenoble, France

*Dr. Soichi Wakatsuki, ESRF, Grenoble, France

Report: 1. Abstract of our paper accepted in *Structure*.

The ribosome is a ribonucleoprotein complex which performs the crucial function of protein biosynthesis. Its role is to decode mRNAs within the cell and to synthesize the corresponding proteins. Ribosomal protein *S7* is located at the head of the small (30s) subunit of the ribosome and faces into the decoding center. *S7* is one of the primary 16s rRNA-binding proteins responsible for initiating the assembly of the head of the 30s subunit. In addition, *S7* has been shown to be the major protein component to cross-link with tRNA molecules bound at both the aminoacyl-tRNA (A) and peptidyl-tRNA (P) sites of the ribosome. The ribosomal protein *S7* clearly plays an important role in ribosome function. It was hoped that an atomic-resolution structure of this protein would aid our understanding of ribosomal mechanisms.

The structure of ribosomal protein *S7* from *Bacillus stearothermophilus* has been solved at 2.5 Å resolution using multiwavelength anomalous diffraction and selenomethionyl-substituted proteins. The molecule consists of a helical hydrophobic core domain and a β -ribbon arm extending from the hydrophobic core. Highly conserved basic and aromatic residues are clustered on one face of the *S7* molecule and create a 16s rRNA contact surface.

The X-ray data presented in this paper are those collected during the in house search beamtime from 20.FEB.97 to 21.FEB.97.

2. Summary of the results obtained during this beamtime.

During this beam-time, we concentrated on measuring crystals of selenomethionyl-substituted proteins. In order to determine the crystal structure using multiple wavelength diffraction method, all diffraction data sets were collected from a single crystal with four different wavelengths (0.90007Å (e0), 0.97881Å (e1), 0.97906Å (e2) and 0.97981Å (e3)). Data collection statistics are given in Table. The wavelengths were optimized to obtain a larger anomalous signal based on the fluorescence spectrum. All diffraction data were recorded on a Princeton CCD detector coupled to an image intensifier and processed with the HKL package.

Table Crystallographic data.

Data	e0	e1	e2	e3
Wavelength (Å)	0.90007	0.97881	0.97906	0.97981
Resolution (Å)	30.0-2.5	30.0-2.5	30.0-2.5	30.0-2.5
R_{merge}^*	0.048 (0.138)	0.041 (0.171)	0.039 (0.176)	0.050 (0.431)
Observed reflections	53,236	45,531	45,666	42,500
Independent reflections	7,558	7,427	7,424	7,529
Completeness (%)	97.6 (92.9)	96.6 (88.2)	96.5 (87.3)	95.9 (85.5)
Multiplicity	2.8 (2.2)	2.5 (1.9)	2.5 (1.9)	2.3 (1.6)
$R_{\text{lambda}}^\dagger$		0.064	0.098	0.098
f'^\ddagger	-1.6	-6.6	-10.8	-4.7
f''^\S	3.3	5.1	5.5	0.7

Values within parentheses are for the highest resolution shell (2.54-2.50 Å). $*R_{\text{merge}} = \sum \sum_i | \langle I(h) \rangle - I(h) | / \sum \sum_i \langle I(h) \rangle$, where $\langle I(h) \rangle$ is the mean intensity of symmetry-equivalent reflections. Friedel pairs were merged as individual data. $^\dagger R_{\text{lambda}} = \sum \sum_i | |F_{\lambda_i}| - |F_{\lambda_0}| | / \sum \sum_i |F_{\lambda_0}|$, where F_{λ_i} is the structure factor of the data collected at λ_i and F_{λ_0} is the structure factor of the data collected at e0 (0.90007Å). ‡ The real part of the anomalous scattering factor of the selenium atom refined by SHARP. § Imaginary part of the anomalous scattering factor of the selenium atom refined by SHARP.

Out of six independent Se atoms, five were located from the Bijvoet anomalous difference Patterson map of the e2 data using the real-space Patterson search program RSPS. The atomic model was first built using the electron-density map from the MLPHARE but at the later stages the map from SHARP was used. The atomic model was built using the graphics program O. At the final stage of refinement, the model has an R factor of 21.6% for 90% of the data between 8 Å and 2.5 Å, including 139 residues (9-147) and 25 water molecules, a total of 1145 atoms. The free R factor for the remaining 10% of the data within this resolution range is 27.0%. The Ramachandran plot of the model shows that 94.5% of the residues lie within the most favored region with no residues in disallowed regions of the plot. The root mean square (rms) deviations from standard values of bond lengths and angles are 0.02281 and 2.083° respectively.