



ESRF

Experiment title:
x-ray structure of acceptor stem of
E.coli tRNA^{ALA}-iodine derivative

Experiment
number:

15573

Beamline:	Date of Experiment:	Date of Report:
D14	from: 07.08.96 to: 09.08.96	21.08.1996
Shifts:	Local contact(s):	Received at ESRF
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Report:

During the diffraction experiment at beamline D 14 a complete dataset up to 1.9 Å maximum resolution could be collected. The spacegroup of the crystal is C2 with a= 33.3 Å , b= 47.52 Å , c= 26.37 Å , $\alpha=\gamma=90^\circ$, $\beta=101.4^\circ$.

The dataset statistics are shown below.:

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By 45INTW/LASQ bins (all statistics use <!*>,<I->etc)

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TABLE: Analysis against resolution:
SGRAPH:Factor v Resolution:1.2,4,6:
Average I,ed and Sigma (h:2,0,0,1):I/sigma:1.2,10: $S
h kcp Delta(A) Rfac Rcruc Nanom Nanom Av_1 SIGMA I/sigma sd Pmean Nref Ncount FRACIAS Mbias $S
$S
1 0.0145 0.30 0.049 0.049 0.000 0 49262. 4439.8 11.1 2870.59 101 32 5 -0.0291 28
2 0.0207 2.93 0.052 0.052 0.000 0 41919. 3967.8 10.6 2666.81 214 67 6 0.0438 79
3 0.0428 4.82 0.046 0.049 0.000 0 46912. 3577.1 12.1 3011.60 278 88 9 -0.0044 121
4 0.0569 4.19 0.050 0.049 0.000 0 57056. 4899.2 13.6 3592.99 397 98 5 -0.0285 145
5 0.0710 3.75 0.048 0.049 0.000 0 65684. 6181.9 10.6 4104.78 349 118 10 -0.0243 149
6 0.0852 3.43 0.051 0.050 0.000 0 60098. 8723.2 6.9 3721.85 388 124 7 -0.0157 150
7 0.0993 3.17 0.052 0.050 0.000 0 37316. 4327.9 7.1 3039.27 404 137 9 -0.0183 186
8 0.1134 2.90 0.050 0.050 0.000 0 37193. 3733.2 10.0 2401.18 448 150 9 -0.0229 187
9 0.1275 2.80 0.052 0.050 0.000 0 19615. 1845.1 10.6 1355.98 485 160 7 -0.0308 196
10 0.1417 2.66 0.060 0.051 0.000 0 16496. 1592.0 10.4 1194.30 493 165 10 -0.0453 218
11 0.1558 2.53 0.058 0.051 0.000 0 11755. 1061.7 11.1 880.36 535 180 8 -0.0017 222
12 0.1699 2.33 0.062 0.052 0.000 0 11062. 1021.4 10.8 857.85 499 163 2 -0.0308 196
13 0.1840 2.23 0.061 0.052 0.000 0 10483. 1091.9 9.8 844.61 581 199 10 -0.0007 180
14 0.1982 2.25 0.068 0.052 0.000 0 6458. 884.3 9.6 719.70 534 184 6 0.0007 180
15 0.2123 2.17 0.060 0.053 0.000 0 9047. 950.0 9.5 779.52 559 190 6 -0.0149 208
16 0.2264 2.10 0.075 0.054 0.000 0 7817. 998.1 7.9 723.24 585 197 4 -0.0299 227
17 0.2406 2.04 0.076 0.054 0.000 0 6354. 792.1 0.0 610.90 675 224 12 -0.0221 260
18 0.2547 1.98 0.080 0.055 0.000 0 4556. 551.1 0.0 492.63 624 287 4 -0.0036 226
19 0.2689 1.92 0.083 0.055 0.000 0 5323. 714.6 7.4 557.99 320 120 2 -0.0149 121
20 0.2829 1.88 0.087 0.055 0.000 0

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Tab.1: Agrovata-output of diffraction experiment of acceptor stem of E.coli tRNA^{ALA}-iodine derivative

Unfortunately these data are not isomorphous to the native crystal. Therefore single isomorphous replacement techniques can not be used for solving the structure. A molecular replacement approach with a canonical A-RNA as the search model will be performed .