

Some Important points from last time

Entrez searches many databases at once.

Pubmed provides access to journal articles.

PMC access to full journal articles.

Boolean searches, filters, and/or advanced tab provide search focus.

Know the syntax and result of boolean searches.

Know the major searchable fields.

Important points from last time

Pubmed is your
knowledge source
friend

Sequence File Formats

Major File Formats

- GenBank
- EMBL
- FASTA / Pearson
- FASTQ
- Phylip
- GDE
- Nexus
- ASN.1
- VCF
- PDB
- SAM/BAM
- GFF

GenBank

- Developed for a single nucleic sequence
- Does not display homology information
- Can display more than one gene, but only one primary sequence
- Large amount of details
 - organism
 - references
 - features

Position Content

-----	-----
01-05	'LOCUS'
06-12	spaces
13-28	Locus name
29-29	space
30-40	Length of sequence, right-justified
41-41	space
42-43	bp
44-44	space
45-47	spaces, ss- (single-stranded), ds- (double-stranded), or ms- (mixed-stranded)
48-53	NA, DNA, RNA, tRNA (transfer RNA), rRNA (ribosomal RNA), mRNA (messenger RNA), uRNA (small nuclear RNA), snRNA, snoRNA. Left justified.
54-55	space
56-63	'linear' followed by two spaces, or 'circular'
64-64	space
65-67	The division code (see Section 3.3)
68-68	space
69-79	Date, in the form dd-MMM-yyyy (e.g., 15-MAR-1991)

LOCUS MPU28721 2283 bp DNA linear ROD 15-OCT-2001
 DEFINITION Mus pahari adenine phosphoribosyltransferase (APRT) gene, complete cds.
 ACCESSION U28721
 VERSION U28721.1 GI:881573
 KEYWORDS .
 SOURCE Mus pahari (shrew mouse)
 ORGANISM [Mus pahari](#)
 Eukaryota; Metazoa; Chordata; Craniata; Vertebrata; Euteleostomi; Mammalia; Eutheria; Euarchontoglires; Glires; Rodentia; Sciurognathi; Muroidea; Muridae; Murinae; Mus.
 REFERENCE 1 (bases 1 to 2283)
 AUTHORS Fieldhouse,D., Yazdani,F. and Golding,G.B.
 TITLE Substitution rate variation in closely related rodent species
 JOURNAL Heredity 78 (Pt 1), 21-31 (1997)
 PUBMED [9023989](#)
 REFERENCE 2 (bases 1 to 2283)
 AUTHORS Fieldhouse,D.
 TITLE Direct Submission
 JOURNAL Submitted (07-JUN-1995) Dan Fieldhouse, Biology, McMaster University, 1280 Main Street West, Hamilton, ON, L8S 4K1, Canada
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 /codon_start=1
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DEFINITION [TITL]

Brief description of the sequence proceeds from general to specific should include:

organism

gene/protein name

description of sequence function (non-coding)

presence of a CDS

(complete / partial)

no limit in number of lines but the last line must ends by a period.

DETERMINED BY THE AUTHORS, MAY VARY

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ACCESSION [ACCN]

Unique identifier

1 letter followed by 5 digits

U28721

2 letters followed by 6 digits

AF123456

(3 letters would indicate a protein)

ACCESSION NUMBERS DO NOT CHANGE, ENTRIES ARE JUST UPDATED

for the RefSeq database:

2 letters, underscore and then 6 or more digits:

NT_ genomic contigs

NM_ mRNAs

NP_ proteins

NC_ chromosomes


```

LOCUS      MPU28721                2283 bp    DNA     linear   ROD 15-OCT-2001
DEFINITION Mus pahari adenine phosphoribosyltransferase (APRT) gene, complete
            cds.
ACCESSION  U28721
VERSION   U28721.1   GI:881573
KEYWORDS  .
SOURCE    Mus pahari (shrew mouse)
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            Eukaryota; Metazoa; Chordata; Craniata; Vertebrata; Euteleostomi;
            Mammalia; Eutheria; Euarchontoglires; Glires; Rodentia;
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  AUTHORS  Fieldhouse,D.
  TITLE    Direct Submission
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KEYWORDS [KYWD]

Words or sentence describing the sequence

Each keyword is separated by a semicolon

The last line should end by a period

NOT PRESENT IN EVERY RECORD

LOCUS MPU28721 2283 bp DNA linear ROD 15-OCT-2001
 DEFINITION Mus pahari adenine phosphoribosyltransferase (APRT) gene, complete cds.
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 VERSION U28721.1 GI:881573
 KEYWORDS .
 SOURCE Mus pahari (shrew mouse)
 ORGANISM [Mus pahari](#)
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 /EC_number="[2.4.2.7](#)"
 /note="purine salvage enzyme"
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 /product="adenine phosphoribosyltransferase"
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ORGANISM [ORGN] Scientific name of the organism following the NCBI Taxonomy Database

- first line:

Genus species

- second line:

Full formal classification

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REFERENCE

Information about the publication of the sequence, divided into optional parts:

Author(s) name(s) [AUTH]

Title [TITL]

Journal of submission [JOUR]

PUBMED reference

REMARK

The reference field contains the number and the range of bases used in the citation

The last publication field may contain information about the submitter.

LOCUS MPU28721 2283 bp DNA linear ROD 15-OCT-2001
 DEFINITION Mus pahari adenine phosphoribosyltransferase (APRT) gene, complete cds.
 ACCESSION U28721
 VERSION U28721.1 GI:881573
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 Eukaryota; Metazoa; Chordata; Craniata; Vertebrata; Euteleostomi; Mammalia; Eutheria; Euarchontoglires; Glires; Rodentia; Sciurognathi; Muroidea; Muridae; Murinae; Mus.
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FEATURES

Information about genes and genes products
 Regions of biological significance


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LOCUS      MPU28721                2283 bp    DNA     linear   ROD 15-OCT-2001
DEFINITION Mus pahari adenine phosphoribosyltransferase (APRT) gene, complete
           cds.
ACCESSION  U28721
VERSION   U28721.1  GI:881573
KEYWORDS   .
SOURCE     Mus pahari (shrew mouse)
  ORGANISM Mus pahari
           Eukaryota; Metazoa; Chordata; Craniata; Vertebrata; Euteleostomi;
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  JOURNAL  Heredity 78 (Pt 1), 21-31 (1997)
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REFERENCE  2 (bases 1 to 2283)
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Keys

Gives the biological nature of the annotated feature

source
 promoter
 mRNA
 CDS

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KEYWORDS .
SOURCE Mus pahari (shrew mouse)
ORGANISM [Mus pahari](#)
Eukaryota; Metazoa; Chordata; Craniata; Vertebrata; Euteleostomi;
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DEFINITION Mus pahari adenine phosphoribosyltransferase (APRT) gene, complete
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VERSION   U28721.1   GI:881573
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  JOURNAL  Submitted (07-JUN-1995) Dr. Fieldhouse, Biology, McMaster
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Locations

Region of the sequence where the feature is located

“<” indicates that the start is unknown

“>” indicates that the end is unknown

Different operators

complement

join

order

LOCUS MPU28721 2283 bp DNA linear ROD 15-OCT-2001
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Qualifiers

Always in the form:
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ORIGIN

ORIGIN

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GenBank format can display more than one gene in a single sequence

RefSeq Genbank Format

- A more formalized recording for “reference” sequences. For example the accession prefixes ...

Accession prefix	Molecule type	Comment
AC_	Genomic	Complete genomic molecule, usually alternate assembly
NC_	Genomic	Complete genomic molecule, usually reference assembly
NG_	Genomic	Incomplete genomic region
NT_	Genomic	Contig or scaffold, clone-based or WGS
NW_	Genomic	Contig or scaffold, primarily WGS
NS_	Genomic	Environmental sequence
NZ_	Genomic	Unfinished WGS
NM_	mRNA	
NR_	RNA	
XM_	mRNA	Predicted model
XR_	RNA	Predicted model
AP_	Protein	Annotated on AC_ alternate assembly
NP_	Protein	Associate with an N_ or NC_ accession
YP_	Protein	
XP_	Protein	Predicted model, associated with an XM_ accession
ZP_	Protein	Predicted model, annotated on NZ_ genomic records

EMBL Format

- Developed for a single nucleic sequence
- Can display more than one gene
- Large amount of detail
- Same as GenBank format but with 2 letters codes

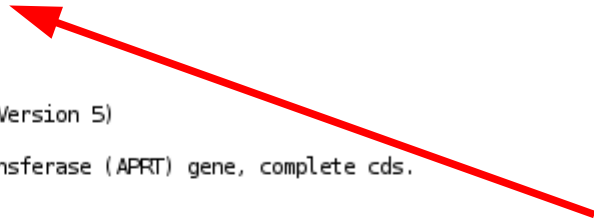
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 DT 17-APR-2005 (Rel. 83, Last updated, Version 5)
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 DE Mus pahari adenine phosphoribosyltransferase (APRT) gene, complete cds.
 XX
 KW .
 XX
 OS Mus pahari (shrew mouse)
 OC Eukaryota; Metazoa; Chordata; Craniata; Vertebrata; Euteleostomi; Mammalia;
 OC Eutheria; Euarchontoglires; Glires; Rodentia; Sciurognathi; Muroidea;
 OC Muridae; Murinae; Mus.
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 RL Heredity 78(1):21-31(1997).
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 RT ;
 RL Submitted (07-JUN-1995) to the EMBL/GenBank/DDBJ databases.
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Line codes

ID - identification
AC - accession number
PR - project identifier
DT - date
DE - description
KW - keyword
OS - organism species
OC - organism classification
OG - organelle
RN - reference number
RC - reference comment
RP - reference positions
RX - reference cross-reference
RG - reference group
RA - reference author(s)

RT - reference title
RL - reference location
DR - database cross-reference
CC - comments or notes
AH - assembly header
AS - assembly information
FH - feature table header
FT - feature table data
XX - spacer line
SQ - sequence header
CO - contig/construct line
bb - (blanks) sequence data
// - termination line

ID U28721; SV 1; linear; genomic DNA; STD; ROD; 2283 BP.
 XX
 AC U28721;
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 DT 17-APR-2005 (Rel. 83, Last updated, Version 5)
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 DE Mus pahari adenine phosphoribosyltransferase (APRT) gene, complete cds.
 XX
 KW .
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 OS Mus pahari (shrew mouse)
 OC Eukaryota; Metazoa; Chordata; Craniata; Vertebrata; Euteleostomi; Mammalia;
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DATA CLASS

How the data was generated

CON	fragments of entered sequences
ANN	fragment of entries sequences with its own annotation
PAT	Patent
EST	Expressed Sequence Tag
GSS	Genome Survey Sequence
HTC	High throughput cDNA
HTG	High throughput genomic
MGA	Mass Genome Annotation
WGS	Whole Genome Shotgun
TPA	Third Party Annotation
STS	Sequence Tag Site
STD	Standard

ID U28721; SV 1; linear; genomic DNA; STD; ROD; 2283 BP.
 XX
 AC U28721;
 XX
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TAXONOMIC DIVISION

PHG Bacteriophage
 ENV Environmental
 FUN Fungal
 HUM *Homo sapiens*
 INV Invertebrates
 MAM Other mammals
 VRT Vertebrate
 MUS *Mus musculus*
 PLN Plant
 PRO Prokaryote
 ROD Other rodents
 SYN Synthetic
 TGN Transgenic
 UNC Unclassified
 VRL Viral

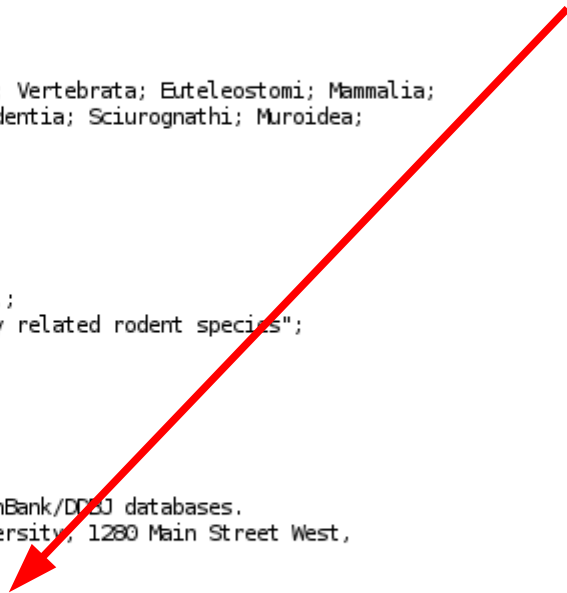
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ID U28721; SV 1; linear; genomic DNA; STD; ROD; 2283 BP.
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OC Eukaryota; Metazoa; Chordata; Craniata; Vertebrata; Euteleostomi; Mammalia;
OC Eutheria; Euarchontoglires; Glires; Rodentia; Sciurognathi; Muroidea;
OC Muridae; Murinae; Mus.
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RX DOI; 10.1038/sj.hdy.6881150
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RL Dan Fieldhouse, Biology, McMaster University, 1280 Main Street West,
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**Qualifiers:
SAME FORMAT AS FOR GenBank**



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XX
SQ

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Sequence 2283 BP; 485 A; 696 C; 590 G; 512 T; 0 other;
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gtgaggttta caactcctga aatgctcagc ctcagaaatg ctccaggcta gggaggtggc 1800
cacttgttag catctactct ctcttaacgc tacttctctgt ctgcaggctg agctggaaat 1860
ccagaaagat gccttagaac ccgggcagag agtggctatt gtggatgacc tcctggccac 1920
tggaggtaaa gaccagccc aagacaaca ggcttcaag ggccaggccc tgtctgggtg 1980
gctgactaaa aaaagcctt gaatacctc tctttctctg tccctcccc ccccccccc 2040
caggaacctt gtttgcagcc tgtgatctgc tgcaccagct acgggctgag gtggtggagt 2100
gtgtgacctt ggtggagctg acctcgtga agggcaggga gaggctagga cctataccat 2160
tctttctct cctccagtat gactgagctg gctagatggt cacaccctg ctcacagcag 2220
cagtaactgc gcggtggctc agccctgggc gcctaagtga cctttgtgag ctacctgctg 2280
2283

```

End of the entry, always //

//

FASTA / Pearson

- Simplest format used
- No feature information is stored in this format
- Each sequence start with “>” and a sequence title
- Can be used for single sequences or multiple sequences (aligned or not)
- Information for homologous sites can be available (“-”).
- used by many software codes

```
>Mus_pahari          607 Weight: 0.75
-----CCTGCGGATACT-C
ACCTCCTCCTTGTCTCCTACAAGCACGCGGCCATGTCCGAGTCTGAGTTG
AAACTGGTGGCGCGGCATCCGCAGCTTCCCCGACTTCCCCATCCCGGG
CGTGCTGTTCAAGTGCAGTGCAGGCGCGGAGGCGTTGGCGCCGTAATC
TCATCCC-CCGGCGCAGGCGCGTGGGCAGCCTTGGGGATCTTGCGGGGCC
TCTGCCCCGCCACACGCGG-TCACTCTCCTGTCTTGTCCCAGGGATAT
CTCGCCCCTCTTGAAAGATCCGGACTCCTTCCGAGCTTCCATCCGCCTCC
TGGCCAGTCACTGAAGTCCACGCACAGCGGCAAGATCGACTATATCGCA
GGGCAAGGTGGCCTTGTAGGCCGTAATCATCCCCACGGTCTATCCCC
TATCCCCTTTCCCC-TCGTGTACCCACAGTCTACCCACACCCATCCAT
TCTTTCTTAACTCTGACTCTTCTCCTTGGTTTCTCACTGCCTTGGAC
GCTTGTTACCCCGGATGAACTCCGTAGGCGTCTCCCTTCCCTGCTTGGT
```

```
>Mus_spicilegus     632 Weight: 0.75
-----TC--GGGATTGACGTGAATTTAGCGTGCTGATACC-T
ACCTCCTCCTTGCCTCCTACACGCACGCGGCCATGTCCGAACCTGAGTTG
AAACTGGTGGCGCGGCATCCGCAGCTTCCCCGACTTCCAATCCCGGG
CGTGCTGTTCAAGTGCAGTGCAGGCGCGGAGGCGTTGGCGCCGTACGC
TCATCCC-CCGGCGCAGGCGCGTAGGCAGCCTCGGGGATCTTGCGGGGCC
TCTGCCCCGCCACACGCGGGTCACTCTCCTGTCTTGTCCCAGGGATAT
CTCGCCCCTCTTGAAAGACCCGGACTCCTTCCGAGCTTCCATCCGCCTCT
TGGCCAGTCACTGAAGTCCACGCACAGCGGCAAGATCGACTACATCGCA
GG-CGAG-TGGCCTTGTAGGCCGTGCTCGTCCCCACGGTCTAGCCCC
TATCCCCTTTCCCCCTCGTGTACCCACAGTCTGCCCCACACCCATCCAT
TCTTTCTTCAACTCTGACTTCTCCTTGGTTCTCACTGCCTTGGAC
GCTTGTTACCCCGGATGAACTATGTAGGAGTCTCCCTTCCCTGCTAGGT
ACCCTAAGGCATCTGCCCTCGGTGCTTGTCTA---GAGACGAACTCTG
CTCT
```

```
>Gerbillus_campestris 615 Weight: 1.49
CCTCCGCCCTTGTTCCTGGGACAGGCTTGACCCTAGCCAGTTGACACCTC
ACCTCCGCCCTTCTC--TCACGCACGCGGCCATGGCGGAACCCGAGTTG
CAGCTGGTGGCGCGGCATCCGCAGCTTCCCCGACTTCCCCATCCCGGG
CGTGCTGTTCAAGTGCAGTGCAGGCGCGGAGGCGTTGGCGCTGCGTCC
TCAGCCCTCCGGCGCAGGCGCGTAGCTGTCTCCGGGATCTTGCGGGGCC
TCCGCCCAGCCATACCCAAGTCAACATCCTGT----GTTCCCAGGGATAT
CTCGCCCCTCTTGAAAGACCCGGACTCCTTCCGAGCTTCCATCCGTCTCC
TGGCCAACCATCTGAAGTCCAAGCATGGCGGCAAAATCGACTACATCGCA
GG-CGAG-TGTTCTTGTAGGCCGTGCCCGTCCC-ACTGTCAGGGCCGC
CATCCCGTGTCCCT--TTTC-----GTGTACCCACACCCACCCCT
CCTTTCTCTGACA-CTCCCAAGTTC-CCT--GTTCTCTCTGCCTTGGTC
CCATATTACCCCGGATGA-CTGCG--GAGTCTCC-----
ACCCTCTGACCTCTGCTCTCAAAGCCTGTCCCTACTAGAGAGGAACTCTG
CTCT
```

Mus pahari, Mus spicilegus and Gerbillus campestris partial APRT gene sequences

>Mus_pahari

607 Weight: 0.75

```

-----CCTGCGGATACT-C
ACCTCCTCCTTGTCTCCTACAAGCACGCGGCCATGTCCGAGTCTGAGTTG
AAACTGGTGGCGGGCGCATCCGCAGCTTCCCCGACTTCCCCATCCCGGG
CGTGCTGTT CAGGTGCGGT CACGAGCCGGCGAGGCGTTGGCGCGTACTC
TCATCCC-CCGGCGCAGGCGCGTGGGCAGCCTTGGGGATCTTGCGGGGCC
TCTGCCCCGCCACACGCGG-TCACTCTCCTGTCTTGTCCCAGGGATAT
CTCGCCCCTCTTGAAAGATCCGGACTCCTTCCGAGCTTCCATCCGCTCC
TGCCAGTCACTGAAGTCCACGCACAGCGGCAAGATCGACTATATCGCA
GGCAAGGTGGCCTTGCTAGGCCGTA CTATCCCCACGGTCTATCCCC
TATCCCCTTTCCCC-TCGTGTACCCACAGTCTACCCACACCCATCCAT
TCTTTCTTAACTCTGACTCTTCTCCTTGGTTTCTCACTGCCTTGGAC
GCTTGTTACCCCCGGATGAACTCCGTAGGCGTCTCCCTTCCCTGCTTGGT

```

Non-essential information

Identifier of the sequence

>Mus_spicilegus 632 Weight: 0.75

```

-----C--GGGATTGACGTGAATTTAGCGTGCTGATACC-T
ACCTCCTCCTTGCCTCCTACACGCACGCGGCCATGTCCGAACCTGAGTTG
AAACTGGTGGCGGGCGCATCCGCAGCTTCCCCGACTTCCCAATCCCGGG
CGTGCTGTT CAGGTGCGGT CACGAGCCGGCGAGGCGTTGGCGCGTACGC
TCATCCC-CCGGCGCAGGCGCGTAGGCAGCCTCGGGGATCTTGCGGGGCC
TCTGCCCCGCCACACGCGGGTCACTCTCCTGTCTTGTCCCAGGGATAT
CTCGCCCCTCTTGAAAGACCCGGACTCCTTCCGAGCTTCCATCCGCTCT
TGCCAGTCACTGAAGTCCACGCACAGCGGCAAGATCGACTACATCGCA
GG-CGAG-TGGCCTTGCTAGGCCGTGCTCGTCCCCACGGTCTAGCCCC
TATCCCCTTTCCCCCTCGTGTACCCACAGTCTGCCACACCCATCCAT
TCTTTCTTCAACTCTGACTTCTCCTTGGTTCTCACTGCCTTGGAC
GCTTGTTACCCCCGGATGAACTATGTAGGAGTCTCCCTTCCCTGCTAGGT
ACCCTAAGGCATCTGCCCTCGGTGCTTGTTCCTA---GAGACGAACTCTG
CTCT

```

" - " symbol for a gap

>Gerbillus campestris 615 Weight: 1.49

```

CCTCCGCCCTTGTTCCTGGGACAGGCTTGACCCTAGCCAGTTGACACCTC
ACCTCCGCCCTTCTC--TCACGCACGCGGCCATGGCGGAACCCGAGTTG
CAGCTGGTGGCGGGCGCATCCGCAGCTTCCCCGACTTCCCCATCCCGGG
CGTGCTGTT CAGGTGCGTCCACGAGCCGCCAGGCGTTGGCGTGCCTCC
TCAGCCCTCCGGCGCAGGCGCGTGAGCTGTCTCCGGGATCTTGCGGGGCC
TCCGCCCAGCCATACCCAAGTCACCATCCTGT----GTTCCCAGGGATAT
CTCGCCCCTCTTGAAAGACCCGGACTCCTTCCGAGCTTCCATCCGTCTCC
TGCCAACCATCTGAAGTCCAAGCATGGCGGCAAAATCGACTACATCGCA
GG-CGAG-TGTTCTTGCTAGGCCGTGCCCGTCCC-ACTGTCAGGGCCGC
CATCCCGTGTTCCTT--TTTC-----GTGTCACCCACACCCACCCCT
CCTTTCTCTGACA-CTCCCAAGTTC-CCT--GTTCTCTCTGCCTTGGTC
CCATATTACCCCCGGATGA-CTGCG---GAGTCTCC-----
ACCCTCTGACCTCTGCTCTCAAAGCCTGTCCCTACTAGAGAGGAACTCTG
CTCT

```

FASTQ

- Format adapted for high-throughput short reads
- Only sequence and quality information is stored in this format
- Each sequence start with “@” and a sequence title (usually machine generated)
- Sequences are on one line
- Third line starts with “+”
- Fourth line stores base quality score

(Phred = ord(Q) - 33)

@HWI-EAS038:8:1:8:697#0/1
AGACTGGCTGGAGCATGTCTATGACGGACTATGATG

+

aaa'[['a' ^ [^U ^ _YPU[['ZU ^VSTZVX_ TBBBB
@HWI-EAS038:8:1:8:1326#0/1

AGACTACCGTGTCGTCACGACACGGTCGACGACCAC

+

a^a^\aa'\ZUZVPV\ 'SP\]aSPQSRNXWBBBBBB
@HWI-EAS038:8:1:8:1305#0/1

AGACTCGAAACGCCTTTCTGGAACACGAAAGGTCTC

+

aXa'_ ^ 'aaa_W[\ \ ^ ^ ^ ^VT]a_ '[T ^ ' 'WSW^W[

Beginning of a new sequence

@HWI-EAS038:8:1:8:697#0/1

AGACTGGCTGGAGCATGTCTATGACGGACTATGATG

+

aaa'[['a' ^ [^U ^ _YPU[['ZU ^VSTZVX_ TBBBB

@HWI-EAS038:8:1:8:1326#0/1

AGACTACCGTGTCGTCACGACACGGTCGACGACCAC

+

a ^ a ^ \aa' \ZUZVPV\ 'SP\]aSPQSRNXWBBBBBB


@HWI-EAS038:8:1:8:1305#0/1

AGACTCGAAACGCCTTTCTGGAACACGAAAGGTCTC

+

aXa' _ ^ 'aaa_W[\ \ ^ ^ ^ ^VT]a_ '[T ^ ' 'WSW ^W[

Sequence title: often machine name, flow cell, x, y coord, etc.


@HWI-EAS038:8:1:8:697#0/1

AGACTGGCTGGAGCATGTCTATGACGGACTATGATG

+

aaa'[['a' ^ [^U ^ _YPU[['ZU ^VSTZVX_ TBBBB

@HWI-EAS038:8:1:8:1326#0/1

AGACTACCGTGTCGTCACGACACGGTCGACGACCAC

+

a ^ a ^ \aa' \ZUZVPV\ 'SP\]aSPQSRNXWBBBBBB

@HWI-EAS038:8:1:8:1305#0/1

AGACTCGAAACGCCTTTCTGGAACACGAAAGGTCTC

+

aXa' _ ^ 'aaa_W[\ \ ^ ^ ^ ^VT]a_ '[T ^ ' 'WSW ^W[

Start of quality scores

@HWI-EAS038:8:1:8:697#0/1

AGACTGGCTGGAGCATGTCTATGACGGACTATGATG

+

aaa'[['a' ^ [^U ^ _YPU[['ZU ^VSTZVX_ TBBBB

@HWI-EAS038:8:1:8:1326#0/1

AGACTACCGTGTCGTCACGACACGGTCGACGACCAC

+

a^a^\aa'\ZUZVPV\ 'SP\]aSPQSRNXWBBBBBB

@HWI-EAS038:8:1:8:1305#0/1

AGACTCGAAACGCCTTTCTGGAACACGAAAGGTCTC

+

aXa'_ ^ 'aaa_W[\ \ ^ ^ ^ ^VT]a_ '[T ^ ' 'WSW^W[

Quality scores for each base

@HWI-EAS038:8:1:8:697#0/1
AGACTGGCTGGAGCATGTCTATGACGGACTATGATG

+

aaa'[['a' ^ [^U ^ _YPU[['ZU ^VSTZVX_ TBBBB

@HWI-EAS038:8:1:8:1326#0/1

AGACTACCGTGTCGTCACGACACGGTCGACGACCAC

+

a^a^\aa'\ZUZVPV\ 'SP\[aSPQSRNXWBBBBBB

@HWI-EAS038:8:1:8:1305#0/1

AGACTCGAAACGCCTTTCTGGAACACGAAAGGTCTC

+

aXa'_ ^ 'aaa_W[\ \ ^ ^ ^ ^VT]a_ '[T ^ ' 'WSW^W[

@HWI-EAS038:8:1:8:697#0/1
AGACTGGCTGGAGCATGTCTATGACGGACTATGATG

+

aaa'[['a' ^ [^U ^ _YPU[['ZU ^VSTZVX_ TBBBB
@HWI-EAS038:8:1:8:1326#0/1

AGACTACCGTGTCGTCACGACACGGTCGACGACCAC

+

a ^ a ^ \aa' \ZUZVPV\ 'SP\]aSPQSRNXWBBBBBB
@HWI-EAS038:8:1:8:1305#0/1

AGACTCGAAACGCCTTTCTGGAACACGAAAGGTCTC

+

aXa' _ ^ 'aaa_W[\ \ ^ ^ ^ ^VT]a_ '[T ^ ' 'WSW ^W[

ASCII Table

	30	40	50	60	70	80	90	100	110	120
0		(2	<	F	P	Z	d	n	x
1)	3	=	G	Q	[e	o	y
2		*	4	>	H	R	\	f	p	z
3	!	+	5	?	I	S]	g	q	{
4	"	,	6	@	J	T	^	h	r	
5	#	-	7	A	K	U	_	i	s	}
6	\$.	8	B	L	V	`	j	t	~
7	%	/	9	C	M	W	a	k	u	DEL
8	&	0	:	D	N	X	b	l	v	
9	'	1	;	E	O	Y	c	m	w	

Fastq-sanger

$$Q = \text{ord}(q) - 33$$

Fastq-solexa

$$Q = 10 * \log_{10}(1 + 10^{((\text{ord}(q) - 64) / 10)})$$

Fastq-illumina

$$Q = \text{ord}(q) - 64$$

As of CASAVA 1.8, the Illumina FASTQ variant use 33-offset quality encoding (ASCII '!' = 0) and have a stylized format:

```
@<instrument>:<run number>:<flowcell ID>:<lane>:<tile>:<x-pos>:<y-pos>  
<read>:<is filtered>:<control number>:<index sequence>
```

Specific example:

```
@EAS139:136:FC706VJ:2:5:1000:12850 1:Y:18:ATCACG  
AAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAA  
+  
BBBBCCCC?<A?BC?7@@????????DBBA@@@@A@@
```

Example: Casava 1.8

If $q = \text{'?'}$ then $\text{ord}(q) = 63$

$$\text{Fastq-sanger} = 63 - 33 = 30$$

$$\text{Fastq-solexa} = 10 * \log_{10}(1 + 10^{-0.1}) = 2$$

$$\text{Fastq-illumina} = 63 - 64 = \text{"undefined"}$$

Example: older Illumina

If $q = \text{'a'}$ then $\text{ord}(q) = 97$

Fastq-sanger = $97 - 33 = \text{"undefined"}$

Fastq-solexa = $10 * \log_{10}(1 + 10^{3.3}) = 33$

Fastq-illumina = $97 - 64 = 33$

GFF file format; General feature format

Example:

```
##gff-version 3
#!gff-spec-version 1.20
#!processor NCBI annotwriter
##sequence-region NC_004354.3 1 22422827
##species http://www.ncbi.nlm.nih.gov/Taxonomy/Browser/wwwtax.cgi?id=7227
NC_004354.3 RefSeq region 1 22422827 . + .
ID=id0;Dbxref=taxon:7227;chromosome=X;gbkey=Src;genome=chromosome;genotype=y%5B1%5D%3B cn%5B1%5D bw
%5B1%5D sp%5B1%5D%3B Rh6%5B1%5D;mol_type=genomic DNA;old-lineage=Eukaryota%3B Metazoa%3B Arthropoda
%3B Hexapoda%3B Insecta%3B Pterygota%3B Neoptera%3B Endopterygota%3B Diptera%3B Brachycera%3B
Muscomorpha%3B Ephydroidea%3B Drosophilidae%3B Drosophila%3B Sophophora

NC_004354.3 RefSeq region 1 4229 . + . \
ID=id1;Dbxref=FLYBASE:FBti0102096;gbkey=mobile_element
NC_004354.3 RefSeq sequence_variant 148 148 . + . \
ID=id2;Dbxref=dbSNP:207064200;gbkey=variation

NC_004354.3 RefSeq region 10396 10433 . + . \
ID=id888;Dbxref=FLYBASE:FBti0063564;gbkey=mobile_element
```


GFF file format; General feature format

Example:

```
NC_004354.3      RefSeq   region   10396    10433    \
.                +          .        \
ID=id888;Dbxref=FLYBASE:FBti0063564;gbkey=mobile_element
```

A tab delimited file.

#1 "Name" sequence, #2 Source (program/database), #3 name of feature (gene/exon), #4 start, #5 end, #6 confidence value ('.' undefined), #7 strand, #8 frame/phase, #9 description

SAM/BAM format

@SQ SN:NC_009456 LN:1108250

@SQ SN:NC_009457 LN:3024069

HWUSI-EAS1786:60:FC62MTAAXX:1:1:5522:1000 0 NC_009456

267580 25 32M * 0 0

NGGACGGGTTGGATGCCGACGATCTCAATTTG

#111166446@@@@C@CCCC@C@@@@CCCC

XT:A:U NM:i:2 X0:i:1 X1:i:0 XM:i:2 XO:i:0 XG:i:0 MD:Z:0T0T30

HWUSI-EAS1786:60:FC62MTAAXX:1:1:1955:1000 0 NC_009456

875747 0 30M * 0 0

NCATCGCGGCTCAATGGGACTGGAAACGCC

#223054535@@@@@@@@@@@@CCCC@8CC

XT:A:R NM:i:1 X0:i:2 X1:i:44 XM:i:1 XO:i:0 XG:i:0 MD:Z:0C29

HWUSI-EAS1786:60:FC62MTAAXX:1:1:9547:1001 16 NC_009457

2485619 0 48M * 0 0

ATCCAGCGCCAGGTTCCCCTAGCGCTACCTTGTTACGACTTCCCCCN

@?@C@@C@@@@@CCCC@C@@@@@@@@@@@@@@@@@@@@@44003//30#

XT:A:R NM:i:2 X0:i:8 X1:i:0 XM:i:2 XO:i:0 XG:i:0 MD:Z:42A4A0

Tab-delimited

1. QNAME Query template/pair NAME
2. FLAG bitwise FLAG
3. RNAME Reference sequence NAME
4. POS The left most coordinate of the read using the number of the sequence in the reference genome.
5. MAPQ MAPping Quality
The map quality is Phred-scaled. A value of 255 is used for an unknown map quality.
6. CIAGR extended CIGAR string
This string describes features of the match between the read and the reference sequence. In the cases above it is '[0-9M' indicating a perfect match for the length of the read. The format is a number followed by a letter. The number indicates the number of bases and the letter designates a category; M for match, I for an insert in the read, D for a deletion in the read, N for a region skipped, etc.

7. MRNM Mate Reference sequence NaMe

In the cases above it is '*' meaning that there is no mate; these were unpaired reads.

8. MPOS Mate POSition

The bp location in the reference genome where the leftmost bp of the mate read maps.

9. TLEN inferred Template LENgth

The length of the insert between mate pairs.

10. SEQ query SEQuence

The sequence of the read.

11. QUAL query QUALity

The quality is given is $\text{ord}(\text{ASCII}) - 33$ (Sanger Phred scores).

12. OPT variable OPTional fields

GDE

- Tagged file format storing all the information about a sequence (similar to GenBank format)
- Can contain alignment information
- Text enclosed in “{ }”
- All tagged values are enclosed in “”

Offset value

```
{
name "MPU28721"
type "DNA"
longname Mus pahari
sequence-ID "U28721"
descrip "Mus pahari adenine phosphoribosyltransferase (APRT) gene, complete cds"
creator "Fieldhouse,D. and Golding,G.B."
offset 36
creation-date 1/31/98 14:18:24
direction 1
strandedness 1
comments "
NID g881573
KEYWORDS.
SOURCE shrew mouse.
Eukaryotae; mitochondrial eukaryotes; Metazoa; Chordata;
Vertebrata; Eutheria; Rodentia; Sciurognathi; Myomorpha; Muridae;
Murinae; Mus.
REFERENCE 1 (bases 1 to 2283)
TITLE Rates of substitution in closely related rodent species
JOURNAL Unpublished
REFERENCE 2 (bases 1 to 2283)
TITLE Direct Submission
JOURNAL Submitted (07-JUN-1995) Dan Fieldhouse, Biology, McMaster
University, 1280 Main Street West, Hamilton, ON, L8S 4K1, Canada
FEATURES Location/Qualifiers
source 1..2283
/organism=?Mus pahari?
/db_xref=?taxon:10093?
gene join(46..125,256..362,1509..1642,1847..1925,2044..2186)
/gene=?APRT?
```

```

CDS          join(46..125,256..362,1509..1642,1847..1925,2044..2186)
              /gene=?APRT?
              /EC_number=?2.4.2.7?
              /note=?purine salvage enzyme?
              /codon_start=1
              /product=?adenine phosphoribosyltransferase?
              /db_xref=?PID:g881574?
              /translation=?MSESELKLVARRIRSFDFPIPGVLFRRDISPLLKDPDSFRASIR
              LLASHLKSTHSGKIDYIAGLDSRGFLFGPSLAQELGVGCVLIRKQGKLPGPTISASYA
              LEYGKAELEIQKDALEPGQRVVIVDDLLATGGTMFAACDLLHQLRAEVVECVSVELT
              SLKGRERLGPPIFFSLLQYD?

```

```

BASE COUNT   485 a    696 c    590 g    512 t
"

```

```

sequence "CCTGCGGATACTCACCTCCTCCTT
GTCTCCTACAAGCACGCGGCCATGTCCGAGTCTGAGTTGAAACTGGTGGCGCGGCGCATC
CGCAGCTTCCCCGACTTCCCCATCCCGGGCGTGCTGTTCAGGTGCGGTCACGAGCCGGCG
AGGCGTTGGCGCCGTACTCTCATCCC-CCGGCGCAGGCGCGTGGGCAGCCTTGGGGATCT
TGCGGGGCCTCTGCCC GGCCACACGCGG-TCACTCTCCTGTCCTTGTTCCCAGGGATATC
TCGCCCCTCTTGAAAGATCCGGACTCCTTCCGAGCTTCCATCCGCCTCCTGGCCAGTCAC
CTGAAGTCCACGCACAGCGGCAAGATCGACTATATCGCAGGGCAAGGTGGCCTTGCTAGG
CCGTA CT CATCCCCACGGTCCTATCCCCTATCCCCTTTCCCC-TCGTGTCACCCACAGT
CTACCCACACCCATCCATTCTTTCTTTAACCTCTGACTCTTCCTCCTTGGTTTCTCACT
GCCTTGGACGCTTGTTACCCCGGATGAACTCCGTAGGCGTCTCCCTTCCCTGCTTGGTA
CCCTAAGG----TGCCCTCGGTGCTTGTTTCGTAGAGACGAACTCTGCTCT"
}

```


Phylip

- Used by a large number of programs (PHYLIP)
- Two different formats
 - sequential format
 - interleaved : 2 numbers on the first line (number of sequences, sequence length)
- No more than 10 characters for the names of the sequences (warning)
- Can store alignment information

Interleaved format

Number of sequences / taxa

Sequence length

3

650

```
Mus_pahari -----
Mus_spicil -----
Gerbillus_ CCTCCGCCCT

TGTCTCCTAC AAGCACGCGG CCATGTCCGA GTCTGAGTTG AAAGTGGTGG CGCGGCGCAT
TGCCTCCTAC ACGCACGCGG CCATGTCCGA ACCTGAGTTG AAAGTGGTGG CGCGGCGCAT
TTCCTC--TC ACGCACGCGG CCATGGCGGA ACCCGAGTTG CAGCTGGTGG CGCGGCGCAT

CCGCAGCTTC CCCGACTTCC CCATCCCGGG CGTGCTGTTC AGGTGCGGTC ACGAGCCGGC
CCGCAGCTTC CCCGACTTCC CAATCCCGGG CGTGCTGTTC AGGTGCGGTC ACGAGCCGGC
CCGCAGCTTC CCCGACTTCC CCATCCCGGG CGTGCTGTTC AGGTGCGTCC ACGAGCCGGC

GAGGCGTTGG CGCCGTACTC TCATCCC-CC GGCAGGCG CGTGGGCAGC CTTGGGGATC
GAGGCGTTGG CGCCGTACGC TCATCCC-CC GGCAGGCG CGTAGGCAGC CTCGGGGATC
CAGGCGTTGG CGCTGCGTCC TCAGCCCTCC GGCAGGCG CGTGAGCTGT CTCCGGGATC

TTGCGGGGCC TCTGCCCGGC CACACGCGG- TCACTCTCCT GTCCTTGTTT CCAGGGATAT
TTGCGGGGCC TCTGCCCGGC CACACGCGGG TCACTCTCCT GTCCTTGTTT CCAGGGATAT
TTGCGGGGCC TCCGCCCAGC CATACCAAG TCACCATCCT GT----GTTT CCAGGGATAT

CTCGCCCCTC TTGAAAGATC CGGACTCCTT CCGAGCTTCC ATCCGCCTCC TGGCCAGTCA
CTCGCCCCTC TTGAAAGACC CGGACTCCTT CCGAGCTTCC ATCCGCCTCT TGGCCAGTCA
CTCGCCCCTC CTGAAAGACC CGGACTCCTT CCGAGCTTCC ATCCGTCTCC TGGCCAACCA

CCTGAAGTCC ACGCACAGCG GCAAGATCGA CTATATCGCA GGGCAAGGTG GCCTTGCTAG
CCTGAAGTCC ACGCACAGCG GCAAGATCGA CTACATCGCA GG-CGAG-TG GCCTTGCTAG
TCTGAAGTCC AAGCATGGCG GCAAAATCGA CTACATCGCA GG-CGAG-TG TTCTTGCTAG
```

Sequential format

3 650

Mus_pahari

-----CCTGCGGATACT-CACCTCCTCCT
TGTCTCCTACAAGCACGCGGCCATGTCCGAGTCTGAGTTGAAACTGGTGGCGCGGCCGCAT
CCGCAGCTTCCCCGACTTCCCATCCCGGGCGTGCTGTTTCCAGGTGCGGTCACGAGCCGGC
GAGGCGTTGGCGCCGTAATCTCATCCC-CCGGCGCAGGCGCGTGGGCAGCCTTGGGGATC
TTGCGGGGCCTCTGCCCCGGCCACACGCGG-TCACTCTCCTGTCTTGTTCAGGGATAT
CTCGCCCCCTTTGAAAGATCCGGACTCCTTCCGAGCTTCCATCCGCCTCCTGGCCAGTCA
CCTGAAGTCCACGCACAGCGGCAAGATCGACTATATCGCAGGGCAAGGTGGCCTTGTAG
GCCGTACTCATCCCCACGGTCCTATCCCCTATCCCCTTTCCCC-TCGTGTCACCCACAG
TCTACCCACACCCATCCATTCTTTCTTAACCTCTGACTCTTCCCTCCTTGGTTTCTCAC
TGCCCTTGACGCTTGTTCACCCCGGATGAACTCCGTAGGCGTCTCCCTTCCCTGCTTGGT
ACCCTAAGG----TGCCCTCGGTGCTTGTTCGTA---GAGACGAACTCTG

Mus_spicil

-----TC--GGGATTGACGTGAATTTAGCGTGCTGATACC-TACCTCCTCCT
TGCCCTCCTACACGCACGCGGCCATGTCCGAACCTGAGTTGAAACTGGTGGCGCGGCCGCAT
CCGCAGCTTCCCCGACTTCCCAATCCCGGGCGTGCTGTTTCCAGGTGCGGTCACGAGCCGGC
GAGGCGTTGGCGCCGTAATCTCATCCC-CCGGCGCAGGCGCGTAGGCAGCCTCGGGGATC
TTGCGGGGCCTCTGCCCCGGCCACACGCGGGTCACTCTCCTGTCTTGTTCAGGGATAT
CTCGCCCCCTTTGAAAGACCCGGACTCCTTCCGAGCTTCCATCCGCCTCCTTGGCCAGTCA
CCTGAAGTCCACGCACAGCGGCAAGATCGACTACATCGCAGG-CGAG-TGGCCTTGTAG
GCCGTGCTCGTCCCCACGGTCCTAGCCCCCTATCCCCTTTCCCCCTCGTGTACCCACAG
TCTGCCCCACACCCATCCATTCTTTCTTAACCTCTGACACTTCCCTCCTTGGTTCTCTCAC
TGCCCTTGACGCTTGTTCACCCCGGATGAACTATGTAGGAGTCTCCCTTCCCTGCTAGGT
ACCCTAAGGCATCTGCCCTCGGTGCTTGTTCCTA---GAGACGAACTCTG

Gerbillus_

CCTCCGCCCTTGTTCCTGGGACAGGCTTGACCCTAGCCAGTTGACACCTCACCTCCGCC
TTCTC--TCACGCACGCGGCCATGGCGGAACCCGAGTTGCAGCTGGTGGCGCGGCCGCAT
CCGCAGCTTCCCCGACTTCCCATCCCGGGCGTGCTGTTTCCAGGTGCGTCCACGAGCCGGC
CAGGCGTTGGCGCTGCGTCTCAGCCCTCCGGCGCAGGCGCGTGAGCTGTCTCCGGGATC
TTGCGGGGCCTCCGCCAGCCATAACCAAGTACCATCCTGT---GTTCCAGGGATAT
CTCGCCCCCTTGAAGACCCGGACTCCTTCCGAGCTTCCATCCGTCTCCTGGCCAACCA
TCTGAAGTCCAAGCATGGCGGCAAAATCGACTACATCGCAGG-CGAG-TGTTCTTGTAG
GCCGTGCCCGTTCCC-ACTGTCAGGGCCGCCATCCCGTGTTCCTT--TTTC-----G
TGTACCCACACCCACCCCTCCTTTCTCTGACA-CTCCCAAGTTC-CCT--GTTCTCTC
TGCCCTTGGTCCCATATTCACCCCGGATGA-CTGCG---GAGTCTCC-----
ACCCTCTGACCTCTGCTCTCAAAGCCTGTCCCTACTAGAGAGGAACTCTG

NEXUS

- Madison et al. 1997. *Syst. Biol.* 46: 590-621
- Format used with PAUP, McClade and Mr. Bayes
- Composed of different modules
 - starting with “ BEGIN XXXXX:”
 - ending with “END;”
- Standard blocks: TAXA, CHARACTERS, TREE
- Comments are enclosed within “[]”

#NEXUS

[Name: Mus_pahar. Len: 680 Check: 70E718C]
[Name: Mus_spici Len: 680 Check: D5E622FB]
[Name: Gerbillus Len: 680 Check: FBE40A58]

BEGIN TAXA;
DIMENSIONS NTAX=3;
TAXLABELS Mus_pahar Mus_spici Gerbillus;
END;

BEGIN CHARACTERS;
DIMENSIONS NCHAR=680;
FORMAT MISSING=? DATATYPE=DNA INTERLEAVE GAP=-;
MATRIX

Mus_pahari	-----	-----CCTG	CGGATACT-CACCTCCTCT	TGTCTCCTACAAGCACGCGG	CCATGTCCGAGTCTGAGTTG
Mus_spicilegus	-----TC--GGG	ATTGACGTGAATTTAGCGTG	CTGATACC-TACCTCCTCT	TGCCTCCTACACGCACGCGG	CCATGTCCGAACCTGAGTTG
Gerbillus_campestris	CCTCCGCCCTTGTTCTGGG	ACAGGCTTGACCTAGCCAG	TTGACACCTCACCTCCGCC	TTCTCT--TCACGCACGCGG	CCATGGCGGAACCCGAGTTG
Mus_pahari	AAACTGGTGGCGGGCGCAT	CCGCAGCTTCCCCGACTTCC	CCATCCCGGGCGTGCTGTTT	AGGTGCGGTACAGAGCCGGC	GAGGCGTTGGCGCCGTAATC
Mus_spicilegus	AAACTGGTGGCGGGCGCAT	CCGCAGCTTCCCCGACTTCC	CAATCCCGGGCGTGCTGTTT	AGGTGCGGTACAGAGCCGGC	GAGGCGTTGGCGCCGTACGC
Gerbillus_campestris	CAGCTGGTGGCGGGCGCAT	CCGCAGCTTCCCCGACTTCC	CCATCCCGGGCGTGCTGTTT	AGGTGCGGTACAGAGCCGGC	GAGGCGTTGGCGCCGTACGC
Mus_pahari	TCATCCC-CCGGCGCAGGCG	CGTGGGCAGCCTTGGGGATC	TTGCGGGGCTCTGCCCGGC	CACACGCGG-TCACTCTCT	GTCCTTGTTCCAGGGATAT
Mus_spicilegus	TCATCCC-CCGGCGCAGGCG	CGTAGGCAGCCTCGGGGATC	TTGCGGGGCTCTGCCCGGC	CACACGCGGGTCACTCTCT	GTCCTTGTTCCAGGGATAT
Gerbillus_campestris	TCAGCCCTCCGGCGCAGGCG	CGTGAGCTGTCTCCGGGATC	TTGCGGGGCTCCGCCAGC	CATACCCAAGTCACCATCT	GT----GTTCCAGGGATAT
Mus_pahari	CTCGCCCCTCTTGAAAGATC	CGGACTCCTTCCGAGCTTCC	ATCCGCTCCTGGCCAGTCA	CCTGAAGTCCACGCACAGCG	GCAAGATCGACTATATCGCA
Mus_spicilegus	CTCGCCCCTCTTGAAAGACC	CGGACTCCTTCCGAGCTTCC	ATCCGCTCCTGGCCAGTCA	CCTGAAGTCCACGCACAGCG	GCAAGATCGACTACATCGCA
Gerbillus_campestris	CTCGCCCCTCTTGAAAGACC	CGGACTCCTTCCGAGCTTCC	ATCCGTCTCCTGGCCAACCA	TCTGAAGTCCAAGCATGGCG	GCAAAATCGACTACATCGCA
Mus_pahari	GGGCAAGGTGGCCTTGCTAG	GCCGTACTCATCCCCACGG	TCCTATCCCCTATCCCCTTT	CCCC-TCGTGTACCCACAG	TCTACCCACACCCATCCAT
Mus_spicilegus	GG-CGAG-TGGCCTTGCTAG	GCCGTGCTCGTCCCCACGG	TCCTAGCCCCTATCCCCTTT	CCCCCTCGTGTACCCACAG	TCTGCCCCACACCCATCCAT
Gerbillus_campestris	GG-CGAG-TGTTCTTGCTAG	GCCGTGCCCCGTTCCC-ACTG	TCAGGGCCGCATCCCCTGT	TCCCTT--TTTC-----G	TGTACCCACACCCACCCCT

File identifier

#NEXUS

```
[Name: Mus_pahar.      Len:   680  Check: 70E718C]
[Name: Mus_spici      Len:   680  Check: D5E622FB]
[Name: Gerbillus      Len:   680  Check: FBE40A58]
```

Sequences information

```
BEGIN TAXA;
  DIMENSIONS NTAX=3;
  TAX LABELS Mus_pahar Mus_spici Gerbillus;
END;
```

Block of information

```
BEGIN CHARACTERS;
  DIMENSIONS NCHAR=680;
  FORMAT MISSING=? DATATYPE=DNA INTERLEAVE GAP=-;
  MATRIX
```

```
Mus_pahari      -----
Mus_spicilegus  -----TC--GGG
Gerbillus_campestris  CCTCCGCCCTTGTTCCTGGG

Mus_pahari      AAACTGGTGGCGCGGCGCAT  CCGCAGCTTCCCCGACTTCC  CCATCCCGGGCGTGCTGTTC  AGGTGCGGTACAGAGCCGGC  GAGGCGTTGGCGCCGTACTC
Mus_spicilegus  AAACTGGTGGCGCGGCGCAT  CCGCAGCTTCCCCGACTTCC  CAATCCCGGGCGTGCTGTTC  AGGTGCGGTACAGAGCCGGC  GAGGCGTTGGCGCCGTACGC
Gerbillus_campestris  CAGCTGGTGGCGCGGCGCAT  CCGCAGCTTCCCCGACTTCC  CCATCCCGGGCGTGCTGTTC  AGGTGCGGTACAGAGCCGGC  GAGGCGTTGGCGCCGTACGC

Mus_pahari      TCATCCC-CCGGCGCAGGCG  CGTGGGCAGCCTTGGGGATC  TTGCGGGGCTCTGCCCGGC  CACACGCGG-TCACTCTCCT  GTCCTTGTTCAGGGATAT
Mus_spicilegus  TCATCCC-CCGGCGCAGGCG  CGTAGGCAGCCTCGGGGATC  TTGCGGGGCTCTGCCCGGC  CACACGCGGTCCTCTCCT  GTCCTTGTTCAGGGATAT
Gerbillus_campestris  TCAGCCCTCCGGCGCAGGCG  CGTGAGCTGTCTCCGGGATC  TTGCGGGGCTCCGCCAGC  CATACCCAAGTACCATCCT  GT----GTTCCAGGGATAT

Mus_pahari      CTCGCCCCTCTTAAAAGATC  CGGACTCCTTCCGAGCTTCC  ATCCGCCTCTTGCCAGTCA  CCTGAAGTCCACGCACAGCG  GCAAGATCGACTATATCGCA
Mus_spicilegus  CTCGCCCCTCTTAAAAGACC  CGGACTCCTTCCGAGCTTCC  ATCCGCCTCTTGCCAGTCA  CCTGAAGTCCACGCACAGCG  GCAAGATCGACTACATCGCA
Gerbillus_campestris  CTCGCCCCTCTTAAAAGACC  CGGACTCCTTCCGAGCTTCC  ATCCGTCTCTTGCCAAACCA  TCTGAAGTCCAAGCATGGCG  GCAAAATCGACTACATCGCA

Mus_pahari      GGGCAAGGTGGCCTTGCTAG  GCCGTAATCATCCCCACGG  TCCTATCCCCTATCCCCTTT  CCCC-TCGTGTACCCACAG  TCTACCCACACCCATCCAT
Mus_spicilegus  GG-CGAG-TGGCCTTGCTAG  GCCGTGCTCGTCCCCACGG  TCCTAGCCCCTATCCCCTTT  CCCCCTCGTGTACCCACAG  TCTGCCCCACACCCATCCAT
Gerbillus_campestris  GG-CGAG-TGTTCTTGCTAG  GCCGTGCCCCTTCCC-ACTG  TCAGGGCCGCCATCCCCTGT  TCCCTT--TTT-----G  TGTCACCCACACCCACCCCT
```

```

Mus_pahari      GGGCAAGGTGGCCTTGCTAG  GCCGTA CT CATCCCCACGG  TCCTATCCCCTATCCCCTTT  CCCC-TCGTGTCACCCACAG  TCTACCCACACCCATCCAT
Mus_spicilegus  GG-CGAG-TGGCCTTGCTAG  GCCGTGCTCGTCCCCACGG  TCCTAGCCCCTATCCCCTTT  CCCCCTCGTGTACCCACAG  TCTGCCCCACCCATCCAT
Gerbillus_campestris  GG-CGAG-TGTTCTTGCTAG  GCCGTGCCCGTTCCC-ACTG  TCAGGGCCGCCATCCCCTGT  TCCCTT--TTTC-----G  TGTACCCACACCCACCCCT

Mus_pahari      TCTTTCTTTAACCTCTGACT  CTTCTCCTTGTTTCTCAC  TGCCTTGGACGCTTGTTTAC  CCCGGATGAACTCCGTAGGC  GTCTCCCTTCCCTGCTTGGT
Mus_spicilegus  TCTTTCTTCAACCTCTGACA  CTTCTCCTTGTTTCTCAC  TGCCTTGGACGCTTGTTTAC  CCCGGATGAACTATGTAGGA  GTCTCCCTTCCCTGCTAGGT
Gerbillus_campestris  CCTTTCTCTGACA-CTCCCA  AGTTC-CCT--GTTCTCTC  TGCCTTGGTCCCATATTAC  CCCGGATGA-CTGCG---GA  GTCTCC-----

Mus_pahari      ACCCTAAGG---TGCCCTC  GGTGCTTGTTCTGTA---GAG  ACGAACTCTGCTCTGTCCCTT  GTGTCCAGAACCAAGCCTTC
Mus_spicilegus  ACCCTAAGGCATCTGCCCTC  GGTGCTTGTTCTGTA---GAG  ACGAACTCTGCTCTGTCCCTT  GTGTCCAGAACCAGGCCTCC
Gerbillus_campestris  ACCCTCTGACCTCTGCTCTC  AAAGCCTGTCCCTACTAGAG  AGGAACTCTGCTCTGTCCAT  GTGTGCAGGGCCAGCTCTTC

```

```

;
END;
BEGIN TREES:
.   TREE tree1 = (Mus_pahar, (Mus_spici,Gerbillus));
.   TREE tree2 = (Mus_spici, (Mus_pahar,Gerbillus));
END;
BEGIN NOTES:
.   PICTURE TAXON=3 FORMAT=GIF SOURCE=FILE
.   PICTURE=a_rodent.gif
END;

```

} Tree

ASN1

- Abstract Syntax Notation
- developed to aid computer access
- made to be read/written by computers


```
Seq-entry ::= set {
  level 1 ,
  class nuc-prot ,
  descr {
    title "Mus pahari adenine phosphoribosyltransferase (APRT) gene, and
translated products" ,
    source {
      org {
        taxname "Mus pahari" ,
        common "shrew mouse" ,
        db {
          {
            db "taxon" ,
            tag
            id 10093 } } ,
        orgname {
          name
          binomial {
            genus "Mus" ,
            species "pahari" } ,
          lineage "Eukaryota; Metazoa; Chordata; Craniata; Vertebrata;
Euteleostomi; Mammalia; Eutheria; Euarchontoglires; Glires; Rodentia;
Sciurognathi; Muroidea; Muridae; Murinae; Mus" ,
          gcode 1 ,
          mgcode 2 ,
          div "ROD" } } } ,
    create-date
    std {
```

```
year 1995 ,
month 6 ,
day 28 } ,
pub {
  pub {
    article {
      title {
        name "Substitution rate variation in closely related rodent
species." } ,
      authors {
        names
        std {
          {
            name
            name {
              last "Fieldhouse" ,
              initials "D." } } ,
          {
            name
            name {
              last "Yazdani" ,
              initials "F." } } ,
          {
            name
            name {
              last "Golding" ,
              initials "G.B." } } } ,
```

```
    affil
      str "Department of Biology, McMaster University, Hamilton,
Ontario, Canada." } ,
    from
      journal {
        title {
          iso-jta "Heredity" ,
          ml-jta "Heredity" ,
          issn "0018-067X" ,
          name "Heredity." } ,
        imp {
          date
            std {
              year 1997 ,
              month 1 } ,
          volume "78" ,
          issue " Pt 1" ,
          pages "21-31" ,
          language "eng" } } ,
        ids {
          pubmed 9023989 ,
          medline 97176443 } } ,
        pmid 9023989 ,
        muid 97176443 ,
        gen {
          serial-number 1 } } } ,
    pub {
```

```
pub {
  gen {
    serial-number 2 } ,
  sub {
    authors {
      names
      std {
        {
          name
          name {
            last "Fieldhouse" ,
            initials "D." } } } ,
      affil
      str "Dan Fieldhouse, Biology, McMaster University, 1280 Main
Street West, Hamilton, ON, L8S 4K1, Canada" } ,
      medium other ,
      date
      std {
        year 1995 ,
        month 6 ,
        day 7 } } } } ,
  update-date
  std {
    year 2001 ,
    month 10 ,
    day 15 } } ,
  seq-set {
    seq {
```

```
id {
  genbank {
    name "MPU28721" ,
    accession "U28721" ,
    version 1 } ,
  gi 881573 } ,
descr {
  title "Mus pahari adenine phosphoribosyltransferase (APRT) gene,
complete cds." ,
  molinfo {
    biomol genomic } } ,
inst {
  repr raw ,
  mol dna ,
  length 2283 ,
  seq-data
```

```
ncbi2na
'5E68C745D75FB75C4246694ED62DE2F807AE99A64D649F5587D54D5A9B9EF4AE6B4
625A629BE996C774D55A64A66EA497EA8DF9AA5DE5694466B4775ED7EF54A8CDD95
77E0235A1D7D627D4D65D7A52D1782D46449A42361CCD92A42BA5F9CA5B1D35546
B5CD57355FD576ED1512DC55115353DFDFC177877D75FAFDD1E5FA19FBD1568E075
B29B757D5E7EB15C2B95DAE7EF6C8860779DED7EED481425F5DFF2A4429E94935E1
24A7A885E8D75238684D7C7CAAC977A8E07233C00F2B05FAA6E5EA485D0B7AC9F4A
A79F755287116A91DF77ED7551554427EE701079ECC529D4E7E27D20115CA92783B5
14A2ED48A8AB8915422048BA572C0E74A851207FE54751F5CFAC55694E552034A93B
FB15D5461276A597A0785EC84B9D7AB239E4FE02BA422A7AE23A749AF2891E1E77D4
0AD78BD035490513AE9D1051712712EC444CC300C0C040DF00000008080AE908945
32E88292B28D5429C239C58B0534BBDF72532EA42172EF5CB43BE177531F97769D4D
5115F575F15C12B721D4AA7D7BFA57D5C9D289EA6EA79B9D35A092A82796A551CCD
25D739DE8B3A82B0A89EEAC8A0A92ADF3C51A714B9728B03BAB9D222BE213EAB8AF
C41D780E7497480E7529CA8AE947EF24DC8777C19C7D7B7929E27A035202397C815
A9222EB4FBA385D7A51E8AC08149508404A7D02A5295EDEAB9E1C04099F8317DDFD
DED5F5555554A053BF925EE379E45271A9E2BAE8BBB897AE89E176782A4A88A7285
CC53DF7775D4B38789E9C8EB4455E744924B0799AE9D257A9970B85FEE27179E54'H
}
```

```
annot {
  {
    data
      ftable {
        {
          data
            rna {
              type mRNA ,
              ext
```

```
    name "adenine phosphoribosyltransferase" } ,
partial TRUE ,
location
  mix {
    int {
      from 45 ,
      to 124 ,
      id
      gi 881573 ,
      fuzz-from
      lim It } ,
    int {
      from 255 ,
      to 361 ,
      id
      gi 881573 } ,
    int {
      from 1508 ,
      to 1641 ,
      id
      gi 881573 } ,
    int {
      from 1846 ,
      to 1924 ,
      id
      gi 881573 } ,
```

```
int {
  from 2043 ,
  to 2185 ,
  id
  gi 881573 ,
  fuzz-to
  lim gt } } } ,
{
  data
  gene {
    locus "APRT" } ,
  partial TRUE ,
  location
  int {
    from 45 ,
    to 2185 ,
    strand plus ,
    id
    gi 881573 ,
    fuzz-from
    lim lt ,
    fuzz-to
    lim gt } } } } } } ,
seq {
  id {
    genbank {
      accession "AAA68957" ,
```



```
version 1 } ,
gi 881574 } ,
descr {
  molinfo {
    biomol peptide ,
    tech concept-trans } ,
  title "adenine phosphoribosyltransferase [Mus pahari]" } ,
inst {
  repr raw ,
  mol aa ,
  length 180 ,
  seq-data
  ncbieaa
```

```
"MSESELKLVARRIRSFDFPIPGVLFRRDISPLLKDPDSFRASIRLLASHLKSTHSGKID
YIAGLDSRGFLFGPSLAQELGVGCVLIRKQGKLPGPTISASYALEYGKAELEIQKDALEPGQRVIVD
DLLATGGTMF
AACDLLHQLRAEVVECVSLVELTSLKGRERLGPIPFSSLLQYD" } ,
```

```
annot {
  {
    data
    ftable {
      {
        data
        prot {
          name {
            "adenine phosphoribosyltransferase" } ,
```

```
        ec {
            "2.4.2.7" } } ,
    location
    whole
    gi 881574 } } } ,
{
db other ,
name "Annot:CDD" ,
desc {
    name "CDDSearch" ,
    create-date
    std {
        year 2007 ,
        month 6 ,
        day 18 ,
        hour 23 ,
        minute 46 ,
        second 57 } } ,
data
    ftable {
        {
            data
                region "PRK02304" ,
                comment "adenine phosphoribosyltransferase" ,
                location
                    int {
                        from 5 ,
                        to 178 ,
```

```
id
  gi 881574 } ,
ext {
  type
    str "cddScoreData" ,
  data {
    {
      label
        str "definition" ,
      data
        str "PRK02304" } ,
    {
      label
        str "short_name" ,
      data
        str "PRK02304" } ,
    {
      label
        str "score" ,
      data
        int 575 } ,
    {
      label
        str "evaluate" ,
      data
        real { 307765, 10, -64 } } ,
```

```

        {
            label
                str "bit_score" ,
            data
                real { 225315, 10, -3 } } } } ,
    dbxref {
        {
            db "CDD" ,
            tag
                id 74170 } } } } } } } } } ,
annot {
    {
        data
            ftable {
                {
                    data
                        cdregion {
                            frame one ,
                            code {
                                id 1 } } ,
                        comment "purine salvage enzyme" ,
                        product
                            whole

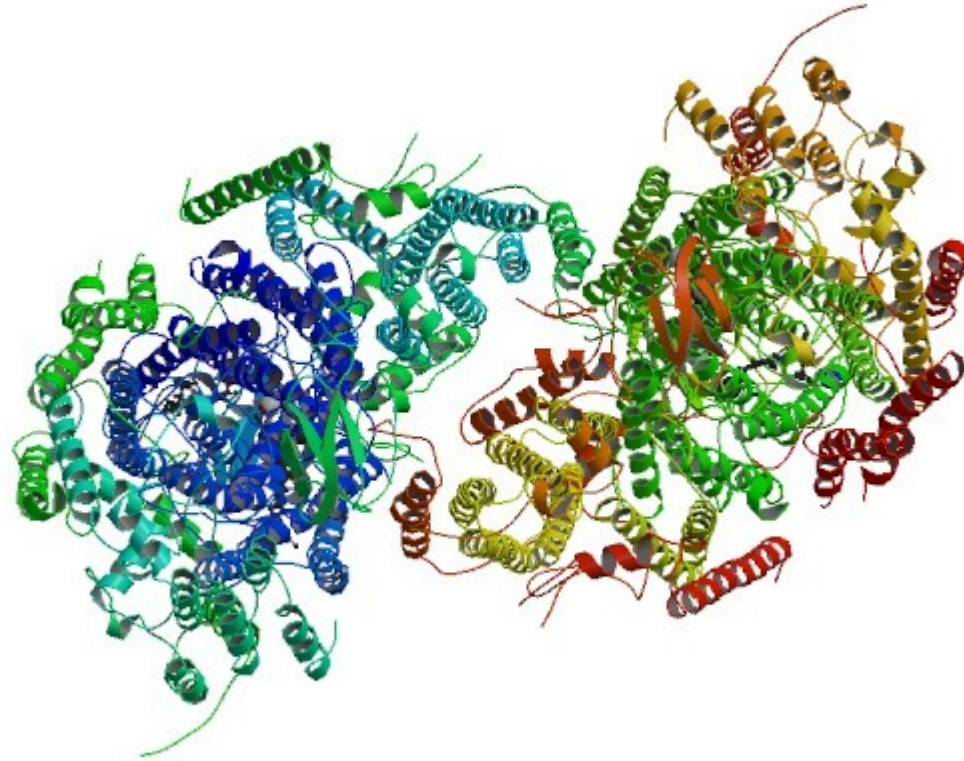
```

```
gi 881574 ,
  location
  mix {
    int {
      from 45 ,
      to 124 ,
      id
      gi 881573 } ,
    int {
      from 255 ,
      to 361 ,
      id
      gi 881573 } ,
    int {
      from 1508 ,
      to 1641 ,
      id
      gi 881573 } ,
    int {
      from 1846 ,
      to 1924 ,
      id
      gi 881573 } ,
    int {
      from 2043 ,
      to 2185 ,
      id
      gi 881573 } } } } } } }
```

PDB

- Protein file
- Store the 3D position of each amino acid
- Primary and secondary structures
- Crystallographic experiments and parameters

CYTOCHROME C OXIDASE



HEADER OXIDOREDUCTASE 26-MAY-98 20CC
TITLE BOVINE HEART CYTOCHROME C OXIDASE AT THE FULLY OXIDIZED
TITLE 2 STATE
COMPND MOL_ID: 1;
COMPND 2 MOLECULE: CYTOCHROME C OXIDASE;
COMPND 3 CHAIN: A, N;
COMPND 4 SYNONYM: FERROCYTOCHROME C\ :OXYGEN OXIDOREDUCTASE;
COMPND 5 EC: 1.9.3.1;
COMPND 6 OTHER_DETAILS: THIS ENZYME IS A HYBRID PROTEIN COMPLEX AND
COMPND 7 IS A HOMODIMER. ONE MONOMER IS COMPOSED OF 13 DIFFERENT
COMPND 8 SUBUNITS AND SEVEN METAL CENTERS, HEME A, HEME A3, CUA,
COMPND 9 CUB, MG, NA AND ZN.;

SOURCE MOL_ID: 1;
SOURCE 2 ORGANISM_SCIENTIFIC: BOS TAURUS;
SOURCE 3 ORGANISM_COMMON: BOVINE;
SOURCE 4 ORGAN: HEART;
SOURCE 5 TISSUE: HEART MUSCLE;
SOURCE 6 ORGANELLE: MITOCHONDRION;

KEYWDS OXIDOREDUCTASE, CYTOCHROME(C)-OXYGEN, CYTOCHROME C OXIDASE
EXPDTA X-RAY DIFFRACTION
AUTHOR T.TSUKIHARA, M.YAO
REVDAT 1 13-JAN-99 20CC 0
JRNL AUTH S.YOSHIKAWA, K.SHINZAWA-ITOH, R.NAKASHIMA, R.YAONO,
JRNL AUTH 2 E.YAMASHITA, N.INOUE, M.YAO, M.J.FEI, C.P.LIBEU,
JRNL AUTH 3 T.MIZUSHIMA, H.YAMAGUCHI, T.TOMIZAKI, T.TSUKIHARA
JRNL TITL REDOX-COUPLED CRYSTAL STRUCTURAL CHANGES IN BOVINE
JRNL TITL 2 HEART CYTOCHROME C OXIDASE.
JRNL REF SCIENCE V. 280 1723 1998
JRNL REFN ASTM SCIEAS US ISSN 0036-8075

REMARK 1
REMARK 1 REFERENCE 1
REMARK 1 AUTH T.TSUKIHARA, H.AOYAMA, E.YAMASHITA, T.TOMIZAKI,
REMARK 1 AUTH 2 H.YAMAGUCHI, K.SHINZAWA-ITOH, R.NAKASHIMA, R.YAONO,
REMARK 1 AUTH 3 S.YOSHIKAWA
REMARK 1 TITL THE WHOLE STRUCTURE OF THE 13-SUBUNIT OXIDIZED
REMARK 1 TITL 2 CYTOCHROME C OXIDASE AT 2.8 A
REMARK 1 REF SCIENCE V. 272 1136 1996
REMARK 1 REFN ASTM SCIEAS US ISSN 0036-8075
REMARK 1 REFERENCE 2

REMARK 2 RESOLUTION. 2.30 ANGSTROMS.
REMARK 3
REMARK 3 REFINEMENT.
REMARK 3 PROGRAM : X-PLOR 3.84
REMARK 3 AUTHORS : BRUNGER
REMARK 3
REMARK 3 DATA USED IN REFINEMENT.
REMARK 3 RESOLUTION RANGE HIGH (ANGSTROMS) : 2.30
REMARK 3 RESOLUTION RANGE LOW (ANGSTROMS) : 15.00
REMARK 3 DATA CUTOFF (SIGMA(F)) : 2.000
REMARK 3 DATA CUTOFF HIGH (ABS(F)) : 100000.000
REMARK 3 DATA CUTOFF LOW (ABS(F)) : 0.1000
REMARK 3 COMPLETENESS (WORKING+TEST) (%) : 88.9
REMARK 3 NUMBER OF REFLECTIONS : 278049
REMARK 3
REMARK 3 FIT TO DATA USED IN REFINEMENT.
REMARK 3 CROSS-VALIDATION METHOD : THROUGHOUT
REMARK 3 FREE R VALUE TEST SET SELECTION : RANDOM
REMARK 3 R VALUE (WORKING SET) : 0.209

REMARK 4
 REMARK 4 20CC COMPLIES WITH FORMAT V. 3.0, 1-DEC-2006
 REMARK 4
 REMARK 4 THIS IS THE REMEDIATED VERSION OF THIS PDB ENTRY.
 REMARK 4 REMEDIATED DATA FILE REVISION 3.101 (2007-05-01)
 REMARK 200
 REMARK 200 EXPERIMENTAL DETAILS
 REMARK 200 EXPERIMENT TYPE : X-RAY DIFFRACTION
 REMARK 200 DATE OF DATA COLLECTION : MAY-1996
 REMARK 200 TEMPERATURE (KELVIN) : 283.0
 REMARK 200 PH : 6.80
 REMARK 200 NUMBER OF CRYSTALS USED : 32
 REMARK 200
 REMARK 200 SYNCHROTRON (Y/N) : Y
 REMARK 200 RADIATION SOURCE : PHOTON FACTORY
 REMARK 200 BEAMLINE : BL-6B
 REMARK 200 X-RAY GENERATOR MODEL : NULL
 REMARK 200 MONOCHROMATIC OR LAUE (M/L) : M

DBREF	20CC	A	1	514	UNP	P00396	COX1_BOVIN	1	514
DBREF	20CC	B	1	227	UNP	P00404	COX2_BOVIN	1	227
DBREF	20CC	C	1	261	UNP	P00415	COX3_BOVIN	1	261
DBREF	20CC	D	1	147	UNP	P00423	COX4_BOVIN	23	169
DBREF	20CC	E	1	109	UNP	P00426	COXA_BOVIN	1	109
DBREF	20CC	F	1	98	UNP	P00428	COXB_BOVIN	1	98
DBREF	20CC	G	1	84	UNP	P07471	COXD_BOVIN	13	96
DBREF	20CC	H	1	85	UNP	P00429	COXG_BOVIN	1	85
DBREF	20CC	I	1	73	UNP	P04038	COXH_BOVIN	1	73
DBREF	20CC	J	1	59	UNP	P07470	COXK_BOVIN	22	80
DBREF	20CC	K	1	56	UNP	P13183	COXM_BOVIN	33	88
DBREF	20CC	L	1	47	UNP	P00430	COXO_BOVIN	17	63

DBREF	20CC	M	1	46	UNP	P10175	COXQ_BOVIN	25	70
DBREF	20CC	N	1	514	UNP	P00396	COX1_BOVIN	1	514
DBREF	20CC	O	1	227	UNP	P00404	COX2_BOVIN	1	227
DBREF	20CC	P	1	261	UNP	P00415	COX3_BOVIN	1	261
DBREF	20CC	Q	1	147	UNP	P00423	COX4_BOVIN	23	169
DBREF	20CC	R	1	109	UNP	P00426	COXA_BOVIN	1	109
DBREF	20CC	S	1	98	UNP	P00428	COXB_BOVIN	1	98
DBREF	20CC	T	1	84	UNP	P07471	COXD_BOVIN	13	96
DBREF	20CC	U	1	85	UNP	P00429	COXG_BOVIN	1	85
DBREF	20CC	V	1	73	UNP	P04038	COXH_BOVIN	1	73
DBREF	20CC	W	1	59	UNP	P07470	COXK_BOVIN	22	80
DBREF	20CC	X	1	56	UNP	P13183	COXM_BOVIN	33	88
DBREF	20CC	Y	1	47	UNP	P00430	COXO_BOVIN	17	63
DBREF	20CC	Z	1	46	UNP	P10175	COXQ_BOVIN	25	70

SEQRES	1	A	514	MET	PHE	ILE	ASN	ARG	TRP	LEU	PHE	SER	THR	ASN	HIS	LYS
SEQRES	2	A	514	ASP	ILE	GLY	THR	LEU	TYR	LEU	LEU	PHE	GLY	ALA	TRP	ALA
SEQRES	3	A	514	GLY	MET	VAL	GLY	THR	ALA	LEU	SER	LEU	LEU	ILE	ARG	ALA
SEQRES	4	A	514	GLU	LEU	GLY	GLN	PRO	GLY	THR	LEU	LEU	GLY	ASP	ASP	GLN
SEQRES	5	A	514	ILE	TYR	ASN	VAL	VAL	VAL	THR	ALA	HIS	ALA	PHE	VAL	MET
SEQRES	6	A	514	ILE	PHE	PHE	MET	VAL	MET	PRO	ILE	MET	ILE	GLY	GLY	PHE
SEQRES	7	A	514	GLY	ASN	TRP	LEU	VAL	PRO	LEU	MET	ILE	GLY	ALA	PRO	ASP
SEQRES	8	A	514	MET	ALA	PHE	PRO	ARG	MET	ASN	ASN	MET	SER	PHE	TRP	LEU

SEQRES	1	B	227	MET	ALA	TYR	PRO	MET	GLN	LEU	GLY	PHE	GLN	ASP	ALA	THR
SEQRES	2	B	227	SER	PRO	ILE	MET	GLU	GLU	LEU	LEU	HIS	PHE	HIS	ASP	HIS
SEQRES	3	B	227	THR	LEU	MET	ILE	VAL	PHE	LEU	ILE	SER	SER	LEU	VAL	LEU
SEQRES	4	B	227	TYR	ILE	ILE	SER	LEU	MET	LEU	THR	THR	LYS	LEU	THR	HIS
SEQRES	5	B	227	THR	SER	THR	MET	ASP	ALA	GLN	GLU	VAL	GLU	THR	ILE	TRP
SEQRES	6	B	227	THR	ILE	LEU	PRO	ALA	ILE	ILE	LEU	ILE	LEU	ILE	ALA	LEU
SEQRES	7	B	227	PRO	SER	LEU	ARG	ILE	LEU	TYR	MET	MET	ASP	GLU	ILE	ASN

HET HEA A 515 60
 HET HEA A 516 60
 HET PER A 520 2
 HET HEA N 515 60
 HET HEA N 516 60
 HET PER N 520 2
 HETNAM CU COPPER (II) ION
 HETNAM MG MAGNESIUM ION
 HETNAM NA SODIUM ION
 HETNAM ZN ZINC ION
 HETNAM HEA HEME-A
 HETNAM PER PEROXIDE ION
 FORMUL 27 CU 6(CU 2+)
 FORMUL 28 MG 2(MG 2+)
 FORMUL 29 NA 2(NA 1+)
 FORMUL 32 ZN 2(ZN 2+)
 FORMUL 39 HEA 4(C49 H56 FE N4 O6)
 FORMUL 41 PER 2(O2 2-)

HELIX	1	1	PHE A	2	TRP A	6	1	
HELIX	2	2	HIS A	12	LEU A	41	1	
HELIX	3	3	ASP A	51	ILE A	87	1	
HELIX	4	4	PRO A	95	MET A	117	1	
HELIX	5	5	ALA A	141	ASN A	170	1	
HELIX	6	6	LEU A	183	ASN A	214	1	

5
 30
 37
 23
 30
 32

SHEET	1	A 5	LEU B 116	SER B 120	0			
SHEET	2	A 5	TYR B 105	TYR B 110	-1	N	TYR B 110	0 LEU B 116
SHEET	3	A 5	LEU B 95	HIS B 102	-1	N	HIS B 102	0 TYR B 105
SHEET	4	A 5	ILE B 150	SER B 156	1	N	ARG B 151	0 LEU B 95
SHEET	5	A 5	ASN B 180	LEU B 184	-1	N	LEU B 184	0 ILE B 150
SHEET	1	B 3	VAL B 142	PRO B 145	0			
SHEET	2	B 3	ILE B 209	VAL B 214	1	N	GLU B 212	0 VAL B 142
SHEET	3	B 3	GLY B 190	GLY B 194	-1	N	GLY B 194	0 ILE B 209
SHEET	1	C 2	HIS B 161	VAL B 165	0			
SHEET	2	C 2	LEU B 170	ALA B 174	-1	N	ALA B 174	0 HIS B 161
SHEET	1	D 3	ASN F 47	SER F 51	0			

SHEET	2	D 3	GLY F	86	PRO F	93	1	N	LYS F	90	0	ASN F	47
SHEET	3	D 3	GLN F	80	CYS F	82	-1	N	CYS F	82	0	GLY F	86
SHEET	1	E 2	LYS F	55	CYS F	60	0						
SHEET	2	E 2	ILE F	70	HIS F	75	-1	N	LEU F	74	0	ARG F	56
SHEET	1	F 5	LEU 0	116	SER 0	120	0						
SHEET	2	F 5	TYR 0	105	TYR 0	110	-1	N	TYR 0	110	0	LEU 0	116
SHEET	3	F 5	LEU 0	95	HIS 0	102	-1	N	HIS 0	102	0	TYR 0	105
SHEET	4	F 5	ILE 0	150	SER 0	156	1	N	ARG 0	151	0	LEU 0	95
SHEET	5	F 5	ASN 0	180	LEU 0	184	-1	N	LEU 0	184	0	ILE 0	150
SHEET	1	G 3	VAL 0	142	PRO 0	145	0						
SHEET	2	G 3	ILE 0	209	VAL 0	214	1	N	GLU 0	212	0	VAL 0	142
SHEET	3	G 3	GLY 0	190	GLY 0	194	-1	N	GLY 0	194	0	ILE 0	209
SHEET	1	H 2	HIS 0	161	VAL 0	165	0						
SHEET	2	H 2	LEU 0	170	ALA 0	174	-1	N	ALA 0	174	0	HIS 0	161
SHEET	1	I 3	ASN S	47	SER S	51	0						
SHEET	2	I 3	GLY S	86	PRO S	93	1	N	LYS S	90	0	ASN S	47
SHEET	3	I 3	GLN S	80	CYS S	82	-1	N	CYS S	82	0	GLY S	86
SHEET	1	J 2	LYS S	55	CYS S	60	0						
SHEET	2	J 2	ILE S	70	HIS S	75	-1	N	LEU S	74	0	ARG S	56
SSBOND	1	CYS H	29		CYS H	64							
SSBOND	2	CYS H	39		CYS H	53							
SSBOND	3	CYS U	29		CYS U	64							
SSBOND	4	CYS U	39		CYS U	53							
LINK		FE	HEA A	515					NE2 HIS A	61			
LINK		FE	HEA A	515					NE2 HIS A	378			
LINK		FE	HEA A	516					NE2 HIS A	376			
LINK		FE	HEA A	516					O1 PER A	520			
LINK		CU	CU A	517					ND1 HIS A	240			
LINK		CU	CU A	517					NE2 HIS A	290			

ATOM	1	N	MET A	1	55.242	340.693	224.088	1.00	68.90				N
ATOM	2	CA	MET A	1	54.908	339.282	224.487	1.00	71.09				C
ATOM	3	C	MET A	1	54.673	338.307	223.329	1.00	66.66				C
ATOM	4	O	MET A	1	55.350	337.285	223.238	1.00	67.66				O

ATOM	5	CB	MET	A	1	53.723	339.248	225.450	1.00	79.30	C
ATOM	6	CG	MET	A	1	54.110	339.452	226.915	1.00	87.90	C
ATOM	7	SD	MET	A	1	55.300	338.229	227.515	1.00	97.07	S
ATOM	8	CE	MET	A	1	54.166	336.799	228.014	1.00	96.59	C
ATOM	9	N	PHE	A	2	53.673	338.579	222.494	1.00	61.89	N
ATOM	10	CA	PHE	A	2	53.412	337.739	221.322	1.00	56.50	C
ATOM	11	C	PHE	A	2	54.569	337.917	220.303	1.00	53.31	C
ATOM	12	O	PHE	A	2	55.076	336.947	219.739	1.00	53.84	O
ATOM	13	CB	PHE	A	2	52.077	338.127	220.683	1.00	55.21	C
ATOM	14	CG	PHE	A	2	51.737	337.334	219.459	1.00	54.54	C
ATOM	15	CD1	PHE	A	2	51.050	336.138	219.565	1.00	55.24	C
ATOM	16	CD2	PHE	A	2	52.126	337.775	218.200	1.00	55.62	C
ATOM	17	CE1	PHE	A	2	50.756	335.388	218.432	1.00	58.99	C
ATOM	18	CE2	PHE	A	2	51.839	337.035	217.059	1.00	57.84	C
ATOM	19	CZ	PHE	A	2	51.155	335.840	217.171	1.00	58.36	C
ATOM	20	N	ILE	A	3	55.010	339.158	220.116	1.00	47.37	N

HETATM28635	CU	CU	A	517	67.173	310.978	190.358	1.00	16.27	CU
HETATM28636	MG	MG	A	518	62.605	315.176	179.115	1.00	19.26	MG
HETATM28637	NA	NA	A	519	42.250	318.661	179.405	1.00	26.18	NA
HETATM28638	CU	CU	B	228	57.527	320.742	171.423	1.00	21.99	CU
HETATM28639	CU	CU	B	229	56.638	319.970	173.568	1.00	24.27	CU
HETATM28640	ZN	ZN	F	99	71.521	300.480	232.843	1.00	33.09	ZN

CONNECT 35128637
CONNECT 47428647
CONNECT 183628635
CONNECT 223928635
CONNECT 224928635
CONNECT 283428636
CONNECT 284228636
CONNECT 290228707
CONNECT 292328647
CONNECT 343128637

CONNECT2888828880
CONNECT288892882928890
CONNECT288902864128889
MASTER 425 0 18 98 30 0 2 928864 26 308 292
END