

Anatomy of a PDB file

Compound/Molecule
Keywords
Method used (also NMR, simulation)
Date Deposited
PDB Identifier

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HEADER      TRANSCRIPTION/DNA
TITLE      CRYSTAL STRUCTURE OF THE LAC REPRESSOR DIMER BOUND TO
TITLE      2 OPERATOR AND THE ANTI-INDUCER ONPF
COMPND     LAC REPRESSOR/DNA COMPLEX
KEYWDS     PROTEIN-DNA COMPLEX, HELIX-TURN-HELIX, GENE REGULATION,
EXPDTA     X-RAY DIFFRACTION
AUTHOR     C.E.BELL, M.LEWIS
JRNL       AUTH  C.E.BELL, M.LEWIS
JRNL       TITL  A CLOSER VIEW OF THE CONFORMATION OF THE LAC
JRNL       TITL 2 REPRESSOR BOUND TO OPERATOR.
JRNL       REF   NAT.STRUCT.BIOL.          V.   7   209 2000
REMARK     1 REFERENCE 1
REMARK     1 AUTH  M.LEWIS, G.CHANG, N.C.HORTON, M.A.KERCHER, H.C.PACE
REMARK     1 TITL  CRYSTAL STRUCTURE OF THE LACTOSE OPERON REPRESSOR
REMARK     1 TITL 2 AND ITS COMPLEXES WITH DNA AND INDUCER
REMARK     1 REF   SCIENCE                  V. 271 1247 1996
REMARK     1 REFN  ASTM SCIEAS  US ISSN 0036-8075
SEQRES     1 D  21   G  A  A  T  T  G  T  G  A  G  C  G  C
SEQRES     2 D  21   T  C  A  C  A  A  T  T
...
SEQRES     1 A 333  MET LYS PRO VAL THR LEU TYR ASP VAL ALA GLU TYR ALA
SEQRES     2 A 333  GLY VAL SER TYR GLN THR VAL SER ARG VAL VAL ASN GLN
SEQRES     3 A 333  ALA SER HIS VAL SER ALA LYS THR ARG GLU LYS VAL GLU
...
SEQRES     1 B 333  MET LYS PRO VAL THR LEU TYR ASP VAL ALA GLU TYR ALA
SEQRES     2 B 333  GLY VAL SER TYR GLN THR VAL SER ARG VAL VAL ASN GLN
...
HETNAM     NPF ORTHONITROPHENYL-BETA-D-FUCOPYRANOSIDE
FORMUL     6 NPF   3(C12 H15 N1 O7)
HELIX      1  1 THR A   5  TYR A  12  1
HELIX      2  2 SER A  16  ASN A  25  1
HELIX      3  3 ALA A  32  ASN A  46  1
HELIX      4  4 ASN A  50  ALA A  57  1
HELIX      5  5 LEU A  73  LEU A  90  1
...
SHEET      1  A 4 SER A  93  MET A  98  0
SHEET      2  A 4 LEU A  63  THR A  68  1  N  ILE A  64  O  SER A  93
SHEET      3  A 4 GLY A 121  ASN A 125  1  O  GLY A 121  N  GLY A  65
SHEET      4  A 4 ALA A 145  PHE A 147  1  O  LEU A 146  N  ILE A 124
...

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Title of this PDB submission

Authors of this PDB submission

Primary Literature Reference

Other Literature Reference(s)

Sequence of DNA chain D

Sequence of protein chain A

Sequence of protein chain B

Heteroatom (non-protein/DNA) declaration

Heteroatom definition

Define where the author thinks helices are

Define where the author thinks beta-sheets are

CISPPEP 1 ILE C 283 PRO C 284 1 -0.51

This molecule has a cis-proline

CRYST1 251.438 251.438 204.791 90.00 90.00 120.00 H 3 2
ORIGX1 1.000000 0.000000 0.000000 0.000000

54 Crystallographic rotation and scaling matrices

SCALE1 0.003977 0.002296 0.000000 0.000000

ATOM 1 O5* T D 5 -6.441 91.288 -22.163 1.00136.32
ATOM 2 C5* T D 5 -6.339 92.635 -21.685 1.00136.72

O sugar atoms
C

ATOM 12 N3 T D 5 -11.923 96.235 -21.510 1.00137.53
ATOM 13 C4 T D 5 -12.400 95.306 -20.603 1.00137.44

N base atoms
C

Nucleic acid residue atom coordinates

ATOM 18 P G D 6 -4.758 96.798 -21.981 1.00137.50
ATOM 19 O1P G D 6 -3.345 96.432 -21.701 1.00137.33

P backbone atoms
O

TER 696 A E 18 Indicates end of a chain

ATOM 699 C LYS A 2 7.988 103.719 -3.783 1.00105.99
ATOM 700 O LYS A 2 8.319 103.402 -4.923 1.00106.22
ATOM 701 N PRO A 3 7.446 102.838 -2.929 1.00106.03
ATOM 702 CA PRO A 3 7.183 101.430 -3.245 1.00106.19
ATOM 703 C PRO A 3 6.592 101.207 -4.633 1.00106.39

C Amino acid residue atom coordinates
O
N
C (parts of residues 2 and 3 of chain A are shown)
C

TER 5575 ALA B 331 Indicates end of a chain

HETATM 5576 C1 NPF 901 -13.446 87.461 32.376 1.00 58.71
HETATM 5577 C2 NPF 901 -12.756 88.680 32.106 1.00 59.04

C Heteroatom atom coordinates
C

HETATM 5616 O HOH 1 1.628 87.097 33.699 1.00 35.03

O Water atom coordinates

CONECT 5576 5577 5581 5585 Instructions for connecting heteroatom atoms
CONECT 5577 5576 5578

MASTER 30 0 0 36 36 0 0 6 7838 5 40 82

Some wrap-up thing

END Signals end of the entire file (subsequent lines ignored)

"ATOM"	Atom No	Atom Name	Residue Name	Chain	Residue Seq No	Atom x-coord (Å)	Atom y-coord (Å)	Atom z-coord (Å)	Occupancy	Temperature Factor	Element Symbol	Charge
1-4	7-11	13-16	17	18-20	22 23-26 27	31-38	39-46	47-54	55-60	61-66	77-78	79-80
ATOM	702	CA	PRO	A	3	7.183	101.430	-3.245	1.00	106.19	C	

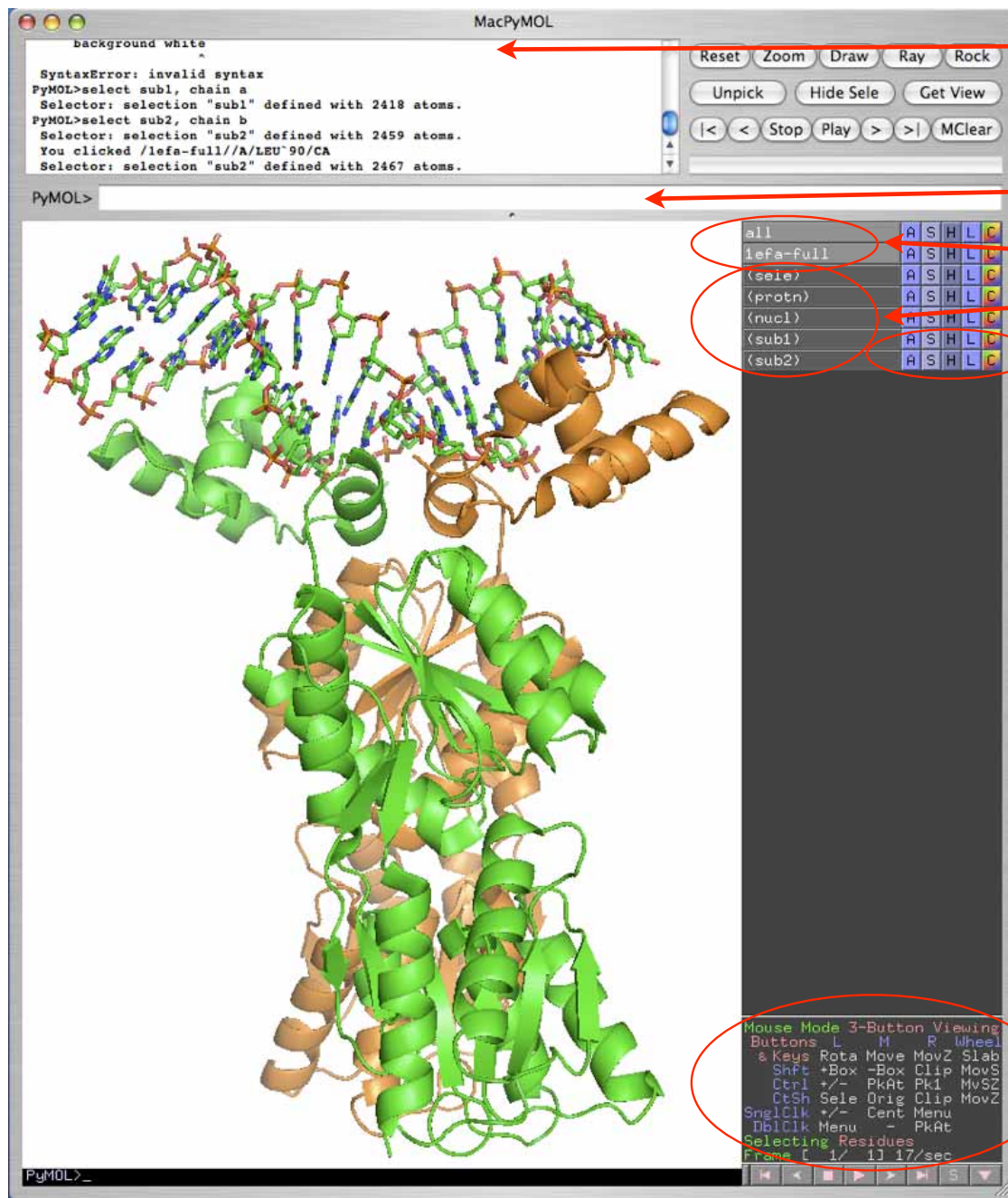
1234567890123456789012345678901234567890123456789012345678901234567890
10 20 30 40 50 60 70 80

Official Coordinate File Format

"ATOM"	Atom No	Atom Name	Residue Name	Chain	Residue Seq No	Insert Code	Atom x-coord (Å)	Atom y-coord (Å)	Atom z-coord (Å)	Occupancy	Temperature Factor	Element Symbol	Charge
1-4	7-11	13-16	18-20	22	23-26	27	31-38	39-46	47-54	55-60	61-66	77-78	79-80
ATOM	702	CA	PRO	A	3		7.183	101.430	-3.245	1.00	106.19	C	

12345678901234567890123456789012345678901234567890123456789012345678901234567890

10 20 30 40 50 60 70 80



Messages show up here
(press <esc> to see more)

Enter your commands here

Objects (not in parenthesis)

Selections (in parenthesis)

Actions (applied to object/selection):

A: Misc actions

S: Show

H: Hide

L: Label

C: Color

Mousing reminders

PyMol