Coordinate Section

The Coordinate Section contains the collection of atomic coordinates as well as the MODEL and ENDMDL records.

MODEL

Overview
The MODEL record specifies the model serial number when multiple structures are presented in a single coordinate entry, as is often the case with structures determined by NMR.
Record Format

```
COLUMNS      DATA TYPE       FIELD       DEFINITION
-------------------------------------------------------------
 1 - 6       Record name     "MODEL "
11 - 14      Integer         serial      Model serial number.
```

Details

This record is used only when more than one model appears in an entry. Generally, it is employed only for NMR structures. The chemical connectivity should be the same for each model. ATOM, HETATM, SIGATM, SIGUIJ, ANISOU, and TER records for each model structure are interspersed as needed between MODEL and ENDMDL records.
The numbering of models is sequential beginning with 1.
If a collection contains more than 99,999 total atoms, then more than one entry must be made. In such a case the collection is divided between models (between an ENDMDL and the following MODEL record) and the model numbering is sequential throughout such a set of entries.

Verification/Validation/Value Authority Control
Entries with multiple structures in the EXPDTA record are checked for corresponding pairs of MODEL/ENDMDL records, and for consecutively numbered models.
Relationships to Other Record Types
Each MODEL must have a corresponding ENDMDL record.
In the case of an NMR entry the EXPDTA record states the number of model structures that are present in the individual entry.
Example

```
         1         2         3         4         5         6         7
8
12345678901234567890123456789012345678901234567890123456789012345678901234567
890
MODEL        1
ATOM      1  N   ALA     1      11.104   6.134  -6.504  1.00  0.00
N
ATOM      2  CA  ALA     1      11.639   6.071  -5.147  1.00  0.00
C
...
...
ATOM    293 1HG  GLU    18     -14.861  -4.847   0.361  1.00  0.00
H
ATOM    294 2HG  GLU    18     -13.518  -3.769   0.084  1.00  0.00
H
```

```
TER     295      GLU    18
ENDMDL
MODEL        2
ATOM    296  N   ALA     1      10.883   6.779  -6.464  1.00  0.00
N
ATOM    297  CA  ALA     1      11.451   6.531  -5.142  1.00  0.00
C
...
...
ATOM    588 1HG  GLU    18     -13.363  -4.163  -2.372  1.00  0.00
H
ATOM    589 2HG  GLU    18     -12.634  -3.023  -3.475  1.00  0.00
H
TER     590      GLU    18
ENDMDL
```

ATOM

Overview

The ATOM records present the atomic coordinates for standard residues (see http://deposit.pdb.org/public-component-erf.cif). They also present the occupancy and temperature factor for each atom. Heterogen coordinates use the HETATM record type. The element symbol is always present on each ATOM record; segment identifier and charge are optional.

Record Format

COLUMNS	DATA TYPE	FIELD	DEFINITION
1 - 6	Record name	"ATOM "	
7 - 11	Integer	serial	Atom serial number.
13 - 16	Atom	name	Atom name.
17	Character	altLoc	Alternate location indicator.
18 - 20	Residue name	resName	Residue name.
22	Character	chainID	Chain identifier.
23 - 26	Integer	resSeq	Residue sequence number.
27	AChar	iCode	Code for insertion of residues.
31 - 38	Real(8.3)	x	Orthogonal coordinates for X in Angstroms
39 - 46	Real(8.3)	y	Orthogonal coordinates for Y in Angstroms
47 - 54	Real(8.3)	z	Orthogonal coordinates for Z in Angstroms
55 - 60	Real(6.2)	occupancy	Occupancy.
61 - 66	Real(6.2)	tempFactor	Temperature factor.
77 - 78	LString(2)	element	Element symbol, right-justified.
79 - 80	LString(2)	charge	Charge on the atom.

Details

ATOM records for proteins are listed from amino to carboxyl terminus.

Nucleic acid residues are listed from the 5' to the 3' terminus.
No ordering is specified for polysaccharides.
The list of ATOM records in a chain is terminated by a TER record.
If more than one model is present in the entry, each model is delimited by MODEL and ENDMDL records.
If an atom is provided in more than one position, then a non-blank alternate location indicator must be used as the alternate location indicator for each of the positions. Within a residue all atoms that are associated with each other in a given conformation are assigned the same alternate position indicator.
For atoms that are in alternate sites indicated by the alternate site indicator, sorting of atoms in the ATOM/HETATM list uses the following general rules:

In the simple case that involves a few atoms or a few residues with alternate sites, the coordinates occur one after the other in the entry.

In the case of a large heterogen groups which are disordered, the atoms for each conformer are listed together.

The insertion code is commonly used in sequence numbering
If the depositor provides the data, then the isotropic B value is given for the temperature factor.
If there are neither isotropic B values from the depositor, nor anisotropic temperature factors in ANISOU, then the default value of 0.0 is used for the temperature factor.
Columns 77 - 78 contain the atom's element symbol (as given in the periodic table), right-justified.
Columns 79 - 80 indicate any charge on the atom, e.g., 2+, 1-. In most cases these are blank.

Verification/Validation/Value Authority Control
PDB checks ATOM/HETATM records for PDB format, sequence information, and packing. The PDB reserves the right to return deposited coordinates to the author for transformation into PDB format.
Relationships to Other Record Types
The ATOM records are compared to the corresponding sequence database. Residue discrepancies appear in the SEQADV record. Missing atoms are annotated in the remarks. HETATM records are formatted in the same way as ATOM records. The sequence implied by ATOM records must be identical to that given in SEQRES, with the exception that residues that have no coordinates, e.g., due to disorder, must appear in SEQRES.
Example

```
         1         2         3         4         5         6         7
8
12345678901234567890123456789012345678901234567890123456789012345678901234567
890
ATOM    145  N   VAL A  25      32.433  16.336  57.540  1.00 11.92
N
ATOM    146  CA  VAL A  25      31.132  16.439  58.160  1.00 11.85
C
ATOM    147  C   VAL A  25      30.447  15.105  58.363  1.00 12.34
C
ATOM    148  O   VAL A  25      29.520  15.059  59.174  1.00 15.65
O
ATOM    149  CB AVAL A  25      30.385  17.437  57.230  0.28 13.88
C
ATOM    150  CB BVAL A  25      30.166  17.399  57.373  0.72 15.41
C
ATOM    151  CG1AVAL A  25      28.870  17.401  57.336  0.28 12.64
C
ATOM    152  CG1BVAL A  25      30.805  18.788  57.449  0.72 15.11
C
```

```
ATOM    153  CG2AVAL A  25      30.835  18.826  57.661  0.28 13.58
C
ATOM    154  CG2BVAL A  25      29.909  16.996  55.922  0.72 13.25
C
```

Known Problems

No distinction is made between ribo- and deoxyribonucleotides in the SEQRES records. These residues are identified with the same residue name (i.e., A, C, G, T, U).