ATOM

Overview

The ATOM records present the atomic coordinates for standard amino acids and nucleotides. They also present the occupancy and temperature factor for each atom. Non-polymer chemical coordinates use the HETATM record type. The element symbol is always present on each ATOM record; charge is optional.

Changes in ATOM/HETATM records result from the standardization atom and residue nomenclature. This nomenclature is described in the Chemical Component Dictionary (ftp://ftp.wwpdb.org/pub/pdb/data/monomers).

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' → 3' terminus.
* Alignment of one-letter atom name such as C starts at column 14, while two-letter atom name such as FE starts at column 13.
* Atom nomenclature begins with atom type.
* No ordering is specified for polysaccharides.
* Non-blank alphanumerical character is used for chain identifier.
* 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.

* AltLoc is the place holder to indicate alternate conformation. The alternate conformation can be in the entire polymer chain, or several residues or partial residue (several atoms within one residue). If an atom is provided in more than one position, then a non-blank alternate location indicator must be used for each of the atomic positions. Within a residue, all atoms that are associated with each other in a given conformation are assigned the same alternate position indicator. There are two ways of representing alternate conformation- either at atom level or at residue level (see examples).

* 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.

* Alphabet letters are commonly used for insertion code. The insertion code is used when two residues have the same numbering. The combination of residue numbering and insertion code defines the unique residue.

* 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 79 - 80 indicate any charge on the atom, e.g., 2+, 1-. In most cases, these are blank.

Verification/Validation/Value Authority Control

The ATOM/HETATM records are checked for PDB file format, sequence information, and packing.

Relationships to Other Record Types

The ATOM records are compared to the corresponding sequence database. Sequence 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.

Examples

```
         1         2         3         4         5         6         7         8
12345678901234567890123456789012345678901234567890123456789012345678901234567890

ATOM     32  N  AARG A  -3      11.281  86.699  94.383  0.50 35.88           N
ATOM     33  N  BARG A  -3      11.296  86.721  94.521  0.50 35.60           N
ATOM     34  CA AARG A  -3      12.353  85.696  94.456  0.50 36.67           C
ATOM     35  CA BARG A  -3      12.333  85.862  95.041  0.50 36.42           C
ATOM     36  C  AARG A  -3      13.559  86.257  95.222  0.50 37.37           C
ATOM     37  C  BARG A  -3      12.759  86.530  96.365  0.50 36.39           C
ATOM     38  O  AARG A  -3      13.753  87.471  95.270  0.50 37.74           O
ATOM     39  O  BARG A  -3      12.924  87.757  96.420  0.50 37.26           O
ATOM     40  CB AARG A  -3      12.774  85.306  93.039  0.50 37.25           C
ATOM     41  CB BARG A  -3      13.428  85.746  93.980  0.50 36.60           C
ATOM     42  CG AARG A  -3      11.754  84.432  92.321  0.50 38.44           C
ATOM     43  CG BARG A  -3      12.866  85.172  92.651  0.50 37.31           C
ATOM     44  CD AARG A  -3      11.698  84.678  90.815  0.50 38.51           C
ATOM     45  CD BARG A  -3      13.374  85.886  91.406  0.50 37.66           C
ATOM     46  NE AARG A  -3      12.984  84.447  90.163  0.50 39.94           N
ATOM     47  NE BARG A  -3      12.644  85.487  90.195  0.50 38.24           N
ATOM     48  CZ AARG A  -3      13.202  84.534  88.850  0.50 40.03           C
ATOM     49  CZ BARG A  -3      13.114  85.582  88.947  0.50 39.55           C
ATOM     50  NH1AARG A  -3      12.218  84.840  88.007  0.50 40.76           N
ATOM     51  NH1BARG A  -3      14.338  86.056  88.706  0.50 40.23           N
ATOM     52  NH2AARG A  -3      14.421  84.308  88.373  0.50 40.45           N

         1         2         3         4         5         6         7         8
12345678901234567890123456789012345678901234567890123456789012345678901234567890
ATOM     32  N  AARG A  -3      11.281  86.699  94.383  0.50 35.88           N
ATOM     33  CA AARG A  -3      12.353  85.696  94.456  0.50 36.67           C
ATOM     34  C  AARG A  -3      13.559  86.257  95.222  0.50 37.37           C
ATOM     35  O  AARG A  -3      13.753  87.471  95.270  0.50 37.74           O
ATOM     36  CB AARG A  -3      12.774  85.306  93.039  0.50 37.25           C
ATOM     37  CG AARG A  -3      11.754  84.432  92.321  0.50 38.44           C
ATOM     38  CD AARG A  -3      11.698  84.678  90.815  0.50 38.51           C
ATOM     39  NE AARG A  -3      12.984  84.447  90.163  0.50 39.94           N
ATOM     40  CZ AARG A  -3      13.202  84.534  88.850  0.50 40.03           C
ATOM     41  NH1AARG A  -3      12.218  84.840  88.007  0.50 40.76           N
ATOM     42  NH2AARG A  -3      14.421  84.308  88.373  0.50 40.45           N
ATOM     43  N  BARG A  -3      11.296  86.721  94.521  0.50 35.60           N
ATOM     44  CA BARG A  -3      12.333  85.862  95.041  0.50 36.42           C
ATOM     45  C  BARG A  -3      12.759  86.530  96.365  0.50 36.39           C
ATOM     46  O  BARG A  -3      12.924  87.757  96.420  0.50 37.26           O
ATOM     47  CB BARG A  -3      13.428  85.746  93.980  0.50 36.60           C
ATOM     48  CG BARG A  -3      12.866  85.172  92.651  0.50 37.31           C
ATOM     49  CD BARG A  -3      13.374  85.886  91.406  0.50 37.66           C
ATOM     50  NE BARG A  -3      12.644  85.487  90.195  0.50 38.24           N
ATOM     51  CZ BARG A  -3      13.114  85.582  88.947  0.50 39.55           C
ATOM     52  NH1BARG A  -3      14.338  86.056  88.706  0.50 40.23           N
```