

## HETATM

### Overview

Non-polymer or other “non-standard” chemical coordinates, such as water molecules or atoms presented in HET groups use the HETATM record type. They also present the occupancy and temperature factor for each atom. The ATOM records present the atomic coordinates for standard residues. The element symbol is always present on each HETATM record; charge is optional.

Changes in ATOM/HETATM records will require standardization in 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	"HETATM"	
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.
39 - 46	Real(8.3)	y	Orthogonal coordinates for Y.
47 - 54	Real(8.3)	z	Orthogonal coordinates for Z.
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.