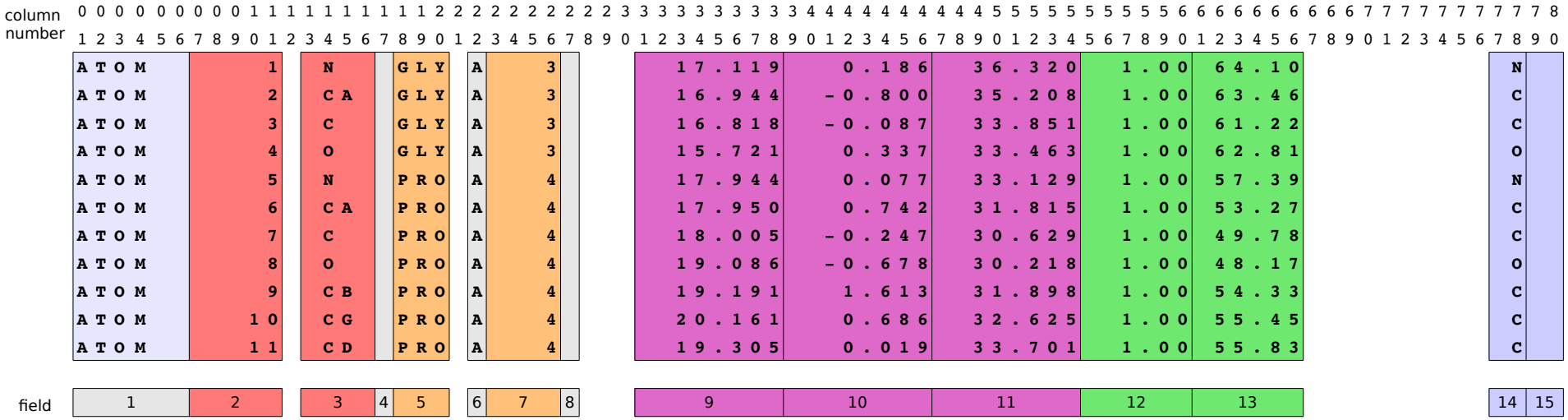
PDB file format 3.3



field	definition	length	format	range	Python extraction
1	'ATOM ' or 'HETATM'	6	{:6s}	01—06	[0:6]
2	atom serial number	5	{:5d}	07—11	[6:11]
		1			
3	atom name	4	{:^4s}	13—16	[12:16]
4	alternate location indicator	1	{:1s}	17	[16:17]
5	residue name	3	{:3s}	18—20	[17:20]
		1			
6	chain identifier	1	{:1s}	22	[21:22]
7	residue sequence number	4	{:4d}	23—26	[22:26]
8	code for insertion of residues	1	{:1s}	27	[26:27]
		3			
9	orthogonal coordinates for X in Angstrom	8	{:8.3f}	31—38	[30:38]
10	orthogonal coordinates for Y in Angstrom	8	{:8.3f}	39—46	[38:46]
11	orthogonal coordinates for Z in Angstrom	8	{:8.3f}	47—54	[46:54]
12	occupancy	6	{:6.2f}	55—60	[54:60]
13	temperature factor	6	{:6.2f}	61—66	[60:66]
		10			
14	element symbol	2	{:>2s}	77—78	[76:78]
15	charge on the atom	2	{:2s}	79—80	[78:80]

Python formated string (old): `'%-6s%5d %4s%1s%3s %1s%4d%1s %8.3f%8.3f%8.3f%6.2f%6.2f %2s%2s'`

Python formated string (Python 2.7 and Python 3.x): `'{:6s}{:5d} {:^4s}{:1s}{:3s} {:1s}{:4d}{:1s} {:8.3f}{:8.3f}{:8.3f}{:6.2f}{:6.2f} {:>2s}{:2s}'`

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reference taken from http://www.wwpdb.org/documentation/file-format-content/format33/sect9.html#ATOM

PP 04/09/2016