

### PDB file format 3.3

column number	1	2	3	4	5	6	7	8
ATOM	1	N	GLY	A	3			
ATOM	2	CA	GLY	A	3			
ATOM	3	C	GLY	A	3			
ATOM	4	O	GLY	A	3			
ATOM	5	N	PRO	A	4			
ATOM	6	CA	PRO	A	4			
ATOM	7	C	PRO	A	4			
ATOM	8	O	PRO	A	4			
ATOM	9	CB	PRO	A	4			
ATOM	10	CG	PRO	A	4			
ATOM	11	CD	PRO	A	4			

field	1	2	3	4	5	6	7	8
1	17.1119	0.186	36.320	1.00	64.10			
2	16.944	-0.800	35.208	1.00	63.46			
3	16.818	-0.087	33.851	1.00	61.22			
4	15.721	0.337	33.463	1.00	62.81			
5	17.944	0.077	33.129	1.00	57.39			
6	17.950	0.742	31.815	1.00	53.27			
7	18.005	-0.247	30.629	1.00	49.78			
8	19.086	-0.678	30.218	1.00	48.17			
9	19.191	1.613	31.898	1.00	54.33			
10	20.161	0.686	32.625	1.00	55.45			
11	19.305	0.019	33.701	1.00	55.83			

field	9	10	11	12	13
14	15	16	17	18	19

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]
3	atom name	1	{: ^ 4s}	13-16	[12:16]
4	alternate location indicator	4	{:1s}	17	[16:17]
5	residue name	3	{:3s}	18-20	[17:20]
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]
9	orthogonal coordinates for X in Angstrom	3	{: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]
14	element symbol	10	{: > 2s}	77-78	[76:78]
15	charge on the atom	2	{: > s}	79-80	[78:80]

Python formatted string (old): %s-%s%d %s%1s%3s %1s%4d%1s %8.3f%8.3f%8.3f%6.2f%6.2f %2s%2s'

```
Python formatted string (Python 2.7 and Python 3.x):
```



PP 04/09/2016

PDB File Format - Contents Guide Version 3.30 (Nov. 21, 2012)

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

FIGURE A.2 – Format PDB et les différents champs de coordonnées.