

## INPUT FILE FORMAT

A	B	C	D	E	F	G	H
ATOM	1	N	GLU	1	18.194	18.496	-16.196
ATOM	2	H1	GLU	1	17.459	18.327	-16.875
ATOM	3	H2	GLU	1	18.999	17.965	-16.497
ATOM	4	H3	GLU	1	18.391	19.483	-16.133
ATOM	5	CA	GLU	1	17.729	17.975	-14.894
ATOM	6	HA	GLU	1	18.521	18.006	-14.148
ATOM	7	CB	GLU	1	16.540	18.768	-14.368
ATOM	8	HB2	GLU	1	15.812	18.885	-15.171
ATOM	9	HB3	GLU	1	16.098	18.198	-13.564
ATOM	10	CG	GLU	1	16.993	20.125	-13.814
ATOM	11	HG2	GLU	1	17.510	19.961	-12.866
ATOM	12	HG3	GLU	1	17.700	20.574	-14.514
ATOM	13	CD	GLU	1	15.846	21.113	-13.598
ATOM	14	OE1	GLU	1	16.182	22.277	-13.299
ATOM	15	OE2	GLU	1	14.684	20.714	-13.819
ATOM	16	C	GLU	1	17.348	16.531	-15.092
ATOM	17	O	GLU	1	16.923	16.202	-16.193
ATOM	18	N	PHE	2	17.617	15.704	-14.092
ATOM	19	H	PHE	2	17.992	16.056	-13.217
ATOM	20	CA	PHE	2	17.524	14.256	-14.180
ATOM	21	HA	PHE	2	17.061	13.967	-15.125
ATOM	22	CB	PHE	2	18.929	13.651	-14.114
ATOM	23	HB2	PHE	2	19.362	13.852	-13.133
ATOM	24	HB3	PHE	2	18.849	12.568	-14.222
ATOM	25	CG	PHE	2	19.845	14.187	-15.187
ATOM	26	CD1	PHE	2	20.589	15.360	-14.962
ATOM	27	HD1	PHE	2	20.521	15.838	-13.996
ATOM	28	CE1	PHE	2	21.382	15.900	-15.989
ATOM	29	HE1	PHE	2	21.941	16.806	-15.820
ATOM	30	CZ	PHE	2	21.454	15.244	-17.231

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Note: The spacing between any two columns may vary. The format of atoms in column C should strictly be the same as described above. Any columns after H are acceptable.

## FORMAT DESCRIPTION

COLUMNS	FIELD	DEFINITION
A	"ATOM "	
B	serial	Atom serial number.
C	name	Atom name.
D	resName	Residue name.
E	resSeq	Residue sequence number.
F	x	Orthogonal coordinates for X in Angstroms.
G	y	Orthogonal coordinates for Y in Angstroms.
H	z	Orthogonal coordinates for Z in Angstroms.