Different Files in MD Simulation

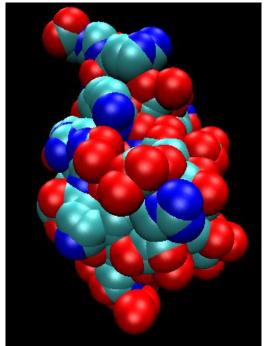
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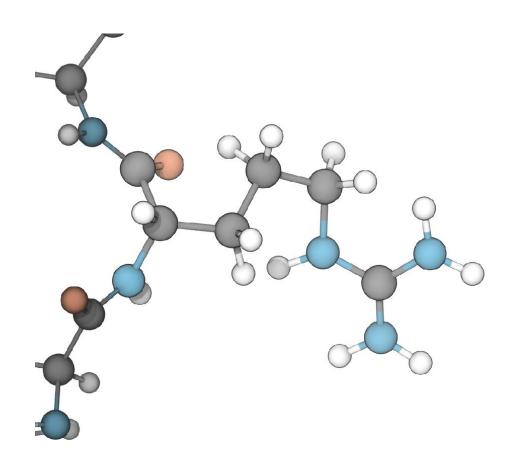
Protein Data Bank (PDB) File

- The Protein Data Bank (pdb) file format is a textual file format describing the three-dimensional structures of molecules held in the Protein Data Bank.
- The pdb format accordingly provides for description and annotation of protein and nucleic acid structures including atomic coordinates, secondary structure assignments, as well as atomic connectivity. In addition experimental metadata are stored.



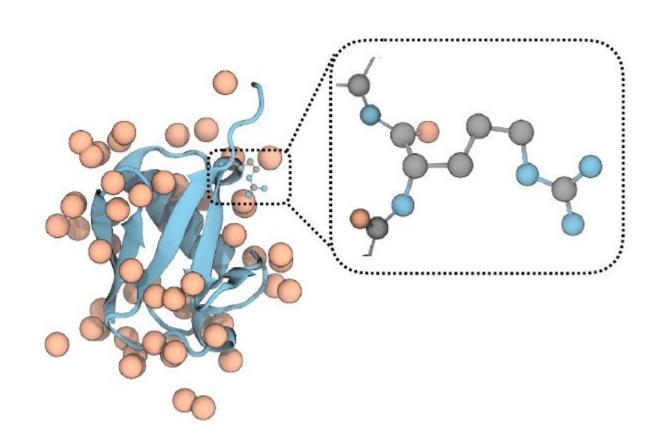
Protein Data Bank (PDB) File

ATOM	1	N	MET	A	1	27.340	24.430	2.614	1.00	9.67	N
ATOM	2	CA	MET	A	1	26.266	25.413	2.842	1.00	10.38	C
MOTA	3	C	MET	A	1	26.913	26.639	3.531	1.00	9.62	C
MOTA	4	0	MET	A	1	27.886	26.463	4.263	1.00	9.62	0
MOTA	5	CB	MET	A	1	25.112	24.880	3.649	1.00	13.77	C
ATOM	6	CG	MET	A	1	25.353	24.860	5.134	1.00	16.29	C
MOTA	7	SD	MET	A	1	23.930	23.959	5.904	1.00	17.17	S
MOTA	8	CE	MET	A	1	24.447	23.984	7.620	1.00	16.11	C
MOTA	9	N	GLN	A	2	26.335	27.770	3.258	1.00	9.27	N
ATOM	10	CA	GLN	A	2	26.850	29.021	3.898	1.00	9.07	C
ATOM	11	С	GLN	A	2	26.100	29.253	5.202	1.00	8.72	C
ATOM	12	0	GLN	A	2	24.865	29.024	5.330	1.00	8.22	0
ATOM	13	CB	GLN	A	2	26.733	30.148	2.905	1.00	14.46	C
ATOM	14	CG	GLN	A	2	26.882	31.546	3.409	1.00	17.01	C
ATOM	15	CD	GLN	A	2	26.786	32.562	2.270	1.00	20.10	C
MOTA	16	OE1	GLN	A	2	27.783	33.160	1.870	1.00	21.89	0
ATOM	17	NE2	GLN	A	2	25.562	32.733	1.806	1.00	19.49	N
ATOM	18	N	ILE	A	3	26.849	29.656	6.217	1.00	5.87	N
ATOM	19	CA	ILE	A	3	26.235	30.058	7.497	1.00	5.07	С
MOTA	20	С	ILE	A	3	26.882	31.428	7.862	1.00	4.01	С
ATOM	21	0	ILE	A	3	27.906	31.711	7.264	1.00	4.61	0
ATOM	22	CB	ILE	A	3	26.344	29.050	8.645	1.00	6.55	C
ATOM	23	CG1	ILE	A	3	27.810	28.748	8.999	1.00	4.72	С
ATOM	24	CG2	ILE	A	3	25.491	27.771	8.287	1.00	5.58	С
ATOM	25	CD1	ILE	A	3	27.967	28.087	10.417	1.00	10.83	C
ATOM	26	N	PHE	A	4	26.214	32.097	8.771	1.00	4.55	N
ATOM	27	CA	PHE	A	4	26.772	33.436	9.197	1.00	4.68	C
ATOM	28	С	PHE	A	4	27.151	33.362	10.650	1.00	5.30	С
ATOM	29	0	PHE	A	4	26.350	32.778	11.395	1.00	5.58	0
ATOM	30	CB	PHE	A	4	25.695	34.498	8.946	1.00	4.83	C
ATOM	31	CG	PHE	A	4	25.288	34.609	7.499	1.00	7.97	C
ATOM	32	CD1	PHE	A	4	24.147	33.966	7.038	1.00	6.69	C
ATOM	33	CD2	PHE	Α	4	26.136	35.346	6.640	1.00	8.34	С
ATOM	34	CE1	PHE	Α	4	23.812	34.031	5.677	1.00	9.10	C
ATOM	35	CE2	PHE	Α	4	25.810	35.392	5.267	1.00	10.61	С
ATOM	36	CZ	PHE	Α	4	24.620	34.778	4.853	1.00	8.90	С
ATOM	37	N	VAL	Α	5	28.260	33.943	11.096	1.00	4.44	N



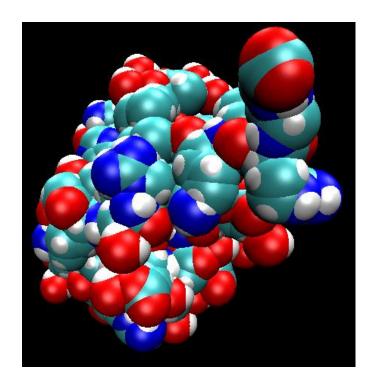
Protein Data Bank (PDB) File

- Things to know about the PDB files:
- No Hydrogen Atoms
- Crystallographic Water Molecules and Ions
- Other Molecules
- Missing residues (Possible Sequence Gaps)
- Poorly Defined Atom's Position



Protein Structure File (PSF)

- The PSF file contains all of the basic molecular details needed to apply a specific force field to a molecular system. And stores structural information of the protein, such as various types of bonding interactions.
- In addition, a PSF often contains hydrogens and other atoms that may be missing from a crystal pdb file to automatically assign coordinates



PSF file has the information of connectivity

Protein Structure File (PSF)

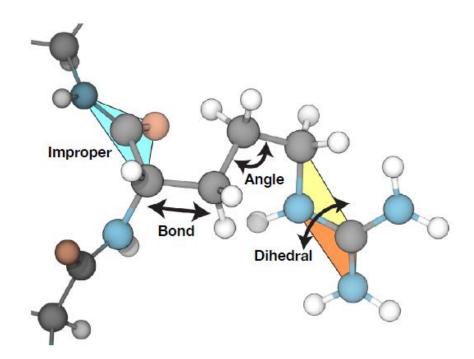
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17 API 1 MET HE3 HA3 0.090000 1.0080 0 2257 !NTHETA: angles 18 API 1 MET C C 0.510000 12.0110 0 1 5 6 1 5 18 2 1 5 20 API 2 GLN N NH1 -0.470000 14.0070 0 3 1 4 4 4 1 5 5 5 18 19 21 API 2 GLN HN H 0.310000 1.0080 0 5 7 9 5 7 8 22 API 2 GLN CA CTI 0.070000 12.0110 0 5 7 10 12 7 10 11 23 API 2 GLN HA HB1 0.090000 1.0080 0 7 10 13 7 5 6 7 5 18 24 API 2 GLN CB CT2 -0.180000 12.0110 0 7 5 1 8 7 9 10 13 14 24 API 2 GLN HB1 HA2 0.090000 1.0080 0 7 5 1 8 7 9 10 13 14 24 API 2 GLN HB1 HA2 0.090000 1.0080 0 1.0080 0 13 14 17 13 14 16 13 14 15 26 API 2 GLN HB2 HA2 0.090000 1.0080 0 13 10 12 13 10 11 15 14 17 27 API 2 GLN CG CT2 -0.180000 12.0110 0 13 10 12 13 10 11 15 14 17 27 API 2 GLN HG2 HA2 0.090000 1.0080 0 13 10 12 13 10 11 15 14 17 27 API 2 GLN CG CT2 -0.180000 12.0110 0 15 14 16 16 14 17 18 5 6 28 API 2 GLN HG1 HA2 0.090000 1.0080 0 20 22 23 20 22 35 20 18 19 29 API 2 GLN CG CT2 -0.180000 12.0110 0 15 14 16 16 14 17 18 5 6 28 API 2 GLN HG2 HA2 0.090000 1.0080 0 20 22 23 20 22 35 20 18 19 29 API 2 GLN CC CT2 -0.180000 12.0110 0 22 23 20 22 35 36 30 API 2 GLN CC CT2 -0.180000 1.0080 0 21 20 18 21 20 18 21 20 22 22 35 36 30 API 2 GLN CC CT2 -0.180000 1.0080 0 22 23 20 22 35 20 22 35 36 30 API 2 GLN CC CT2 -0.180000 1.0080 0 21 20 18 21 20 18 21 20 22 22 35 36 30 API 2 GLN CC CT2 -0.180000 1.0080 0 22 24 27 28 24 26 22 24 26 22 24 26 22 24 26 22 24 26 22 24 26 22 24 26 22 24 26 22 24 26 22 24 27 28 24 26 22 24 26 22 24 26 22 24 26 22 24 26 22 24 27 28 24 27 28 24 27 29 30 32 27 24 26 34 API 2 GLN HE21 H 0.300000 1.0080 0 27 30 31 27 30 31 27 30 32 27 24 26 34 API 2 GLN HE21 H 0.300000 1.0080 0 27 30 31 27 24 26 34 API 2 GLN HE21 H 0.300000 1.0080 0 27 30 31 27 24 26 34 API 2 GLN HE22 H 0.300000 1.0080 0 27 24 25 28 27 29 30 32 27 24 26 34 API 2 GLN HE22 H 0.300000 1.0080 0 27 24 25 28 27 29 30 32 27 24 26 34 API 2 GLN HE22 H 0.300000 1.0080 0 27 24 25 28 27 29 30 32 27 24 26 34 API 2 GLN HE22 H 0.300000 1.0080 0 27 24 25 28 27 29 30 32 27 24 26 34 API 2 GLN HE21 H 0.300000 1.0080 0 27 24 25 28 27 29	15 AP1	1	MET	HE1	HA3	0.090000	1.0080	0										
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19 AP1 1 MET O O -0.510000 15.9990 0 2 1 4 2 1 3 3 3 1 5 5 20 AP1 2 GLN N NH1 -0.470000 14.0070 0 3 1 4 4 4 1 5 5 5 18 19 21 AP1 2 GLN HN H O.310000 1.0080 0 5 18 20 5 7 9 5 7 8 8 12 AP1 2 GLN CA CT1 0.070000 12.0110 0 7 10 11 7 10 11 7 10 11 13 7 5 6 7 10 11 13 7 5 6 7 18 11 10 12 13 AP1 2 GLN CB CT2 -0.180000 12.0110 0 10 7 10 13 7 5 6 7 9 10 13 14 14 15 15 AP1 2 GLN CB CT2 -0.180000 12.0110 0 10 7 9 10 7 8 11 10 12 25 AP1 2 GLN HB1 HA2 0.090000 1.0080 0 13 14 17 13 14 16 13 14 15 12 13 10 11 15 14 17 17 17 18 5 6 AP1 2 GLN CB CT2 -0.180000 12.0110 0 13 14 17 13 14 16 13 14 15 14 17 17 17 18 15 6 AP1 2 GLN CB CT2 -0.180000 12.0110 0 13 10 12 13 10 11 15 14 17 17 18 15 6 AP1 2 GLN HB1 HA2 0.090000 1.0080 0 13 10 12 13 10 11 15 14 17 17 18 15 6 AP1 2 GLN HB2 HA2 0.090000 1.0080 0 13 10 12 13 10 11 15 14 17 17 18 15 6 AP1 2 GLN HB1 HA2 0.090000 1.0080 0 12.0110 0 15 14 16 16 14 17 18 5 6 AP1 2 GLN HB1 HA2 0.090000 1.0080 0 20 22 23 20 22 35 20 18 19 19 19 19 19 19 19 19 19 19 19 19 19	17 AP1	1	MET	HE3	HA3	0.090000	1.0080	0	225	7 !!	NTHETA: a	ngles						
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21 AP1 2 GLN HN H 0.310000 1.0080 0 5 18 20 5 7 9 5 7 8 22 AP1 2 GLN CA CT1 0.070000 12.0110 0 5 7 10 12 7 10 11 23 AP1 2 GLN HA HB1 0.090000 1.0080 0 7 10 13 7 5 6 7 5 18 23 AP1 2 GLN CB CT2 -0.180000 12.0110 0 10 7 9 10 7 8 11 10 12 25 AP1 2 GLN HB1 HA2 0.090000 1.0080 0 13 14 17 13 14 16 13 14 15 26 AP1 2 GLN HB2 HA2 0.090000 1.0080 0 13 14 17 13 14 16 13 14 15 26 AP1 2 GLN CB CT2 -0.180000 12.0110 0 13 14 17 13 14 16 13 14 15 27 AP1 2 GLN CG CT2 -0.180000 12.0110 0 13 14 17 18 5 6 28 AP1 2 GLN HG1 HA2 0.090000 1.0080 0 13 10 12 13 10 11 15 14 17 27 AP1 2 GLN CG CT2 -0.180000 12.0110 0 15 14 16 16 14 17 18 5 6 28 AP1 2 GLN HG1 HA2 0.090000 1.0080 0 20 22 23 20 22 35 20 18 19 29 AP1 2 GLN HG2 HA2 0.090000 1.0080 0 21 20 18 21 20 22 22 35 36 30 AP1 2 GLN CD CC 0.550000 12.0110 0 22 24 27 28 24 26 22 24 25 31 AP1 2 GLN NE2 NH2 -0.620000 14.0070 0 24 27 28 24 27 20 18 24 27 29 31 AP1 2 GLN NE2 NH2 -0.620000 14.0070 0 24 22 35 24 26 22 24 26 33 AP1 2 GLN HE21 H 0.320000 1.0080 0 27 30 31 27 30 32 27 24 26 34 AP1 2 GLN HE22 H 0.300000 1.0080 0 27 30 31 27 30 32 27 24 26 34 AP1 2 GLN HE21 H 0.320000 1.0080 0 27 30 31 27 30 32 27 24 26 34 AP1 2 GLN HE22 H 0.300000 1.0080 0 27 30 31 27 30 32 27 24 26 34 AP1 2 GLN HE22 H 0.300000 1.0080 0 27 30 31 27 30 32 27 24 26	19 AP1	1	MET	0	0	-0.510000	15.9990	0		2	1	4	2	1	3			
21 API 2 GLN HN H 0.310000 1.0080 0 5 7 10 12 7 10 11 2 2 API 2 GLN CA CT1 0.070000 12.0110 0 7 10 13 7 5 6 7 5 18 23 API 2 GLN HA HBI 0.090000 1.0080 0 7 5 1 8 7 9 10 13 14 10 12 25 API 2 GLN HBI HA2 0.090000 1.0080 0 13 14 17 13 14 16 13 14 15 14 17 13 14 16 13 14 15 14 17 17 18 10 11 15 14 17 17 18 10 11 15 14 17 17 18 10 11 15 14 17 17 18 10 11 15 14 17 17 18 10 11 15 14 17 17 18 10 11 15 14 17 17 18 10 11 15 14 17 18 10 11 11 15 14 11 17 18 10 11 11 15 14 17 18 10 11 11 15 14 17 18 10 11 11 15 14 11	20 AP1	2	GLN	N	NHl	-0.470000	14.0070	0					_					
22 API 2 GLN CA CTI 0.070000 12.0110 0 7 10 13 7 5 6 7 5 18 23 API 2 GLN HA HB1 0.090000 12.0110 0 10 7 9 10 7 8 11 10 12 25 API 2 GLN HB1 HA2 0.090000 1.0080 0 13 14 17 13 14 16 13 14 15 12 26 API 2 GLN HB2 HA2 0.090000 1.0080 0 13 14 17 13 14 16 13 14 17 17 18 15 14 17 17 18 15 14 17 17 18 15 14 17 17 18 15 14 17 18 15 14 17 17 18 15 14 16 18 API 2 GLN HB1 HA2 0.090000 1.0080 0 13 14 16 16 16 14 17 18 15 16 17 17 18 17 18 18 19 18 API 2 GLN HB1 HA2 0.090000 1.0080 0 12.0110 0 15 14 16 16 16 14 17 18 15 16 17 18 19 19 19 19 19 19 19 19 19 19 19 19 19	21 AP1	2	GLN	HN	H	0.310000	1.0080	0					_	-		_		
23 AP1 2 GLN HA HB1 0.090000 1.0080 0 7 5 1 8 7 9 10 13 14 24 AP1 2 GLN CB CT2 -0.180000 12.0110 0 10 7 9 10 7 8 11 10 12 2 AP1 2 GLN HB1 HA2 0.090000 1.0080 0 13 14 17 13 14 16 13 14 15 14 15 15 14 17 13 10 11 15 14 17 17 18 15 14 16 16 16 14 17 18 18 5 6 18 AP1 2 GLN HG1 HA2 0.090000 1.0080 0 12.0110 0 15 14 16 16 16 14 17 18 5 6 18 AP1 2 GLN HG1 HA2 0.090000 1.0080 0 20 22 23 20 22 35 20 18 19 19 19 19 19 19 19 19 19 19 19 19 19	22 AP1	2	GLN	CA	CT1	0.070000	12.0110	0										
24 API 2 GLN CB CT2 -0.180000 12.0110 0 10 7 9 10 7 8 11 10 12 25 API 2 GLN HB1 HA2 0.090000 1.0080 0 13 14 17 13 14 16 13 14 15 26 API 2 GLN HB2 HA2 0.090000 1.0080 0 13 10 12 13 10 11 15 14 17 27 API 2 GLN CG CT2 -0.180000 1.0080 0 12.0110 0 15 14 16 16 14 17 18 5 6 8 API 2 GLN HG1 HA2 0.090000 1.0080 0 20 22 23 20 22 35 20 18 19 29 API 2 GLN HG2 HA2 0.090000 1.0080 0 21 20 18 21 20 22 22 35 36 37 22 24 26 22 24 25 30 API 2 GLN CD CC 0.550000 12.0110 0 22 24 27 28 24 26 22 24 25 31 API 2 GLN NE2 NH2 -0.620000 14.0070 0 24 27 28 24 27 29 20 18 24 27 29 31 API 2 GLN NE2 NH2 -0.620000 14.0070 0 24 22 35 24 26 22 24 26 33 API 2 GLN HE21 H 0.320000 1.0080 0 27 30 31 27 30 32 27 24 26 34 API 2 GLN HE22 H 0.300000 1.0080 0 27 24 25 28 27 29 30 32 34 API 2 GLN HE22 H 0.300000 1.0080 0 27 24 25 28 27 29 30 32 34 34 API 2 GLN HE22 H 0.300000 1.0080 0	23 AP1	2	GLN	HA	HB1	0.090000	1.0080	0										
25 API 2 GLN HB1 HA2 0.090000 1.0080 0 13 14 17 13 14 16 13 14 15 26 API 2 GLN HB2 HA2 0.090000 1.0080 0 13 10 12 13 10 11 15 14 17 27 API 2 GLN CG CT2 -0.180000 12.0110 0 15 14 16 16 14 17 18 5 6 28 API 2 GLN HG1 HA2 0.090000 1.0080 0 20 22 23 20 22 35 20 18 19 29 API 2 GLN HG2 HA2 0.090000 1.0080 0 21 20 18 21 20 18 21 20 22 23 35 36 API 2 GLN CD CC 0.550000 12.0110 0 22 24 27 22 20 18 24 27 29 31 API 2 GLN OEI 0 -0.550000 15.9990 0 24 27 28 24 27 30 24 22 23 34 API 2 GLN HE21 H 0.320000 1.0080 0 27 30 31 27 30 32 27 24 26 34 API 2 GLN HE22 H 0.300000 1.0080 0 27 24 25 28 27 29 30 32 34 API 2 GLN HE22 H 0.300000 1.0080 0 27 24 25 28 27 29 30 32 34 34 API 2 GLN HE22 H 0.300000 1.0080 0 27 24 25 28 27 29 30 32 34 34 API 2 GLN HE22 H 0.300000 1.0080 0 27 24 25 28 27 29 30 32 37 38	24 AP1	2	GLN	CB	CT2	-0.180000	12.0110	0					_		_			
26 API 2 GLN HB2 HA2 0.090000 1.0080 0 13 10 12 13 10 11 15 14 17 27 API 2 GLN CG CT2 -0.180000 12.0110 0 15 14 16 16 14 17 18 5 6 28 API 2 GLN HG1 HA2 0.090000 1.0080 0 20 22 23 20 22 35 20 18 19 29 API 2 GLN HG2 HA2 0.090000 1.0080 0 21 20 18 21 20 22 22 35 36 30 API 2 GLN CD CC 0.550000 12.0110 0 22 35 37 22 24 26 22 24 25 31 API 2 GLN OE1 0 -0.550000 15.9990 0 24 27 28 24 27 30 24 22 23 32 API 2 GLN NE2 NH2 -0.620000 14.0070 0 24 27 28 24 22 20 25 24 26 33 API 2 GLN HE21 H 0.320000 1.0080 0 27 30 31 27 30 32 27 24 26 34 API 2 GLN HE22 H 0.300000 1.0080 0 27 24 25 28 27 29 30 32 34 34 API 2 GLN HE22 H 0.300000 1.0080 0	25 AP1	2	GLN	HB1	HA2	0.090000	1.0080	0			14	17	13	14	16			
27 AP1 2 GLN CG CT2 -0.180000 12.0110 0 15 14 16 16 14 17 18 5 6 28 AP1 2 GLN HG1 HA2 0.090000 1.0080 0 20 22 23 20 22 35 20 22 35 20 18 19 29 AP1 2 GLN HG2 HA2 0.090000 1.0080 0 21 20 18 21 20 22 22 22 35 36 30 AP1 2 GLN CD CC 0.550000 12.0110 0 22 35 37 22 24 26 22 24 25 31 AP1 2 GLN OE1 0 -0.550000 15.9990 0 24 27 28 24 27 30 24 22 23 32 AP1 2 GLN NE2 NH2 -0.620000 14.0070 0 24 22 35 24 22 20 25 24 26 33 AP1 2 GLN HE21 H 0.320000 1.0080 0 27 30 31 27 30 32 27 24 26 34 AP1 2 GLN HE22 H 0.300000 1.0080 0 27 24 25 25 28 27 29 30 32 34	26 AP1	2	GLN	HB2	HA2	0.090000		0	1	.3	10	12	13	10	11	15	14	
28 API 2 GLN HG1 HA2 0.090000 1.0080 0 20 22 23 20 22 35 20 18 19 29 API 2 GLN HG2 HA2 0.090000 1.0080 0 21 20 18 21 20 22 22 35 36 30 API 2 GLN CD CC 0.550000 12.0110 0 22 24 27 22 20 18 24 27 29 31 API 2 GLN OE1 0 -0.550000 15.9990 0 24 27 28 24 27 30 24 22 23 32 API 2 GLN NE2 NH2 -0.620000 14.0070 0 24 22 35 24 22 20 25 24 26 33 API 2 GLN HE21 H 0.320000 1.0080 0 27 30 31 27 30 32 27 24 26 34 API 2 GLN HE22 H 0.300000 1.0080 0 27 24 25 28 27 29 30 32 37 30 32 37	27 AP1	2	GLN	CG	CT2	-0.180000		0	1	.5	14	16	16	14	17	18	5	
29 AP1 2 GLN HG2 HA2 0.090000 1.0080 0 21 20 18 21 20 22 22 35 36 36 30 AP1 2 GLN CD CC 0.550000 12.0110 0 22 24 27 22 20 18 24 27 29 31 AP1 2 GLN OE1 O -0.550000 15.9990 0 24 27 28 24 27 30 24 22 23 32 AP1 2 GLN NE2 NH2 -0.620000 14.0070 0 24 22 35 24 26 22 24 26 33 AP1 2 GLN HE21 H 0.320000 1.0080 0 27 30 31 27 30 32 27 24 26 34 AP1 2 GLN HE22 H 0.300000 1.0080 0 27 24 25 28 27 29 30 32 37 38 AP1 2 GLN HE22 H 0.300000 1.0080 0 27 24 25 28 27 29 30 32 34 AP1 2 GLN HE22 H 0.300000 1.0080 0 27 24 25 28 27 29 30 32 34 AP1 2 GLN HE22 H 0.300000 1.0080 0	28 AP1	2	GLN	HG1	HA2	0.090000	1.0080	0										
30 API 2 GLN CD CC 0.550000 12.0110 0 22 24 27 22 20 18 24 27 29 31 API 2 GLN OE1 0 -0.550000 15.9990 0 24 27 28 24 27 30 24 22 23 32 API 2 GLN NE2 NH2 -0.620000 14.0070 0 24 22 35 24 22 20 25 24 26 33 API 2 GLN HE21 H 0.320000 1.0080 0 27 30 31 27 30 32 27 24 26 34 API 2 GLN HE22 H 0.300000 1.0080 0 27 24 25 28 27 29 30 32 34 39 API 2 GLN HE22 H 0.300000 1.0080 0 27 24 25 28 27 29 30 32 34	29 AP1	2	GLN					0										
31 AP1 2 GLN OE1 O -0.550000 15.9990 0 24 27 28 24 27 30 24 22 23 32 AP1 2 GLN NE2 NH2 -0.620000 14.0070 0 24 22 35 24 22 20 25 24 26 33 AP1 2 GLN HE21 H 0.320000 1.0080 0 27 30 31 27 30 32 27 24 26 34 AP1 2 GLN HE22 H 0.300000 1.0080 0 27 24 25 28 27 29 30 32 34 AP1 2 GLN HE22 H 0.300000 1.0080 0 27 24 25 28 27 29 30 32 34																		
32 AP1 2 GLN NE2 NH2 -0.620000 14.0070 0 24 22 35 24 22 20 25 24 26 33 AP1 2 GLN HE21 H 0.320000 1.0080 0 27 30 31 27 30 32 27 24 26 34 AP1 2 GLN HE22 H 0.300000 1.0080 0 27 24 25 28 27 29 30 32 34																		
33 AP1 2 GLN HE21 H 0.320000 1.0080 0 27 30 31 27 30 32 27 24 26 34 AP1 2 GLN HE22 H 0.300000 1.0080 0 27 24 25 28 27 29 30 32 34					_			_										
34 AP1 2 GLN HE22 H 0.300000 1.0080 0 27 24 25 28 27 29 30 32 34								_										
20 22 22 20 27 20 20 27 20											24			27				
	35 AP1	2	GLN	C	C	0.510000	12.0110	0	3	30	32	33	30	27	29	30	27	28

Topology Files (TOP)

We read the connectivity from here to convert .pdb to .psf file

- A CHARMM forcefield topology file contains all of the information needed to convert a list of residue names into a complete PSF structure file.
- In addition, a PSF often contains internal coordinates that allow hydrogen and other atoms that may be missing from a crystal pdb file to automatically assign coordinates

```
MASS
        31 H
                  1.00800 ! polar H
        32 HC
                  1.00800 ! N-ter H
        34 HP
                  1.00800 ! aromatic H
MASS
        35 HB1
                 1.00800 ! backbone H
        36 HB2
                 1.00800 ! aliphatic backbone H, to CT2
        37 HR1
                 1.00800 ! his hel, (+) his HG, HD2
MASS
        38 HR2
                 1.00800 ! (+) his HE1
MASS
        39 HR3
                 1.00800 ! neutral his HG, HD2
MASS
        40 HS
                  1.00800 ! thiol hydrogen
        41 HE1
                 1.00800 ! for alkene; RHC=CR
        42 HE2
                 1.00800 ! for alkene; H2C=CR
        43 HA1
                 1.00800 ! alkane, CH, new LJ params (see toppar all22 prot aliphatic c27.str)
                 1.00800 ! alkane, CH2, new LJ params (see toppar all22 prot aliphatic c27.str)
        45 HA3
                 1.00800 ! alkane, CH3, new LJ params (see toppar all22 prot aliphatic c27.str)
MASS
        46 C
                 12.01100 ! carbonyl C, peptide backbone
                12.01100 ! aliphatic sp3 C, new LJ params, no hydrogens
               12.01100 ! aliphatic sp3 C for
                12.01100 ! aliphatic sp3 C for CH2
        51 CT2A 12.01100 ! from CT2 (asp, glu, hsp chil/chi2 fitting)
        53 CPH1 12.01100 ! his CG and CD2 carbons
        54 CPH2 12.01100 ! his CE1 carbon
```



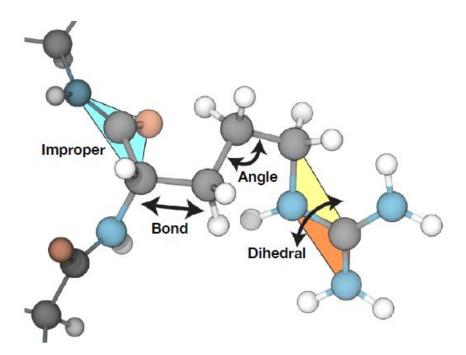
Topology Files (TOP)

```
MASS
       31 H
                1.00800 ! polar H
MASS
       32 HC
                1.00800 ! N-ter H
       33 HA
                1.00800 ! nonpolar H
MASS
       34 HP
                1.00800 ! aromatic H
MASS
                1.00800 ! backbone H
       35 HB1
       36 HB2
                1.00800 ! aliphatic backbone H, to CT2
                1.00800 ! his hel, (+) his HG, HD2
MASS
       37 HR1
       38 HR2
                1.00800 ! (+) his HE1
       39 HR3
                1.00800 ! neutral his HG, HD2
MASS
       40 HS
                1.00800 ! thiol hydrogen
MASS
                1.00800 ! for alkene; RHC=CR
       41 HE1
MASS
       42 HE2
                1.00800 ! for alkene; H2C=CR
                1.00800 ! alkane, CH, new LJ params (see toppar all22 prot aliphatic c27.str)
MASS
               1.00800 ! alkane, CH2, new LJ params (see toppar all22 prot aliphatic c27.str)
               1.00800 ! alkane, CH3, new LJ params (see toppar all22 prot aliphatic c27.str)
MASS
                12.01100 ! carbonvl C, peptide backbone
MASS
       47 CA 12.01100 ! aromatic C
                12.01100 ! aliphatic sp3 C, new LJ params, no hydrogens
       49 CT1 12.01100 ! aliphatic sp3 C for CH
       50 CT2 12.01100 ! aliphatic sp3 C for CH2
       51 CT2A 12.01100 ! from CT2 (asp, glu, hsp chil/chi2 fitting)
       52 CT3 12.01100 ! aliphatic sp3 C for CH3
       53 CPH1 12.01100 ! his CG and CD2 carbons
       54 CPH2 12.01100 ! his CE1 carbon
```

```
RESI ASN
                 0.00
GROUP
ATOM N
                -0.47 !
         NH1
ATOM HN
                 0.31 ! HN-N
ATOM CA CT1
                 0.07 !
                                HB1 OD1
                                           HD21 (cis to OD1)
ATOM HA
                 0.09 !
                                    11
GROUP
                         HA-CA--CB--CG--ND2
ATOM CB
                -0.18 !
ATOM HB1 HA2
                 0.09 !
                                HB2
                                           HD22 (trans to OD1)
ATOM HB2 HA2
                 0.09 !
                          O=C
GROUP
ATOM CG CC
                 0.55
ATOM OD1 O
                -0.55
GROUP
ATOM ND2 NH2
                -0.62
ATOM HD21 H
                 0.32
ATOM HD22 H
                 0.30
GROUP
ATOM C
                 0.51
ATOM O
                -0.51
BOND CB CA CG CB
                  ND2 CG
BOND N HN N CA
                  С
                      CA
                            C +N
BOND CA HA CB HB1 CB HB2 ND2 HD21 ND2 HD22
DOUBLE C O
             CG OD1
IMPR N
        -C CA
                 HN
                       C
                          CA +N
IMPR CG ND2 CB
                 OD1
                       CG CB ND2 OD1
IMPR ND2 CG HD21 HD22 ND2 CG HD22 HD21
CMAP - C N CA C N CA C + N
DONOR HN N
DONOR HD21 ND2
DONOR HD22 ND2
ACCEPTOR OD1 CG
```

Parameter Files – Force Fields (PRM)

- Force field parameter file is a mathematical expression of the potential which atoms in the system experience
- The parameter file defines bond strengths, equilibrium lengths and contains all of the numerical constants required to determine forces and energies, given that a PSF structure file and atomic coordinates have been provided .pdb file

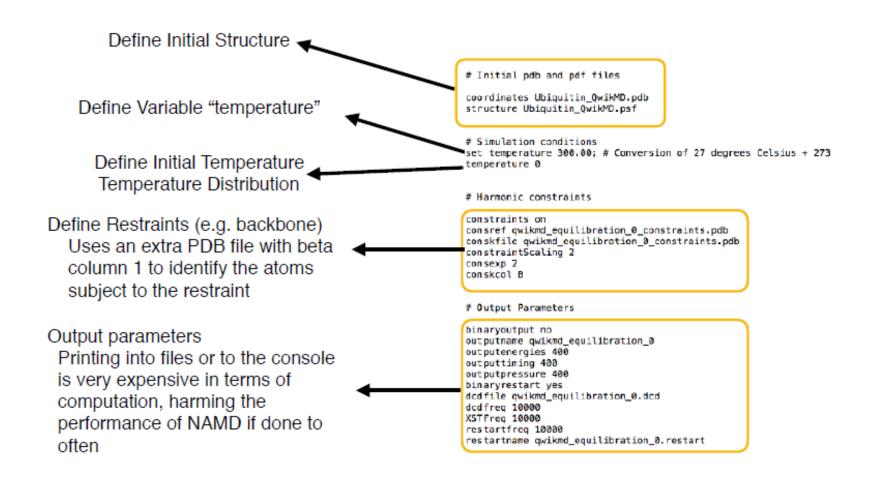


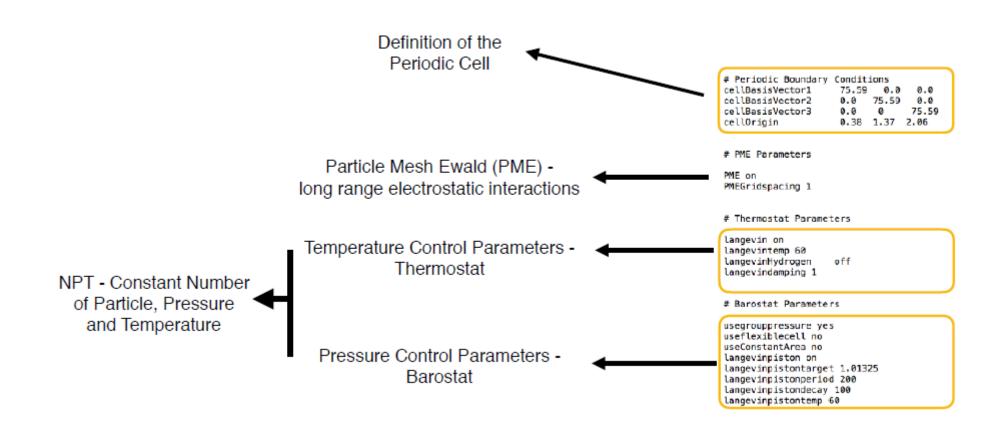
Parameter Files – Force Fields (PRM)

```
BONDS
!V(bond) = Kb(b - b0)**2
!Kb: kcal/mole/A**2
!b0: A
!atom type Kb
                      1.4550 ! From LSN NH2-CT2
NH2 CT1 240.000
!Indole/Tryptophan
          305.000
                      1.3750 ! from CA CA
CAI CAI 305.000
                      1.3750 ! atm, methylindole, fit CCDSS
          300.000
                      1.3600 ! atm, methylindole, fit CCDSS
          300.000
                      1.3600 ! atm, methylindole, fit CCDSS
          360.000
                      1.3850 ! atm, methylindole, fit CCDSS
CPT CPT
          350.000
                      1.3650 ! trj, adm jr., 5/08/91, indole CCDB structure search
          350.000
                      1.3650 ! from CY CA
          350.000
    CPT
                      1.4300 ! atm, methylindole, fit CDS data
   CT3
          375.000
                      1.4920 ! atm, methylindole, fit CDS data
          375.000
                      1.4920 ! atm, methylindole, fit CDS data
          340.000
                      1.0800 ! from HP CA
    CAI
    CY
          350.000
                      1.0800 ! trp, adm jr., 12/30/91
```

```
ANGLES
!V(angle) = Ktheta(Theta - Theta0) **2
!V(Urey-Bradley) = Kub(S - S0)**2
!Ktheta: kcal/mole/rad**2
!Theta0: degrees
!Kub: kcal/mole/A**2 (Urey-Bradley)
!S0: A
                         Theta0 Kub
                                         SO
!atom types
               Ktheta
    NH2 CT1
               50.000
                         111.00
                                            ! From LSN HC-NH2-CT2
                         110.00
NH2 CT1 CT1
               67.700
                                            ! From LSN NH2-CT2-CT2
NH2 CT1 CT2
               67.700
                         110.00
                                            ! From LSN NH2-CT2-CT2
NH2 CT1 CT3
               67.700
                         110.00
                                            ! From LSN NH2-CT2-CT2
CT1 CD OH1
               55.000
                         110.50
                                            ! From ASPP CT2-CD-OH1
CT3 CT1 CD
               52.000
                         108.00
                                            ! Ala cter
               38.000
                                         2.1400 ! From LSN NH2-CT2-HA
NH2 CT1 HB1
                         109.50
NH2 CT1 C
               50.000
                         107.00
                                            ! From ALA Dipep. NH1-CT2-C
!Indole/Tryptophan
                                         2.41620 ! from CA CA CA
CAI CAI CA
               40.000
                         120.00
                                  35.00
                                        2.41620 ! from CA CA CA
CAI CA CA
               40.000
                         120.00
                                  35.00
CPT CA CA
               50.000
                         113.20 ! atm, methylindole, 1/17/04
CPT CPT CA
               50.000
                         110.00 ! atm, methylindole, 1/17/04
CPT CAI CA
               50.000
                         113.20 ! atm, methylindole, 1/17/04
CPT CPT CAI
               50.000
                         110.00 ! atm, methylindole, 1/17/04
```

- The user defines all the options that NAMD should consider while running the simulation
- The configuration file tells NAMD how the simulation should be run
- NAMD Configuration File is a TCL Script File
- NAMD Configuration File Manual: https://www.ks.uiuc.edu/Training/Tutorials/namd/namd-tutorial-unix-html/node26.html





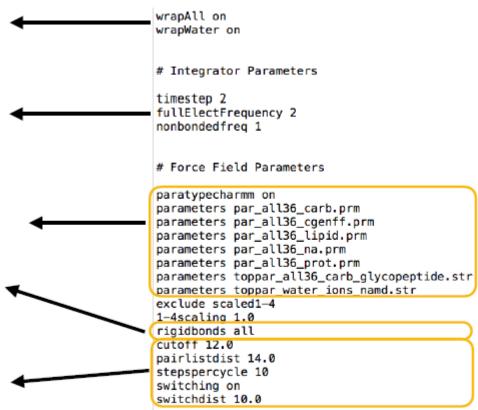
Keep Molecules Inside the Periodic Cell. No Physical Value Changes, Only Its Representation

Multi Time Stepping Integration time 2fs Short Non-Bonded Interaction (2fs) Full Electrostatics (PME - 4 fs)

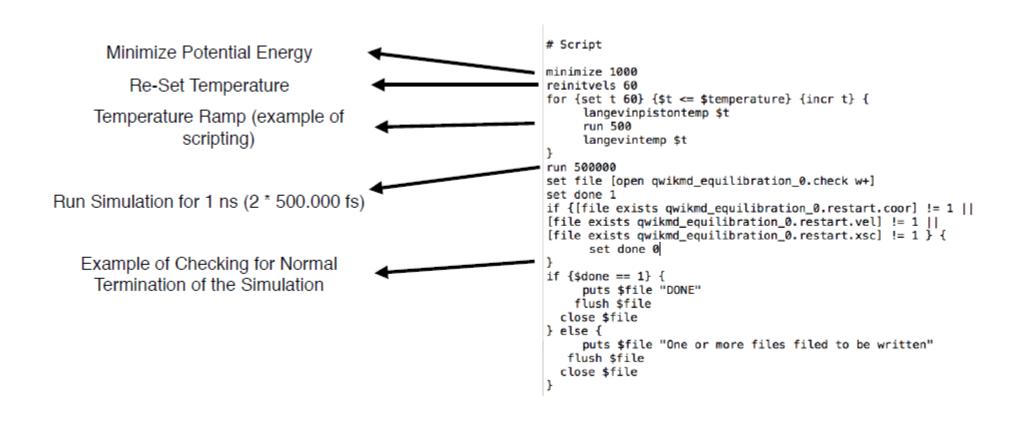
Input Parameters Files

What Allows the 2fs Integration Step
Water Oxygen-Hydrogen bonds (opt = water)
Heavy Atom-Hydrogen bonds (opt = all)

Non-Bonded Parameters
Cutoff - VDW interaction
Switching - Smoothly Tend to 0
Pairlistdist - Dist. To Pair of Atoms in VDW
Interactions
Stepspercyle - Cycles between evaluating PairList



PBC: https://www.ks.uiuc.edu/Research/namd/2.13/ug/node33.html
Temperature Control: https://www.ks.uiuc.edu/Research/namd/2.13/ug/node36.html
Pressure Control: https://www.ks.uiuc.edu/Research/namd/2.13/ug/node37.html
Non-Bonded Int.: https://www.ks.uiuc.edu/Research/namd/2.13/ug/node23.html
Pair List: https://www.ks.uiuc.edu/Research/namd/2.13/ug/node92.html



Modifications for NAMD Configuration File (CONF)

.log => Energies, timing .dcd => trajectory file

- Add: *stepspercycle 10 or stepspercycle 20* to Minimization.conf, Annealing.conf, Equalibration.conf, and MD.conf
- Modify Output parameters to an appropriate frequencies:
- Recommended is 1000 all for Minimization
- And 1000 for energy related, and 50000 for coordinates related output

For other procedures: Annealing, Equilibration, MD

```
# Output Parameters

binaryoutput no
outputname Minimization
outputenergies 1000
outputtiming 1000
outputpressure 1000
binaryrestart yes
XSTFreq 1000
restartfreq 1000
restartname Minimization.restart
```

```
# Output Parameters

binaryoutput no
outputname MD
outputenergies 1000
outputtiming 1000
outputpressure 1000
binaryrestart yes
dcdfile MD.dcd
dcdfreq 50000
XSTFreq 50000
restartfreq 50000
restartname MD.restart
```

```
#Implicit Solvent Parameters
gbis off
alphaCutoff
                    14.0
ionConcentration
                    0.15
stepspercycle 10
# Script
minimize 2000
set file [open Minimization.check w+]
set done 1
if {[file exists Minimization.restart.coor] !=
     set done 0
if {$done == 1} {
    puts $file "DONE"
    flush Sfile
  close $file
} else {
    puts $file "One or more files failed to be
  flush Sfile
  close $file
```

Restart/Resume or Continue a NAMD Simulation

- If you want Restart/Resume a NAMD simulation that stopped due to any reason, you do the following:
- Go to the .conf file of the last step
- Make a Copy of that with a new name (e.g.: MD2.conf)
- In the bin---- part, You need to use the .restart files from the last step in this step

Xxxx.restart.coor

Xxxx.restart.vel

Xxxx.restart.xsc

• To know the remaining time, go for the .log file of the last step, in the last line that contains the word "TIMING". Remaining time = Original time – TIMING_{last}

Restart/Resume or Continue a NAMD Simulation

- If you want increase the time for a NAMD simulation that has already finished, you do the following:
- Go to the .conf file of the last step
- Copy that
- You need to use the files from the last step in your new .conf file, without .restart

Xxxx.coor

Xxxx.vel

Xxxx.xsc

• You also decide the run time