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Support Information Material

Updating atomic charges parameters of aliphatic amino acids: A quest to improve the performance of molecular modeling via sequential molecular dynamics and DFT-GIAO-NMR calculations

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ABSTRACT

In this work we observe the behavior of the dipole moment, atomic charges, solute-solvent interactions and NMR spectroscopy of aliphatic amino acids in water solution through computational simulations of classical molecular dynamics and DFT quantum calculations. Our results show that the convergence of the atomic charge of the solute, from an iterative process, together with the dipole moment of the amino acid, alters the lifetime of the hydrogen bonds present in the first solvation shell, modifying its structure and dynamics. Using GIAO-DFT-NMR calculations, we assessed the impact of these structural solute-solvent modifications on the magnetic shielding constants of the solute's carbon atoms. In this sense, we evaluate the importance of an update in the parameters that describe the atomic charges present in the CHARMM36 force field.

Table S1

Original CHARMM36 atomic charges (S1) and updated atomic charges (S4) for alanine (Ala) in water solution.

Alanine Atoms	*Atomic charges (q)*		
	Original CHARMM36.ff	*Updated CHARMM36.ff*	$\|\Delta q\|$ *(%)*
N1	-0.30	-0.584338	95%
H1	0.33	0.412795	25%
H2	0.33	0.413343	25%
H3	0.33	0.410494	24%
C1	0.21	0.137255	35%
H4	0.10	0.073979	26%
C2	-0.27	-0.271780	1%
H5	0.09	0.096421	7%
H6	0.09	0.095631	6%
H7	0.09	0.098902	10%
C3	0.34	0.976132	187%
O1	-0.67	-0.920562	37%
O2	-0.67	-0.938274	40%

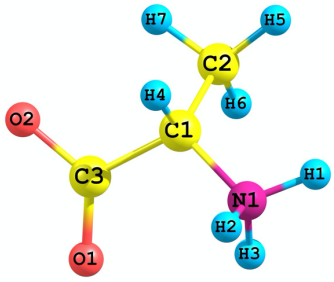


Table S2

Original CHARMM36 atomic charges (S1) and updated atomic charges (S4) for glycine (Gly) in water solution.

Glycine Atoms	*Atomic charges (q)*		
	Original CHARMM36.ff	*Updated CHARMM36.ff*	$\|\Delta q\|$ *(%)*
N1	-0.30	-0.302125	1%
H1	0.33	0.353656	7%
H2	0.33	0.354866	8%
H3	0.33	0.353980	7%
C1	0.13	-0.168448	230%
H4	0.09	0.122561	36%
H5	0.09	0.119051	32%
C3	0.34	1.091121	221%
O1	-0.67	-0.940203	40%
O2	-0.67	-0.984460	47%

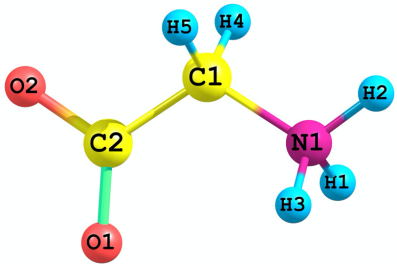


Table S3

Original CHARMM36 atomic charges (S1) and updated atomic charges (S4) for isoleucine (Ile) in water solution.

Isoleucine Atoms	*Atomic charges (q)*		
	Original CHARMM36.ff	*Updated CHARMM36.ff*	$\|\Delta q\|$ *(%)*
N1	-0.30	-0.603732	101%
H1	0.33	0.413942	25%
H2	0.33	0.418826	27%
H3	0.33	0.415861	26%
C1	0.21	-0.014785	107%
H4	0.10	0.080907	19%
C2	-0.09	0.310981	446%
H5	0.09	-0.004705	105%
C3	-0.27	-0.419443	55%
H6	0.09	0.105674	17%
H7	0.09	0.103343	15%
H8	0.09	0.103197	15%
C4	-0.18	-0.015311	91%
H9	0.09	0.009439	90%
H10	0.09	0.037036	59%
C5	-0.27	-0.213746	21%
H11	0.09	0.054092	40%
H12	0.09	0.054335	40%
H13	0.09	0.051478	43%
C6	0.34	1.017883	199%
O1	-0.67	-0.951464	42%
O2	-0.67	-0.953807	42%

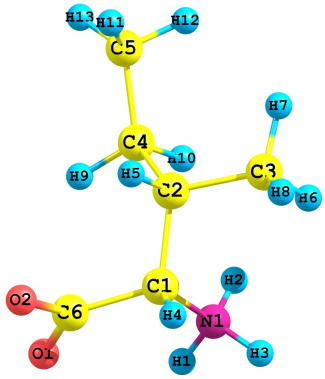


Table S4

Original CHARMM36 atomic charges (S1) and updated atomic charges (S4) for leucine (Leu) in water solution.

Leucine Atoms	*Atomic charges (q)*		
	Original CHARMM36.ff	*Updated CHARMM36.ff*	*$\|\Delta q\|$ (%)*
N1	-0.30	-0.593067	98%
H1	0.33	0.407199	23%
H2	0.33	0.414261	26%
H3	0.33	0.412714	25%
C1	0.21	0.108926	48%
H4	0.10	0.069366	31%
C2	-0.18	-0.253899	41%
H5	0.09	0.072629	19%
H6	0.09	0.079818	11%
C3	-0.09	0.504626	661%
H7	0.09	-0.059512	166%
C4	-0.27	-0.394217	46%
H8	0.09	0.085138	5%
H9	0.09	0.087400	3%
H10	0.09	0.082613	8%
C5	-0.27	-0.414079	53%
H11	0.09	0.089594	0%
H12	0.09	0.094440	5%
H13	0.09	0.088531	2%
C6	0.34	0.977581	188%
O1	-0.67	-0.930695	39%
O2	-0.67	-0.929365	39%

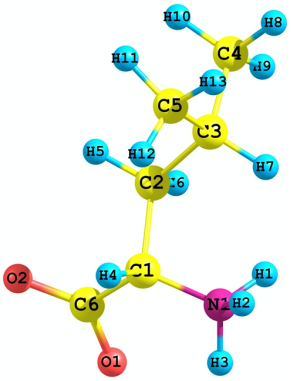


Table S5

Original CHARMM36 atomic charges (S1) and updated atomic charges (S4) for proline (Pro) in water solution.

Proline Atoms	*Atomic charges (q)*		
	Original CHARMM36.ff	*Updated CHARMM36.ff*	*$\|\Delta q\|$ (%)*
N1	-0.07	-0.109977	57%
H1	0.24	0.325234	36%
H2	0.24	0.295551	23%
C1	0.16	-0.024555	115%
H3	0.09	0.084721	6%
H4	0.09	0.088657	1%
C2	0.16	-0.069996	144%
H5	0.09	0.095824	6%
C3	-0.18	-0.023012	87%
H6	0.09	0.048323	46%
H7	0.09	0.039358	56%
C4	-0.18	0.042010	123%
H8	0.09	0.036651	59%
H9	0.09	0.033564	63%
C5	0.34	1.019092	200%
O1	-0.67	-0.944638	41%
O2	-0.67	-0.936808	40%

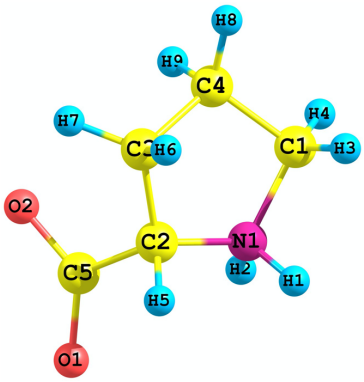
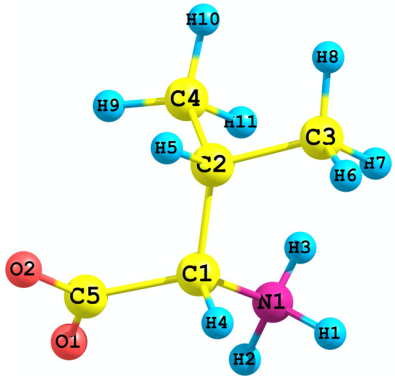


Table S6

Original CHARMM36 atomic charges (S1) and updated atomic charges (S4) for valine (Val) in water solution.

Valine Atoms	*Atomic charges (q)*		
	Original CHARMM36.ff	*Updated CHARMM36.ff*	*$\|\Delta q\|$ (%)*
N1	-0.30	-0.442198	47%
H1	0.33	0.376901	14%
H2	0.33	0.380043	15%
H3	0.33	0.381646	16%
C1	0.21	-0.083391	140%
H4	0.10	0.076902	23%
C2	-0.09	0.404919	550%
H5	0.09	-0.008321	109%
C3	-0.27	-0.403742	50%
H6	0.09	0.096686	7%
H7	0.09	0.100019	11%
H8	0.09	0.096036	7%
C4	-0.27	-0.364971	35%
H9	0.09	0.092570	3%
H10	0.09	0.091495	2%
H11	0.09	0.088054	2%
C5	0.34	1.046798	208%
O1	-0.67	-0.954834	43%
O2	-0.67	-0.974611	45%



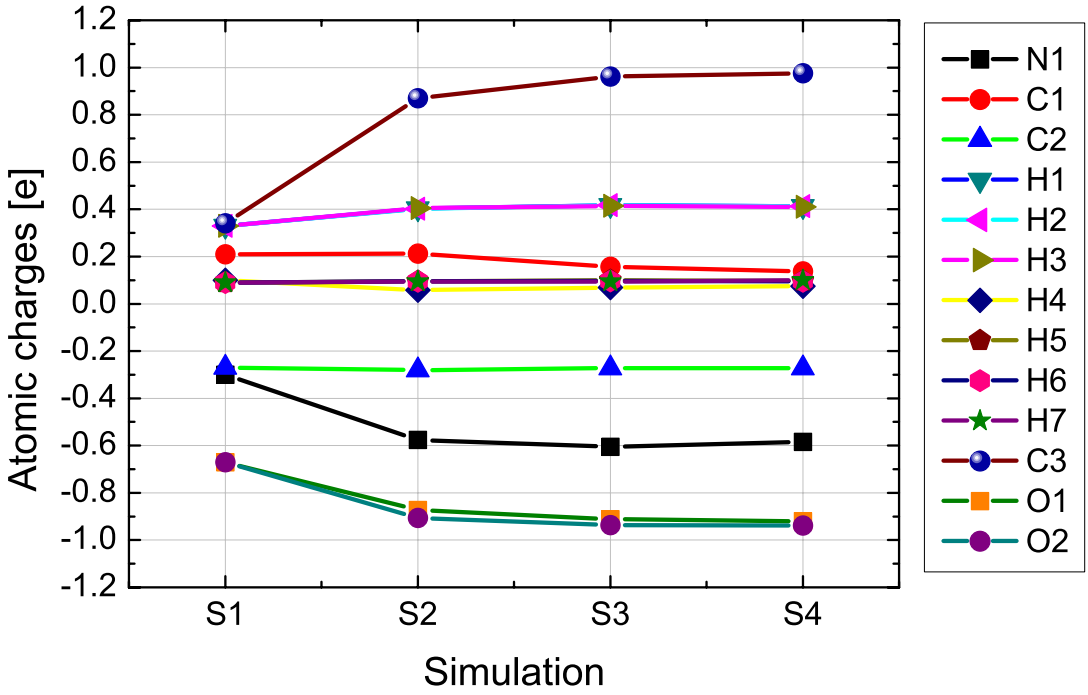


Figure S1: Convergence of atomic charge values [in e] during the dipole moment convergence process. S1 corresponds to the MD-simulation performed with CHARMM36 atomic charges and S4 corresponds to the MD-simulation performed with updated atomic charges. Results for Alanine.

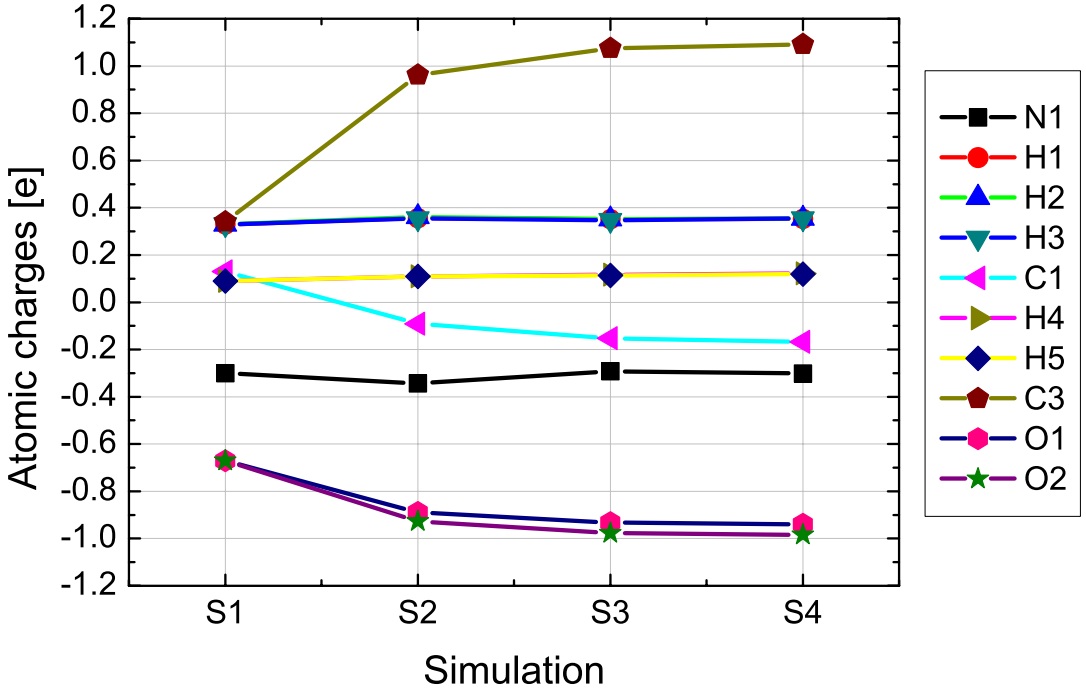


Figure S2: Convergence of atomic charge values [in e] during the dipole moment convergence process. S1 corresponds to the MD-simulation performed with CHARMM36 atomic charges and S4 corresponds to the MD-simulation performed with updated atomic charges. Results for Glycine.

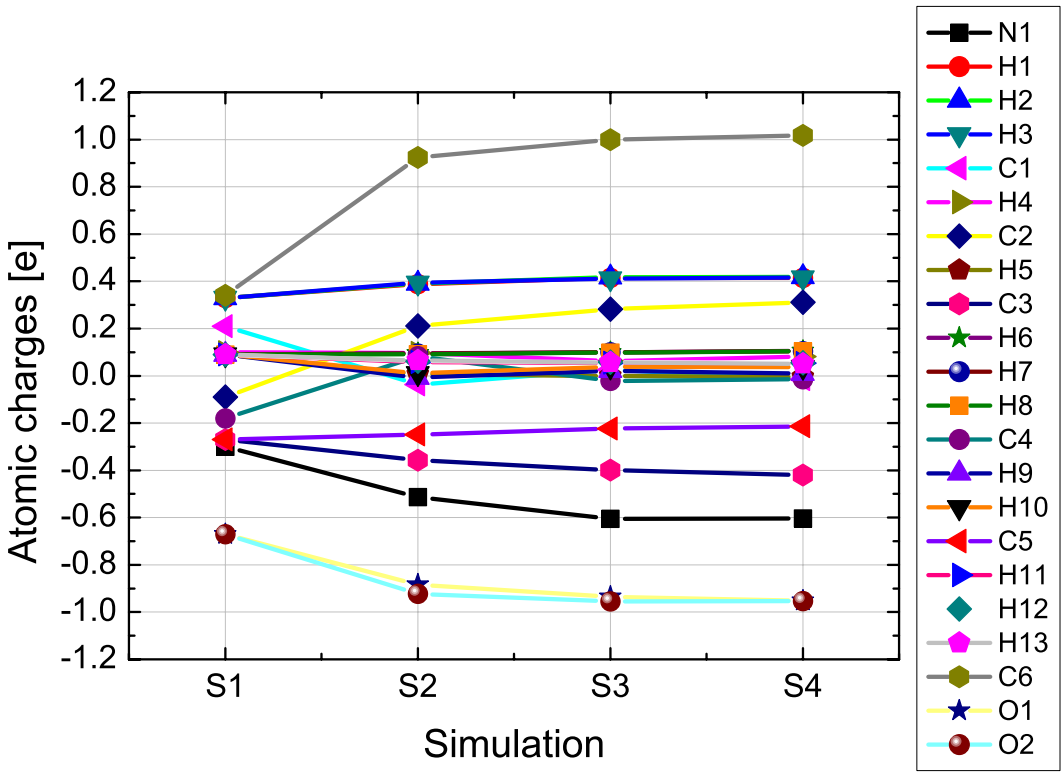


Figure S3: Convergence of atomic charge values [in e] during the dipole moment convergence process. S1 corresponds to the MD-simulation performed with CHARMM36 atomic charges and S4 corresponds to the MD-simulation performed with updated atomic charges. Results for Isoleucine.

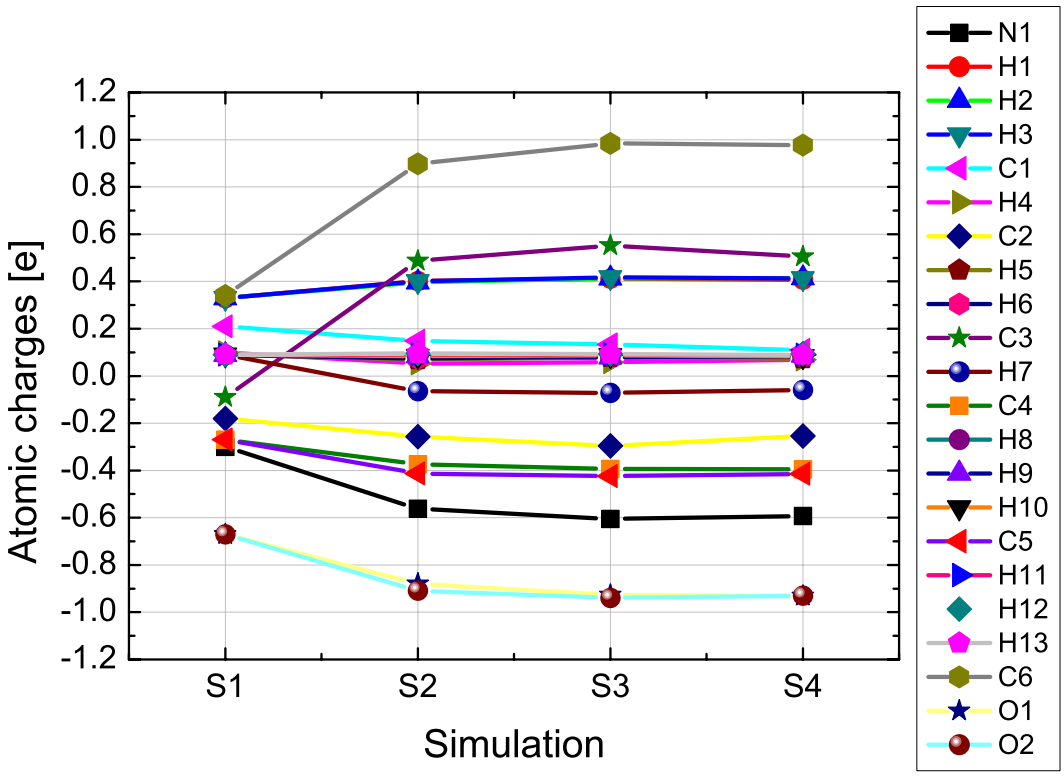


Figure S4: Convergence of atomic charge values [in e] during the dipole moment convergence process. S1 corresponds to the MD-simulation performed with CHARMM36 atomic charges and S4 corresponds to the MD-simulation performed with updated atomic charges. Results for Leucine.

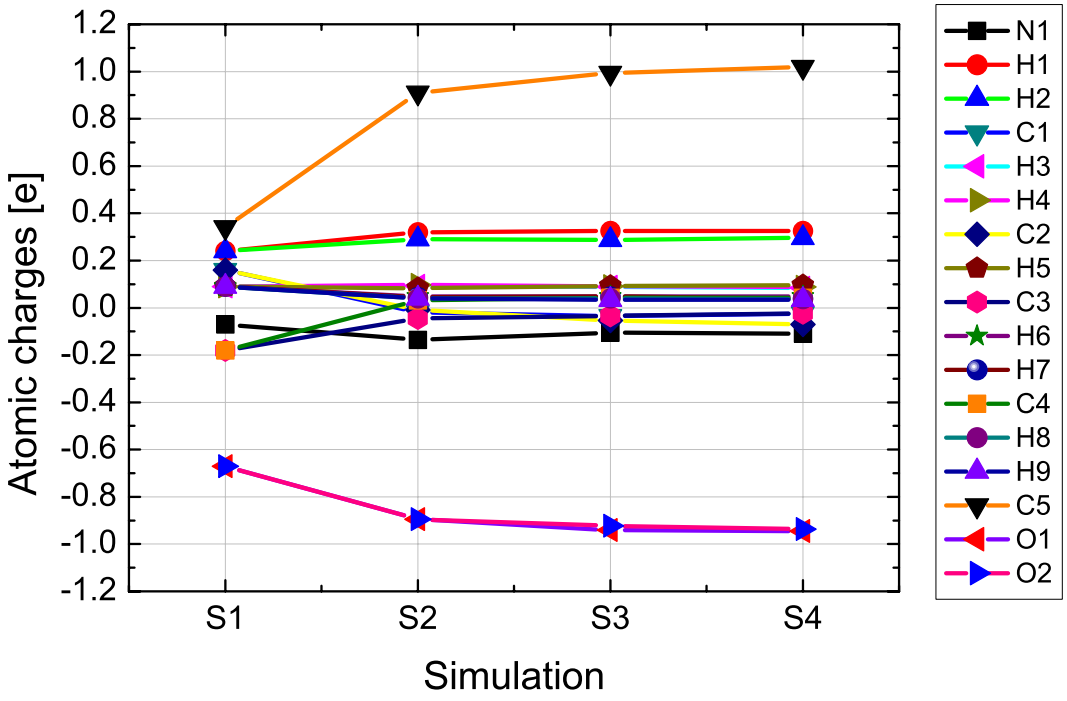


Figure S5: Convergence of atomic charge values [in e] during the dipole moment convergence process. S1 corresponds to the MD-simulation performed with CHARMM36 atomic charges and S4 corresponds to the MD-simulation performed with updated atomic charges. Results for Proline.

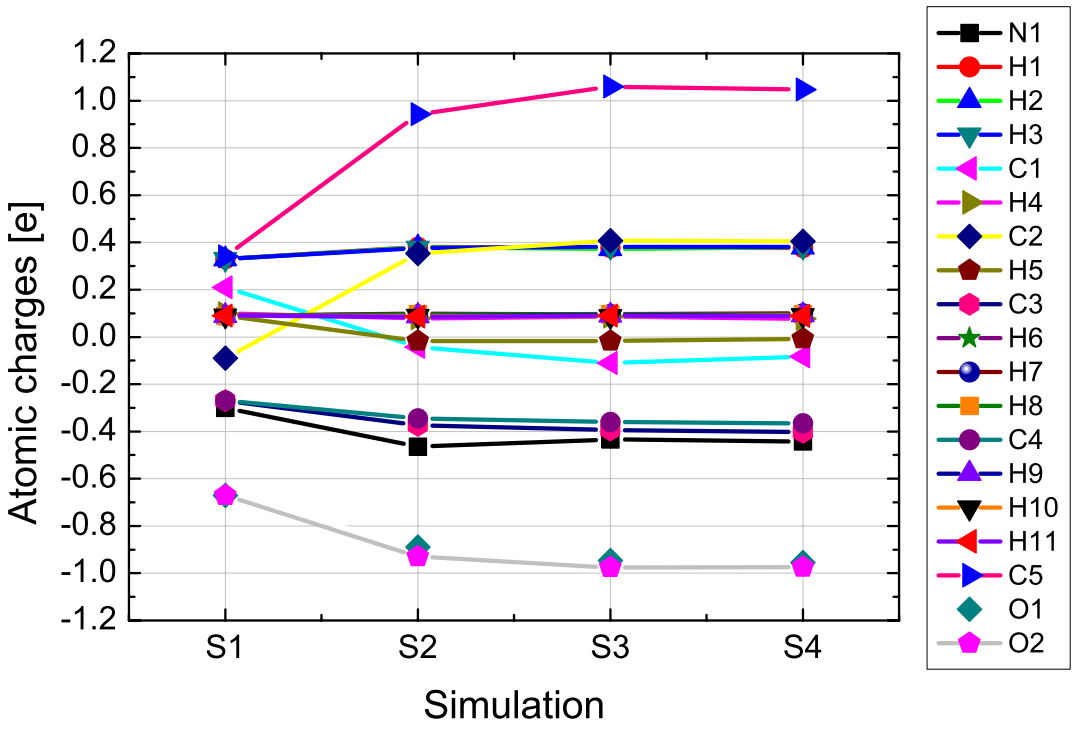


Figure S6: Convergence of atomic charge values [in e] during the dipole moment convergence process. S1 corresponds to the MD-simulation performed with CHARMM36 atomic charges and S4 corresponds to the MD-simulation performed with updated atomic charges. Results for Valine.