Supplementary Text

Parameterisation of Compounds.

Initial parameterisation. The parameterization of the local anaesthetic drug models were performed with the Force Field Toolkit (FFTK)(1) implemented in VMD(2). FFTK does not support the parameterization of LJ parameters and the Urey-Bradley term, and these parameters were obtained by analogy from the CGenFF program (https://cgenff.paramchem.org/)(3, 4).

The potential energy function of the additive CHARMM force field(5) is expressed as

$$\begin{aligned} U_{tot} = & \sum_{bonds} K_b(b-b_0)^2 + \sum_{angles} K_\theta(\theta-\theta_0)^2 \\ & + \sum_{UB} K_{UB}(S-S_0)^2 + \sum_{dihedrals} K_\chi(1+cos(n\chi-\delta)) \\ & + \sum_{impropers} K_{imp}(\Theta-\Theta_0)^2 \\ & + \sum_{\substack{nonbonded \\ i\neq j}} \left(\epsilon_{ij} \left[\left(\frac{R_{min}}{r_{ij}} \right)^{12} - 2 \left(\frac{R_{min}}{r_{ij}} \right)^{6} \right] + \frac{q_i q_j}{\epsilon_i r_{ij}} \right) \end{aligned} \tag{1}$$

U_{tot} is the sum of bonding and non-bonding interaction potentials. The bonding interaction terms involve the bonds, valence angles, a Urey-Bradley term, dihedral angles, and an improper dihedral angles term (the first four terms in Equation 1) . The quantity K corresponds to the force constants; b_0, θ_0, Φ_0, and S_0 are the bond, angle, improper and Urey-Bradley equilibrium terms; n and δ are the dihedral multiplicity and dihedral phase. The non-bonding interactions are represented by the last term in Equation 1, which includes the Lennard-Jones (LJ) interactions and electrostatic interactions. ϵ_{ij} is the strength (well depth) of the LJ potential between atoms i and j. R_{min} implicitly depends on i and j and is the distance at the minimum of the LJ potential. Finally, q_i is the partial charge on atom i and ϵ_l is the dielectric constant. Parameters of all compounds are below.

Octanol-water and cyclohexane-water partitioning. To validate the drug models, we calculated the octanol-water and cyclohexane-water partitioning coefficients, which were compared with available experimental data. The octanol-water and cyclohexane-water partitioning free energies for neutral drugs were determined using the Bennett Acceptance Ratio (BAR) approach(6), as implemented in GROMACS4.5.4(7). In this approach, the free energy difference between two close states is derived as:

$$\begin{aligned} A_1 - A_2 &= -k_B T ln \frac{\int e^{-\beta U_2(r^N)} dr^N}{\int e^{-\beta U_1(r^N)} dr^N} \\ &= -k_B T ln \left(\frac{\int e^{-\beta U_2(r^N)} dr^N}{\int \omega(r^N) e^{-\beta U_1(r^N) - \beta U_2(r^N)} dr^N} \right) \\ &\quad * \left(\frac{\int \omega(r^N) e^{-\beta U_1(r^N) - \beta U_2(r^N)} dr^N}{\int e^{-\beta U_1(r^N)} dr^N} \right) \\ &= -k_B T ln \frac{\langle \omega e^{-\beta U_2} \rangle_1}{\langle \omega e^{-\beta U_1} \rangle_2} \end{aligned} \tag{2}$$

where k_B is the Boltzmann constant, T is the temperature, N is the number of atoms, and $\omega(r^N)$ is an arbitrary weighting function. The strategy in BAR method is to try to find an optimal ω value that minimizes the expected statistical error in the calculated free energy difference. The optimal weighting function has the form,

$$\omega(r^N) \propto (n_1^{-1} e^{-\beta A_1 - \beta U_2(r^N)} + n_2^{-1} e^{-\beta A_2 - \beta U_1(r^N)})^{-1} \tag{3}$$

The variables n_1 and n_2 give the number of trajectory configurations used in the free energy average for states 1 and 2. If we assume that these are the same, we have that,

$$\omega(r^N) \propto (e^{-\beta A_1 - \beta U_2(r^N)} + e^{-\beta A_2 - \beta U_1(r^N)})^{-1} \tag{4}$$

Finally, the following equation is derived:

$$\Delta A_{1\to 2} = k_B T ln \frac{\langle \frac{1}{1+e^{-\beta \Delta U + \beta \Delta A_{1\to 2}}} \rangle_1}{\langle \frac{1}{1+e^{-\beta \Delta U + \beta \Delta A_{1\to 2}}} \rangle_2} \tag{5}$$

Equation (5) can be solved by iterating until the free energy difference converges. However, the free energy value cannot converge if the two states are separated in the configurational space. In practice, many intermediate states represented by λ are needed to bridge the two-end states. And hence, the free energy difference between state A and B can be expressed as:

$$\Delta A_{1\to 2} = \sum \Delta A_{\lambda i \to \lambda(i+1)} \tag{6}$$

The resulting free energy difference can be used to calculate the partitioning coefficient, P, using the relation:

$$LogP = \frac{\Delta A_{1\to 2}}{2.303RT} \tag{7}$$

where R is the universal gas constant and T is the simulation temperature.

The simulations were carried out at a constant isotropic pressure of 1 atm and a temperature of 300 K. The Nosé-Hoover thermostat(8, 9) and the Parrinello-Rahman barostat(10) were used. Integration of equation of motion was performed using the stochastic dynamics. A series of 51 windows with the λ equally spaced between 0 and 1 were constructed for both water and octanol or cyclohexane phases. Each window was simulated for 1,000 ps and the first 200 ps simulation was discarded for equilibration. A soft core potential with α=1, σ=0.3 nm and λ-power of 1 was used in order to avoid singularities. The two-step procedure for decoupling LJ and electrostatic interactions independently was employed. The CHARMM general force field(11) was used for the octanol and cyclohexane and the TIP3P model(12) was used for water. Each box contained 1500 explicit waters, and either 512 octanol molecules, or 512 cyclohexane molecules, with periodic boundary conditions present, and PME used for electrostatics.

Water-lipid bilayer partitioning. Steered molecular dynamics (MD) and umbrella sampling simulations(13) were carried out to obtain the water-to-DPPC bilayer potentials of mean force (PMF) for the 9 drugs. In steered MD simulations, one drug was inserted into the water phase and a harmonic potential with a force constant of 1000 kJ/mol/nm^2 was applied between the center of mass of the drug and the center of mass of the lipid bilayer. The drug was then pulled along the z-axis (perpendicular to the bilayer/water interface) at a rate of 0.01 nm/ps to generate a number of configurations. The generated configurations were selected every 0.1 nm along the z-axis and used as starting points for subsequent umbrella sampling

simulations. In each umbrella sampling window, we carried out 50 ns umbrella sampling simulations. During umbrella sampling simulations, a biased harmonic potential with a force constant of 3000 kJ/mol/nm^2 was used to confine the drug within the sampling window. The free energy profiles and error estimates were determined using the weighted histogram analysis method (WHAM)(14). The first 20 ns within each window was discarded to allow for appropriate equilibration at the new solute position, and the free energy profile was determined from the remaining 30 ns.

All PMF calculations were performed using the GROMACS 4.5.5 package.(7) The simulation systems contain 0.15 M concentration of NaCl and the systems are electrostatically neutral. The CHARMM36 lipid models(15) were used for the DPPC lipid bilayer. The system was 6.3 x 6.4 x 92 nm^3, with 128 DPPC molecules, 7100 explicit waters and 0.1 M NaCl. All lipid bilayer simulations were performed at 323K, and the molecular species were independently coupled to the Nosé-Hoover thermostat(8, 9) with a coupling time constant of 0.5 ps. The system's volume was allowed to fluctuate according to the semi-isotropic pressure coupling method at 1atm, with a coupling time constant of 2 ps and compressibility of 4.5×10-5 bar^{-1}. The PME method was used for electrostatic calculations. Periodic boundary conditions were employed in all our simulations. All bonds lengths in molecules apart from water were constrained using the LINCS algorithm(16). The TIP3P water molecule bonds were constrained using the SETTLE algorithm(17). The simulation time step was 2 fs. Other simulation parameters are found in (18).

REST simulations.

REST Theory. Replica Exchange molecular dynamics (REMD) is a method used to speed up conformational sampling by running a number of simulations in parallel at different temperatures. The high temperature simulations allow for transitions over barriers to be sped up, while the low temperature simulations explore the conformations in the energetic valleys. By regularly swapping coordinates between the replicas, the high temperature simulations help the simulation at the low temperature to more rapidly explore the conformational landscape. For large systems, REMD requires a very large number of simulations to be run to allow for overlap between the potential energies of adjacent replicas and smooth swaps in conformations. Replica Exchange Solute Scaling/Tempering (REST2) is the second iteration of REST1, a method used to reduce the number of replicas required for large systems. In these methods the idea is to only change the temperature in part of the system, while the temperature in the other parts remains constant. To achieve this, the potential surface for replica m was rescaled as follows:

$$E^{REST1}(T_m) = E_{pp}(T_m) + \left(\frac{\beta_0}{\beta_m}\right) E_{ww}(T_m) + \left(\frac{\beta_0 + \beta_m}{2\beta_m}\right) E_{pw}(T_m) \quad (8)$$

where $\beta_m = \frac{1}{k_B T_m}$, $\beta_0 = \frac{1}{k_B T_0}$, E_{T_m} is the energy of the entire system at temperature T_m, E_{pp}, is the interaction energies within the group(s) of interest, E_{pw} is the interaction energies between the group of interest and the other parts of the system, and E_{ww} is the interaction energies within the other parts of the system(19). Note that when $\beta_m = \beta_0$, the original energy surface is recovered.

The exchange rate between two replicas m and n is calculated as

$$\Delta_{nm}(REST1) = (\beta_n - \beta_m)\left[(E_{pp}(T_m) + \frac{1}{2}E_{pw}(T_m)) - (E_{pp}(T_n) + \frac{1}{2}E_{pw}T_n)\right] \quad (9)$$

where the subscripts m and n are used to denote two neighbouring temperatures(19).

When the first implementation of REST was benchmarked, it was found that as the number of particles in the system increased, the scaling was poorer than expected(20). Therefore, a more efficient method of REST was implemented by (21) as previously suggested(22, 23). This iteration of REST uses the law of corresponding states, or that "the thermodynamic properties of a system with potential energy E_m at temperature T_m, are the same as those for a system with potential energy $(\frac{T_0}{T_m})E_m$ at temperature T_0." Therefore, instead of using different potential energies and different temperatures for each replica, each replicate would be run at the same temperature, but the potential surface for each replicate would still be different(24, 25).

This resultant potential energy surface for temperature T_m is

$$E^{REST2}(T_m) = \left(\frac{\beta_m}{\beta_0}\right) E_{pp}(T_m) + \sqrt{\frac{\beta_m}{\beta_0}} E_{pw}(T_m) + E_{ww}(T_m) \quad (10)$$

where $\beta_m = \frac{1}{k_B T_m}$, $\beta_0 = \frac{1}{k_B T_0}$, E_{T_m} is the energy of the entire system at temperature T_m, E_{pp} is the interaction energies within the group(s) of interest, E_{pw} is the interaction energies between the group of interest and the other parts of the system, and E_{ww} is the interaction energies within the other parts of the system(21).

The exchange rate between two replicas m and n is calculated as

$$\Delta_{nm}(REST2) = (\beta_m - \beta_0)\left[(E_{pp}(T_n) - E_{pp}(T_m) + \frac{\sqrt{\beta_0}}{\sqrt{\beta_m} + \sqrt{\beta_n}}(E_{pw}(T_n) - E_{pw}(T_m))\right] \quad (11)$$

where subscripts m and n denote two neighbouring temperatures. This method was implemented in NAMD2.10(26), and found to have more efficient scaling with larger systems than REST1. This implementation was used for all REST simulations.

Simulation Parameters. The NavAb pore domain (residues 146-230 in the sequence, x-ray crystallographic coordinates from pdb 3rvy(27)) and NavMs pore domain (residues 129-213 in the sequence, x-ray crystallographic coordinates from pdb 4p9o(28)) were embedded in a bilayer of 126 and 129 all-atom 1-Palmitoyl-2-oleoylphosphatidylcholine (POPC) lipids, respectively. Explicit TIP3P water molecules (10500) were used, as well as an ion concentration of 150mM NaCl. These two systems were the starting point of our equilibration simulations, and each system was 54500 particles. For the NavPas systems,

cryo-EM coordinates of the pore domain from pdb 5x0m(29) were embedded into a bilayer of 151 all-atom 1-Palmitoyl-2-oleoylphosphatidylcholine (POPC) lipids, with 16000 explicity TIP3P water molecules, and an ion concentration of 150mM NaCl with an overall system size of 78000 atoms. Note that for all systems associated with the REST simulations, NAMD2.10(http://www.ks.uiuc.edu/Research/namd/)(30) was used to run all equilibration and unbiased simulations, NAMD2.10+REST2 patch(26) was used for all REST simulations, with VMD(2) used for visualisation and analysis. Local scripts were written for additional analysis, such as for the energy landscape and volume analysis.

Equilibration of 3rvy, 4p9o and 5x0m Systems. All equilibrations were run at a temperature of 310K, with a 1fs timestep. Langevin dynamics were used, as well as PME, with a grid spacing of 1.0 Å. The simulations were run at NPT, with the dcd frequency set at 1ps, with the pressure set at 1 atm. In the first equilibration step, a minimization of 1 ps was run, followed by a 10 ns production run with all protein atoms fixed. The second equilibration was run for 6 ns, with constraints placed only on the backbone. These constraints were relaxed slowly from 10 kcal/mol/Å^2 down to 0.1 kcal/mol/Å^2, with a 1 ps minimisation, followed by a production run for 1 ns for each constraint. The final frame from the second equilibration of each system was used as the starting point for REST simulations of 3rvy and 4p9o, and the last frame of a 375 ns unrestrained simulation was used as a starting point for the 5x0m system.

Addition of Compounds Into the Equilibrated Systems. The final pdb structure from the second equilibration step was visualised in VMD, and the pdb structure of the parameterised drug was placed into the middle of the pore. Care was taken to place the drug in such a manner that there were no steric clashes. The drug pdb and pore+lipid system pdb were combined, and if the drug was charged, the system re-neutralised. This final pdb system was used as a starting point for both the unbiased and the REST simulations.

Parameters of the Unbiased and REST2 protein+drug simulations. Both the unbiased and REST2 simulations were run at 310K, with a 2 fs time step. The pressure was 1 atm, and the system was NPT. PME was used with a 1 Å cutoff, and langevin dynamics was used. For the unbiased simulation, the temperature was set to 310K. For the REST2 simulations, 21 parallel simulations were run, with the effective temperature of the protein and the drug system ranging from 310K-410K. Only the protein and the drug were used as the 'hot' parts of the system, whilst the lipids, waters and ions were used as the 'cool' parts of the system. Tbe temperature of the ith replica for the hot region was determined by the equation

$$T_i = T_0 \exp\left[ln\left(\frac{T_{max}}{T_0}\right)\left(\frac{i}{N_{rep}-1}\right)\right] \qquad (12)$$

where T_0 and T_{max} are the lowest and the highest temperature used in the simulation, and N_{rep} is the total number of interactions. It should be noted that among the bonded interactions, only the dihedrals are scaled(26). Exchanges were attempted every 2ps, to allow the drug to more efficiently sample its position before exchange. Constraints were added onto the backbone at 0.1 kcal/mol/Å^2, and a collective variable was added to the drug to keep it from exiting the pore, with a radius of 37 Å from the pore center, and a constant of 20 kcal/mol/Å^2.

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Supplementary Figures

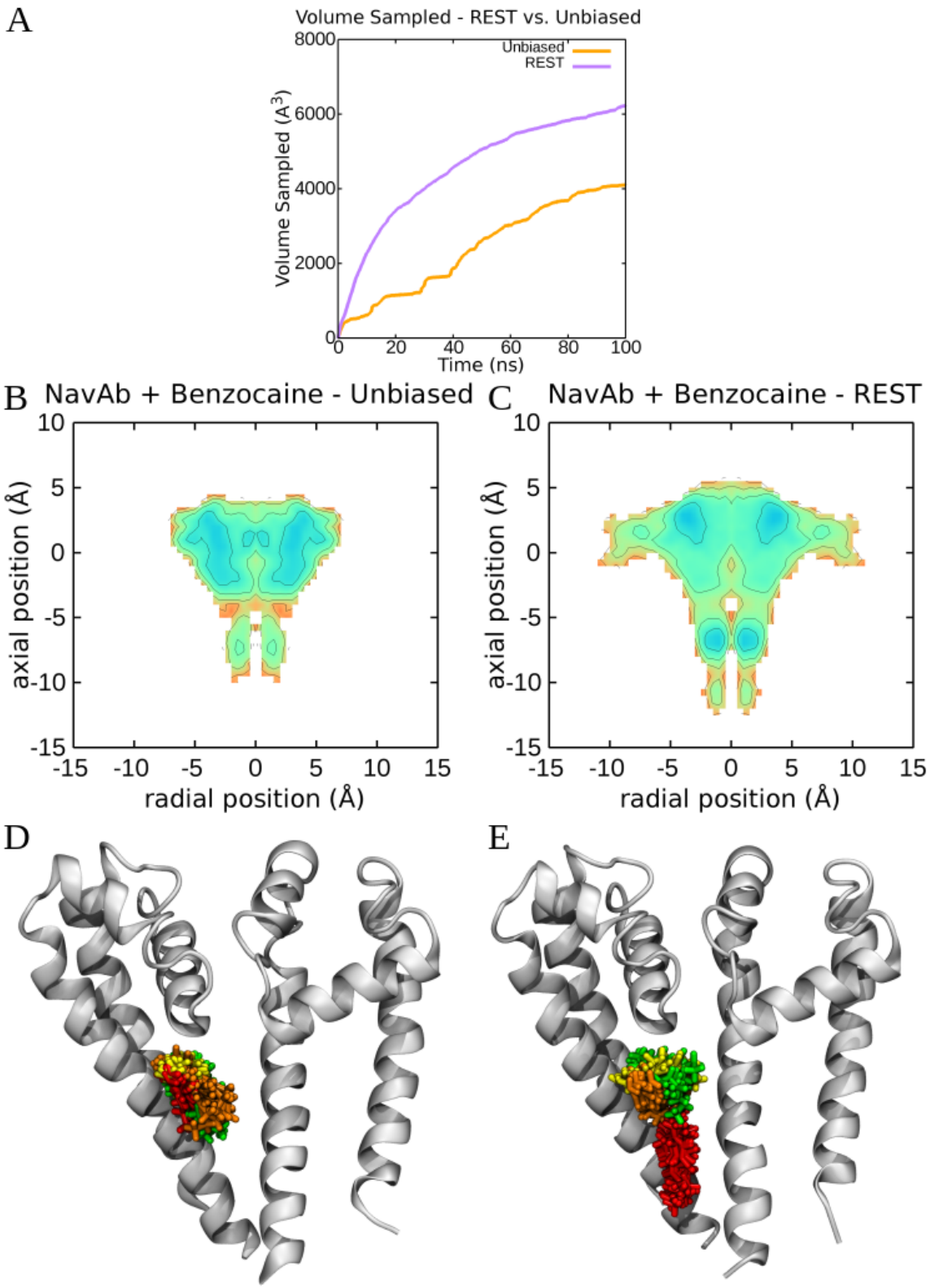

Fig. S1. REST increases conformational sampling. A) Volume sampled by the unbiased vs. REST simulations of test systems NavAb (pdb ID 3RVY) and Benzocaine. The unbiased simulation is represented by an orange line, and the REST simulation is represented by a purple line. Energy landscapes of unbiased (B) vs. REST (C) simulations. Energies are in kCal/mol. Four most populous clusters of the unbiased (D) vs. REST (E) simulations. Two subunits of NavAb are in grey surface representation, and the four most populous clusters are in red, orange, yellow and green licorice.

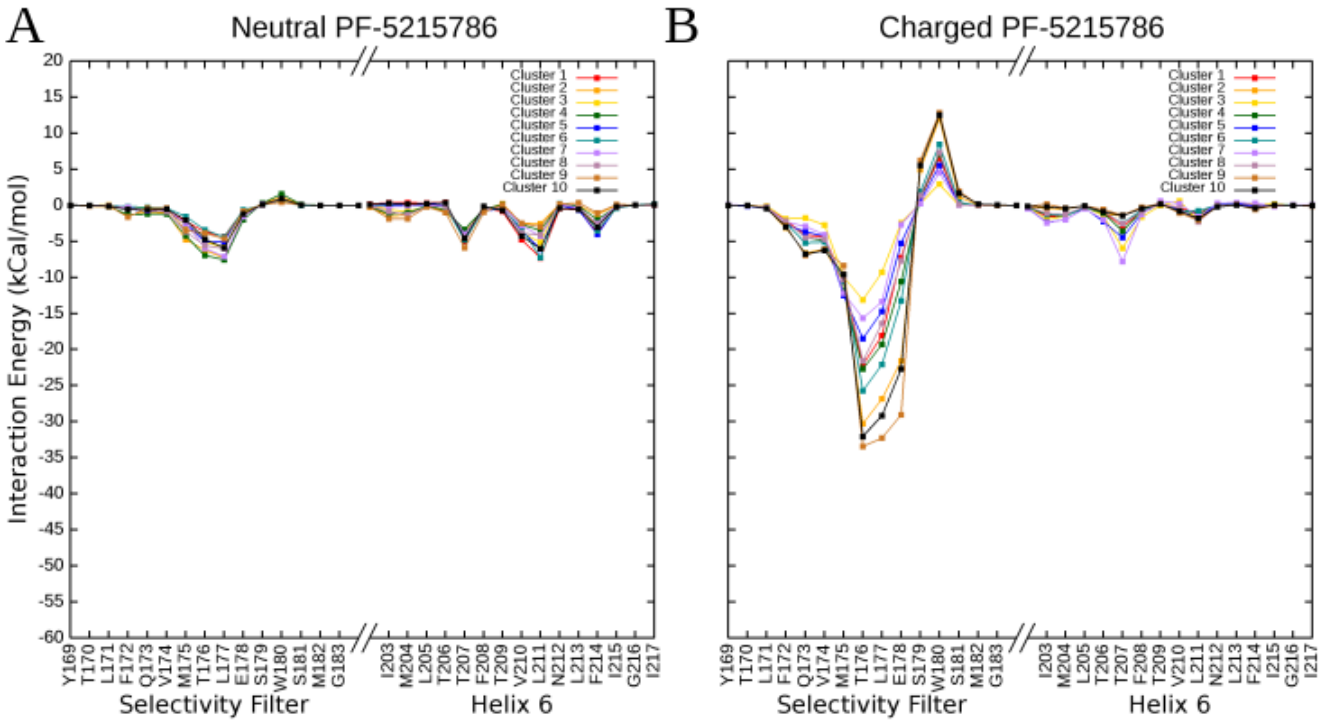

Fig. S2. Interaction energies of specific NavMs residues with each of the 10 most populated clusters of neutral PF-5215786 (A) and charged PF-5215786 (B). Each cluster is shown as a separate line, and only residues from the selectivity filter (left half) and the S6 helix (right half) are shown.

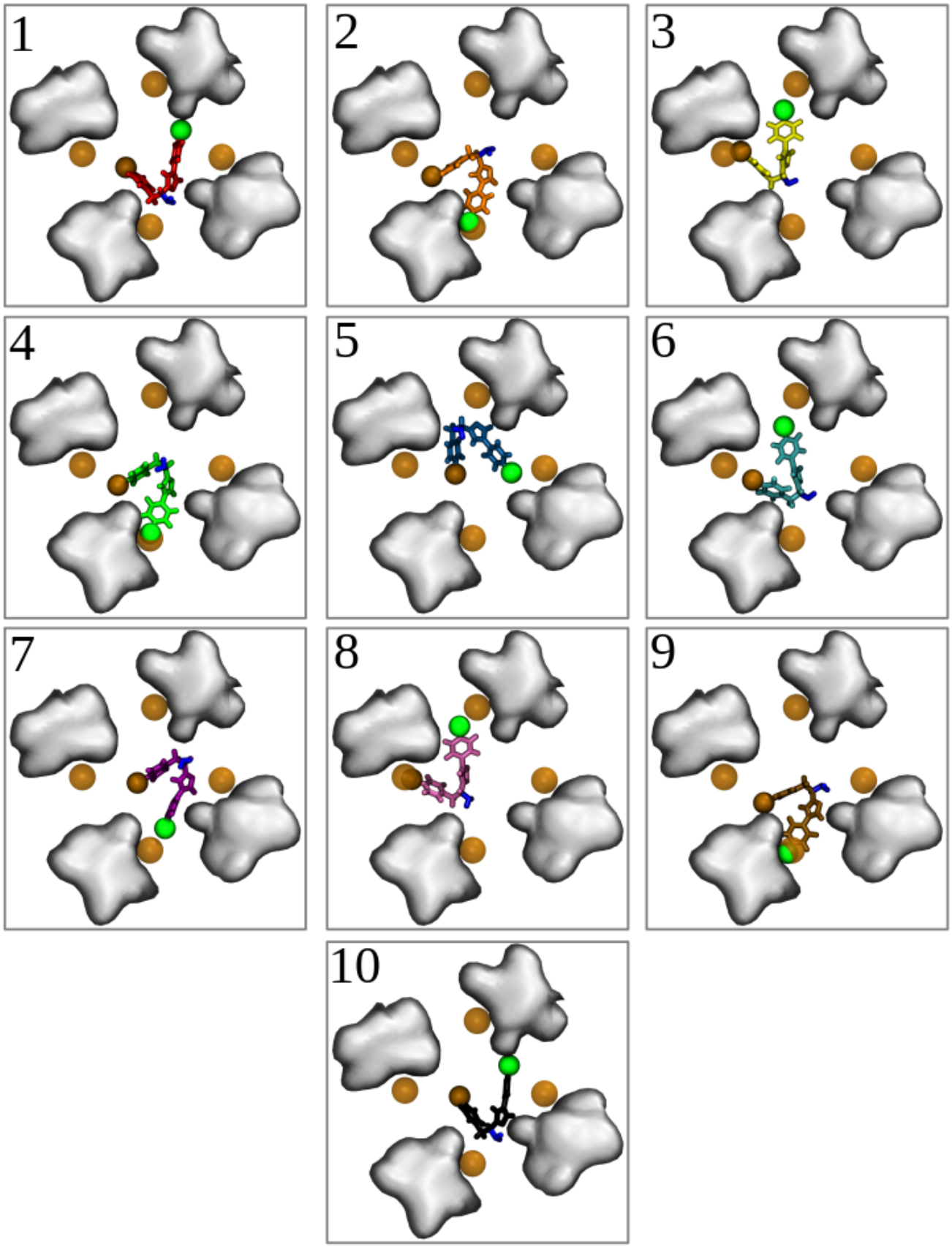

Fig. S3. Representative images of all 10 clusters of neutral PF-5215786. Each cluster is shown as a different panel and labelled with their cluster number, and PF-5215786 a different colour for each cluster. In all panels, part of the S6 helix is shown as a grey surface, and the crystallographic bromine atoms are shown in brown transparent spheres. The bromine and chlorine atom on the drug is shown as a brown and green solid sphere, respectively.

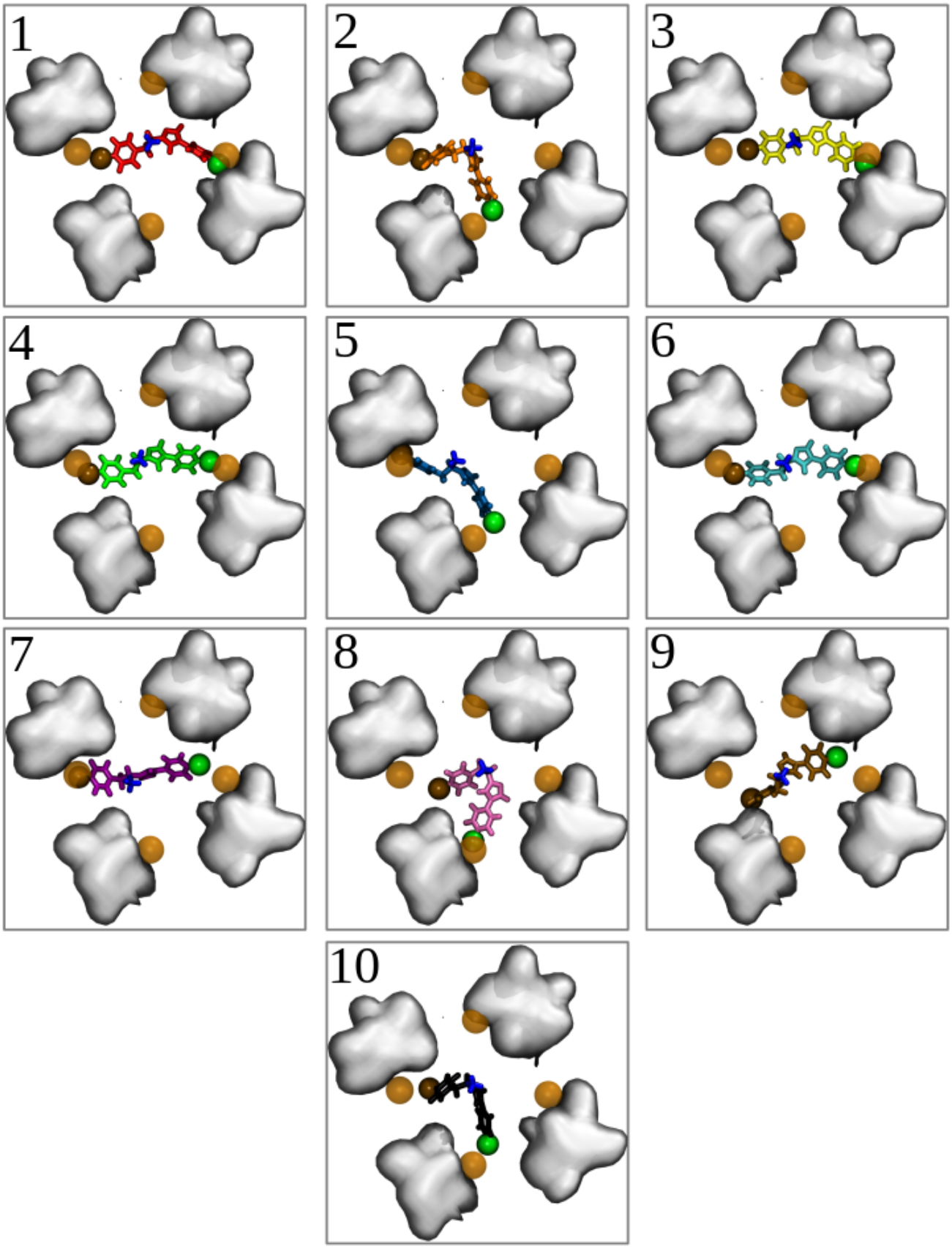

Fig. S4. Representative images of all 10 clusters of charged PF-5215786. Each cluster is shown as a different panel and labelled with their cluster number, and PF-5215786 a different colour for each cluster. In all panels, part of the S6 helix is shown as a grey surface, and the crystallographic bromine atoms are shown in brown transparent spheres. The bromine and chlorine atom on the drug is shown as a brown and green solid sphere, respectively.

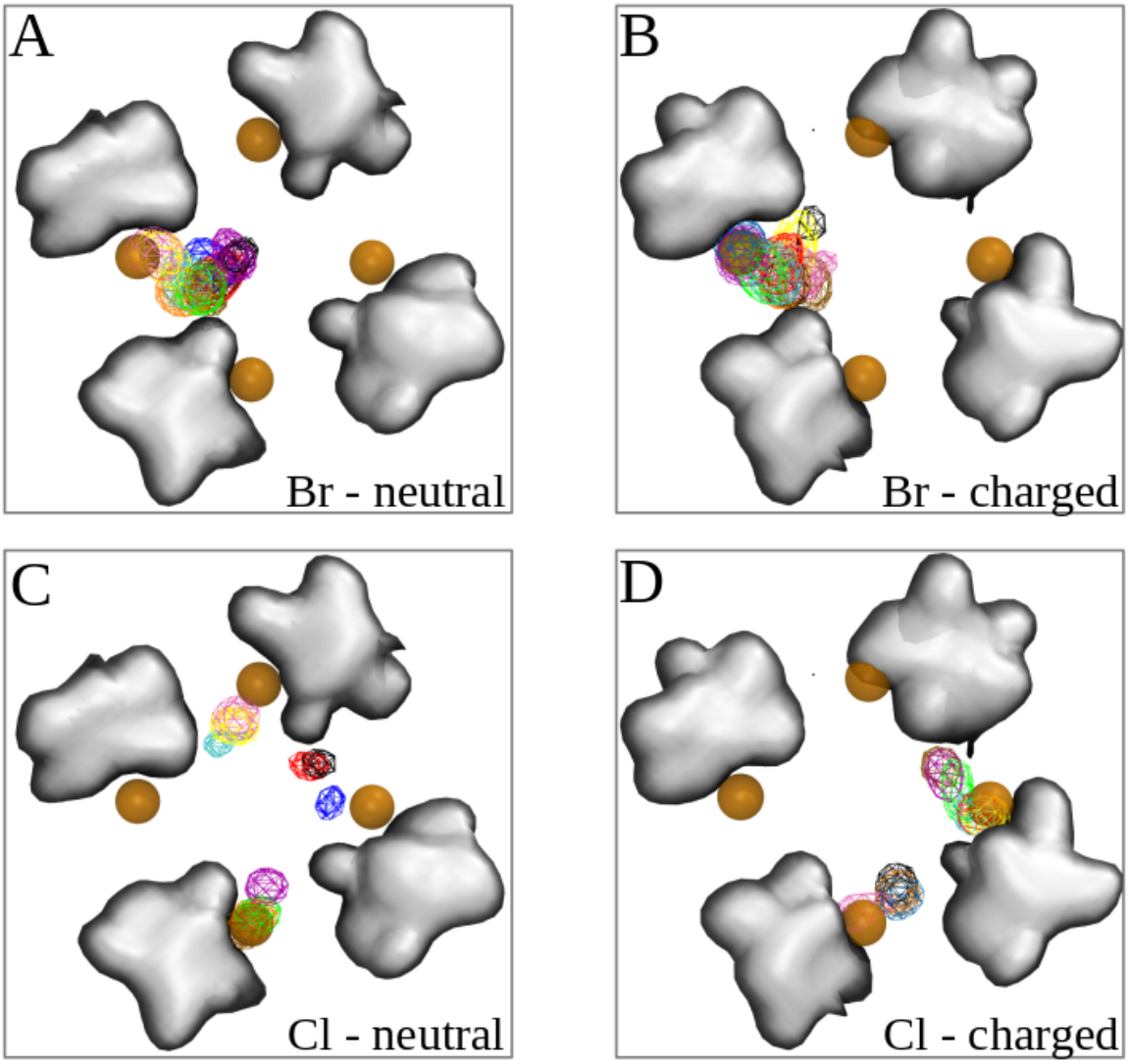

Fig. S5. Densities of Bromine and Chlorine atoms for the neutral (left) and the charged (right) versions of PF-5215786. Bromine atom densities are shown in (A) and (B), and chlorine atom densities are shown in (C) and (D). The densities are shown as mesh, with each color representing a different cluster. Part of the S6 helix is shown in grey surface, and the crystallographic bromine atoms are shown in brown transparent spheres.

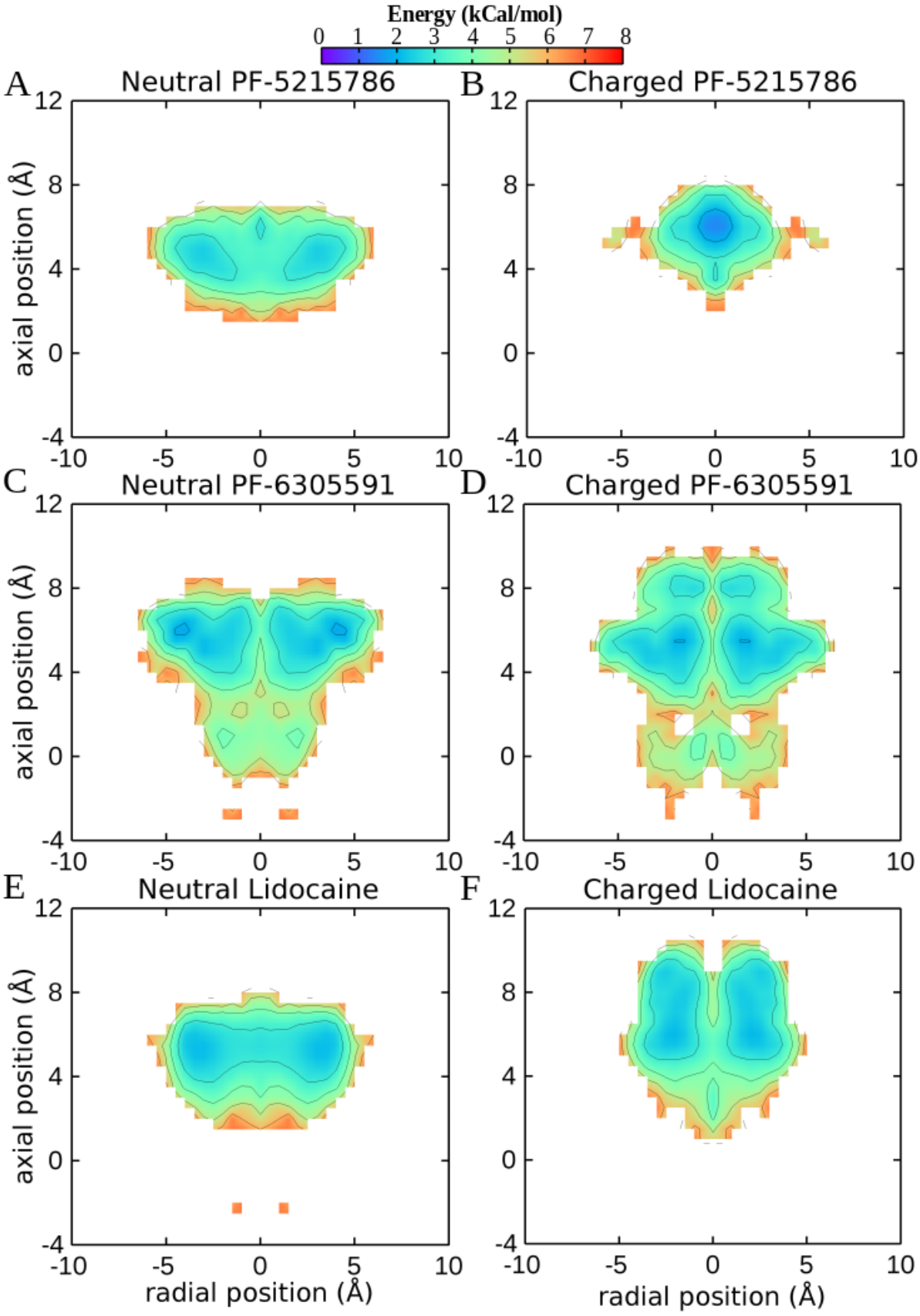

Fig. S6. Energy landscapes of the centre of mass of neutral PF-5215786 (A), charged PF-5215786 (B), neutral PF-6305591 (C), charged PF-6305591 (D), neutral lidocaine (E), and charged lidocaine (F) inside the pore of NavMs. Energies are shown in kCal/mol.

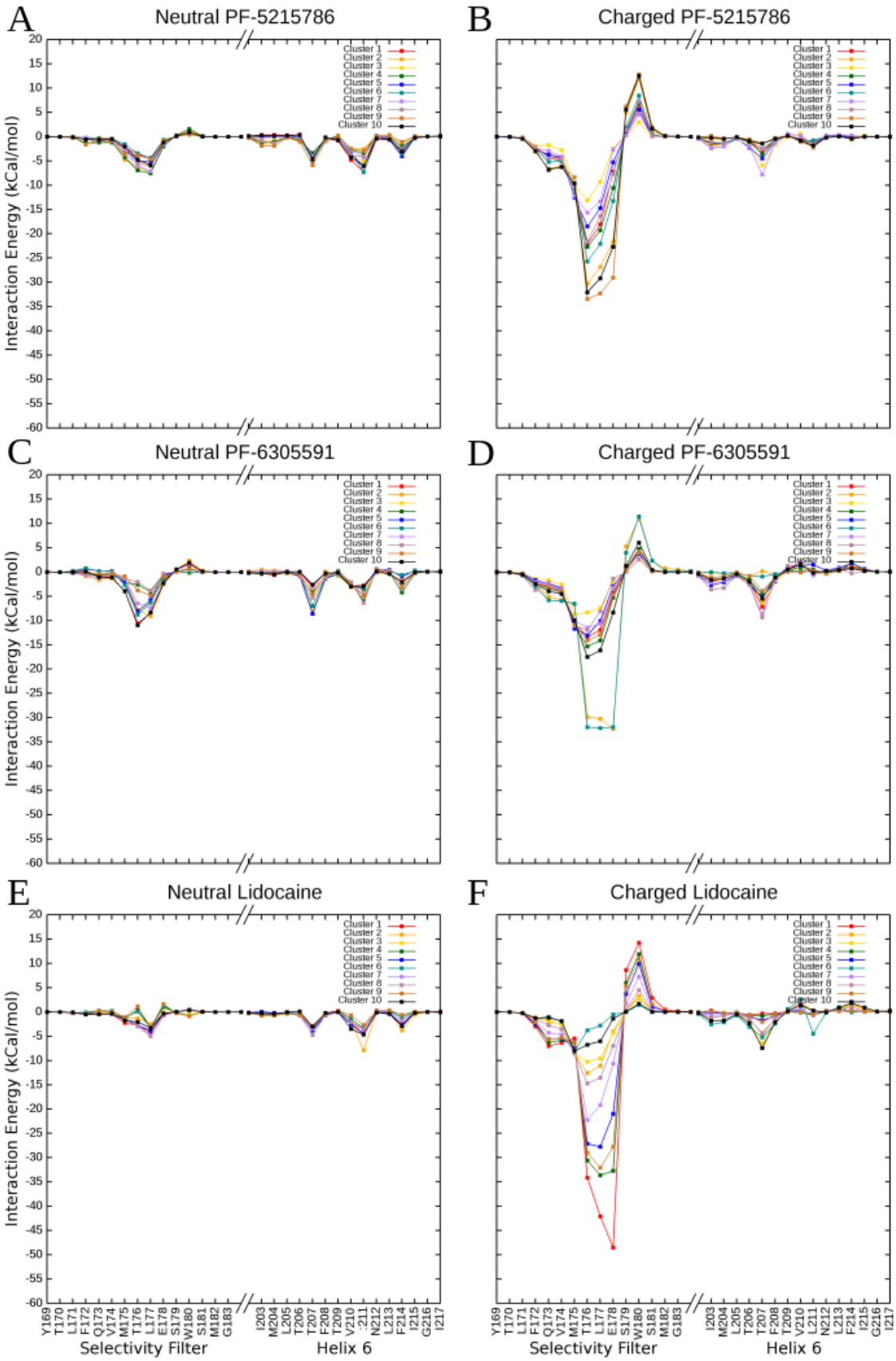

Fig. S7. Drug-protein interaction energies of specific protein residues with each of the 10 most populated clusters of neutral PF-5215786 (A), charged PF-5215786 (B), neutral PF-6305591 (C), charged PF-6305591 (D), neutral lidocaine (E), and charged lidocaine (F). Each cluster is shown as a separate line, and only residues from the selectivity filter (left half) and the S6 helix (right half) are shown.

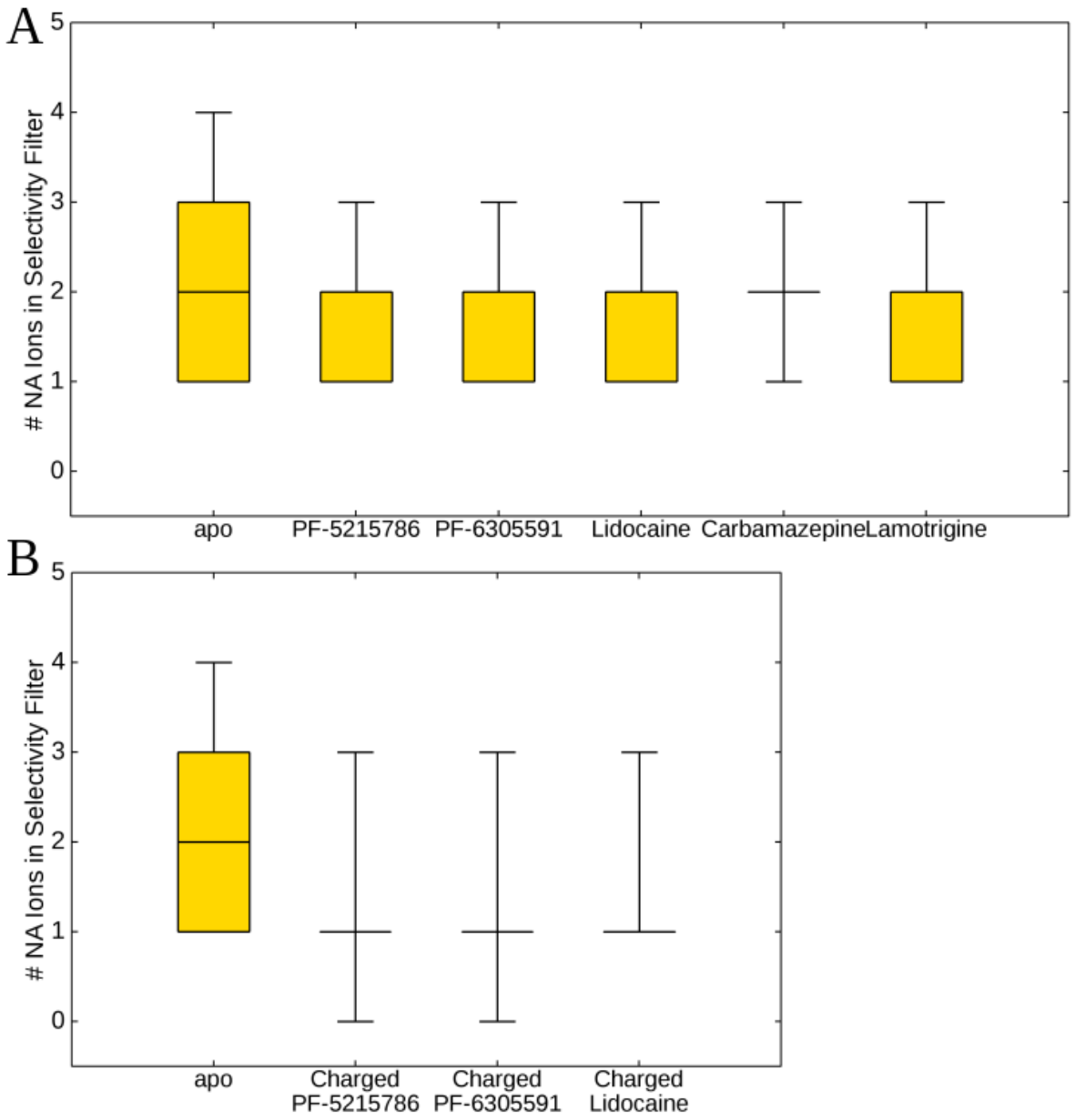

Fig. S8. Number of sodium ions in the selectivity filter for all frames of the neutral compounds (A) and charged (B) compounds as compared to an apo simulation.

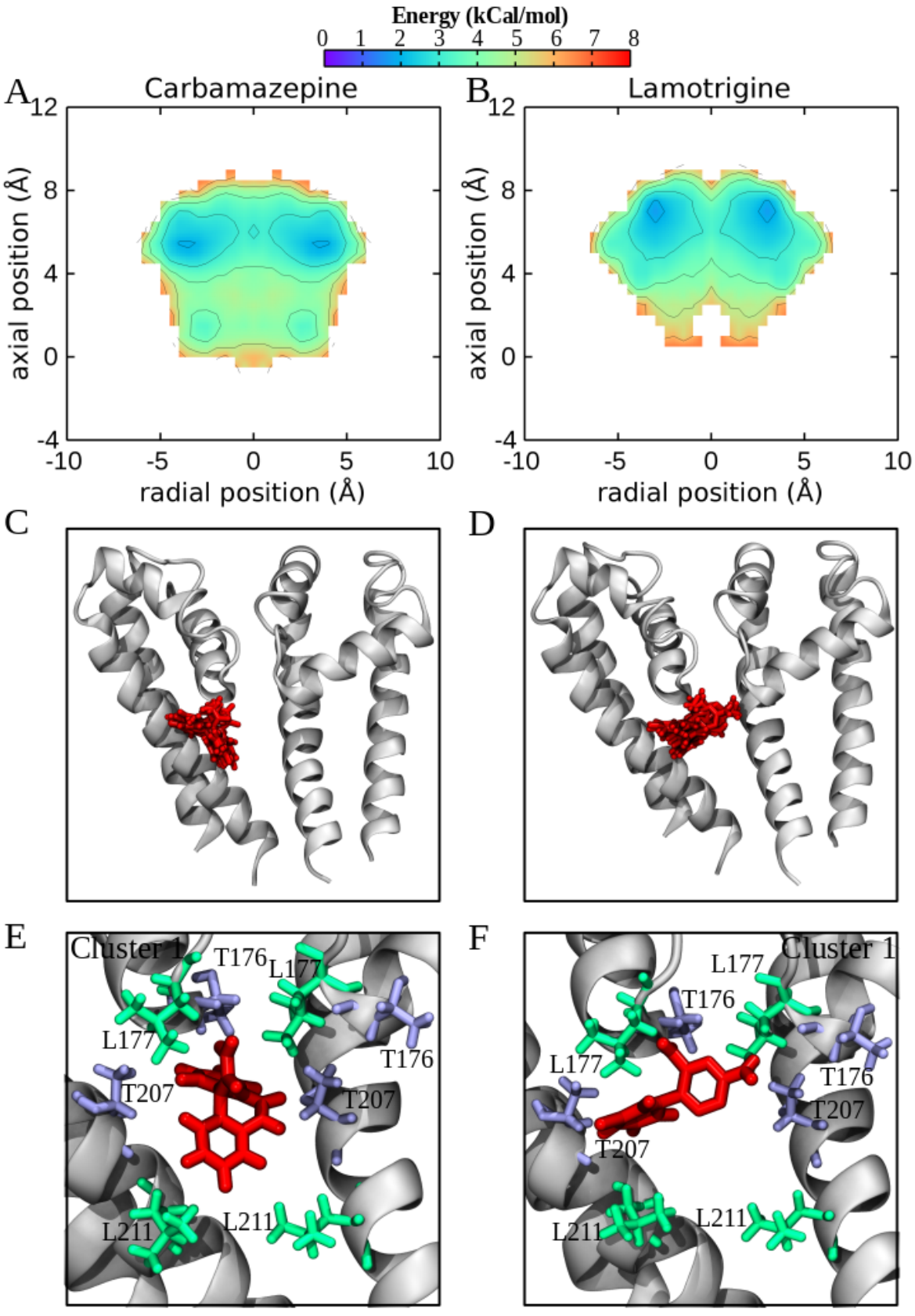

Fig. S9. Binding of perpetually neutral compounds in the pore. Energy landscapes (in kCal/mol) of the centres of mass of Carbamazepine (A) and Lamotrigine (B) inside the central cavity of the pore. The most populated clusters are shown for both Carbamazepine (C) and Lamotrigine (D), with the channel in grey cartoon, and the compound in red licorice. A representative frame from the most populated cluster of Carbamazepine (E) and Lamotrigine (F) are shown in red licorice, and surrounding residues (176T, 177L, 207T, 211L) shown in iceblue (T) and green (L).

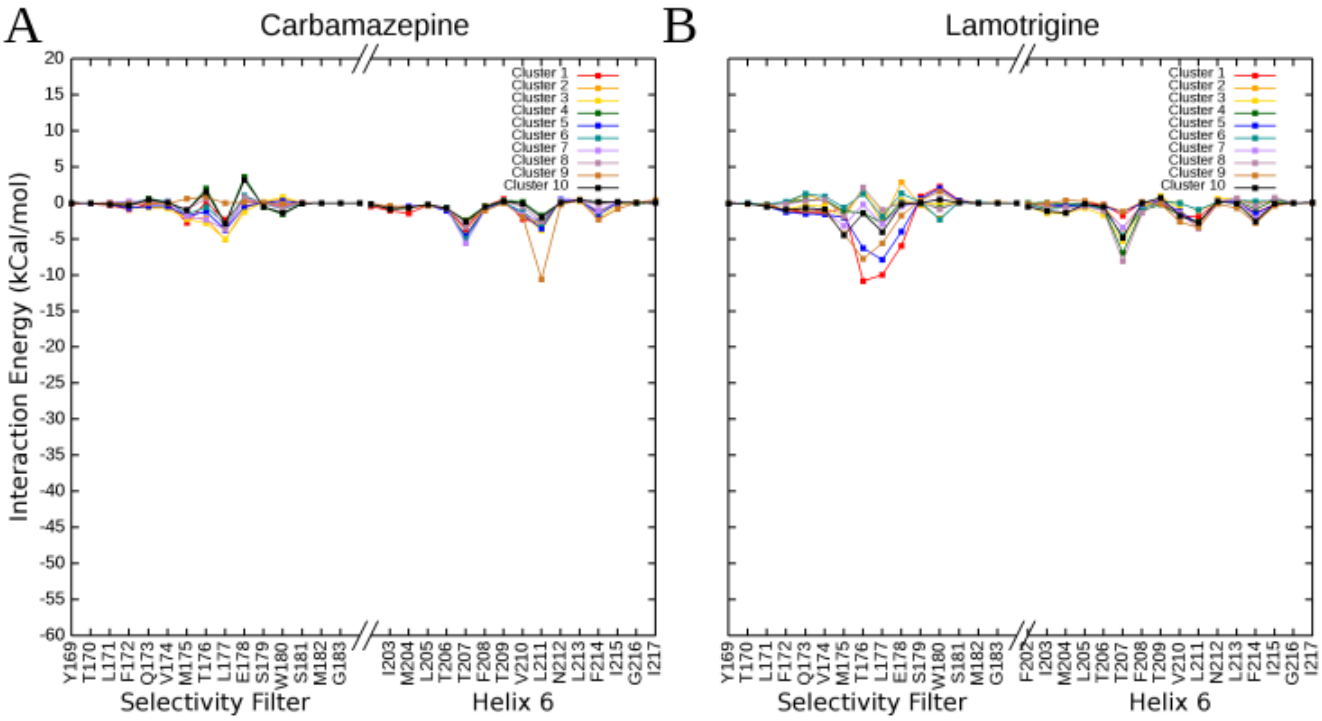

Fig. S10. Drug-protein interaction energies of specific protein residues with each of the 10 most populated clusters of Carbamazepine (A) and Lamotrigine (B). Each cluster is shown as a separate line, and only residues from the selectivity filter (left half) and the S6 helix (right half) are shown.

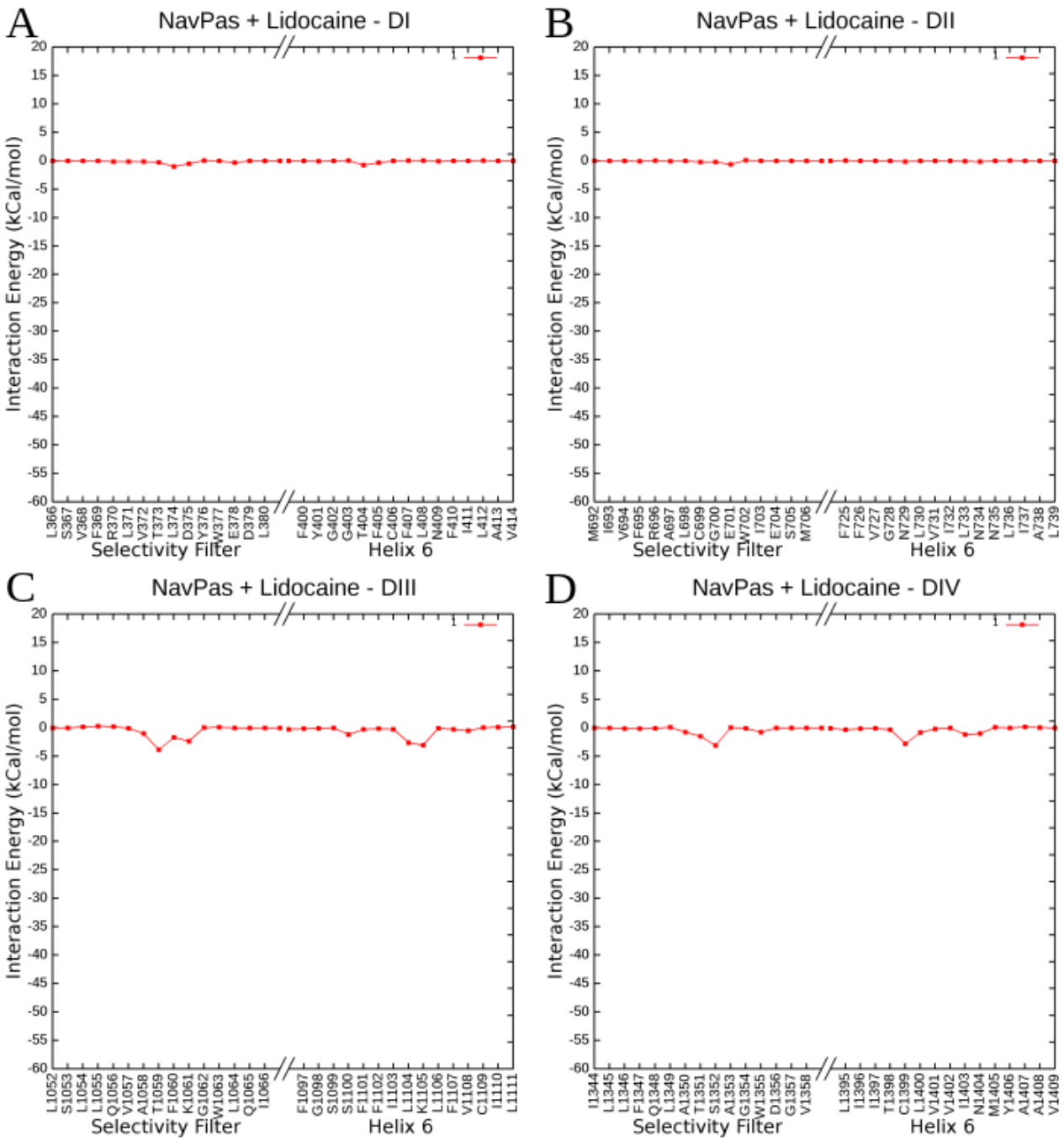

Fig. S11. Drug-protein interaction energies of the most populous cluster of lidocaine with specific protein residues on DI-IV of NavPas (A-D, respectively). Only residues from the selectivity filter (left half) and the S6 helix (right half) are shown.

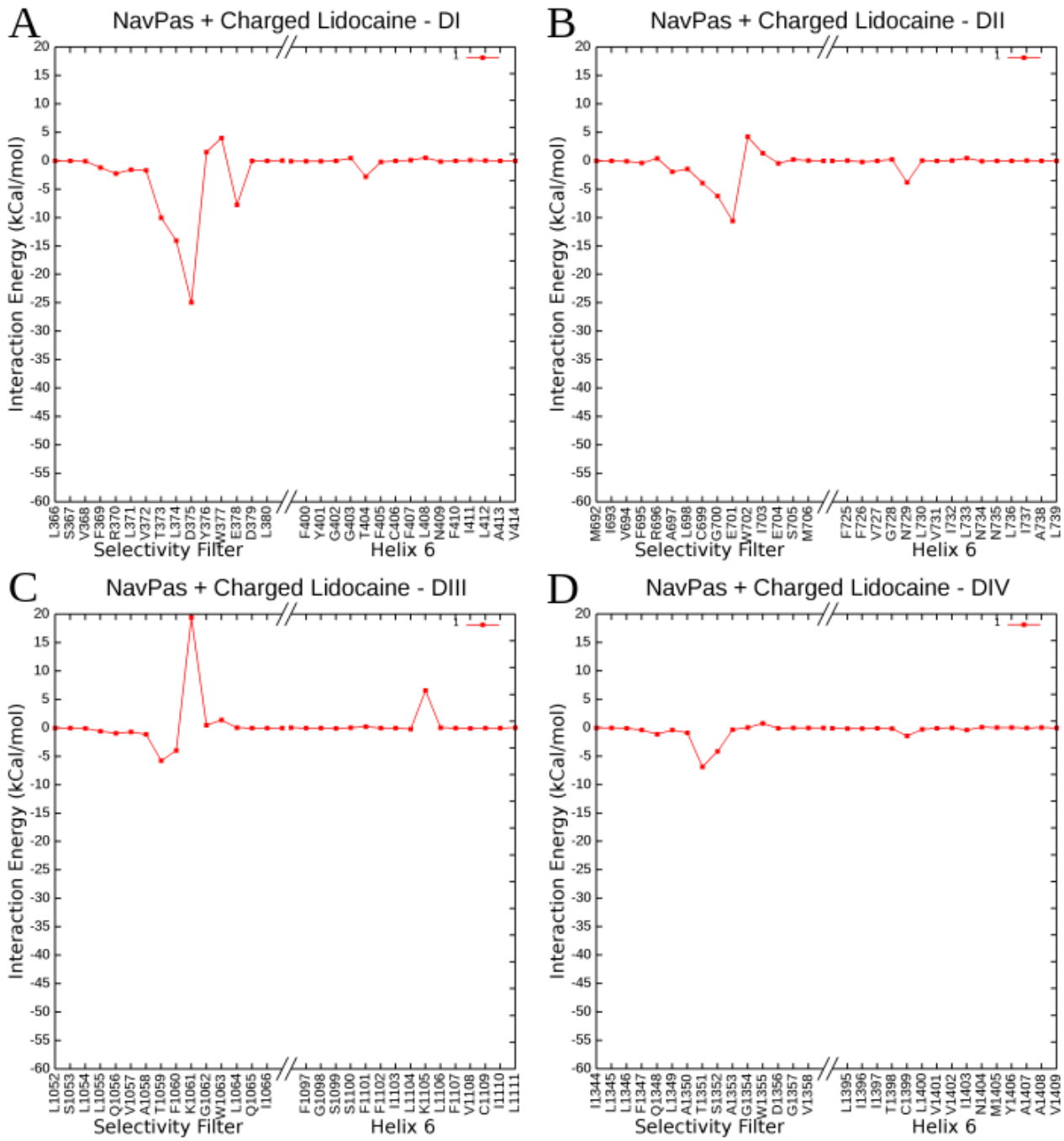

Fig. S12. Drug-protein interaction energies of the most populous cluster of charged lidocaine with specific protein residues on DI-IV of NavPas (A-D, respectively). Only residues from the selectivity filter (left half) and the S6 helix (right half) are shown.

Supplementary Tables

Compounds	Octanol-water partitioning			Cyclohexane-water partitioning		
	Free energies (kCal/mol)	Log P		Free energies (kCal/mol)	Log P	
	MD	MD	Exp	MD	MD	Exp
Benzocaine	3.6 ± 0.1	2.61 ± 0.07	1.86	0.56 ± 0.08	0.41 ± 0.06	0.27
Carbamazepine	4.4± 0.2	3.2± 0.2	2.45	-0.1 ± 0.2	-0.1± 0.1	NA
Lamotrigine	3.0 ± 0.7	2.2± 0.5	1.87	-6.31 ± 0.08	-4.59± 0.06	NA
Lidocaine	7.9 ± 0.1	5.73± 0.09	2.44	6.9 ± 0.2	5.0± 0.1	NA
PF-5215786	9.3 ± 0.1	6.79± 0.07	NA	6.79 ± 0.08	4.95± 0.06	NA
PF-6305591	5.8 ± 0.1	4.22± 0.07	NA	-3.9 ± 0.1	-2.84± 0.08	NA

Table S1. Comparison of simulated octanol-water partitionings and associated partition coefficients (logP) with experimental values. Units are in kcal/mol. Numbers are shown for simulations in GROMACS.

Simulation	Duration
NavAb Simulations	
NavAb+Benzocaine-Unbiased	1x100ns
NavAb+Benzocaine-REST	1x100ns (21x100ns)
NavMs Simulations	
NavMs-apo	1x100ns (Unbiased)
NavMs+PF-5215786	1x100ns (21x100ns)
NavMs+charged PF-5215786	1x100ns (21x100ns)
NavMs+Carbamazepine	1x100ns (21x100ns)
NavMs+Lamotrigine	1x100ns (21x100ns)
NavMs+PF-6215591	1x100ns (21x100ns)
NavMs+charged PF-6315591	1x100ns (21x100ns)
NavMs+Lidocaine	1x100ns (21x100ns)
NavMs+charged Lidocaine	1x100ns (21x100ns)
NavPas+Lidocaine	1x100ns (25x100ns)
NavPas+charged Lidocaine	1x100ns (25x100ns)

Table S2. Channel and drug systems used in the REST simulations.

System	Cluster Number	Number of Frames Per Cluster	Mean Number of Sodium Ions in SF
NavAb+Benzocaine - Unbiased	1	8661	2.17±0.82
	2	4521	2.98±0.60
	3	3601	2.33±0.94
	4	3012	3.15±0.83
	5	2178	1.99±0.61
	6	1918	2.60±0.89
	7	1629	2.72±0.82
	8	1357	2.29±0.70
	9	1252	2.95±0.81
	10	1218	2.97±0.84
	leftover	20653	X
NavAb+Benzocaine - REST	1	7828	3.05±0.77
	2	3640	2.28±0.86
	3	3411	2.15±0.80
	4	2097	2.14±0.77
	5	1443	2.08±1.00
	6	1261	2.75±0.74
	7	1203	1.89±0.61
	8	1167	2.21±0.69

Continued on next page

Table S3 – continued from previous page

System	Cluster Number	Number of Frames Per Cluster	Mean Number of Sodium Ions in SF
	9	1099	1.97±0.73
	10	1069	2.20±0.70
	leftover	25782	X
NavMs+PF-5215786	1	9688	1.61±0.49
	2	6657	1.23±0.43
	3	6185	1.61±0.50
	4	2872	1.36±0.48
	5	2618	1.31±0.46
	6	1837	1.69±0.47
	7	1434	1.59±0.49
	8	1416	1.66±0.47
	9	1076	1.63±0.49
	10	997	1.59±0.49
	leftover	15220	X
NavMs+charged PF-5215786	1	25344	1.01±0.1
	2	5994	0.96±0.37
	3	5505	1.36±0.48
	4	4265	1.00±0.07
	5	2505	1.00±0.06
	6	1076	1.04±0.19
	7	756	1.00±0.05
	8	675	1.08±0.27
	9	649	0.97±0.23
	10	626	0.78±0.46
	leftover	2605	X
NavMs+PF-6305591	1	6516	1.29±0.45
	2	3646	1.24±0.43
	3	3463	1.90±0.30
	4	3180	1.96±0.23
	5	2263	1.29±0.46
	6	2097	1.73±0.44
	7	1761	1.61±0.49
	8	125	1.42±0.49
	9	1424	1.96±0.30
	10	1368	1.32±0.48
	leftover	22757	X
NavMs+charged PF-6305591	1	5496	X1.10±0.31
	2	3253	0.99±0.23
	3	3194	1.18±0.39
	4	2660	1.10±0.30
	5	2283	1.03±0.16
	6	2248	1.00±0.05
	7	1830	1.17±0.38
	8	1807	1.19±0.40
	9	1647	1.19±0.39
	10	1349	1.14±0.35
	leftover	24233	X
NavMs+Lidocaine	1	7170	1.48±0.50
	2	4022	1.58±0.52
	3	2753	1.79±0.44
	4	2743	1.75±0.50
	5	2277	1.29±0.45
	6	1994	1.69±0.49
	7	1969	1.54±0.50
	8	1296	1.47±0.50
	9	1168	1.74±0.52
	10	1036	1.38±0.49

Continued on next page

Table S3 – continued from previous page

System	Cluster Number	Number of Frames Per Cluster	Mean Number of Sodium Ions in SF
	leftover	23572	X
NavMs+charged Lidocaine	1	10910	1.02±0.14
	2	7855	1.07±0.26
	3	5651	1.02±0.15
	4	4167	1.04±0.20
	5	3265	1.04±0.20
	6	2115	1.93±0.26
	7	1771	1.03±0.16
	8	1219	1.02±0.14
	9	1100	1.03±0.16
	10	1050	1.32±0.47
	leftover	10897	X
NavMs+Lamotrigine	1	10997	1.75±0.46
	2	5974	1.91±0.29
	3	4227	1.90±0.32
	4	3968	1.72±0.46
	5	2440	1.67±0.47
	6	2013	1.86±0.37
	7	1633	1.80±0.41
	8	1546	1.95±0.25
	9	1372	1.37±0.48
	10	1277	1.48±0.50
	leftover	14553	X
NavMs+Carbamazepine	1	7705	2.07±0.39
	2	5452	1.82±0.49
	3	2896	1.63±0.56
	4	2815	1.96±0.29
	5	2437	1.89±0.44
	6	2279	1.64±0.52
	7	1858	1.60±0.53
	8	1662	1.98±0.34
	9	1601	1.83±0.39
	10	1426	1.98±0.31
	leftover	19869	X
NavPas+Lidocaine	1	10551	1.4±0.6
	2	6778	1.2±0.6
	3	4870	1.5±0.5
	4	2956	1.2±0.6
	5	2579	1.5±0.6
	6	2292	1.7±0.7
	7	2047	1.3±0.6
	8	1654	1.2±0.5
	9	1362	2.0±0.3
	10	1255	1.4±0.6
	leftover	13656	X
NavPas+Charged Lidocaine	1	21261	0.4±0.5
	2	6286	0.5±0.6
	3	3263	0.3±0.5
	4	2345	0.5±0.6
	5	2336	0.6±0.7
	6	1908	0.6±0.6
	7	1735	0.6±0.6
	8	1693	0.3±0.5
	9	1030	0.3±0.5
	10	922	0.4±0.5
	leftover	7221	X

Continued on next page

Table S3 – continued from previous page

System	Cluster Number	Number of Frames Per Cluster	Mean Number of Sodium Ions in SF

Table S3. List of the top 10 clusters for each pore+drug simulation, along with the number of frames in each cluster and the mean number of sodium ions in the selectivity filter (with standard deviation)

Parameters of Compounds. All topologies were generated by CHARMM General Force Field (CGenFF) program version 1.0.0 and modified by Delin Sun.

```
# Benzocaine
#
# Topology
36 1
RESI          BNZ       0.000
GROUP
ATOM C1       CG2R61   −0.115  !
ATOM H1       HGR61     0.115  !
ATOM C2       CG2R61   −0.115  !
ATOM H2       HGR61     0.115  !
ATOM C3       CG2R61   −0.095  !
ATOM C4       CG2R61   −0.115  !
ATOM H3       HGR61     0.115  !
ATOM C5       CG2R61   −0.115  !
ATOM H4       HGR61     0.115  !
ATOM C6       CG2R61    0.249  !
ATOM N        NG2S3    −0.861  !
ATOM H5       HGP4      0.365  !
ATOM H6       HGP4      0.365  !
ATOM C7       CG2O2     0.726  !
ATOM O1       OG2D1    −0.551  !
ATOM O2       OG3O2    −0.391  !
ATOM C8       CG321     0.013  !
ATOM H7       HGA2      0.090  !
ATOM H8       HGA2      0.090  !
ATOM C9       CG331    −0.270  !
ATOM H9       HGA3      0.090  !
ATOM H10      HGA3      0.090  !
ATOM H11      HGA3      0.090  !
                               !  Bond order
BOND H10      C9               !  1
BOND H8       C8               !  1
BOND H9       C9               !  1
BOND C9       C8               !  1
BOND C9       H11              !  1
BOND C8       O2               !  1
BOND C8       H7               !  1
BOND O2       C7               !  1
BOND H5       N                !  1
BOND H2       C2               !  1
BOND C7       O1               !  2
BOND C7       C3               !  1
BOND C2       C3               !  1
BOND C2       C1               !  2
BOND H6       N                !  1
BOND C3       C4               !  2
BOND H1       C1               !  1
BOND C1       C6               !  1
BOND C4       H3               !  1
BOND C4       C5               !  1
```

```
BOND C6         C5                !  2
BOND C6         N                 !  1
BOND C5         H4                !  1
IMPR N          H5        H 6     C6
IMPR C7         C3        O 1     O2

END

# Parameters
BONDS
CG2O2           CG2R61     340.897     1.454   !
CG2O2           OG2D1      713.430     1.238   !
CG2O2           OG302      420.251     1.337   !
CG2R61          CG2R61     296.826     1.355   !
CG2R61          NG2S3      414.059     1.408   !
CG2R61          HGR61      370.887     1.085   !
CG321           CG331      350.852     1.523   !
CG321           OG302      328.640     1.427   !
CG321           HGA2       364.822     1.085   !
CG331           HGA3       405.939     1.095   !
NG2S3           HGP4       460.285     1.022   !

ANGLES
CG2R61   CG2O2    OG2D1      115.338     125.259      20.00      2.442 00 !
CG2R61   CG2O2    OG302      113.594     111.696      20.00      2.360 00 !
OG2D1    CG2O2    OG302      172.080     123.070     160.00      2.257 60 !
CG2O2    CG2R61   CG2R61     105.789     120.000                            !
CG2R61   CG2R61   CG2R61     189.243     120.156      35.00      2.416 20 !
CG2R61   CG2R61   NG2S3      104.758     120.284                            !
CG2R61   CG2R61   HGR61       74.692     120.091      22.00      2.152 50 !
CG331    CG321    OG302      141.711     106.502                            !
CG331    CG321    HGA2       173.176     112.437      22.53      2.179 00 !
OG302    CG321    HGA2       108.596     108.835                            !
HGA2     CG321    HGA2        85.438     107.644       5.40      1.802 00 !
CG321    CG331    HGA3       150.388     110.348      22.53      2.179 00 !
HGA3     CG331    HGA3        62.798     108.547       5.40      1.802 00 !
CG2R61   NG2S3    HGP4        91.270     113.956                            !
HGP4     NG2S3    HGP4        71.538     111.240                            !
CG2O2    OG302    CG321      134.158     114.402      30.00      2.265 10 !

DIHEDRALS
OG2D1       CG2O2    CG2R61   CG2R61      2.1330   2      180.00    !
OG302       CG2O2    CG2R61   CG2R61      0.4770   2      180.00    !
OG302       CG2O2    CG2R61   CG2R61      0.4590   4      180.00    !
CG2R61      CG2O2    OG302    CG321       2.5060   2      180.00    !
CG2R61      CG2O2    OG302    CG321       2.7590   3        0.00    !
CG2R61      CG2O2    OG302    CG321       0.9580   4        0.00    !
CG2R61      CG2O2    OG302    CG321       0.0670   6      180.00    !
OG2D1       CG2O2    OG302    CG321       1.2410   2      180.00    !
CG2O2       CG2R61   CG2R61   CG2R61      2.1250   3        0.00    !
CG2O2       CG2R61   CG2R61   HGR61       1.0870   2      180.00    !
CG2R61      CG2R61   CG2R61   CG2R61      2.9980   2      180.00    !
CG2R61      CG2R61   CG2R61   NG2S3       2.5020   3        0.00    !
CG2R61      CG2R61   CG2R61   HGR61       2.9160   2      180.00    !
NG2S3       CG2R61   CG2R61   HGR61       1.0050   3      180.00    !
HGR61       CG2R61   CG2R61   HGR61       2.9990   2      180.00    !
HGR61       CG2R61   CG2R61   HGR61       2.4850   3      180.00    !
CG2R61      CG2R61   NG2S3    HGP4        1.1260   2      180.00    !
OG302       CG321    CG331    HGA3        0.6640   2        0.00    !
HGA2        CG321    CG331    HGA3        0.2570   3        0.00    !
CG331       CG321    OG302    CG2O2       1.6340   1      180.00    !
CG331       CG321    OG302    CG2O2       0.9220   2      180.00    !
CG331       CG321    OG302    CG2O2       1.3230   3      180.00    !
CG331       CG321    OG302    CG2O2       0.9230   4      180.00    !
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HGA2        CG321    OG302    CG2O2       0.0220   2          0.00    !
HGA2        CG321    OG302    CG2O2       0.0370   3          0.00    !
HGA2        CG321    OG302    CG2O2       0.3020   4        180.00    !

IMPROPERS
CG2O2       CG2R61   OG2D1    OG302      72.0000   0          0.00 !
NG2S3       HGP4     HGP4     CG2R61     -2.5000   0          0.00 !

END
RETURN


# PF-5215786
#
# Topology
36 1
RESI           PF1        0.000
GROUP
ATOM C1        CG2R61    -0.036!
ATOM BR        BRGR1      0.020!
ATOM C2        CG2R61    -0.094!
ATOM H2        HGR62      0.129!
ATOM C3        CG2R61    -0.115!
ATOM H3        HGR61      0.115!
ATOM C4        CG2R61    -0.078!
ATOM C5        CG2R61    -0.115!
ATOM H5        HGR61      0.115!
ATOM C6        CG2R61    -0.094!
ATOM H6        HGR62      0.129!
ATOM C7        CG321     -0.176!
ATOM H71       HGA2       0.090!
ATOM H72       HGA2       0.090!
ATOM C8        CG311     -0.193!
ATOM H8        HGA1       0.090!
ATOM N1        NG321     -0.181!
ATOM HN1       HGPAM2     0.151!
ATOM HN2       HGPAM2     0.151!
ATOM C9        CG2R53    -0.012!
ATOM N2        NG2R50    -0.313!
ATOM C10       CG2R51    -0.091!
ATOM H10       HGR52      0.144!
ATOM C11       CG2R51    -0.154!
ATOM N3        NG2R51     0.186!
ATOM HN3       HGP1       0.215!
ATOM C12       CG2R61     0.047!
ATOM C13       CG2R61    -0.115!
ATOM H13       HGR61      0.115!
ATOM C14       CG2R61    -0.033!
ATOM H14       HGR62      0.105!
ATOM C15       CG2R61     0.008!
ATOM CL        CLGR1     -0.172!
ATOM C16       CG2R61    -0.033!
ATOM H16       HGR62      0.105!
ATOM C17       CG2R61    -0.115!
ATOM H17       HGR61      0.115!
                                 !  Bond order
BOND HN1       N1                !  1
BOND H8        C8                !  1
BOND H17       C17               !  1
BOND N1        C8                !  1
BOND N1        HN2               !  1
BOND H16       C16               !  1
```

```
BOND HN3       N3              !  1
BOND C17       C16             !  1
BOND C17       C12             !  2
BOND C16       C15             !  2
BOND C8        C9              !  1
BOND C8        C7              !  1
BOND N3        C9              !  1
BOND N3        C11             !  1
BOND C9        N2              !  2
BOND C11       C12             !  1
BOND C11       C10             !  2
BOND C12       C13             !  1
BOND C15       CL              !  1
BOND C15       C14             !  1
BOND H3        C3              !  1
BOND N2        C10             !  1
BOND C10       H10             !  1
BOND C13       C14             !  2
BOND C13       H13             !  1
BOND C14       H14             !  1
BOND H2        C2              !  1
BOND H72       C7              !  1
BOND C3        C2              !  1
BOND C3        C4              !  2
BOND C7        C4              !  1
BOND C7        H71             !  1
BOND C2        C1              !  2
BOND C4        C5              !  1
BOND C1        BR              !  1
BOND C1        C6              !  1
BOND C5        C6              !  2
BOND C5        H5              !  1
BOND C6        H6              !  1

END

# Parameters
BONDS
CG2R51         CG2R51     420.659     1.389   !
CG2R51         CG2R61     357.252     1.459   !
CG2R51         NG2R50     394.053     1.370   !
CG2R51         NG2R51     433.025     1.376   !
CG2R51         HGR52      391.017     1.083   !
CG2R53         CG311      308.073     1.501   !
CG2R53         NG2R50     469.156     1.332   !
CG2R53         NG2R51     419.850     1.366   !
CG2R61         CG2R61     406.299     1.385   !
CG2R61         CG321      331.736     1.498   !
CG2R61         CLGR1      276.071     1.740   !
CG2R61         BRGR1      200.092     1.906   !
CG2R61         HGR61      373.664     1.088   !
CG2R61         HGR62      376.042     1.086   !
CG311          CG321      293.330     1.546   !
CG311          NG321      339.659     1.460   !
CG311          HGA1       347.160     1.098   !
CG321          HGA2       346.550     1.096   !
NG2R51         HGP1       484.675     1.015   !
NG321          HGPAM2     446.047     1.021   !

ANGLES
CG2R51   CG2R51   CG2R61      27.499     133.048                    !
CG2R51   CG2R51   NG2R50     263.766     110.381                    !
CG2R51   CG2R51   NG2R51     276.467     104.009                    !
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CG2R51   CG2R51   HGR52      63.792    127.307     15.00      2.215 00 !
CG2R61   CG2R51   NG2R51    104.514    122.776!
NG2R50   CG2R51   HGR52      66.025    121.485     20.00      2.140 00 !
CG311    CG2R53   NG2R50    129.590    124.507                        !
CG311    CG2R53   NG2R51    156.195    124.492                        !
NG2R50   CG2R53   NG2R51    228.498    110.711                        !
CG2R51   CG2R61   CG2R61    117.411    120.711                        !
CG2R61   CG2R61   CG2R61     88.091    119.989     35.00      2.416 20 !
CG2R61   CG2R61   CG321     105.919    120.440                        !
CG2R61   CG2R61   CLGR1     106.226    119.532                        !
CG2R61   CG2R61   BRGR1     109.474    119.317                        !
CG2R61   CG2R61   HGR61      72.520    119.524     22.00      2.152 50 !
CG2R61   CG2R61   HGR62      69.218    120.459     22.00      2.152 50 !
CG2R53   CG311    CG321     252.719    110.263                        !
CG2R53   CG311    NG321     148.874    113.395                        !
CG2R53   CG311    HGA1       74.644    108.763                        !
CG321    CG311    NG321     162.020    108.551                        !
CG321    CG311    HGA1       82.252    107.689     22.53      2.179 00 !
NG321    CG311    HGA1       75.906    107.878     50.00      2.140 00 !
CG2R61   CG321    CG311     265.812    110.311                        !
CG2R61   CG321    HGA2       86.240    111.291                        !
CG311    CG321    HGA2       80.362    108.165     22.53      2.179 00 !
HGA2     CG321    HGA2       73.730    107.633      5.40      1.802 00 !
CG2R51   NG2R50   CG2R53    184.088    105.499                        !
CG2R51   NG2R51   CG2R53    239.308    108.404                        !
CG2R51   NG2R51   HGP1       68.722    125.185     20.00      2.150 00 !
CG2R53   NG2R51   HGP1       72.654    125.893     20.00      2.140 00 !
CG311    NG321    HGPAM2     57.476    107.614                        !
HGPAM2   NG321    HGPAM2     67.729    104.661                        !

DIHEDRALS
CG2R61     CG2R51   CG2R51   NG2R50     3.0000   2      180.00  !
CG2R61     CG2R51   CG2R51   HGR52      0.4750   2      180.00  !
NG2R50     CG2R51   CG2R51   NG2R51     1.9450   3        0.00  !
NG2R50     CG2R51   CG2R51   NG2R51     2.9930   6      180.00  !
NG2R51     CG2R51   CG2R51   HGR52      3.0000   3        0.00  !
CG2R51     CG2R51   CG2R61   CG2R61     0.4460   2      180.00  !
CG2R51     CG2R51   CG2R61   CG2R61     0.3450   4        0.00  !
CG2R51     CG2R51   CG2R61   CG2R61     0.1800   6        0.00  !
NG2R51     CG2R51   CG2R61   CG2R61     0.0000   1        0.00  !
CG2R51     CG2R51   NG2R50   CG2R53     2.1100   3      180.00  !
CG2R51     CG2R51   NG2R50   CG2R53     2.9970   6      180.00  !
HGR52      CG2R51   NG2R50   CG2R53     3.0000   2      180.00  !
CG2R51     CG2R51   NG2R51   CG2R53     2.9870   3        0.00  !
CG2R51     CG2R51   NG2R51   CG2R53     2.9400   6      180.00  !
CG2R51     CG2R51   NG2R51   HGP1       0.1700   2      180.00  !
CG2R61     CG2R51   NG2R51   CG2R53     2.4520   2      180.00  !
CG2R61     CG2R51   NG2R51   HGP1       2.6970   2      180.00  !
NG2R50     CG2R53   CG311    CG321      1.4600   2        0.00  !
NG2R50     CG2R53   CG311    NG321      1.6690   2        0.00  !
NG2R50     CG2R53   CG311    HGA1       1.2300   2        0.00  !
NG2R51     CG2R53   CG311    CG321      1.2970   1        0.00  !
NG2R51     CG2R53   CG311    CG321      1.0160   3        0.00  !
NG2R51     CG2R53   CG311    NG321      1.0590   2      180.00  !
NG2R51     CG2R53   CG311    NG321      1.3910   3      180.00  !
NG2R51     CG2R53   CG311    HGA1       0.2270   3        0.00  !
CG311      CG2R53   NG2R50   CG2R51     0.6110   3      180.00  !
NG2R51     CG2R53   NG2R50   CG2R51     3.0000   2      180.00  !
CG311      CG2R53   NG2R51   CG2R51     2.9890   2      180.00  !
CG311      CG2R53   NG2R51   CG2R51     2.7790   3        0.00  !
CG311      CG2R53   NG2R51   HGP1       0.7260   2        0.00  !
NG2R50     CG2R53   NG2R51   CG2R51     3.0000   2      180.00  !
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NG2R50      CG2R53   NG2R51   HGP1        1.8440   2        180.00 !
CG2R51      CG2R61   CG2R61   CG2R61      2.9650   3          0.00 !
CG2R51      CG2R61   CG2R61   HGR61       2.3990   2        180.00 !
CG2R61      CG2R61   CG2R61   CG2R61      3.0000   2        180.00 !
CG2R61      CG2R61   CG2R61   CG321       1.3460   3          0.00 !
CG2R61      CG2R61   CG2R61   CLGR1       3.0000   3          0.00 !
CG2R61      CG2R61   CG2R61   BRGR1       3.0000   2        180.00 !
CG2R61      CG2R61   CG2R61   HGR61       2.4250   2        180.00 !
CG2R61      CG2R61   CG2R61   HGR62       2.8430   3          0.00 !
CG321       CG2R61   CG2R61   HGR61       2.9990   2        180.00 !
CLGR1       CG2R61   CG2R61   HGR62       1.2950   2        180.00 !
BRGR1       CG2R61   CG2R61   HGR62       3.0000   2        180.00 !
HGR61       CG2R61   CG2R61   HGR62       3.0000   3        180.00 !
CG2R61      CG2R61   CG321    CG311       0.6600   3          0.00 !
CG2R61      CG2R61   CG321    HGA2        0.2960   2          0.00 !
CG2R53      CG311    CG321    CG2R61      1.0910   1        180.00 !
CG2R53      CG311    CG321    HGA2        0.0450   2        180.00 !
NG321       CG311    CG321    CG2R61      0.8450   1        180.00 !
NG321       CG311    CG321    HGA2        2.9990   1        180.00 !
NG321       CG311    CG321    HGA2        1.8280   2        180.00 !
NG321       CG311    CG321    HGA2        0.6470   3          0.00 !
HGA1        CG311    CG321    CG2R61      0.2750   3        180.00 !
HGA1        CG311    CG321    HGA2        1.9770   1        180.00 !
HGA1        CG311    CG321    HGA2        0.8460   2        180.00 !
HGA1        CG311    CG321    HGA2        0.5260   3          0.00 !
CG2R53      CG311    NG321    HGPAM2      0.4010   1        180.00 !
CG321       CG311    NG321    HGPAM2      0.5080   1          0.00 !
CG321       CG311    NG321    HGPAM2      1.1650   2          0.00 !
CG321       CG311    NG321    HGPAM2      0.4870   3          0.00 !
CG321       CG311    NG321    HGPAM2      0.1460   4        180.00 !
HGA1        CG311    NG321    HGPAM2      0.3250   1          0.00 !

IMPROPERS

END
RETURN


# Charged PF-5215786
#
# Topology
36 1
RESI                    PF1        0.000
GROUP
ATOM C1                 CG2R61     0.269   !
ATOM BR                 BRGR1     −0.188   !
ATOM C2                 CG2R61    −0.163   !
ATOM H2                 HGR62      0.160   !
ATOM C3                 CG2R61    −0.115   !
ATOM H3                 HGR61      0.115   !
ATOM C4                 CG2R61     0.068   !
ATOM C5                 CG2R61    −0.115   !
ATOM H5                 HGR61      0.115   !
ATOM C6                 CG2R61    −0.163   !
ATOM H6                 HGR62      0.160   !
ATOM C7                 CG321     −0.277   !
ATOM H71                HGA2       0.090   !
ATOM H72                HGA2       0.090   !
ATOM C8                 CG314     −0.346   !
ATOM H8                 HGA1       0.090   !
ATOM N1                 NG3P3      0.199   !
ATOM HN1                HGP2       0.255   !
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ATOM HN2              HGP2       0.255   !
ATOM HN3              HGP2       0.255   !
ATOM C9               CG2R53    −0.139   !
ATOM N2               NG2R50    −0.257   !
ATOM C10              CG2R51    −0.004   !
ATOM H10              HGR52      0.163   !
ATOM C11              CG2R51    −0.147   !
ATOM N3               NG2R51     0.041   !
ATOM HN4              HGP1       0.542   !
ATOM C12              CG2R61     0.025   !
ATOM C13              CG2R61    −0.115   !
ATOM H13              HGR61      0.115   !
ATOM C14              CG2R61    −0.259   !
ATOM H14              HGR62      0.063   !
ATOM C15              CG2R61     0.473   !
ATOM CL               CLGR1     −0.059   !
ATOM C16              CG2R61    −0.259   !
ATOM H16              HGR62      0.063   !
ATOM C17              CG2R61    −0.115   !
ATOM H17              HGR61      0.115   !
                                         !  Bond order
BOND H10              C10                !  1
BOND HN2              N1                 !  1
BOND H8               C8                 !  1
BOND HN3              N1                 !  1
BOND C10              N2                 !  1
BOND C10              C11                !  2
BOND N2               C9                 !  2
BOND N1               C8                 !  1
BOND N1               HN1                !  1
BOND C11              C12                !  1
BOND C11              N3                 !  1
BOND C9               C8                 !  1
BOND C9               N3                 !  1
BOND H17              C17                !  1
BOND H3               C3                 !  1
BOND C8               C7                 !  1
BOND C12              C17                !  2
BOND C12              C13                !  1
BOND C17              C16                !  1
BOND H2               C2                 !  1
BOND N3               HN4                !  1
BOND H13              C13                !  1
BOND C13              C14                !  2
BOND C16              H16                !  1
BOND C16              C15                !  2
BOND C14              C15                !  1
BOND C14              H14                !  1
BOND C15              CL                 !  1
BOND C3               C2                 !  1
BOND C3               C4                 !  2
BOND C2               C1                 !  2
BOND H72              C7                 !  1
BOND C7               C4                 !  1
BOND C7               H71                !  1
BOND C4               C5                 !  1
BOND C1               BR                 !  1
BOND C1               C6                 !  1
BOND C5               C6                 !  2
BOND C5               H5                 !  1
BOND C6               H6                 !  1
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END

# Parameters
BONDS
CG2R51          CG2R51      420.316     1.381   !
CG2R51          CG2R61      316.533     1.461   !
CG2R51          NG2R50      338.553     1.372   !
CG2R51          NG2R51      357.380     1.389   !
CG2R51          HGR52       386.738     1.079   !
CG2R53          CG314       330.266     1.508   !
CG2R53          NG2R50      464.892     1.318   !
CG2R53          NG2R51      385.166     1.352   !
CG2R61          CG2R61      433.243     1.383   !
CG2R61          CG321       304.755     1.514   !
CG2R61          CLGR1       251.591     1.746   !
CG2R61          BRGR1       216.129     1.903   !
CG2R61          HGR61       371.674     1.084   !
CG2R61          HGR62       372.107     1.083   !
CG314           CG321       278.396     1.539   !
CG314           NG3P3       293.991     1.528   !
CG314           HGA1        369.782     1.094   !
CG321           HGA2        360.958     1.097   !
NG2R51          HGP1        490.039     1.011   !
NG3P3           HGP2        399.805     1.042   !

ANGLES
CG2R51   CG2R51   CG2R61    102.816    132.277                      !
CG2R51   CG2R51   NG2R50    233.158    110.121                      !
CG2R51   CG2R51   NG2R51    204.644    104.753                      !
CG2R51   CG2R51   HGR52      67.171    128.358     15.00    2.215 00 !
CG2R61   CG2R51   NG2R51     95.933    123.111                      !
NG2R50   CG2R51   HGR52      72.090    121.823     20.00    2.140 00 !
CG314    CG2R53   NG2R50    164.899    119.519                      !
CG314    CG2R53   NG2R51    161.059    129.446                      !
NG2R50   CG2R53   NG2R51    262.891    111.234                      !
CG2R51   CG2R61   CG2R61     98.711    120.508                      !
CG2R61   CG2R61   CG2R61    126.378    119.105     35.00    2.416 20 !
CG2R61   CG2R61   CG321      99.288    120.770                      !
CG2R61   CG2R61   CLGR1     116.846    119.639                      !
CG2R61   CG2R61   BRGR1     107.584    119.665                      !
CG2R61   CG2R61   HGR61      73.202    119.661     22.00    2.152 50 !
CG2R61   CG2R61   HGR62      68.850    120.700     22.00    2.152 50 !
CG2R53   CG314    CG321     117.474    116.912                      !
CG2R53   CG314    NG3P3     209.718    101.716     35.00    2.101 00 !
CG2R53   CG314    HGA1       68.243    110.835                      !
CG321    CG314    NG3P3      99.123    111.155                      !
CG321    CG314    HGA1       66.543    109.074     22.53    2.179 00 !
NG3P3    CG314    HGA1       77.063    106.505                      !
CG2R61   CG321    CG314      83.350    112.061                      !
CG2R61   CG321    HGA2       79.923    110.755                      !
CG314    CG321    HGA2       66.866    108.508     22.53    2.179 00 !
HGA2     CG321    HGA2       51.902    107.578      5.40    1.802 00 !
CG2R51   NG2R50   CG2R53    260.524    106.297                      !
CG2R51   NG2R51   CG2R53    192.783    107.639                      !
CG2R51   NG2R51   HGP1       64.592    126.011     20.00    2.150 00 !
CG2R53   NG2R51   HGP1       74.708    125.979     20.00    2.140 00 !
CG314    NG3P3    HGP2       79.877    109.051     20.00    2.074 00 !
HGP2     NG3P3    HGP2       72.453    109.735                      !

DIHEDRALS
CG2R61      CG2R51   CG2R51   NG2R50      3.0000   3        0.00     !
CG2R61      CG2R51   CG2R51   HGR52       0.5440   2      180.00     !
NG2R50      CG2R51   CG2R51   NG2R51      2.9760   3        0.00     !
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NG2R50      CG2R51   CG2R51   NG2R51      1.0360   6        180.00    !
NG2R51      CG2R51   CG2R51   HGR52       3.0000   3          0.00    !
CG2R51      CG2R51   CG2R61   CG2R61      0.1080   2        180.00    !
NG2R51      CG2R51   CG2R61   CG2R61      1.6750   2        180.00    !
CG2R51      CG2R51   NG2R50   CG2R53      0.7210   3        180.00    !
CG2R51      CG2R51   NG2R50   CG2R53      3.0000   6        180.00    !
HGR52       CG2R51   NG2R50   CG2R53      3.0000   2        180.00    !
CG2R51      CG2R51   NG2R51   CG2R53      3.0000   3        180.00    !
CG2R51      CG2R51   NG2R51   CG2R53      2.6210   6        180.00    !
CG2R51      CG2R51   NG2R51   HGP1        0.7540   2          0.00    !
CG2R61      CG2R51   NG2R51   CG2R53      1.3490   2        180.00    !
CG2R61      CG2R51   NG2R51   HGP1        3.0000   2        180.00    !
NG2R50      CG2R53   CG314    CG321       1.2720   1        180.00    !
NG2R50      CG2R53   CG314    CG321       0.2920   3          0.00    !
NG2R50      CG2R53   CG314    NG3P3       3.0000   2        180.00    !
NG2R50      CG2R53   CG314    NG3P3       1.8620   3        180.00    !
NG2R50      CG2R53   CG314    HGA1        0.7030   2          0.00    !
NG2R51      CG2R53   CG314    CG321       1.0990   1          0.00    !
NG2R51      CG2R53   CG314    NG3P3       3.0000   2          0.00    !
NG2R51      CG2R53   CG314    NG3P3       1.6010   3          0.00    !
NG2R51      CG2R53   CG314    HGA1        0.8270   2        180.00    !
CG314       CG2R53   NG2R50   CG2R51      3.0000   3          0.00    !
NG2R51      CG2R53   NG2R50   CG2R51      2.9590   2        180.00    !
CG314       CG2R53   NG2R51   CG2R51      1.1340   2          0.00    !
CG314       CG2R53   NG2R51   HGP1        0.5270   2        180.00    !
NG2R50      CG2R53   NG2R51   CG2R51      3.0000   1        180.00    !
NG2R50      CG2R53   NG2R51   HGP1        2.4240   1          0.00    !
CG2R51      CG2R61   CG2R61   CG2R61      3.0000   3          0.00    !
CG2R51      CG2R61   CG2R61   HGR61       3.0000   2        180.00    !
CG2R61      CG2R61   CG2R61   CG2R61      0.2530   2          0.00    !
CG2R61      CG2R61   CG2R61   CG321       2.5130   3          0.00    !
CG2R61      CG2R61   CG2R61   CLGR1       3.0000   3          0.00    !
CG2R61      CG2R61   CG2R61   BRGR1       2.8490   3          0.00    !
CG2R61      CG2R61   CG2R61   HGR61       2.2770   3          0.00    !
CG2R61      CG2R61   CG2R61   HGR62       2.8660   3          0.00    !
CG321       CG2R61   CG2R61   HGR61       2.6880   2        180.00    !
CLGR1       CG2R61   CG2R61   HGR62       3.0000   2        180.00    !
BRGR1       CG2R61   CG2R61   HGR62       3.0000   3        180.00    !
HGR61       CG2R61   CG2R61   HGR62       3.0000   3        180.00    !
CG2R61      CG2R61   CG321    CG314       0.5190   2        180.00    !
CG2R61      CG2R61   CG321    HGA2        0.4660   2        180.00    !
CG2R53      CG314    CG321    CG2R61      1.2130   1          0.00    !
CG2R53      CG314    CG321    CG2R61      0.9860   3          0.00    !
CG2R53      CG314    CG321    HGA2        0.0940   2        180.00    !
NG3P3       CG314    CG321    CG2R61      1.0650   1        180.00    !
NG3P3       CG314    CG321    HGA2        0.2500   2        180.00    !
HGA1        CG314    CG321    CG2R61      0.8420   1          0.00    !
HGA1        CG314    CG321    HGA2        0.4030   2        180.00    !
CG2R53      CG314    NG3P3    HGP2        3.0000   1        180.00    !
CG321       CG314    NG3P3    HGP2        1.4790   2          0.00    !
HGA1        CG314    NG3P3    HGP2        0.1170   3        180.00    !

IMPROPERS
CG2O2       CG2R61   OG2D1    OG3O2      72.0000   0          0.00 !
NG2S3       HGP4     HGP4     CG2R61     -2.5000   0          0.00 !

END
RETURN


# PF-6305591
#
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```
# Topology
36 1
RESI           PF3        0.000
GROUP
ATOM CA        CG301      0.018   !
ATOM CB        CG331     -0.288   !
ATOM HB1       HGA3       0.090   !
ATOM HB2       HGA3       0.090   !
ATOM HB3       HGA3       0.090   !
ATOM CC        CG331     -0.288   !
ATOM HC1       HGA3       0.090   !
ATOM HC2       HGA3       0.090   !
ATOM HC3       HGA3       0.090   !
ATOM CD        CG331     -0.288   !
ATOM HD1       HGA3       0.090   !
ATOM HD2       HGA3       0.090   !
ATOM HD3       HGA3       0.090   !
ATOM CE        CG2R61     0.021   !
ATOM CF        CG2R61    -0.040   !
ATOM HF        HGR61      0.115   !
ATOM CG        CG2RC0     0.032   !
ATOM CH        CG2RC0    -0.058   !
ATOM CI        CG2R61    -0.116   !
ATOM HI        HGR61      0.115   !
ATOM CJ        CG2R61    -0.115   !
ATOM HJ        HGR61      0.115   !
ATOM N1        NG2R50    -0.300   !
ATOM CK        CG2R53    -0.003   !
ATOM N2        NG2R51    -0.012   !
ATOM H1        HGP1       0.255   !
ATOM CL        CG311     -0.112   !
ATOM HL        HGA1       0.090   !
ATOM N3        NG321     -0.194   !
ATOM H2        HGPAM2     0.174   !
ATOM H3        HGPAM2     0.174   !
ATOM CM        CG311     -0.072   !
ATOM HM        HGA1       0.090   !
ATOM CN        CG331     -0.279   !
ATOM HN1       HGA3       0.090   !
ATOM HN2       HGA3       0.090   !
ATOM HN3       HGA3       0.090   !
ATOM CO        CG2O1     -0.092   !
ATOM O         OG2D1     -0.458   !
ATOM N4        NG2S2      0.234   !
ATOM H4        HGP1       0.101   !
ATOM H5        HGP1       0.101   !
                                  !  Bond order
BOND HN3       CN                 !  1
BOND HN2       CN                 !  1
BOND HI        CI                 !  1
BOND HD1       CD                 !  1
BOND HN1       CN                 !  1
BOND CN        CM                 !  1
BOND HJ        CJ                 !  1
BOND HD2       CD                 !  1
BOND CI        CJ                 !  1
BOND CI        CH                 !  2
BOND O         CO                 !  2
BOND H1        N2                 !  1
BOND CD        HD3                !  1
BOND CD        CA                 !  1
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```
BOND CJ        CE                !  2
BOND N2        CH                !  1
BOND N2        CK                !  1
BOND CH        CG                !  1
BOND CM        CO                !  1
BOND CM        HM                !  1
BOND CM        CL                !  1
BOND CO        N4                !  1
BOND HC1       CC                !  1
BOND CE        CA                !  1
BOND CE        CF                !  1
BOND CA        CC                !  1
BOND CA        CB                !  1
BOND CK        CL                !  1
BOND CK        N1                !  2
BOND HL        CL                !  1
BOND CG        CF                !  2
BOND CG        N1                !  1
BOND CL        N3                !  1
BOND CF        HF                !  1
BOND CC        HC2               !  1
BOND CC        HC3               !  1
BOND N4        H5                !  1
BOND N4        H4                !  1
BOND HB1       CB                !  1
BOND CB        HB3               !  1
BOND CB        HB2               !  1
BOND N3        H2                !  1
BOND N3        H3                !  1
IMPR CO        CM       N 4      O

END

# Parameters
BONDS
CG2O1          CG311     280.817     1.552   !
CG2O1          NG2S2     483.853     1.353   !
CG2O1          OG2D1     806.694     1.229   !
CG2R53         CG311     307.242     1.505   !
CG2R53         NG2R50    578.916     1.308   !
CG2R53         NG2R51    438.848     1.383   !
CG2R61         CG2R61    468.675     1.397   !
CG2R61         CG2RC0    189.274     1.394   !
CG2R61         CG301     284.947     1.532   !
CG2R61         HGR61     358.125     1.083   !
CG2RC0         CG2RC0    197.363     1.407   !
CG2RC0         NG2R50    107.818     1.393   !
CG2RC0         NG2R51    461.817     1.385   !
CG301          CG331     284.625     1.544   !
CG311          CG311     284.136     1.555   !
CG311          CG331     293.337     1.527   !
CG311          NG321     338.427     1.478   !
CG311          HGA1      341.851     1.099   !
CG331          HGA3      358.269     1.092   !
NG2R51         HGP1      481.999     1.008   !
NG2S2          HGP1      471.056     1.012   !
NG321          HGPAM2    453.708     1.021   !

ANGLES
CG311    CG2O1    NG2S2     150.731     115.219     50.00     2.450 00
CG311    CG2O1    OG2D1     134.096     121.575                       !
NG2S2    CG2O1    OG2D1     130.367     123.169     50.00     2.370 00
CG311    CG2R53   NG2R50    108.803     123.587                       !
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CG311    CG2R53   NG2R51    105.026    123.679                    !
NG2R50   CG2R53   NG2R51    295.471    112.858                    !
CG2R61   CG2R61   CG2R61    282.380    120.862     35.00    2.41620
CG2R61   CG2R61   CG2RC0    286.203    118.131                    !
CG2R61   CG2R61   CG301     161.572    120.601                    !
CG2R61   CG2R61   HGR61      79.164    119.886     22.00    2.15250
CG2RC0   CG2R61   HGR61      74.394    120.337     22.00    2.14600
CG2R61   CG2RC0   CG2RC0    290.038    121.044                    !
CG2R61   CG2RC0   NG2R50    290.611    129.547                    !
CG2R61   CG2RC0   NG2R51    290.985    133.649                    !
CG2RC0   CG2RC0   NG2R50    285.471    110.175                    !
CG2RC0   CG2RC0   NG2R51    291.356    104.604                    !
CG2R61   CG301    CG331     115.817    110.457                    !
CG331    CG301    CG331     105.368    108.549     11.16    2.56100
CG2O1    CG311    CG311     155.388    111.941                    !
CG2O1    CG311    CG331     134.684    109.451                    !
CG2O1    CG311    HGA1       57.492    107.296                    !
CG2R53   CG311    CG311     107.959    112.155                    !
CG2R53   CG311    NG321     125.408    110.393                    !
CG2R53   CG311    HGA1       70.423    108.410                    !
CG311    CG311    CG331     121.480    113.431      8.00    2.56100
CG311    CG311    NG321     129.345    109.949                    !
CG311    CG311    HGA1       69.019    106.893     22.53    2.17900
CG331    CG311    HGA1       65.155    108.502     22.53    2.17900
NG321    CG311    HGA1       83.502    107.860     50.00    2.14000
CG301    CG331    HGA3       57.056    111.132     22.53    2.17900
CG311    CG331    HGA3       64.368    110.741     22.53    2.17900
HGA3     CG331    HGA3       54.065    107.850      5.40    1.80200
CG2R53   NG2R50   CG2RC0    284.618    105.281                    !
CG2R53   NG2R51   CG2RC0    288.701    107.126                    !
CG2R53   NG2R51   HGP1       61.427    126.022     20.00    2.14000
CG2RC0   NG2R51   HGP1       69.159    126.794                    !
CG2O1    NG2S2    HGP1       73.183    117.783                    !
HGP1     NG2S2    HGP1       59.747    121.870                    !
CG311    NG321    HGPAM2     65.900    107.843                    !
HGPAM2   NG321    HGPAM2     62.029    104.986                    !

DIHEDRALS
NG2S2      CG2O1    CG311    CG311      0.4310    2      0.00    !
NG2S2      CG2O1    CG311    CG331      0.8550    1      0.00    !
NG2S2      CG2O1    CG311    HGA1       0.8240    1    180.00    !
NG2S2      CG2O1    CG311    HGA1       0.5390    2      0.00    !
NG2S2      CG2O1    CG311    HGA1       0.8110    3    180.00    !
OG2D1      CG2O1    CG311    CG311      0.6010    1      0.00    !
OG2D1      CG2O1    CG311    CG311      2.2110    2    180.00    !
OG2D1      CG2O1    CG311    CG311      1.6010    3    180.00    !
OG2D1      CG2O1    CG311    CG331      2.4150    1    180.00    !
OG2D1      CG2O1    CG311    CG331      2.1970    2    180.00    !
OG2D1      CG2O1    CG311    CG331      1.4010    3      0.00    !
OG2D1      CG2O1    CG311    CG331      0.5780    4    180.00    !
OG2D1      CG2O1    CG311    HGA1       1.0290    3      0.00    !
CG311      CG2O1    NG2S2    HGP1       0.2820    2    180.00    !
OG2D1      CG2O1    NG2S2    HGP1       1.2630    2      0.00    !
NG2R50     CG2R53   CG311    CG311      1.0320    2    180.00    !
NG2R50     CG2R53   CG311    NG321      0.5410    3      0.00    !
NG2R50     CG2R53   CG311    HGA1       1.3610    1      0.00    !
NG2R50     CG2R53   CG311    HGA1       1.8350    3    180.00    !
NG2R51     CG2R53   CG311    CG311      1.6130    2      0.00    !
NG2R51     CG2R53   CG311    NG321      2.4100    1    180.00    !
NG2R51     CG2R53   CG311    NG321      0.6840    2    180.00    !
NG2R51     CG2R53   CG311    NG321      1.3620    3    180.00    !
NG2R51     CG2R53   CG311    HGA1       1.7570    1    180.00    !
```

CG311	CG2R53	NG2R50	CG2RC0	0.0710	3	0.00	!
NG2R51	CG2R53	NG2R50	CG2RC0	3.0000	3	180.00	!
CG311	CG2R53	NG2R51	CG2RC0	2.7230	3	0.00	!
CG311	CG2R53	NG2R51	HGP1	2.3470	2	180.00	!
NG2R50	CG2R53	NG2R51	CG2RC0	3.0000	3	180.00	!
NG2R50	CG2R53	NG2R51	CG2RC0	3.0000	4	180.00	!
NG2R50	CG2R53	NG2R51	HGP1	1.8880	1	180.00	!
CG2R61	CG2R61	CG2R61	CG2R61	2.8380	2	180.00	!
CG2R61	CG2R61	CG2R61	CG2RC0	2.9990	3	180.00	!
CG2R61	CG2R61	CG2R61	CG301	3.0000	2	0.00	!
CG2R61	CG2R61	CG2R61	HGR61	2.9860	1	0.00	!
CG2RC0	CG2R61	CG2R61	CG301	3.0000	3	0.00	!
CG2RC0	CG2R61	CG2R61	HGR61	3.0000	3	0.00	!
CG301	CG2R61	CG2R61	HGR61	3.0000	3	180.00	!
CG301	CG2R61	CG2R61	HGR61	0.6280	4	180.00	!
HGR61	CG2R61	CG2R61	HGR61	2.9990	1	180.00	!
CG2R61	CG2R61	CG2RC0	CG2RC0	1.4590	1	0.00	!
CG2R61	CG2R61	CG2RC0	NG2R50	2.8520	1	180.00	!
CG2R61	CG2R61	CG2RC0	NG2R51	2.8840	1	0.00	!
HGR61	CG2R61	CG2RC0	CG2RC0	2.6670	3	0.00	!
HGR61	CG2R61	CG2RC0	NG2R50	2.9530	1	180.00	!
HGR61	CG2R61	CG2RC0	NG2R51	2.0760	3	180.00	!
CG2R61	CG2R61	CG301	CG331	0.4380	3	180.00	!
CG2R61	CG2RC0	CG2RC0	CG2R61	2.1380	1	180.00	!
CG2R61	CG2RC0	CG2RC0	NG2R50	2.9970	3	0.00	!
CG2R61	CG2RC0	CG2RC0	NG2R50	1.5690	4	180.00	!
CG2R61	CG2RC0	CG2RC0	NG2R51	2.2120	2	0.00	!
NG2R50	CG2RC0	CG2RC0	NG2R51	3.0000	3	180.00	!
NG2R50	CG2RC0	CG2RC0	NG2R51	2.9990	4	180.00	!
CG2R61	CG2RC0	NG2R50	CG2R53	3.0000	3	0.00	!
CG2R61	CG2RC0	NG2R50	CG2R53	2.1990	4	180.00	!
CG2RC0	CG2RC0	NG2R50	CG2R53	2.9990	2	180.00	!
CG2R61	CG2RC0	NG2R51	CG2R53	3.0000	2	0.00	!
CG2R61	CG2RC0	NG2R51	HGP1	1.3750	1	0.00	!
CG2RC0	CG2RC0	NG2R51	CG2R53	3.0000	2	0.00	!
CG2RC0	CG2RC0	NG2R51	HGP1	0.3840	1	0.00	!
CG2R61	CG301	CG331	HGA3	2.9890	2	180.00	!
CG331	CG301	CG331	HGA3	0.2670	3	0.00	!
CG2O1	CG311	CG311	CG2R53	3.0000	1	0.00	!
CG2O1	CG311	CG311	CG2R53	1.4220	3	0.00	!
CG2O1	CG311	CG311	NG321	1.6300	1	180.00	!
CG2O1	CG311	CG311	HGA1	1.0100	1	180.00	!
CG2O1	CG311	CG311	HGA1	0.7260	2	180.00	!
CG2O1	CG311	CG311	HGA1	0.3510	3	180.00	!
CG2R53	CG311	CG311	CG331	1.6880	1	0.00	!
CG2R53	CG311	CG311	HGA1	1.7360	1	180.00	!
CG2R53	CG311	CG311	HGA1	0.1100	2	0.00	!
CG2R53	CG311	CG311	HGA1	1.1910	3	0.00	!
CG331	CG311	CG311	NG321	1.7010	1	180.00	!
CG331	CG311	CG311	NG321	1.8370	2	0.00	!
CG331	CG311	CG311	NG321	0.5720	3	0.00	!
CG331	CG311	CG311	HGA1	0.9340	1	180.00	!
NG321	CG311	CG311	HGA1	0.3670	3	180.00	!
NG321	CG311	CG311	HGA1	0.6820	4	180.00	!
HGA1	CG311	CG311	HGA1	1.4960	3	180.00	!
CG2O1	CG311	CG331	HGA3	2.9780	2	0.00	!
CG311	CG311	CG331	HGA3	0.1110	3	0.00	!
HGA1	CG311	CG331	HGA3	0.0280	3	0.00	!
CG2R53	CG311	NG321	HGPAM2	1.1340	2	0.00	!
CG311	CG311	NG321	HGPAM2	1.3740	3	180.00	!
HGA1	CG311	NG321	HGPAM2	0.0850	1	0.00	!

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HGA1        CG311    NG321    HGPAM2      2.5840   2        180.00    !
HGA1        CG311    NG321    HGPAM2      1.0110   3          0.00    !

IMPROPERS
CG2O1       CG311    NG2S2    OG2D1     120.0000   0          0.00    !

END
RETURN


# Charged PF-6305591
#
# Topology
36 1
RESI                   PF3       0.000
GROUP
ATOM CA                CG3O1     0.064   !
ATOM CB                CG331    -0.266   !
ATOM HB1               HGA3      0.090   !
ATOM HB2               HGA3      0.090   !
ATOM HB3               HGA3      0.090   !
ATOM CC                CG331    -0.266   !
ATOM HC1               HGA3      0.090   !
ATOM HC2               HGA3      0.090   !
ATOM HC3               HGA3      0.090   !
ATOM CD                CG331    -0.266   !
ATOM HD1               HGA3      0.090   !
ATOM HD2               HGA3      0.090   !
ATOM HD3               HGA3      0.090   !
ATOM CE                CG2R61    0.031   !
ATOM CF                CG2R61   -0.063   !
ATOM HF                HGR61     0.115   !
ATOM CG                CG2RC0   -0.019   !
ATOM CH                CG2RC0    0.003   !
ATOM CI                CG2R61   -0.026   !
ATOM HI                HGR61     0.115   !
ATOM CJ                CG2R61   -0.115   !
ATOM HJ                HGR61     0.115   !
ATOM N1                NG2R52   -0.095   !
ATOM H6                HGP2      0.335   !
ATOM CK                CG2R53    0.041   !
ATOM N2                NG2R52   -0.053   !
ATOM H1                HGP2      0.261   !
ATOM CL                CG311    -0.114   !
ATOM HL                HGA1      0.090   !
ATOM N3                NG321    -0.209   !
ATOM H2                HGPAM2    0.247   !
ATOM H3                HGPAM2    0.247   !
ATOM CM                CG311    -0.090   !
ATOM HM                HGA1      0.090   !
ATOM CN                CG331    -0.192   !
ATOM HN1               HGA3      0.090   !
ATOM HN2               HGA3      0.090   !
ATOM HN3               HGA3      0.090   !
ATOM CO                CG2O1    -0.051   !
ATOM O                 OG2D1    -0.283   !
ATOM N4                NG2S2    -0.126   !
ATOM H4                HGP1      0.200   !
ATOM H5                HGP1      0.200   !
                                         !  Bond order
BOND HB1               CB                !  1
BOND HD2               CD                !  1
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BOND H3               N3               !  1
BOND HL               CL               !  1
BOND H6               N1               !  1
BOND HB3              CB               !  1
BOND HF               CF               !  1
BOND HD3              CD               !  1
BOND CB               HB2              !  1
BOND CB               CA               !  1
BOND CD               HD1              !  1
BOND CD               CA               !  1
BOND H4               N4               !  1
BOND N3               CL               !  1
BOND N3               H2               !  1
BOND N1               CG               !  1
BOND N1               CK               !  1
BOND H5               N4               !  1
BOND CF               CG               !  1
BOND CF               CE               !  2
BOND N4               CO               !  1
BOND CL               CK               !  1
BOND CL               CM               !  1
BOND CG               CH               !  2
BOND CK               N2               !  2
BOND CA               CE               !  1
BOND CA               CC               !  1
BOND CE               CJ               !  1
BOND CH               N2               !  1
BOND CH               CI               !  1
BOND N2               H1               !  1
BOND CO               CM               !  1
BOND CO               O                !  2
BOND CJ               CI               !  2
BOND CJ               HJ               !  1
BOND CM               HM               !  1
BOND CM               CN               !  1
BOND HN2              CN               !  1
BOND CI               HI               !  1
BOND HC2              CC               !  1
BOND CC               HC3              !  1
BOND CC               HC1              !  1
BOND CN               HN1              !  1
BOND CN               HN3              !  1
IMPR CO               CM       N 4     O

END

# Parameters
BONDS
CG2O1          CG311      264.613     1.557   !
CG2O1          NG2S2      508.573     1.359   !
CG2O1          OG2D1      857.401     1.222   !
CG2R53         CG311      279.484     1.513   !
CG2R53         NG2R52     534.193     1.337   !
CG2R61         CG2R61     472.068     1.401   !
CG2R61         CG2RC0     105.178     1.395   !
CG2R61         CG301      300.787     1.533   !
CG2R61         HGR61      394.043     1.079   !
CG2RC0         CG2RC0      84.364     1.405   !
CG2RC0         NG2R52     436.845     1.401   !
CG301          CG331      278.319     1.542   !
CG311          CG311      273.155     1.565   !
CG311          CG331      289.726     1.530   !
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CG311          NG321      352.173    1.458   !
CG311          HGA1       348.246    1.098   !
CG331          HGA3       357.024    1.092   !
NG2R52         HGP2       481.330    1.014   !
NG2S2          HGP1       483.046    1.015   !
NG321          HGPAM2     473.782    1.013   !

ANGLES
CG311    CG2O1    NG2S2      142.128    116.805     50.00     2.450 00 !
CG311    CG2O1    OG2D1      134.480    119.541                        !
NG2S2    CG2O1    OG2D1      134.507    123.653     50.00     2.370 00 !
CG311    CG2R53   NG2R52      94.028    126.290                        !
NG2R52   CG2R53   NG2R52     295.552    107.483                        !
CG2R61   CG2R61   CG2R61     286.249    121.245     35.00     2.416 20 !
CG2R61   CG2R61   CG2RC0     290.597    117.180                        !
CG2R61   CG2R61   CG301       90.073    120.659                        !
CG2R61   CG2R61   HGR61       77.791    119.839     22.00     2.152 50 !
CG2RC0   CG2R61   HGR61       74.127    121.430     22.00     2.146 00 !
CG2R61   CG2RC0   CG2RC0     293.148    121.660                        !
CG2R61   CG2RC0   NG2R52     295.918    132.504                        !
CG2RC0   CG2RC0   NG2R52     285.289    105.878                        !
CG2R61   CG301    CG331      112.327    110.193                        !
CG331    CG301    CG331       95.473    108.784     11.16     2.561 00 !
CG2O1    CG311    CG311      146.882    112.969                        !
CG2O1    CG311    CG331      144.046    108.696                        !
CG2O1    CG311    HGA1        63.224    106.202                        !
CG2R53   CG311    CG311       97.803    111.568                        !
CG2R53   CG311    NG321      106.449    113.177                        !
CG2R53   CG311    HGA1        74.148    105.692                        !
CG311    CG311    CG331      115.816    113.352      8.00     2.561 00 !
CG311    CG311    NG321      115.681    110.787                        !
CG311    CG311    HGA1        69.379    107.294     22.53     2.179 00 !
CG331    CG311    HGA1        64.153    108.308     22.53     2.179 00 !
NG321    CG311    HGA1        79.617    107.404     50.00     2.140 00 !
CG301    CG331    HGA3        60.196    111.189     22.53     2.179 00 !
CG311    CG331    HGA3        55.449    110.698     22.53     2.179 00 !
HGA3     CG331    HGA3        55.848    107.883      5.40     1.802 00 !
CG2R53   NG2R52   CG2RC0     286.699    110.503                        !
CG2R53   NG2R52   HGP2        69.988    123.727     15.00     2.090 00 !
CG2RC0   NG2R52   HGP2        66.660    125.778     15.00     2.130 00 !
CG2O1    NG2S2    HGP1        68.885    119.024                        !
HGP1     NG2S2    HGP1        54.270    120.770                        !
CG311    NG321    HGPAM2      60.020    113.793                        !
HGPAM2   NG321    HGPAM2      50.154    109.943                        !

DIHEDRALS
NG2S2      CG2O1    CG311    CG311      0.0000    1      0.00    !
NG2S2      CG2O1    CG311    CG331      0.0000    1      0.00    !
NG2S2      CG2O1    CG311    CG331      0.0000    1      0.00    !
NG2S2      CG2O1    CG311    CG331      0.0000    1      0.00    !
NG2S2      CG2O1    CG311    HGA1       0.0000    1      0.00    !
NG2S2      CG2O1    CG311    HGA1       0.0000    1      0.00    !
NG2S2      CG2O1    CG311    HGA1       0.0000    1      0.00    !
OG2D1      CG2O1    CG311    CG311      1.4000    1      0.00    !
OG2D1      CG2O1    CG311    CG331      1.4000    1      0.00    !
OG2D1      CG2O1    CG311    CG331      1.4000    1      0.00    !
OG2D1      CG2O1    CG311    CG331      1.4000    1      0.00    !
OG2D1      CG2O1    CG311    CG331      1.4000    1      0.00    !
OG2D1      CG2O1    CG311    HGA1       0.0000    1      0.00    !
OG2D1      CG2O1    CG311    HGA1       0.0000    1      0.00    !
OG2D1      CG2O1    CG311    HGA1       0.0000    1      0.00    !
CG311      CG2O1    NG2S2    HGP1       2.5000    2    180.00    !
CG311      CG2O1    NG2S2    HGP1       2.5000    2    180.00    !
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CG311     CG2O1   NG2S2   HGP1      2.5000   2      180.00   !
OG2D1     CG2O1   NG2S2   HGP1      1.4000   2      180.00   !
NG2R52    CG2R53  CG311   CG311     0.1900   3        0.00   !
NG2R52    CG2R53  CG311   CG311     0.1900   3        0.00   !
NG2R52    CG2R53  CG311   NG321     0.1900   3        0.00   !
NG2R52    CG2R53  CG311   HGA1      0.1900   3        0.00   !
CG311     CG2R53  NG2R52  CG2RC0    2.5000   2      180.00   !
CG311     CG2R53  NG2R52  HGP2      3.0000   2      180.00   !
NG2R52    CG2R53  NG2R52  CG2RC0   12.0000   2      180.00   !
NG2R52    CG2R53  NG2R52  CG2RC0   12.0000   2      180.00   !
NG2R52    CG2R53  NG2R52  HGP2      1.4000   2      180.00   !
CG2R61    CG2R61  CG2R61  CG2R61    3.1000   2      180.00   !
CG2R61    CG2R61  CG2R61  CG2RC0    3.0000   2      180.00   !
CG2R61    CG2R61  CG2R61  CG301     3.1000   2      180.00   !
CG2R61    CG2R61  CG2R61  HGR61     4.2000   2      180.00   !
CG2RC0    CG2R61  CG2R61  CG301     3.1000   2      180.00   !
CG2RC0    CG2R61  CG2R61  HGR61     3.0000   2      180.00   !
CG2RC0    CG2R61  CG2R61  HGR61     3.0000   2      180.00   !
CG301     CG2R61  CG2R61  HGR61     2.4000   2      180.00   !
CG301     CG2R61  CG2R61  HGR61     2.4000   2      180.00   !
HGR61     CG2R61  CG2R61  HGR61     2.4000   2      180.00   !
CG2R61    CG2R61  CG2RC0  CG2RC0    3.0000   2      180.00   !
CG2R61    CG2R61  CG2RC0  NG2R52    1.5000   2      180.00   !
HGR61     CG2R61  CG2RC0  CG2RC0    3.0000   2      180.00   !
HGR61     CG2R61  CG2RC0  CG2RC0    3.0000   2      180.00   !
HGR61     CG2R61  CG2RC0  NG2R52    0.8000   2      180.00   !
CG2R61    CG2R61  CG301   CG331     0.2300   2      180.00   !
CG2R61    CG2RC0  CG2RC0  CG2R61    3.0000   2      180.00   !
CG2R61    CG2RC0  CG2RC0  NG2R52    1.5000   2      180.00   !
NG2R52    CG2RC0  CG2RC0  NG2R52   10.0000   2      180.00   !
CG2R61    CG2RC0  NG2R52  CG2R53   12.0000   2      180.00   !
CG2R61    CG2RC0  NG2R52  HGP2      1.4000   2      180.00   !
CG2RC0    CG2RC0  NG2R52  CG2R53   12.0000   2      180.00   !
CG2RC0    CG2RC0  NG2R52  HGP2      1.4000   2      180.00   !
CG2R61    CG301   CG331   HGA3      0.0400   3        0.00   !
CG331     CG301   CG331   HGA3      0.1600   3        0.00   !
CG2O1     CG311   CG311   CG2R53    0.2000   3        0.00   !
CG2O1     CG311   CG311   CG2R53    0.2000   3        0.00   !
CG2O1     CG311   CG311   CG2R53    0.2000   3        0.00   !
CG2O1     CG311   CG311   NG321     0.2000   3        0.00   !
CG2O1     CG311   CG311   HGA1      0.2000   3        0.00   !
CG2R53    CG311   CG311   CG331     0.0400   3        0.00   !
CG2R53    CG311   CG311   CG331     0.0400   3        0.00   !
CG2R53    CG311   CG311   CG331     0.0400   3        0.00   !
CG2R53    CG311   CG311   HGA1      0.2000   3        0.00   !
CG331     CG311   CG311   NG321     0.2000   3        0.00   !
CG331     CG311   CG311   HGA1      0.1950   3        0.00   !
NG321     CG311   CG311   HGA1      0.1600   3        0.00   !
HGA1      CG311   CG311   HGA1      0.1950   3        0.00   !
CG2O1     CG311   CG331   HGA3      0.2000   3        0.00   !
CG311     CG311   CG331   HGA3      0.2000   3        0.00   !
HGA1      CG311   CG331   HGA3      0.1950   3        0.00   !
CG2R53    CG311   NG321   HGPAM2    0.1600   3        0.00   !
CG311     CG311   NG321   HGPAM2    0.1000   3        0.00   !
HGA1      CG311   NG321   HGPAM2    0.0100   3        0.00   !
HGA1      CG311   NG321   HGPAM2    0.0100   3        0.00   !
HGA1      CG311   NG321   HGPAM2    0.0100   3        0.00   !

IMPROPERS
CG2O1     CG311   NG2S2   OG2D1   120.0000   0        0.00   !
```

```
END
RETURN


# Lidocaine
#
# Topology
36 1
RESI          LDC       0.000
GROUP
ATOM CA       CG2R61   −0.115   !
ATOM HA       HGR61     0.115   !
ATOM CB       CG2R61    0.034   !
ATOM CC       CG2R61   −0.131   !
ATOM CD       CG2R61    0.034   !
ATOM CE       CG2R61   −0.115   !
ATOM HE       HGR61     0.115   !
ATOM CF       CG2R61   −0.115   !
ATOM HF       HGR61     0.115   !
ATOM CG       CG331    −0.270   !
ATOM HG1      HGA3      0.090   !
ATOM HG2      HGA3      0.090   !
ATOM HG3      HGA3      0.090   !
ATOM CH       CG331    −0.270   !
ATOM HH1      HGA3      0.090   !
ATOM HH2      HGA3      0.090   !
ATOM HH3      HGA3      0.090   !
ATOM NA       NG2S1    −0.117   !
ATOM HN       HGP1      0.177   !
ATOM CI       CG2O1     0.673   !
ATOM O        OG2D1    −0.511   !
ATOM CJ       CG321    −0.206   !
ATOM HJ1      HGA2      0.090   !
ATOM HJ2      HGA2      0.090   !
ATOM NB       NG301    −0.369   !
ATOM CK       CG321    −0.062   !
ATOM HK1      HGA2      0.090   !
ATOM HK2      HGA2      0.090   !
ATOM CL       CG331    −0.270   !
ATOM HL1      HGA3      0.090   !
ATOM HL2      HGA3      0.090   !
ATOM HL3      HGA3      0.090   !
ATOM CM       CG321    −0.062   !
ATOM HM1      HGA2      0.090   !
ATOM HM2      HGA2      0.090   !
ATOM CN       CG331    −0.270   !
ATOM HN1      HGA3      0.090   !
ATOM HN2      HGA3      0.090   !
ATOM HN3      HGA3      0.090   !
                                !  Bond order
BOND HL2      CL                !  1
BOND HL1      CL                !  1
BOND CL       HL3               !  1
BOND CL       CK                !  1
BOND HF       CF                !  1
BOND HE       CE                !  1
BOND HH2      CH                !  1
BOND HK1      CK                !  1
BOND HN1      CN                !  1
BOND O        CI                !  2
BOND CF       CE                !  1
BOND CF       CA                !  2
```

```
BOND CE       CD              !  2
BOND CK       NB              !  1
BOND CK       HK2             !  1
BOND HN3      CN              !  1
BOND HA       CA              !  1
BOND CA       CB              !  1
BOND HG2      CG              !  1
BOND CD       CH              !  1
BOND CD       CC              !  1
BOND CH       HH3             !  1
BOND CH       HH1             !  1
BOND CN       HN2             !  1
BOND CN       CM              !  1
BOND NB       CM              !  1
BOND NB       CJ              !  1
BOND CB       CC              !  2
BOND CB       CG              !  1
BOND CC       NA              !  1
BOND CI       NA              !  1
BOND CI       CJ              !  1
BOND CG       HG1             !  1
BOND CG       HG3             !  1
BOND NA       HN              !  1
BOND CM       HM1             !  1
BOND CM       HM2             !  1
BOND CJ       HJ2             !  1
BOND CJ       HJ1             !  1
IMPR CI       CJ         NA     0

END

# Parameters
BONDS
CG2O1          CG321      283.302     1.529   !
CG2O1          NG2S1      447.022     1.378   !
CG2O1          OG2D1      811.230     1.227   !
CG2R61         CG2R61     362.949     1.370   !
CG2R61         CG331      296.511     1.504   !
CG2R61         NG2S1      414.059     1.408   !
CG2R61         HGR61      351.466     1.088   !
CG321          CG331      299.955     1.524   !
CG321          NG301      344.534     1.455   !
CG321          HGA2       335.089     1.099   !
CG331          HGA3       353.752     1.096   !
NG2S1          HGP1       476.127     1.011   !

ANGLES
CG321    CG2O1    NG2S1      105.549     113.166                      !
CG321    CG2O1    OG2D1      112.568     124.575                      !
NG2S1    CG2O1    OG2D1      115.192     122.381                      !
CG2R61   CG2R61   CG2R61      56.245     120.124      35.00     2.41620
CG2R61   CG2R61   CG331       78.777     120.347                      !
CG2R61   CG2R61   NG2S1      104.758     120.284      35.00     2.41620
CG2R61   CG2R61   HGR61       38.995     120.551      22.00     2.15250
CG2O1    CG321    NG301      111.427     112.321                      !
CG2O1    CG321    HGA2        60.577     107.631      30.00     2.16300
CG331    CG321    NG301      103.252     114.594                      !
CG331    CG321    HGA2        62.507     109.296      22.53     2.17900
NG301    CG321    HGA2        71.957     109.154      50.00     2.13000
HGA2     CG321    HGA2        60.371     106.683       5.40     1.80200
CG2R61   CG331    HGA3        34.012     109.403                      !
CG321    CG331    HGA3        65.438     110.764      22.53     2.17900
HGA3     CG331    HGA3        45.274     108.130       5.40     1.80200
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CG2O1    NG2S1    CG2R61     50.000    120.000                    !
CG2O1    NG2S1    HGP1       59.055    118.293                    !
CG2R61   NG2S1    HGP1       34.000    117.000                    !
CG321    NG3O1    CG321     113.117    112.307                    !

DIHEDRALS
NG2S1       CG2O1    CG321    NG3O1       0.2610   1       180.00    !
NG2S1       CG2O1    CG321    NG3O1       0.3360   2       180.00    !
NG2S1       CG2O1    CG321    NG3O1       0.1750   4         0.00    !
NG2S1       CG2O1    CG321    HGA2        1.3850   2         0.00    !
NG2S1       CG2O1    CG321    HGA2        0.1090   3         0.00    !
NG2S1       CG2O1    CG321    HGA2        0.1720   4       180.00    !
OG2D1       CG2O1    CG321    NG3O1       0.3680   1       180.00    !
OG2D1       CG2O1    CG321    NG3O1       0.1740   2       180.00    !
OG2D1       CG2O1    CG321    NG3O1       0.1150   3         0.00    !
OG2D1       CG2O1    CG321    HGA2        0.1540   1       180.00    !
OG2D1       CG2O1    CG321    HGA2        0.4100   2         0.00    !
OG2D1       CG2O1    CG321    HGA2        0.2320   3         0.00    !
CG321       CG2O1    NG2S1    CG2R61      1.4210   1       180.00    !
CG321       CG2O1    NG2S1    CG2R61      2.7860   2       180.00    !
CG321       CG2O1    NG2S1    CG2R61      0.8350   3         0.00    !
CG321       CG2O1    NG2S1    CG2R61      0.2810   6         0.00    !
CG321       CG2O1    NG2S1    HGP1        0.7270   1       180.00    !
CG321       CG2O1    NG2S1    HGP1        2.7860   2       180.00    !
CG321       CG2O1    NG2S1    HGP1        0.9760   3         0.00    !
OG2D1       CG2O1    NG2S1    CG2R61      1.3870   1       180.00    !
OG2D1       CG2O1    NG2S1    CG2R61      3.0000   2       180.00    !
OG2D1       CG2O1    NG2S1    CG2R61      0.6580   3       180.00    !
OG2D1       CG2O1    NG2S1    CG2R61      0.4180   4       180.00    !
OG2D1       CG2O1    NG2S1    CG2R61      0.5920   6         0.00    !
OG2D1       CG2O1    NG2S1    HGP1        3.0000   2       180.00    !
OG2D1       CG2O1    NG2S1    HGP1        0.9820   3       180.00    !
OG2D1       CG2O1    NG2S1    HGP1        1.2130   4       180.00    !
OG2D1       CG2O1    NG2S1    HGP1        0.5120   6         0.00    !
CG2R61      CG2R61   CG2R61   CG2R61      2.9110   2       180.00    !
CG2R61      CG2R61   CG2R61   CG331       1.7120   3         0.00    !
CG2R61      CG2R61   CG2R61   NG2S1       3.0000   3         0.00    !
CG2R61      CG2R61   CG2R61   HGR61       2.6800   3         0.00    !
CG331       CG2R61   CG2R61   NG2S1       0.4040   3         0.00    !
CG331       CG2R61   CG2R61   HGR61       2.9570   3       180.00    !
HGR61       CG2R61   CG2R61   HGR61       0.1890   2       180.00    !
CG2R61      CG2R61   CG331    HGA3        2.9990   2         0.00    !
CG2R61      CG2R61   CG331    HGA3        0.5740   3       180.00    !
CG2R61      CG2R61   NG2S1    CG2O1       0.6460   3       180.00    !
CG2R61      CG2R61   NG2S1    CG2O1       0.4270   4         0.00    !
CG2R61      CG2R61   NG2S1    CG2O1       0.1630   6         0.00    !
CG2R61      CG2R61   NG2S1    HGP1        1.5830   3       180.00    !
CG2R61      CG2R61   NG2S1    HGP1        0.5190   4         0.00    !
NG3O1       CG321    CG331    HGA3        0.4530   3         0.00    !
HGA2        CG321    CG331    HGA3        0.0220   3       180.00    !
CG2O1       CG321    NG3O1    CG321       0.5510   2       180.00    !
CG2O1       CG321    NG3O1    CG321       0.7360   3         0.00    !
CG331       CG321    NG3O1    CG321       0.1190   3         0.00    !
HGA2        CG321    NG3O1    CG321       0.8070   1       180.00    !
HGA2        CG321    NG3O1    CG321       0.5610   2       180.00    !
HGA2        CG321    NG3O1    CG321       0.3270   3         0.00    !

IMPROPERS
CG2O1       CG321    NG2S1    OG2D1     120.0000   0         0.00    !

END
RETURN
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```
# Charged Lidocaine
#
# Topology
36 1
RESI                LDN       0.000
GROUP
ATOM CA             CG2R61   −0.115   !
ATOM HA             HGR61     0.115   !
ATOM CB             CG2R61    0.034   !
ATOM CC             CG2R61   −0.131   !
ATOM CD             CG2R61    0.034   !
ATOM CE             CG2R61   −0.115   !
ATOM HE             HGR61     0.115   !
ATOM CF             CG2R61   −0.115   !
ATOM HF             HGR61     0.115   !
ATOM CG             CG331    −0.270   !
ATOM HG1            HGA3      0.090   !
ATOM HG2            HGA3      0.090   !
ATOM HG3            HGA3      0.090   !
ATOM CH             CG331    −0.270   !
ATOM HH1            HGA3      0.090   !
ATOM HH2            HGA3      0.090   !
ATOM HH3            HGA3      0.090   !
ATOM NA             NG2S1    −0.117   !
ATOM HNA            HGP1      0.209   !
ATOM CI             CG2O1     0.469   !
ATOM O              OG2D1    −0.360   !
ATOM CJ             CG324    −0.023   !
ATOM HJ1            HGA2      0.090   !
ATOM HJ2            HGA2      0.090   !
ATOM NB             NG3P1     0.022   !
ATOM HNB            HGP2      0.031   !
ATOM CK             CG324     0.146   !
ATOM HK1            HGA2      0.090   !
ATOM HK2            HGA2      0.090   !
ATOM CL             CG331    −0.270   !
ATOM HL1            HGA3      0.090   !
ATOM HL2            HGA3      0.090   !
ATOM HL3            HGA3      0.090   !
ATOM CM             CG324     0.146   !
ATOM HM1            HGA2      0.090   !
ATOM HM2            HGA2      0.090   !
ATOM CN             CG331    −0.270   !
ATOM HN1            HGA3      0.090   !
ATOM HN2            HGA3      0.090   !
ATOM HN3            HGA3      0.090   !
                                      !  Bond order
BOND HL2            CL                !  1
BOND HL1            CL                !  1
BOND HL3            CL                !  1
BOND CL             CK                !  1
BOND HF             CF                !  1
BOND HE             CE                !  1
BOND HH2            CH                !  1
BOND O              CI                !  2
BOND CE             CF                !  1
BOND CE             CD                !  2
BOND CF             CA                !  2
BOND HNB            NB                !  1
BOND HN3            CN                !  1
BOND HH3            CH                !  1
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```
BOND CA               HA                !  1
BOND CA               CB                !  1
BOND CD               CH                !  1
BOND CD               CC                !  1
BOND CH               HH1               !  1
BOND CK               HK1               !  1
BOND CK               NB                !  1
BOND CK               HK2               !  1
BOND HM2              CM                !  1
BOND NB               CM                !  1
BOND NB               CJ                !  1
BOND CI               NA                !  1
BOND CI               CJ                !  1
BOND CC               CB                !  2
BOND CC               NA                !  1
BOND CB               CG                !  1
BOND CN               CM                !  1
BOND CN               HN2               !  1
BOND CN               HN1               !  1
BOND HG2              CG                !  1
BOND CM               HM1               !  1
BOND HG1              CG                !  1
BOND NA               HNA               !  1
BOND CG               HG3               !  1
BOND CJ               HJ2               !  1
BOND CJ               HJ1               !  1
IMPR CI               CJ          NA    0

END

# Parameters
BONDS
CG2O1          CG324      323.888     1.535   !
CG2O1          NG2S1      535.640     1.341   !
CG2O1          OG2D1      729.461     1.241   !
CG2R61         CG2R61     332.977     1.370   !
CG2R61         CG331      289.678     1.503   !
CG2R61         NG2S1      338.950     1.440   !
CG2R61         HGR61      360.459     1.086   !
CG324          CG331      323.154     1.512   !
CG324          NG3P1      325.738     1.487   !
CG324          HGA2       352.740     1.092   !
CG331          HGA3       352.341     1.093   !
NG2S1          HGP1       438.739     1.017   !
NG3P1          HGP2       343.255     1.049   !

ANGLES
CG324    CG2O1    NG2S1      96.822    116.009                        !
CG324    CG2O1    OG2D1     149.268    117.737                        !
NG2S1    CG2O1    OG2D1     126.403    126.028                        !
CG2R61   CG2R61   CG2R61     84.906    120.031     35.00    2.416 20 !
CG2R61   CG2R61   CG331      80.855    121.549                        !
CG2R61   CG2R61   NG2S1     154.638    118.312     35.00    2.416 20 !
CG2R61   CG2R61   HGR61      57.543    119.563     22.00    2.152 50 !
CG2O1    CG324    NG3P1     150.551    105.020                        !
CG2O1    CG324    HGA2       67.219    112.119     30.00    2.163 00 !
CG331    CG324    NG3P1     107.723    111.740                        !
CG331    CG324    HGA2       71.584    111.479     22.53    2.179 00 !
NG3P1    CG324    HGA2       85.454    106.888     35.00    2.101 00 !
HGA2     CG324    HGA2       80.115    108.969      5.40    1.802 00 !
CG2R61   CG331    HGA3       66.094    110.852                        !
CG324    CG331    HGA3       71.642    110.758     22.53    2.179 00 !
HGA3     CG331    HGA3       65.907    108.379      5.40    1.802 00 !
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CG2O1    NG2S1    CG2R61     92.346     123.641                    !
CG2O1    NG2S1    HGP1      111.348     118.502                    !
CG2R61   NG2S1    HGP1      101.233     117.959                    !
CG324    NG3P1    CG324     108.858     112.617                    !
CG324    NG3P1    HGP2       78.873     106.051     27.00   2.074 00 !

DIHEDRALS
NG2S1       CG2O1    CG324    NG3P1      2.9920   1        0.00    !
NG2S1       CG2O1    CG324    NG3P1      2.2150   2      180.00    !
NG2S1       CG2O1    CG324    NG3P1      0.3430   4        0.00    !
NG2S1       CG2O1    CG324    HGA2       0.8640   2      180.00    !
OG2D1       CG2O1    CG324    NG3P1      0.5650   3      180.00    !
OG2D1       CG2O1    CG324    HGA2       0.7990   2        0.00    !
CG324       CG2O1    NG2S1    CG2R61     1.0950   1      180.00    !
CG324       CG2O1    NG2S1    CG2R61     0.1810   2      180.00    !
CG324       CG2O1    NG2S1    CG2R61     0.9480   3        0.00    !
CG324       CG2O1    NG2S1    CG2R61     1.3220   4      180.00    !
CG324       CG2O1    NG2S1    HGP1       3.0000   1      180.00    !
CG324       CG2O1    NG2S1    HGP1       3.0000   2      180.00    !
CG324       CG2O1    NG2S1    HGP1       0.9030   3        0.00    !
OG2D1       CG2O1    NG2S1    CG2R61     2.9990   2      180.00    !
OG2D1       CG2O1    NG2S1    CG2R61     1.5540   4      180.00    !
OG2D1       CG2O1    NG2S1    CG2R61     0.6260   6        0.00    !
OG2D1       CG2O1    NG2S1    HGP1       3.0000   2      180.00    !
CG2R61      CG2R61   CG2R61   CG2R61     1.3610   2      180.00    !
CG2R61      CG2R61   CG2R61   CG331      2.7620   3        0.00    !
CG2R61      CG2R61   CG2R61   NG2S1      3.0000   3        0.00    !
CG2R61      CG2R61   CG2R61   HGR61      1.2930   3        0.00    !
CG331       CG2R61   CG2R61   NG2S1      1.0250   3      180.00    !
CG331       CG2R61   CG2R61   HGR61      2.5640   3      180.00    !
HGR61       CG2R61   CG2R61   HGR61      3.0000   3      180.00    !
CG2R61      CG2R61   CG331    HGA3       0.6190   3      180.00    !
CG2R61      CG2R61   CG331    HGA3       0.0450   6        0.00    !
CG2R61      CG2R61   NG2S1    CG2O1      0.1160   2        0.00    !
CG2R61      CG2R61   NG2S1    HGP1       0.7030   2      180.00    !
NG3P1       CG324    CG331    HGA3       0.4210   3        0.00    !
HGA2        CG324    CG331    HGA3       0.0020   3        0.00    !
CG2O1       CG324    NG3P1    CG324      1.4760   1        0.00    !
CG2O1       CG324    NG3P1    HGP2       0.2400   2      180.00    !
CG331       CG324    NG3P1    CG324      0.7060   1        0.00    !
CG331       CG324    NG3P1    CG324      0.8200   2        0.00    !
CG331       CG324    NG3P1    CG324      0.5760   3        0.00    !
CG331       CG324    NG3P1    HGP2       0.1100   3        0.00    !
HGA2        CG324    NG3P1    CG324      0.0220   3        0.00    !
HGA2        CG324    NG3P1    HGP2       1.9910   2      180.00    !

IMPROPERS
CG2O1       CG324    NG2S1    OG2D1    120.0000   0        0.00    !

END
RETURN


# Carbamazepine
#
# Topology
36 1
RESI              CBZ        0.000
GROUP
ATOM C1           CG2R61    −0.108   !
ATOM H1           HGR61      0.115   !
ATOM C2           CG2R61    −0.115   !
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ATOM H2          HGR61     0.115  !
ATOM C3          CG2R61   −0.115  !
ATOM H3          HGR61     0.115  !
ATOM C4          CG2R61   −0.088  !
ATOM H4          HGR61     0.115  !
ATOM C5          CG2R61    0.072  !
ATOM C6          CG2R71   −0.258  !
ATOM H6          HGR71     0.184  !
ATOM C7          CG2R71   −0.258  !
ATOM H7          HGR71     0.184  !
ATOM C8          CG2R61    0.072  !
ATOM C9          CG2R61   −0.088  !
ATOM H8          HGR61     0.115  !
ATOM C10         CG2R61   −0.115  !
ATOM H10         HGR61     0.115  !
ATOM C11         CG2R61   −0.115  !
ATOM H11         HGR61     0.115  !
ATOM C12         CG2R61   −0.108  !
ATOM H12         HGR61     0.115  !
ATOM C13         CG2R61    0.039  !
ATOM N14         NG2S0    −0.097  !
ATOM C15         CG2R61    0.039  !
ATOM C16         CG2O6     0.828  !
ATOM O17         OG2D1    −0.614  !
ATOM N18         NG2S2    −0.941  !
ATOM H181        HGP1      0.341  !
ATOM H182        HGP1      0.341  !
                                  !  Bond order
BOND H2          C2               !  1
BOND H11         C11              !  1
BOND H1          C1               !  1
BOND H12         C12              !  1
BOND C2          C1               !  2
BOND C2          C3               !  1
BOND C11         C12              !  1
BOND C11         C10              !  2
BOND C1          C15              !  1
BOND C12         C13              !  2
BOND H3          C3               !  1
BOND H10         C10              !  1
BOND C3          C4               !  2
BOND C10         C9               !  1
BOND C15         N14              !  1
BOND C15         C5               !  2
BOND C13         N14              !  1
BOND C13         C8               !  1
BOND N14         C16              !  1
BOND C4          C5               !  1
BOND C4          H4               !  1
BOND C9          C8               !  2
BOND C9          H8               !  1
BOND C5          C6               !  1
BOND C8          C7               !  1
BOND C16         O17              !  2
BOND C16         N18              !  1
BOND N18         H181             !  1
BOND N18         H182             !  1
BOND C6          C7               !  2
BOND C6          H6               !  1
BOND C7          H7               !  1
IMPR C16         N14      N18      O17
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IMPR N            H5       H 6      C6
IMPR C7           C3       O 1      O2

END

# Parameters
BONDS
CG2O6          NG2S0      391.169     1.355   !
CG2O6          NG2S2      441.546     1.358   !
CG2O6          OG2D1      767.402     1.241   !
CG2R61         CG2R61     357.930     1.337   !
CG2R61         CG2R71     241.523     1.446   !
CG2R61         NG2S0      279.960     1.400   !
CG2R61         HGR61      361.428     1.078   !
CG2R71         CG2R71     508.209     1.355   !
CG2R71         HGR71      357.536     1.076   !
NG2S2          HGP1       430.906     1.012   !

ANGLES
NG2S0    CG2O6    NG2S2      168.682     114.091                      !
NG2S0    CG2O6    OG2D1      135.886     122.807                      !
NG2S2    CG2O6    OG2D1      132.320     123.396     50.00     2.37000
CG2R61   CG2R61   CG2R61      35.667     120.875     35.00     2.41620
CG2R61   CG2R61   CG2R71     152.183     120.373                      !
CG2R61   CG2R61   NG2S0       52.193     119.348     35.00     2.41620
CG2R61   CG2R61   HGR61       53.543     121.203     22.00     2.15250
CG2R61   CG2R71   CG2R71     128.134     126.881                      !
CG2R61   CG2R71   HGR71       85.272     114.546                      !
CG2R71   CG2R71   HGR71       76.806     118.684                      !
CG2O6    NG2S0    CG2R61      85.103     120.844                      !
CG2R61   NG2S0    CG2R61     151.009     116.746                      !
CG2O6    NG2S2    HGP1       101.309     114.361                      !
HGP1     NG2S2    HGP1        51.136     114.325                      !

DIHEDRALS
NG2S2       CG2O6    NG2S0    CG2R61      2.9980   1      0.00   !
NG2S2       CG2O6    NG2S0    CG2R61      3.0000   2    180.00   !
NG2S2       CG2O6    NG2S0    CG2R61      0.6410   3      0.00   !
NG2S2       CG2O6    NG2S0    CG2R61      0.7230   4      0.00   !
OG2D1       CG2O6    NG2S0    CG2R61      0.0170   3    180.00   !
NG2S0       CG2O6    NG2S2    HGP1        1.1300   2    180.00   !
OG2D1       CG2O6    NG2S2    HGP1        2.4440   1      0.00   !
OG2D1       CG2O6    NG2S2    HGP1        2.9860   2    180.00   !
OG2D1       CG2O6    NG2S2    HGP1        0.4270   3    180.00   !
CG2R61      CG2R61   CG2R61   CG2R61      2.7260   2    180.00   !
CG2R61      CG2R61   CG2R61   CG2R71      0.7890   3      0.00   !
CG2R61      CG2R61   CG2R61   NG2S0       2.4190   3      0.00   !
CG2R61      CG2R61   CG2R61   HGR61       0.8260   3      0.00   !
CG2R71      CG2R61   CG2R61   NG2S0       2.9970   2    180.00   !
CG2R71      CG2R61   CG2R61   HGR61       2.9100   3    180.00   !
NG2S0       CG2R61   CG2R61   HGR61       2.6690   3    180.00   !
HGR61       CG2R61   CG2R61   HGR61       2.9990   2    180.00   !
HGR61       CG2R61   CG2R61   HGR61       1.6090   3    180.00   !
CG2R61      CG2R61   CG2R71   CG2R71      1.5590   2    180.00   !
CG2R61      CG2R61   CG2R71   HGR71       3.0000   2    180.00   !
CG2R61      CG2R61   CG2R71   HGR71       2.9990   3    180.00   !
CG2R61      CG2R61   CG2R71   HGR71       1.5680   4      0.00   !
CG2R61      CG2R61   NG2S0    CG2O6       1.8140   3    180.00   !
CG2R61      CG2R61   NG2S0    CG2R61      1.3370   3      0.00   !
CG2R61      CG2R71   CG2R71   CG2R61      2.1970   2      0.00   !
CG2R61      CG2R71   CG2R71   HGR71       1.0580   3      0.00   !
HGR71       CG2R71   CG2R71   HGR71       3.0000   2    180.00   !

IMPROPERS
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CG206       NG2S0    NG2S2    OG2D1       80.0000    0           0.00 !

END
RETURN


# Lamotrigine
#
# Topology
36 1
RESI            LMT       0.000
GROUP
ATOM C1         CG2R64     0.761   !
ATOM N1         NG2S3     −0.508   !
ATOM H1         HGP4       0.260   !
ATOM H2         HGP4       0.260   !
ATOM N2         NG2R62    −0.698   !
ATOM C2         CG2R64     0.297   !
ATOM N3         NG2S3     −0.335   !
ATOM H3         HGP4       0.284   !
ATOM H4         HGP4       0.284   !
ATOM N4         NG2R62    −0.443   !
ATOM N5         NG2R62    −0.417   !
ATOM C3         CG2R67     0.077   !
ATOM C4         CG2R67     0.401   !
ATOM C5         CG2R61    −0.115   !
ATOM H5         HGR62      0.115   !
ATOM C6         CG2R61    −0.115   !
ATOM H6         HGR61      0.115   !
ATOM C7         CG2R61    −0.115   !
ATOM H7         HGR61      0.115   !
ATOM C8         CG2R61    −0.412   !
ATOM CL         CLGR1     −0.105   !
ATOM C9         CG2R61     0.309   !
ATOM CL2        CLGR1     −0.015   !
                                   !  Bond order
BOND H1         N1                 !  1
BOND CL2        C9                 !  1
BOND CL         C8                 !  1
BOND N1         H2                 !  1
BOND N1         C1                 !  1
BOND C9         C8                 !  1
BOND C9         C5                 !  2
BOND C8         C3                 !  2
BOND C1         N2                 !  2
BOND C1         C4                 !  1
BOND N2         C2                 !  1
BOND H4         N3                 !  1
BOND H5         C5                 !  1
BOND C5         C6                 !  1
BOND C3         C4                 !  1
BOND C3         C7                 !  1
BOND C4         N5                 !  2
BOND C2         N3                 !  1
BOND C2         N4                 !  2
BOND N3         H3                 !  1
BOND C6         C7                 !  2
BOND C6         H6                 !  1
BOND C7         H7                 !  1
BOND N5         N4                 !  1
IMPR C1         C4       N 2       N1
IMPR N1         H1       H 2       C1
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IMPR C2         N2       N 4       N3
IMPR N3         H3       H 4       C2

END

# Parameters
BONDS
CG2R61          CG2R61     390.348     1.375   !
CG2R61          CG2R67     384.918     1.402   !
CG2R61          CLGR1      273.039     1.729   !
CG2R61          HGR61      412.122     1.086   !
CG2R64          CG2R67     442.307     1.381   !
CG2R64          NG2R62     503.979     1.330   !
CG2R64          NG2S3      522.544     1.378   !
CG2R67          CG2R67     431.369     1.476   !
CG2R67          NG2R62     425.802     1.319   !
NG2R62          NG2R62     466.829     1.317   !
NG2S3           HGP4       523.145     1.018   !

ANGLES
CG2R61   CG2R61   CG2R61      70.714     120.206      35.00      2.416 20 !
CG2R61   CG2R61   CG2R67     287.027     120.418                          !
CG2R61   CG2R61   CLGR1      134.935     119.945                          !
CG2R61   CG2R61   HGR61      103.957     120.342      22.00      2.152 50 !
CG2R67   CG2R61   CLGR1      135.126     119.611                          !
CG2R67   CG2R61   HGR61      209.832     118.452                          !
CG2R67   CG2R64   NG2R62     262.195     120.240                          !
CG2R67   CG2R64   NG2S3      231.259     122.622                          !
NG2R62   CG2R64   NG2R62     152.933     127.074                          !
NG2R62   CG2R64   NG2S3      208.081     117.665                          !
CG2R61   CG2R67   CG2R61     124.657     119.795                          !
CG2R61   CG2R67   CG2R67     183.221     119.966                          !
CG2R64   CG2R67   CG2R67     246.276     122.587                          !
CG2R64   CG2R67   NG2R62     154.711     120.273                          !
CG2R67   CG2R67   NG2R62     204.104     115.578                          !
CG2R64   NG2R62   CG2R64     146.416     115.041                          !
CG2R64   NG2R62   NG2R62     145.406     117.331                          !
CG2R67   NG2R62   NG2R62     259.817     117.180                          !
CG2R64   NG2S3    HGP4       102.772     116.945                          !
HGP4     NG2S3    HGP4        87.737     118.061                          !

DIHEDRALS
CG2R61      CG2R61   CG2R61   CG2R61      2.8300   2      180.00     !
CG2R61      CG2R61   CG2R61   CG2R67      2.8300   2      180.00     !
CG2R61      CG2R61   CG2R61   CLGR1       3.0000   2      180.00     !
CG2R61      CG2R61   CG2R61   CLGR1       2.8580   3        0.00     !
CG2R61      CG2R61   CG2R61   CLGR1       0.5300   6        0.00     !
CG2R61      CG2R61   CG2R61   HGR61       1.9720   2      180.00     !
CG2R67      CG2R61   CG2R61   CLGR1       2.8860   3        0.00     !
CG2R67      CG2R61   CG2R61   HGR61       2.9940   3        0.00     !
CLGR1       CG2R61   CG2R61   CLGR1       3.0000   3      180.00     !
HGR61       CG2R61   CG2R61   HGR61       3.0000   3      180.00     !
CG2R61      CG2R61   CG2R67   CG2R61      2.9680   2        0.00     !
CG2R61      CG2R61   CG2R67   CG2R67      2.9990   3        0.00     !
CLGR1       CG2R61   CG2R67   CG2R61      2.6520   3      180.00     !
CLGR1       CG2R61   CG2R67   CG2R67      3.0000   3      180.00     !
HGR61       CG2R61   CG2R67   CG2R61      2.8910   3        0.00     !
HGR61       CG2R61   CG2R67   CG2R67      0.9690   2      180.00     !
NG2R62      CG2R64   CG2R67   CG2R67      2.9990   2      180.00     !
NG2R62      CG2R64   CG2R67   NG2R62      1.9720   2        0.00     !
NG2S3       CG2R64   CG2R67   CG2R67      3.0000   3      180.00     !
NG2S3       CG2R64   CG2R67   CG2R67      0.7370   4      180.00     !
NG2S3       CG2R64   CG2R67   NG2R62      3.0000   2      180.00     !
CG2R67      CG2R64   NG2R62   CG2R64      2.3000   3      180.00     !
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NG2R62      CG2R64   NG2R62   CG2R64      3.0000   3        180.00    !
NG2R62      CG2R64   NG2R62   NG2R62      3.0000   2        180.00    !
NG2S3       CG2R64   NG2R62   CG2R64      2.9990   2        180.00    !
NG2S3       CG2R64   NG2R62   NG2R62      1.8400   2        180.00    !
CG2R67      CG2R64   NG2S3    HGP4        0.1070   2        180.00    !
NG2R62      CG2R64   NG2S3    HGP4        0.2750   2        180.00    !
G2R61       CG2R67   CG2R67   CG2R64      3.0000   1        180.00    !
CG2R61      CG2R67   CG2R67   CG2R64      1.1770   2        180.00    !
CG2R61      CG2R67   CG2R67   CG2R64      3.0000   3        180.00    !
CG2R61      CG2R67   CG2R67   NG2R62      2.9930   1          0.00    !
CG2R61      CG2R67   CG2R67   NG2R62      0.9920   2        180.00    !
CG2R61      CG2R67   CG2R67   NG2R62      2.9990   3          0.00    !
CG2R64      CG2R67   NG2R62   NG2R62      3.0000   3        180.00    !
CG2R67      CG2R67   NG2R62   NG2R62      3.0000   2        180.00    !
CG2R64      NG2R62   NG2R62   CG2R67      2.8410   3        180.00    !
HGR61       CG2R61   CG2R61   CLGR1       2.7230   3        180.00    !

IMPROPERS
CG2R64      CG2R67   NG2R62   NG2S3      60.0000   0          0.00    !
CG2R64      NG2R62   NG2R62   NG2S3      40.0000   0          0.00    !
NG2S3       HGP4     HGP4     CG2R64      9.0000   0          0.00    !

END
RETURN
```