Supporting Information

Nov. 8, 2013

Prepared for *JPCB*

Charge Transfer and Polarization for Bounded Chloride Ions in ClC Transport Proteins: Natural Bond Orbital and Energy Decomposition Analyses

Jonathan Church,[†] Soroosh Pezeshki, Christal Davis, and Hai Lin*

Chemistry Department, University of Colorado Denver, Denver, Colorado 80217-3364

[†]Current address: Chemistry Department, University of Colorado at Boulder.

* Email: hai.lin@ucdenver.edu, Phone: 303-352-3889, Fax: 303-556-4776

Table of Contents

Extrapolation of the MP2 Energies to the Complete Basis Set Limit

The geometries of chloride-amino acid model systems were optimized at the MP2/aug-cc-pVTZ level. Additional single-point MP2/aug-cc-pVDZ and MP2/aug-cc-pVQZ energy calculations were performed at the optimized geometries. The MP2 energies at the complete basis set (CBS) limit $E_{\mathrm{MP2}}^{\mathrm{CBS}}$ were extrapolated according to

$$E_{\mathrm{HF}}^{X} = E_{\mathrm{HF}}^{\mathrm{CBS}} + b\exp\left(-cX\right)$$

$$E_{\mathrm{corr}}^{X} = E_{\mathrm{corr}}^{\mathrm{CBS}} + \frac{a}{X^{3}}$$

$$E^{\mathrm{CBS}} = E_{\mathrm{HF}}^{\mathrm{CBS}} + E_{\mathrm{corr}}^{\mathrm{CBS}}$$

Here, E_{HF}^{X} is the Hartree-Fock (HF) energy and E_{corr}^{X} the correlation energy at the aug-cc-pV*X*Z (*X*=D, T, Q) basis set, $E_{\mathrm{HF}}^{\mathrm{CBS}}$ the HF energy and $E_{\mathrm{corr}}^{\mathrm{CBS}}$ the correlation energy at the CBS, *a*, *b*, and *c* are fitted parameters.

Construction of the ClC Active-Site Models

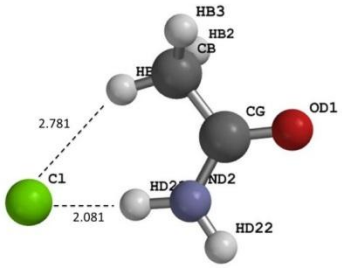
The active-site models were taken from those in our recent publication (Smith and Lin, (2011) *Chem. Phys. Lett.* 502, 112-117) and were modified as follows:

- Removed the benzene ring of F357, capped the methyl group with a hydrogen atom.
- Removed I356 side chain, capped Cα with a hydrogen atom.
- Removed P150, F348, P359, capped the dangling bond with a hydrogen atom.
- No changes to G106, S107, G108, I109, P110, K131, G146, R147, E148 (or Q148 in the mutant), G355, Y445, or the water molecules.

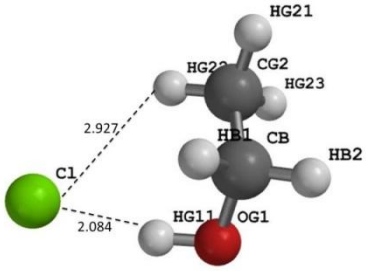
The resulted models are shown in Figure 3 of the paper for E148Q_Cl4 and in Figure S2 for the rest.

Figure S1. Additional Chloride-Amino Acid Complex Models. Color Code: Green, Chlorine; Yellow, Sulfur; Red, Oxygen; Black, Carbon; White, Hydrogen; and Blue, Nitrogen. Distance in Å.

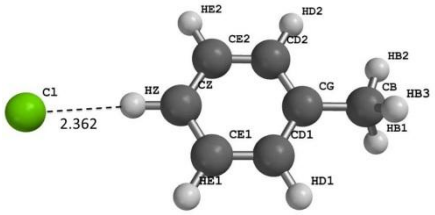
(a) ASN



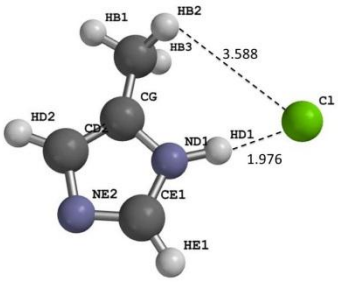
(b) THR



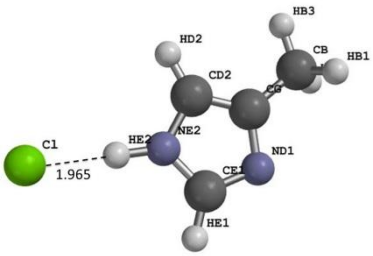
(c) PHE



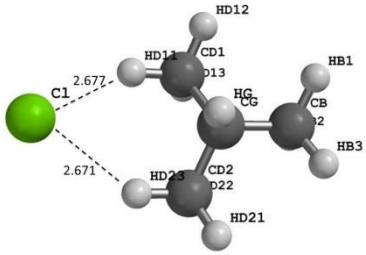
(d) HID



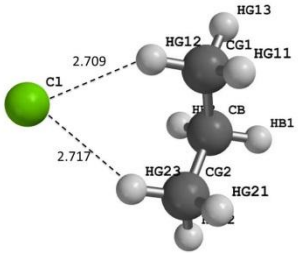
(e) HIE



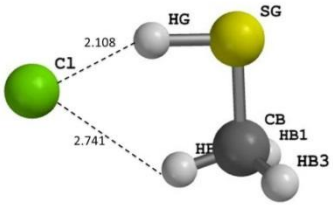
(f) LEU



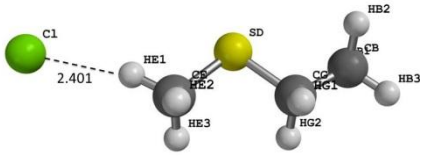
(g) VAL



(h) CYS



(i) MET



(j) LYS

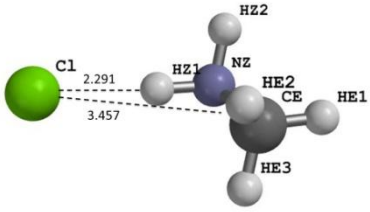


Figure S2. The (a) WT_Cl2, (b) PWT_Cl3, (c) PWT_Cl4, and (d) E148Q_Cl3 Models. Color Code: Green, Chlorine; Red, Oxygen; Black, Carbon; and Blue, Nitrogen.

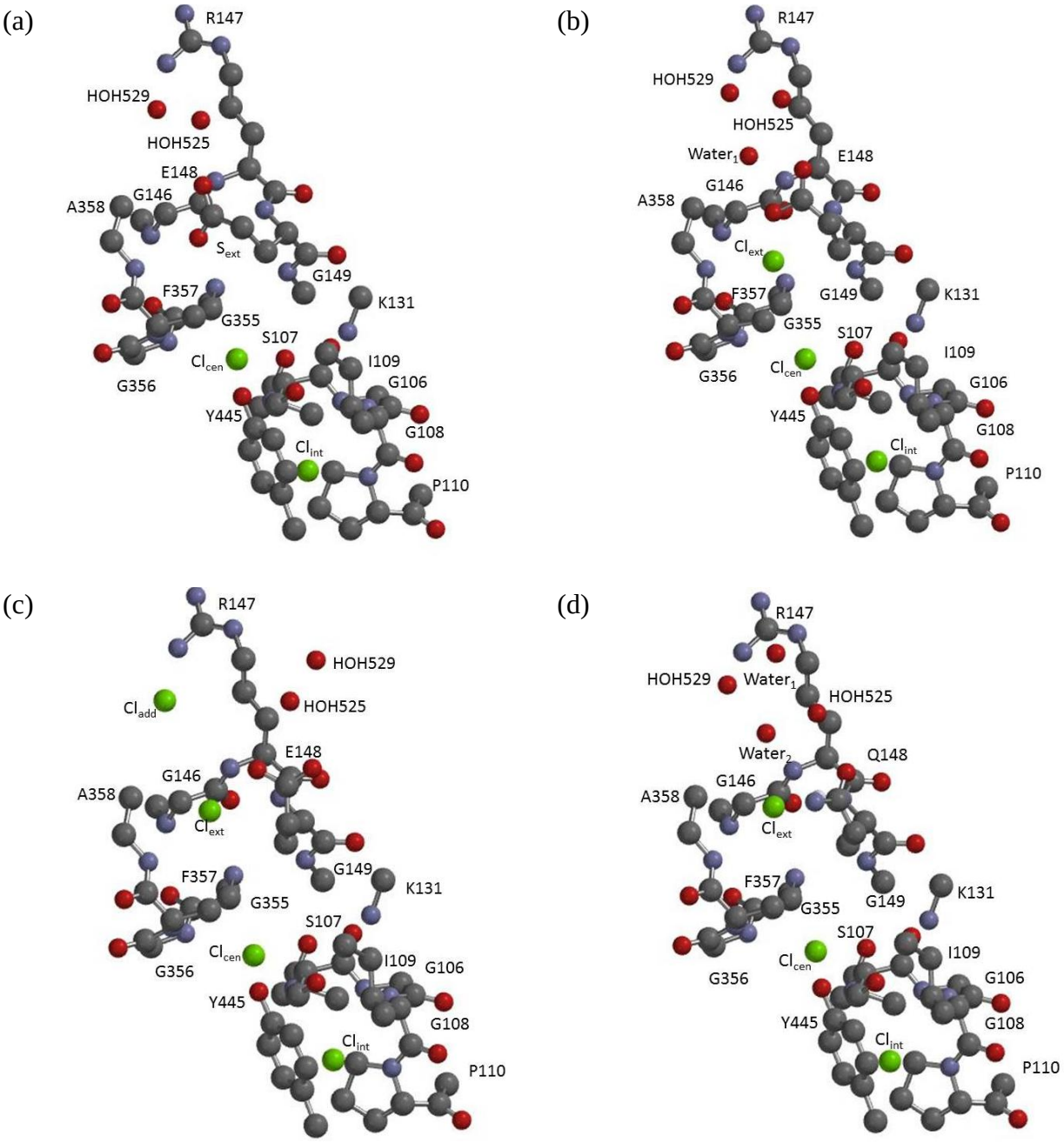


Table S1. NEDA Results for Chloride-Amino Acid Complexes by M06-2X Calculations. [a]

	BBN	ARG^+	LYS^+	GLN	SER	GLU	TYR	ILE
M06-2X/B1								
E_{ES}	-29.4	-96.3	-113.0	-29.6	-22.5	-28.8	-31.3	-6.7
E_{EX}	-8.5	-4.9	-7.3	-9.3	-7.0	-8.2	-9.7	-6.8
E_{PL}	-17.3	-11.0	-7.4	-16.5	-10.8	-12.9	-20.7	-16.4
E_{CT}	-41.8	-37.3	-36.2	-37.2	-32.8	-63.3	-54.7	-11.8
E_{DEF}(AA)	24.2	14.3	13.9	22.6	18.3	26.6	30.8	16.5
E_{DEF}(Cl)	48.7	34.4	37.3	45.3	37.6	63.1	60.1	19.0
E_{SE}(AA)	9.8	6.8	5.8	9.6	6.5	9.0	12.2	8.0
E_{SE}(Cl)	-1.8	-1.6	-2.3	-1.9	-1.5	-3.8	-2.7	-0.1
E_{EL}	-38.7	-102.1	-116.8	-38.4	-28.3	-36.1	-42.4	-15.2
E_{CORE}	56.4	38.7	40.9	50.8	43.9	75.9	71.7	20.8
E_{INT}	-24.2	-100.7	-112.6	-24.8	-17.2	-23.5	-25.5	-6.2
M06-2X/B2								
E_{ES}	-27.4	-96.1	-112.9	-27.3	-22.2	-28.8	-31.6	-5.6
E_{EX}	-4.7	-4.5	-7.4	-8.7	-6.9	-7.8	-9.3	-6.2
E_{PL}	-14.6	-9.9	-6.4	-15.4	-12.3	-15.2	-21.5	-13.3
E_{CT}	-39.2	-35.4	-34.1	-36.3	-33.0	-62.9	-54.2	-11.2
E_{DEF}(AA)	24.7	15.3	15.0	24.7	23.1	33.9	35.5	14.7
E_{DEF}(Cl)	44.2	31.8	34.4	42.6	36.8	61.0	57.9	17.2
E_{SE}(AA)	9.0	6.6	5.8	9.3	7.0	10.0	12.6	6.8
E_{SE}(Cl)	-2.3	-1.9	-2.8	-2.1	-1.2	-3.1	-2.6	-0.4
E_{EL}	-35.3	-101.3	-116.3	-35.5	-28.6	-37.1	-43.0	-12.5
E_{CORE}	54.5	38.0	39.0	51.4	47.1	80.1	74.1	19.2
E_{INT}	-20.0	-98.8	-111.4	-20.4	-14.5	-19.8	-23.1	-4.4
E_{MP2}^{CBS}	-24.7	-99.9	-113.9	-26.2	-17.1	-25.3	-26.2	-6.5

[a] Energy in kcal/mol. B1 denotes 6-31+G(d,p), B2 denotes a combination of 3-21+G* for Cl, 3-21G* for S, and 3-21G for O, N, C, and H. See Equations 2-4 in the main text for term definitions.

Table S2. Significant Occupancy Changes in NBO upon Chloride Binding for Chloride-Amino Acid Complexes by M06-2X Calculations. [a]

	Type [b]	Orbital	q_{comp}		q_{frag}		Δq	
			B1	B2	B1	B2	B1	B2
BBN	CT	*n*(Cl)	7.90	7.91	8.00	8.00	-0.10	-0.09
	CT	σ*(N-H)	0.09	0.09	0.01	0.01	0.08	0.08
	PL	*n*(N)	1.66	1.66	1.72	1.72	-0.06	-0.06
	PL	π*(C-O)	0.34	0.33	0.28	0.28	0.06	0.05
ARG^+	CT	*n*(Cl)	7.88	7.89	8.00	8.00	-0.12	-0.11
	CT	σ*(NH2-HH22)	0.10	0.10	0.00	0.00	0.09	0.10
	PL	*n*(NE)	1.73	1.73	1.69	1.68	0.05	0.05
	PL	*n*(NH1)	1.76	1.74	1.73	1.73	0.02	0.01
	PL	*n*(NH2)	1.66	1.65	1.73	1.73	-0.07	-0.07
	PL	*n**(CZ)	0.82	0.86	0.85	0.85	0.00	0.01
LYS^+	CT	*n*(Cl)	7.88	7.88	8.00	8.00	-0.12	-0.12
	CT	σ*(NZ-HZ3)	0.10	0.10	0.01	0.01	0.09	0.09
GLN	CT	*n*(Cl)	7.91	7.91	8.00	8.00	-0.09	-0.09
	CT	σ*(NE2-HE21)	0.08	0.08	0.01	0.01	0.07	0.07
	PL	*n*(NE2)	1.71	1.71	1.78	1.77	-0.07	-0.07
	PL	π*(CD-OE1)	0.31	0.31	0.25	0.26	0.06	0.06
SER	CT	*n*(Cl)	7.92	7.93	8.00	8.00	-0.08	-0.07
	CT	σ*(OG-HG)	0.07	0.07	0.01	0.01	0.06	0.06
	PL	*n*(OG)	1.96	1.95	1.97	1.96	-0.01	-0.01
	PL	σ*(CB-HB1)	0.02	0.03	0.02	0.02	0.01	0.01
	PL	σ*(CB-HB2)	0.02	0.03	0.02	0.02	0.01	0.01
GLU	CT	*n*(Cl)	7.84	7.85	8.00	8.00	-0.16	-015
	CT	σ*(OE2-HE2)	0.15	0.16	0.02	0.02	0.13	0.14
	PL	*n*(OE2)	1.78	1.76	1.83	1.84	-0.06	-0.08
	PL	π*(CD-OE1)	0.24	0.26	0.20	0.21	0.05	0.05
TYR	CT	*n*(Cl)	7.86	7.87	8.00	8.00	-0.14	-0.13

	CT	σ*(OH-HH)	0.11	0.12	0.01	0.01	0.10	0.11
	PL	$n^{(\pi)}$(OH)	1.84	1.82	1.89	1.87	-0.05	-0.05
	PL	π(CG-CD2)	1.69	1.69	1.67	1.67	0.02	0.02
	PL	π(CZ-CE2)	1.60	1.61	1.67	1.67	-0.06	-0.06
	PL	π(CD1-CE1)	1.70	1.71	1.70	1.71	0.00	0.00
	PL	π*(CG-CD2)	0.41	0.41	0.35	0.35	0.06	0.06
	PL	π*(CZ-CE2)	0.39	0.41	0.38	0.40	0.01	0.01
	PL	π*(CD1-CE1)	0.35	0.35	0.37	0.33	0.02	0.02
	PL	π(ring) [c]	5.00	5.01	5.04	5.05	-0.04	-0.04
	PL	π*(ring) [d]	1.15	1.17	1.06	1.080	0.08	0.09
ILE	CT	*n*(Cl)	7.97	7.97	8.00	8.00	-0.03	-0.03
	CT	σ*(CB-HB1)	0.03	0.02	0.01	0.01	0.01	0.01
	CT	σ*(CD-HD1)	0.02	0.02	0.01	0.01	0.01	0.01

[a] Charge and occupancy in e. Based on NBO analysis, $\Delta q = q_{comp} - q_{frag}$, q_{comp} and q_{frag} the occupancies of the NBO in complex and in fragment, respectively, *n*(Cl) is the sum over all 3p lone pairs of Cl^-. Basis sets B1 denotes 6-31+G(d,p) and B2 denotes a combination of 3-21+G* for Cl, 3-21G* for S, and 3-21G for O, N, C, and H. [b] CT for charge transfer (shifting charges between Cl^- and amino acid NBOs), and PL for polarization (shifting charges between amino acid NBOs). [c] Sum over π(CG-CD1), π(CE1-CZ), and π(CD2-CE2). .[d] Sum over π*(CG-CD1), π*(CE1-CZ), and π*(CD2-CE2).

Table S3. KM-EDA for Additional Chloride-Amino Acid Model Systems. [a]

	ASN	CYS	HID	HIE	LEU	LYS	MET	PHE	THR	VAL
HF/B1										
E_{ES}	-29.6	-22.0	-30.9	-31.2	-6.1	-13.1	-7.1	-7.3	-23.3	-5.7
E_{EX}	22.4	27.0	22.5	26.2	10.5	12.4	10.0	10.8	21.2	9.7
E_{PL}	-7.6	-7.9	-6.8	-8.1	-6.0	-4.2	-4.5	-5.7	-7.3	-5.4
E_{PL}(AA)	-4.5	-4.4	-5.2	-4.7	-4.7	-2.9	-3.7	-4.8	-4.1	-4.2
E_{PL}(Cl)	-2.5	-3.1	-1.1	-2.5	-1.0	-1.1	-0.5	-0.5	-2.7	-1.0
E_{PL}(Coup)	-0.6	-0.4	-0.6	-0.9	-0.3	-0.3	-0.2	-0.3	-0.5	-0.2
E_{CT}	-7.3	-10.3	-7.1	-10.1	-2.7	-3.4	-2.8	-3.1	-6.6	-2.5
E_{CT}(AA)	-1.6	-3.0	-1.4	-1.8	-1.0	-1.0	-0.9	-0.9	-1.6	-0.9
E_{CT}(Cl)	-5.8	-7.2	-5.7	-8.2	-1.7	-2.4	-2.0	-2.2	-5.1	-1.6
E_{MIX}	3.1	4.7	0.0	2.5	2.5	1.9	1.4	1.5	3.5	2.3
E_{INT}	-19.0	-8.4	-22.3	-20.7	-1.9	-6.4	-3.1	-3.8	-12.5	-1.6
HF/B2										
E_{ES}	-27.4	-21.2	-31.1	-30.5	-5.3	-12.7	-6.6	-7.0	-23.0	-5.0
E_{EX}	22.1	26.6	26.1	25.6	10.2	12.1	9.6	10.4	21.6	9.5
E_{PL}	-6.8	-7.3	-7.8	-7.2	-5.5	-3.7	-4.3	-5.2	-6.6	-5.0
E_{PL}(AA)	-4.0	-4.0	-4.4	-4.1	-4.4	-2.5	-3.6	-4.4	-3.5	-3.9
E_{PL}(Cl)	-2.3	-3.0	-2.7	-2.4	-0.9	-1.0	-0.5	-0.5	-2.7	-0.9
E_{PL}(Coup)	-0.5	-0.3	-0.8	-0.8	-0.2	-0.2	-0.2	-0.3	-0.4	-0.2
E_{CT}	-4.9	-8.6	-6.4	-6.5	-1.7	-2.1	-1.9	-1.9	-5.0	-1.5

E_{CT}(AA)	-1.1	-3.1	-1.3	-1.3	-0.4	-0.5	-0.5	-0.3	-1.5	-0.4
E_{CT}(Cl)	-3.8	-5.5	-5.1	-5.2	-1.3	-1.6	-1.4	-1.6	-3.5	-1.1
E_{MIX}	1.7	3.4	1.0	0.4	1.7	1.3	0.7	0.7	2.7	1.6
E_{INT}	-15.2	-7.0	-18.2	-18.2	-0.7	-5.2	-2.3	-3.0	-10.2	-0.4
E_{MP2}^{CBS}	-24.1	-15.2	-27.9	-27.1	-6.6	-10.5	-6.7	-7.4	-18.2	-6.1

[a] Energy in kcal/mol. B1 denotes 6-31+G(d,p), B2 denotes a combination of 3-21+G* for Cl, 3-21G* for S, and 3-21G for O, N, C, and H. E_{PL}(AA) is due to the polarization of amino acid by chloride ion, and E_{PL}(Cl) of chloride ion by amino acid. E_{PL}(Coup) is due to the simultaneous polarization between fragments. E_{CT}(AA) is due to the charge transfer from chloride ion to amino acid, and E_{CT}(Cl) from amino acid to chloride ion. See Equation 1 in the main text for the other term definitions.

Table S4. NEDA for Additional Chloride-Amino Acid Model Systems by B3LYP Calculations. [a]

	ASN	CYS	HID	HIE	LEU	LYS	MET	PHE	THR	VAL
B3LYP/B1										
E_{ES}	-29.5	-22.4	-32.7	-31.5	-7.4	-14.0	-7.8	-7.6	-24.3	-7.0
E_{EX}	-6.2	-7.5	-6.5	-6.2	-4.4	-4.1	-3.3	-3.6	-6.2	-4.2
E_{PL}	-15.0	-16.4	-16.0	-14.8	-15.0	-10.4	-11.3	-14.1	-14.3	-13.6
E_{CT}	-38.1	-35.3	-49.9	-51.0	-10.5	-17.3	-12.8	-14.5	-34.2	-9.7
E_{DEF}(AA)	22.5	26.7	26.2	25.1	15.5	14.5	12.1	14.3	23.2	14.5
E_{DEF}(Cl)	44.6	41.6	54.4	54.4	18.0	22.7	18.2	20.2	40.2	16.6
E_{SE}(AA)	9.1	10.1	10.0	9.4	7.7	5.9	5.8	7.1	8.8	7.0
E_{SE}(Cl)	-2.1	-2.4	-2.8	-2.8	-0.4	-0.9	-0.4	-0.5	-2.0	-0.4
E_{EL}	-37.5	-31.1	-41.4	-39.7	-15.2	-19.5	-13.7	-15.1	-31.9	-14.0
E_{CORE}	53.9	53.1	66.9	66.7	21.8	28.1	21.6	24.3	50.4	20.3
E_{INT}	-21.7	-13.3	-24.4	-24.0	-3.9	-8.6	-4.9	-5.3	-15.7	-3.3
B3LYP/B2										
E_{ES}	-26.8	-21.7	-31.4	-30.7	-6.1	-13.3	-7.1	-7.2	-23.6	-5.8
E_{EX}	-5.8	-7.2	-5.9	-5.7	-3.8	-3.9	-3.0	-3.1	-6.3	-3.7
E_{PL}	-14.2	-14.0	-13.5	-12.8	-12.7	-9.8	-9.6	-11.8	-15.8	-11.6
E_{CT}	-37.1	-32.4	-47.2	-48.5	-10.4	-17.5	-12.0	-13.9	-34.7	-9.4
E_{DEF}(AA)	25.0	26.6	26.9	26.1	14.8	16.2	11.5	13.2	28.8	13.8
E_{DEF}(Cl)	42.4	37.9	50.5	50.9	16.5	21.9	16.6	18.7	39.5	15.3
E_{SE}(AA)	8.8	9.5	9.2	8.9	6.8	5.5	5.2	6.2	9.3	6.2

E_{SE}(Cl)	-2.1	-3.0	-3.2	-3.1	-0.7	-0.9	-0.7	-0.7	-1.6	-0.6
E_{EL}	-34.3	-29.1	-38.9	-37.8	-12.7	-18.4	-12.2	-13.5	-31.8	-11.7
E_{CORE}	54.9	50.7	65.5	65.6	21.4	29.6	20.6	23.2	54.4	19.8
E_{INT}	-16.5	-10.8	-20.6	-20.7	-1.7	-6.4	-3.6	-4.1	-12.1	-1.3
E_{MP2}^{CBS}	-24.1	-15.2	-27.9	-27.1	-6.6	-10.5	-6.7	-7.4	-18.2	-6.1

[a] Energy in kcal/mol. See the footnote (a) of Table S1 for the notations.

Table S5. NEDA for Additional Chloride-Amino Acid Model Systems by M06-2X Calculations. [a]

	ASN	CYS	HID	HIE	LEU	LYS	MET	PHE	THR	VAL
M06-2X/B1										
E_{ES}	-29.2	-21.9	-32.3	-31.4	-6.8	-13.5	-7.6	-7.5	-23.7	-6.3
E_{EX}	-8.6	-9.9	-8.1	-7.2	-6.8	-5.8	-4.3	-4.6	-8.6	-6.6
E_{PL}	-14.7	-16.7	-15.8	-14.4	-14.9	-10.4	-11.1	-13.7	-14.4	-13.6
E_{CT}	-37.2	-33.6	-49.2	-50.3	-10.2	-16.6	-12.3	-13.9	-33.3	-9.3
E_{DEF}(AA)	21.0	25.6	24.6	23.4	14.4	13.5	11.2	13.2	21.7	13.5
E_{DEF}(Cl)	44.2	41.1	54.2	54.3	17.6	22.4	18.0	19.9	39.9	16.2
E_{SE}(AA)	8.7	10.0	9.6	9.0	7.4	5.6	5.5	6.8	8.4	6.7
E_{SE}(Cl)	-1.8	-2.2	-2.5	-2.6	-0.2	-0.7	-0.3	-0.3	-1.7	-0.2
E_{EL}	-37.1	-30.8	-41.0	-39.5	-14.5	-18.9	-13.4	-14.8	-31.4	-13.3
E_{CORE}	50.4	49.0	63.6	64.1	18.1	25.2	19.6	22.0	46.2	16.6
E_{INT}	-23.7	-15.3	-26.6	-25.7	-6.6	-10.4	-6.1	-6.7	-18.5	-6.0
M06-2X/B2										
E_{ES}	-26.9	-21.4	-31.4	-30.9	-5.6	-13.1	-7.0	-7.1	-23.3	-5.2
E_{EX}	-7.4	-9.8	-7.4	-6.5	-6.3	-5.4	-4.1	-4.1	-8.5	-6.3
E_{PL}	-14.1	-14.0	-13.3	-12.6	-12.6	-9.8	-9.6	-11.6	-15.6	-11.5
E_{CT}	-36.5	-30.9	-46.8	-48.0	-10.0	-17.1	-11.6	-13.4	-33.8	-9.0
E_{DEF}(AA)	23.3	25.3	25.3	24.4	13.8	15.1	10.9	12.2	26.5	12.7
E_{DEF}(Cl)	41.9	37.1	50.0	50.5	16.1	21.5	16.3	18.3	38.9	14.9
E_{SE}(AA)	8.4	9.3	8.9	8.5	6.5	5.3	5.0	6.0	8.8	5.9

E_{SE}(Cl)	-1.9	-2.8	-3.0	-2.9	-0.4	-0.7	-0.5	-0.5	-1.4	-0.4
E_{EL}	-34.4	-28.9	-38.8	-37.9	-12.2	-18.2	-12.0	-13.2	-31.4	-11.2
E_{CORE}	51.3	46.1	61.9	62.9	17.4	26.5	18.5	21.0	49.5	15.8
E_{INT}	-19.7	-13.7	-23.6	-23.0	-4.7	-8.7	-5.1	-5.7	-15.8	-4.4
E_{MP2}^{CBS}	-24.1	-15.2	-27.9	-27.1	-6.6	-10.5	-6.7	-7.4	-18.2	-6.1

[a] Energy in kcal/mol. See the footnote (a) of Table S1 for the notations.

Table S6. Significant Occupancy Changes in NBO upon Chloride Binding for Additional Chloride-Amino Acid Complexes by B3LYP Calculations. [a]

	Type [b]	NBO	q_{comp}		q_{frag}		Δq	
			B1	B2	B1	B2	B1	B2
ASN	CT	*n*(Cl)	7.90	7.94	8.00	8.00	-0.10	-0.05
	CT	σ*(ND2-HD2)	0.09	0.06	0.01	0.01	0.08	0.05
	PL	*n*(ND2)	1.69	1.68	1.76	1.75	-0.07	-0.07
	PL	π*(CG-OD1)	0.33	0.34	0.26	0.28	0.07	0.07
CYS	CT	*n*(Cl)	7.88	7.93	8.00	8.00	-0.12	-0.07
	CT	σ*(SG-HG)	0.11	0.07	0.01	0.01	0.10	0.05
HID	CT	*n*(Cl)	7.88	7.93	8.00	8.00	-0.12	-0.07
	CT	σ*(ND1-HD1)	0.12	0.09	0.02	0.02	0.10	0.07
	PL	*n*(ND1)	1.50	1.49	1.59	1.56	-0.09	-0.07
	PL	π*(CG-CD2)	0.35	0.38	0.31	0.34	0.04	0.04
	PL	π*(CE1-NE2)	0.43	0.42	0.38	0.38	0.05	0.04
HIE	CT	*n*(Cl)	7.88	7.93	8.00	8.00	-0.12	-0.07
	CT	σ*(NE2-HE2)	0.12	0.09	0.02	0.02	0.11	0.07
	PL	*n*(NE2)	1.49	1.47	1.58	1.56	-0.09	-0.09
	PL	π*(CG-CD2)	0.35	0.38	0.32	0.34	0.03	0.04
	PL	π*(CE1-ND1)	0.44	0.43	0.39	0.39	0.05	0.04
LEU	CT	*n*(Cl)	7.98	7.99	8.00	8.00	-0.02	-0.01
	CT	σ*(CD1-HD1)	0.02	0.01	0.01	0.01	0.01	0.01
	CT	σ*(CD2-HD2)	0.02	0.01	0.01	0.01	0.01	0.01
LYS	CT	*n*(Cl)	7.95	7.97	8.00	8.00	-0.05	-0.03
	CT	σ*(NZ- HZ1)	0.05	0.03	0.01	0.01	0.04	0.02
MET	CT	*n*(Cl)	7.96	7.98	8.00	8.00	-0.04	-0.02
	CT	σ*(CE-HE1)	0.04	0.02	0.00	0.00	0.03	0.02
PHE	CT	*n*(Cl)	7.96	7.98	8.00	8.00	-0.04	-0.02
	CT	σ*(CZ-HZ)	0.04	0.03	0.01	0.01	0.03	0.02
	PL	π(CG-CD1)	1.68	1.68	1.65	1.66	0.03	0.03
	PL	π(CZ-CE1)	1.63	1.63	1.67	1.67	-0.04	-0.04

	PL	π(CD2-CE2)	1.69	1.69	1.68	1.68	0.01	0.01
	PL	π*(CG-CD1)	0.37	0.37	0.34	0.34	0.03	0.03
	PL	π*(CZ-CE1)	0.29	0.30	0.33	0.33	-0.04	-0.04
	PL	π*(CD2-CE2)	0.33	0.34	0.33	0.33	0.01	0.01
	PL	π(ring) [c]	5.00	5.01	5.00	5.01	0.00	0.00
	PL	π*(ring)[d]	1.00	1.00	1.00	1.00	0.00	0.00
THR	CT	*n*(Cl)	7.91	7.94	8.00	8.00	-0.09	-0.06
	CT	σ*(OG1-HG11)	0.08	0.06	0.01	0.01	0.07	0.05
VAL	CT	*n*(Cl)	7.97	7.99	8.00	8.00	-0.03	-0.01
	CT	σ*(CG1-HG12)	0.02	0.01	0.01	0.01	0.01	0.01
	CT	σ*(CG2-HG23)	0.02	0.01	0.01	0.01	0.01	0.01

[a] Charge and occupancy in e. Based on NBO analysis, $\Delta q = q_{comp} - q_{frag}$, q_{comp} and q_{frag} are the occupancies of the NBO in complex and fragment, respectively, *n*(Cl) is the sum over all 3p lone pairs of Cl^-. Basis sets B1 denotes 6-31+G(d,p) and B2 denotes a combination of 3-21+G* for Cl, 3-21G* for S, and 3-21G for O, N, C, and H. [b] CT for charge transfer (shifting charges between Cl^- and amino acid NBOs), and PL for polarization (shifting charges between amino acid NBOs). [c] Sum over π(CG-CD1), π(CD2-CE2), and π(CE1-CZ). [d] Sum over π*(CG-CD1), π*(CD2-CE2), and π*(CE1-CZ).

Table S7. Significant Occupancy Changes in NBO upon Chloride Binding for Additional Chloride-Amino Acid Complexes by M06-2X Calculations. [a]

	Type [b]	NBO	q_{comp}		q_{frag}		Δq	
			B1	B2	B1	B2	B1	B2
ASN	CT	*n*(Cl)	7.90	7.91	8.00	8.00	-0.10	-0.09
	CT	σ*(ND2-HD2)	0.08	0.08	0.01	0.01	0.08	0.07
	PL	*n*(ND2)	1.70	1.70	1.77	1.77	-0.07	-0.09
	PL	π*(CG-OD1)	0.32	0.32	0.25	0.26	0.07	0.07
CYS	CT	*n*(Cl)	7.88	7.89	8.00	8.00	-0.11	-0.11
	CT	σ*(SG-HG)	0.10	0.09	0.01	0.01	0.09	0.08
HID	CT	*n*(Cl)	7.88	7.88	8.00	8.00	-0.12	-0.12
	CT	σ*(ND1-HD1)	0.12	0.12	0.02	0.02	0.10	0.10
	PL	*n*(ND1)	1.51	1.49	1.59	1.57	-0.08	-0.08
	PL	π*(CG-CD2)	0.35	0.37	0.31	0.33	0.04	0.04
	PL	π*(CE1-NE2)	0.42	0.41	0.37	0.37	0.05	0.04
HIE	CT	*n*(Cl)	7.88	7.88	8.00	8.00	-0.12	-0.12
	CT	σ*(NE2-HE2)	0.12	0.12	0.02	0.01	0.11	0.11
	PL	*n*(NE2)	1.50	1.48	1.58	1.57	-0.08	-0.08
	PL	π*(CG-CD2)	0.35	0.37	0.32	0.34	0.03	0.03
	PL	π*(CE1-ND1)	0.43	0.42	0.38	0.38	0.05	0.04
LEU	CT	*n*(Cl)	7.97	7.97	8.00	8.00	-0.03	-0.03
	CT	σ*(CD1-HD1)	0.02	0.02	0.01	0.01	0.01	0.01
	CT	σ*(CD2-HD2)	0.02	0.02	0.01	0.01	0.01	0.01
LYS	CT	*n*(Cl)	7.96	7.96	8.00	8.00	-0.04	-0.04
	CT	σ*(NZ- HZ1)	0.04	0.04	0.01	0.01	0.04	0.04
MET	CT	*n*(Cl)	7.97	7.97	8.00	8.00	-0.03	-0.03
	CT	σ*(CE-HE1)	0.03	0.03	0.00	0.01	0.03	0.03
PHE	CT	*n*(Cl)	7.96	7.97	8.00	8.00	-0.04	-0.03
	CT	σ*(CZ-HZ)	0.04	0.04	0.01	0.01	0.03	0.03
	PL	π(CG-CD1)	1.69	1.69	1.66	1.66	0.03	0.03
	PL	π(CZ-CE1)	1.63	1.64	1.67	1.67	-0.04	-0.04

	PL	π(CD2-CE2)	1.69	1.69	1.68	1.68	0.01	0.01
	PL	π*(CG-CD1)	0.37	0.37	0.34	0.34	0.03	0.03
	PL	π*(CZ-CE1)	0.29	0.30	0.33	0.33	-0.04	-0.04
	PL	π*(CD2-CE2)	0.33	0.33	0.33	0.33	0.01	0.01
	PL	π(ring) [c]	5.00	5.01	5.01	5.01	0.00	0.00
	PL	π*(ring)[d]	0.99	1.00	1.00	1.00	0.00	0.00
THR	CT	*n*(Cl)	7.92	7.92	8.00	8.00	-0.08	-0.08
	CT	σ*(OG1-HG11)	0.07	0.07	0.01	0.01	0.07	0.07
VAL	CT	*n*(Cl)	7.97	7.98	8.00	8.00	-0.03	-0.02
	CT	σ*(CG1-HG12)	0.02	0.02	0.01	0.01	0.01	0.01
	CT	σ*(CG2-HG23)	0.02	0.02	0.01	0.01	0.01	0.01

[a] Charge and occupancy in e. Based on NBO analysis, $\Delta q = q_{comp} - q_{frag}$, q_{comp} and q_{frag} are the occupancies of the NBO in complex and fragment, respectively, *n*(Cl) is the sum over all 3p lone pairs of Cl^-. Basis sets B1 denotes 6-31+G(d,p) and B2 denotes a combination of 3-21+G* for Cl, 3-21G* for S, and 3-21G for O, N, C, and H. [b] CT for charge transfer (shifting charges between Cl^- and amino acid NBOs), and PL for polarization (shifting charges between amino acid NBOs). [c] Sum over π(CG-CD1), π(CD2-CE2), and π(CE1-CZ). [d] Sum over π*(CG-CD1), π*(CD2-CE2), and π*(CE1-CZ).

Table S8. NEDA Results for the ClC Active-Site Models by M06-2X Calculations. [a]

	WT_Cl2		PWT_Cl3			PWT_Cl4				E148Q_Cl3			E148Q_Cl4			
	Cl_{int}	Cl_{cen}	Cl_{int}	Cl_{cen}	Cl_{ext}	Cl_{int}	Cl_{cen}	Cl_{ext}	Cl_{add}	Cl_{int}	Cl_{cen}	Cl_{ext}	Cl_{int}	Cl_{cen}	Cl_{ext}	Cl_{add}
E_{ES}	-62.6	-82.4	-59.7	-73.9	-106.2	-39.4	-53.5	-52.7	-32.4	-63.3	-85.1	-102.4	-34.2	-40.6	-46.3	-54.5
E_{EX}	-15.9	-28.4	-15.9	-29.2	-43.4	-15.6	-28.0	-36.1	-13.9	-16.0	-28.3	-37.0	-15.4	-28.5	-41.7	-18.3
E_{PL}	-37.6	-72.6	-37.6	-72.1	-87.2	-37.2	-72.7	-75.0	-26.8	-37.7	-73.0	-74.2	-36.9	-72.3	-84.6	-45.0
E_{CT}	-46.5	-96.0	-45.4	-100.6	-126.6	-42.9	-100.9	-107.9	-78.3	-46.6	-97.6	-91.5	-40.9	-105.7	-96.8	-67.7
E_{DEF}(P-S)	46.3	87.9	46.0	89.5	126.7	44.9	88.9	100.8	43.1	46.3	88.5	102.4	44.0	89.8	112.9	56.7
E_{DEF}(Cl)	54.7	124.9	53.7	126.9	167.3	51.0	129.5	149.1	76.9	54.9	126.7	129.5	48.8	132.5	143.3	78.1
E_{SE}(P-S)	21.7	36.9	21.6	37.0	47.9	21.2	37.0	40.1	18.5	21.7	37.1	39.6	21.0	37.1	45.1	24.7
E_{SE}(Cl)	-3.2	0.6	-3.1	0.1	-1.6	-2.9	0.5	-1.0	-5.7	-3.2	0.6	-1.1	-2.8	0.1	-0.5	-2.0
E_{EL}	-81.7	-117.5	-78.8	-109.0	-147.1	-58.3	-88.7	-88.5	-46.5	-82.5	-120.4	-138.0	-52.9	-75.6	-86.3	-76.9
E_{CORE}	66.5	146.9	65.3	150.1	204.4	62.0	152.9	174.7	93.4	66.7	149.3	156.4	59.4	156.5	170.0	93.9
E_{INT}	-61.6	-66.6	-59.0	-59.5	-69.3	-39.3	-36.7	-21.8	-31.4	-62.3	-68.7	-73.2	-34.5	-24.8	-13.1	-50.7

[a] Energy in kcal/mol. Computed at the M06-2X/B2 level, where B2 denotes a combination of 3-21+G* for Cl, 3-21G* for S, and 3-21G for O, N, C, and H. P-S denotes protein-solvent. See Equations 2-4 for term definitions and Figures 3 and S2 for geometries.

Table S9. Significant Occupancy Changes in NBO upon Chloride Binding for the ClC Active-Site Models by M06-2X Calculations. [a]

			WT_Cl2	PWT_Cl3	PWT_Cl4	E148Q_Cl3	E148Q_Cl4
Cl_{add}	CT	*n*(Cl)	n/a	n/a	-0.20	n/a	-0.16
	CT	σ*(R147:NH2-HH2)	n/a	n/a	0.20	n/a	0.10
	CT	σ*(HOH529:O-H1)	n/a	n/a	0.01	n/a	0.02
	CT	σ*(HOH525:O-H1)	n/a	n/a	0.00	n/a	0.02
	PL	*n*(R147:NH2)	n/a	n/a	-0.07	n/a	-0.06
	PL	*n**(R147:CZ)	n/a	n/a	0.01	n/a	0.01
	PL	*n*(R147:NH1)	n/a	n/a	0.05	n/a	0.05
	PL	*n*(R147:NE)	n/a	n/a	0.02	n/a	0.01
Cl_{ext}	CT	*n*(Cl)	n/a	-0.25	-0.22	-0.19	-0.19
	CT	σ*(E/Q148:N-H)	n/a	0.02	0.04	0.04	0.01
	CT	σ*(A358:N-H)	n/a	0.02	0.02	0.01	0.03
	CT	σ*(E148:OE2-HE2)	n/a	0.10	0.10	n/a	n/a
	CT	σ*(Q148:NE2-HE2)	n/a	n/a	n/a	0.01	0.03
	CT	σ*($Water_2$:O-H1)	n/a	n/a	n/a	0.08	n/a
	PL	*n*(E/Q148:N)	n/a	-0.03	-0.04	-0.04	-0.03
	PL	π*(R147:C-O)	n/a	0.04	0.04	0.04	0.03
	PL	*n*(G149:N)	n/a	-0.03	-0.02	-0.02	-0.03
	PL	π*(E/Q148:C-O)	n/a	0.03	0.02	0.02	0.03
	PL	*n*(A358:N)	n/a	-0.02	-0.04	-0.03	-0.03
	PL	π*(F357:C-O)	n/a	0.01	0.04	0.03	0.03
	PL	*n*(E148:OE2)	n/a	-0.04	-0.04	n/a	n/a
	PL	*n*(Q148:NE2)	n/a	n/a	n/a	0.02	-0.04
	PL	π*(E/Q148:CD-OE1)	n/a	0.04	0.05	-0.01	0.04
Cl_{cen}	CT	*n*(Cl)	-0.20	-0.21	-0.21	-0.20	-0.22
	CT	σ*(S107:OG1-HG1)	0.06	0.07	0.07	0.06	0.07
	CT	σ*(Y445:OZ1-HZ1)	0.06	0.06	0.06	0.06	0.07
	CT	σ*(I356:N-H)	0.04	0.04	0.04	0.04	0.04
	PL	*n*(I356:N)	-0.03	-0.02	-0.02	-0.02	-0.02
	PL	π*(G355:C-O)	0.03	0.03	0.02	0.03	0.02

	PL	*n*(F357:N)	-0.02	-0.04	-0.04	-0.03	-0.05
	PL	π*(I356:C-O)	0.02	0.05	0.03	0.03	0.06
	PL	$n^{(\pi)}$(Y445:OH)	-0.03	-0.03	-0.04	-0.03	-0.04
	PL	π(Y445:CG-CD1)	0.01	0.02	0.02	0.01	0.02
	PL	π(Y445:CD2-CE2)	0.02	0.03	0.03	0.02	0.03
	PL	π(Y445:CE1-CZ)	-0.04	-0.05	-0.05	-0.05	-0.06
	PL	π*(Y445:CG-CD1)	0.02	0.03	0.03	0.03	0.03
	PL	π*(Y445:CD2-CE2)	0.02	0.03	0.02	0.02	0.03
	PL	π*(Y445:CE1-CZ)	-0.02	-0.02	-0.02	-0.02	-0.02
Cl_{int}	CT	*n*(Cl)	-0.13	-0.12	-0.12	-0.13	-0.11
	CT	σ*(G108:N-H)	0.05	0.05	0.05	0.05	0.04
	CT	σ*(G107:N-H)	0.05	0.05	0.05	0.05	0.04
	PL	*n*(G108:N)	-0.02	-0.02	-0.02	-0.02	-0.01
	PL	π*(S107:C-O)	0.02	0.02	0.02	0.02	0.01
	PL	*n*(G107:N)	-0.05	-0.05	-0.05	-0.05	-0.05
	PL	π*(S106:C-O)	0.06	0.06	0.06	0.06	0.05

[a] Computed at the M06-2X/B2 level, $\Delta q = q_{comp} - q_{frag}$, q_{comp} and q_{frag} are the occupancies of the NBO in complex and in fragment, respectively. The NBO with large (≥0.03 e) values are listed. See footnotes (a) and (b) of Table S7 for the definitions of the other notations.

Table S10. Sequence Alignment for Select Members of the ClC Family. [a]

	Sequence		UniProt Entry	PDB ID	UniProt Entry Name
134	GGLGTLGGG--MVLG**R**EGPTVQIGGNIGRMVLDIF----------RLKGDEARHTLL	179	P37019	1OTS	CLCA_ECOLI
134	GGMGTLGAG--MVLG**R**EGPTVQIGGNLGRMVLDVF----------RMRSAEARHTLL	179	Q8ZRP8	1KPL	CLCA_SALTY
196	GLICAIGGG--LPVG**W**EGPNVHIACIIAHQFYRLGVFK------EL--CTDRALRLQTL	245	M1UVK6	3ORG	M1UVK6_CYAME
152	GLTVALSAG--FPLG**K**EGPFVHIASICATLLNQLLCFI------SGRREEPYYLRADIL	203	P35522	2D4Z	CICH_TORCA
218	ALTAGLGSG--IPVG**K**EGPFVHIASICAAVLSKFMSVF------CGVYEQPYYY-SDIL	268	P35523	N/A	CLCN1_HUMAN
191	GLTCALGSG--MPLG**K**EGPFVHIASMCAALLSKFLSLF------GGIYENESRN-TEML	241	P51788	N/A	CLCN2_HUMAN
150	GLSCTLATGSTLFLG**K**VGPFVHLSVMIAAYLGRVRTTT------IGEPENKSKQ-NEML	202	P51800	N/A	CLCKA_HUMAN
150	GLSCTLACGSTLFLG**K**VGPFVHLSVMMAAYLGRVRTTT------IGEPENKSKQ-NEML	202	P51801	N/A	CLCKB_HUMAN
268	TLVLAVASG--LSLG**K**EGPLVHVACCCGNIFSYL----------FPKYSTNEAKKREVL	315	P51790	N/A	CLCN3_HUMAN
210	TLVLVVSSG--LSLG**K**EGPLVHVACCCGNFFSSL----------FSKYSKNEGKRREVL	257	P51793	N/A	CLCN4_HUMAN
197	TLVLAVSSG--LSLG**K**EGPLVHVACCCGNILCHC----------FNKYRKNEAKRREVL	244	P51795	N/A	CLCN5_HUMAN
186	GVLFSVAGG--LFVE**K**EGPMIHSGSVVGAGLPQFQSISLRKIQFNFPYFRSDRDKRDFV	243	P51797	N/A	CLCN6_HUMAN
233	GVILSVVGG--LAVG**K**EGPMIHSGSVIAAGISQGRSTSLKRDFKIFEYFRRDTEKRDFV	290	P51798	N/A	CLCN7_HUMAN
	...* *:. * :*..* *: :* : . .:: . .				

[a] Performed by using the Universal Protein Resource (UniProt) service (http://www.uniprot.org).[1] The R147 residue in EcClC and its equivalents are in bold.

1. Consortium, T. U., Update on activities at the Universal Protein Resource (UniProt) in 2013. *Nucleic Acids Res.* **2013**, 41, D43-D47.

Table S11. Cartesian Coordinates (Å) of All the Chloride-Amino Acid Complexes.

ARG^{+} complex

C	-1.765087	0.692783	0.366167
H	-2.796794	0.473557	0.111283
N	-0.914262	-0.279276	-0.297632
H	-1.535124	1.712274	0.054060
H	-1.268006	-0.762404	-1.105313
H	-1.655498	0.605580	1.445764
C	0.407860	-0.330896	-0.093091
N	1.171815	-1.217473	-0.755438
H	2.155715	-1.239051	-0.491859
H	0.763203	-2.064078	-1.109234
N	1.031796	0.475940	0.751142
H	0.545445	1.254129	1.160907
H	2.068957	0.372682	0.953671
Cl	4.225371	0.038463	1.233271

ASN Complex

C	2.505912	-1.203358	1.374598
H	3.487224	-1.662876	1.484767
H	2.386217	-0.392868	2.092541
C	1.388513	-2.199227	1.592480
O	0.196837	-1.870891	1.511225
N	1.803138	-3.445410	1.876033
H	2.806475	-3.692218	1.938569
H	1.094685	-4.142717	2.029374
H	2.397148	-0.780209	0.376716
Cl	4.859560	-4.019718	2.026514

BBN complex

C	-0.565542	0.336004	-0.363824
H	-0.610207	1.400222	-0.602615
H	-1.149892	0.178453	0.544467
H	-0.998395	-0.237458	-1.180167
N	0.796352	-0.101473	-0.188303
C	1.563302	0.426745	0.775665
H	1.170447	-0.847080	-0.804556
O	1.167737	1.310940	1.553989
C	2.963335	-0.139507	0.848744
H	3.117138	-0.548246	1.846963
H	3.673721	0.675079	0.711472
H	3.126847	-0.911381	0.097903
Cl	1.884463	-2.336085	-2.023768

CYS complex

C	1.449329	-1.126863	-0.104910
S	1.387337	0.666362	-0.417669
H	0.040973	0.726607	-0.125406
H	1.749965	-1.661073	-1.004129
H	0.440587	-1.421525	0.183935
H	2.147478	-1.349420	0.699704
Cl	-1.869516	0.033228	0.434745

GLN complex

C	0.757207	-1.810428	-0.448591
H	-0.139000	-1.515915	-0.993295
H	1.609513	-1.839908	-1.129201
C	1.009693	-0.821484	0.691178
H	1.852918	-1.140559	1.302701
H	0.106752	-0.754505	1.298744
C	1.352527	0.540906	0.126881
O	2.523507	0.899882	-0.061019
N	0.280486	1.295460	-0.177982
H	-0.682015	0.926754	-0.083070
H	0.448841	2.165760	-0.653280
H	0.593781	-2.814261	-0.054901
Cl	-2.513806	-0.032603	0.158972

GLU complex

C	2.616516	-1.057068	-0.472750
C	2.247632	0.262228	0.203718
H	2.025748	-1.870311	-0.055801
H	2.415035	-1.006449	-1.543076
H	2.823476	1.087242	-0.211591
H	2.449795	0.193670	1.273655
C	0.774766	0.579896	0.011994
O	0.391925	1.521100	-0.666060
O	0.019968	-0.296377	0.646418
H	-0.999555	-0.157879	0.523454
H	3.674331	-1.286112	-0.336597
Cl	-2.867324	-0.244978	0.545960

HID complex

C	2.568121	-1.392537	0.048250
C	1.807951	-0.113061	0.006831
H	3.636708	-1.182795	0.095657
H	2.285812	-1.990475	0.915014
C	2.205024	1.213256	-0.007210
H	3.214148	1.595511	0.012146
H	-0.962744	1.525038	-0.093571
N	1.116855	2.051761	-0.050775
C	0.071290	1.224188	-0.062281
N	0.442679	-0.077654	-0.028957
H	-0.174446	-0.930886	-0.026489
H	2.366945	-2.000553	-0.834178
Cl	-1.117761	-2.666696	0.002793

HIE complex

C	-3.147479	0.377380	0.248729
C	-1.712337	0.017899	0.058403
H	-3.768942	-0.061878	-0.533402
H	-3.519474	0.012035	1.207382
C	-0.630007	0.859517	-0.133725
N	-1.290537	-1.289107	0.054773
H	-0.552865	1.931981	-0.191479
H	1.459772	0.371958	-0.412340
C	0.029003	-1.218026	-0.137794
N	0.465570	0.054898	-0.255931
H	0.698642	-2.059775	-0.197224

H	-3.278287	1.459523	0.221501
Cl	3.296539	1.006932	-0.701482

ILE complex

C	-1.156641	-0.767500	0.587709
C	-1.061915	-1.563723	-0.709206
H	-0.152629	-0.659114	1.008138
C	-1.744072	0.628798	0.388069
H	-1.799703	1.121645	1.362399
H	-2.773199	0.549375	0.014772
C	-0.904167	1.490944	-0.551442
H	0.138709	1.479833	-0.224263
H	-1.266950	2.521096	-0.567268
H	-0.944397	1.113374	-1.574517
H	-0.733498	-2.585868	-0.515531
H	-0.332795	-1.113386	-1.381629
H	-2.027196	-1.608620	-1.223530
H	-1.774308	-1.315619	1.306624
Cl	2.253359	0.360885	0.962752

LEU complex

C	2.634479	-0.295506	0.111736
C	0.690134	1.293492	0.280688
H	3.013469	-1.214491	-0.341885
C	1.204950	-0.002779	-0.332783
H	1.184272	0.116537	-1.419646
H	2.673586	-0.418952	1.198166
C	0.269834	-1.152870	0.020105
H	0.621695	-2.093983	-0.411044
H	-0.728787	-0.936844	-0.365132
H	0.221793	-1.277230	1.107130
H	1.342969	2.134298	0.031405
H	0.656566	1.204602	1.371769
H	-0.313269	1.498296	-0.098208
H	3.310581	0.520248	-0.155431
Cl	-2.166098	0.746535	-1.869864

LYS complex

C	2.023190	-0.216055	0.075927
H	2.997799	0.247945	0.245734
H	1.756493	-0.808848	0.957363
N	1.034278	0.802033	-0.277956
H	0.127436	0.319708	-0.330714
H	0.930535	1.432399	0.509667
H	2.127409	-0.909213	-0.758104
Cl	-1.578557	-1.143953	0.112461

LYS^{+} complex

C	-0.782450	0.100586	0.418448
H	-1.453754	-0.108596	-0.408779
H	-0.906213	-0.597542	1.237861
H	-0.911155	1.102309	0.810978
N	0.628097	-0.013837	-0.051861
H	0.838500	0.655163	-0.787763
H	0.840865	-0.948932	-0.389132
H	1.237681	0.191910	0.776314
Cl	1.212224	0.707661	2.914854

MET complex

C	3.280952	-0.835810	0.074172
C	2.253817	0.284830	0.126638
H	3.111712	-1.548820	0.881015
H	3.212039	-1.374862	-0.870693
H	2.424292	1.001829	-0.679450
H	2.318671	0.822741	1.075019
S	0.583018	-0.393305	-0.042707
C	-0.349722	1.150047	0.059380
H	-1.422048	0.934075	-0.027369
H	-0.056430	1.811386	-0.755244
H	-0.159738	1.630566	1.018665
H	4.293473	-0.440766	0.171152
Cl	-3.800277	1.204731	-0.209887

PHE complex

C	3.677483	-0.184352	0.058758
C	2.175918	-0.087765	0.026275
H	4.093473	0.404189	0.878378
H	3.998316	-1.217943	0.189496
C	-0.644447	0.106883	-0.058114
C	1.542219	1.158984	-0.004106
C	1.377316	-1.233665	0.015396
C	-0.015361	-1.137255	-0.026601
C	0.151772	1.254004	-0.046273
H	2.146424	2.061203	0.006218
H	1.852677	-2.209319	0.040566
H	-0.619597	-2.036403	-0.033917
H	-0.327116	2.225377	-0.069276
H	-1.732933	0.192179	-0.090793
H	4.117823	0.188535	-0.868303
Cl	-4.062760	0.560461	-0.220577

SER complex

C	2.163302	-0.428142	-0.006111
O	1.496031	0.811095	0.041269
H	1.838339	-1.098749	0.795320
H	2.000246	-0.947705	-0.956196
H	0.531948	0.586010	-0.017211
H	3.233012	-0.239968	0.107244
Cl	-1.330886	-0.305334	-0.111097

THR complex

C	1.553129	0.341992	-0.411418
O	0.768182	1.185884	0.405131
C	1.720520	-1.043916	0.194095
H	1.101867	0.245992	-1.404964
H	-0.156443	0.842824	0.304995
H	2.343720	-1.677206	-0.443781
H	0.736709	-1.500235	0.299681
H	2.185459	-0.969543	1.178133
H	2.527222	0.826610	-0.527624
Cl	-1.855957	-0.244097	-0.217446

TRP complex

C	1.901993	-2.096374	0.349150
C	1.680443	-0.643175	0.082857
H	2.088250	-2.271213	1.410773
H	1.016902	-2.689467	0.106276
C	2.610991	0.291487	-0.313704
C	0.447082	0.070158	0.240810
H	3.658369	0.164142	-0.541889
N	2.025723	1.543125	-0.392235
C	0.693941	1.436210	-0.063669
H	2.480420	2.378581	-0.713458
C	-0.849595	-0.342940	0.597252
C	-0.310102	2.405763	-0.011007
H	-0.111758	3.445730	-0.245635
C	-1.581678	1.979813	0.354494
H	-2.387282	2.703016	0.406078
C	-1.842956	0.625044	0.648869
H	-1.065671	-1.395330	0.791766
H	-2.850506	0.329558	0.914886
Cl	-1.211889	-3.832622	0.889965
H	2.760638	-2.468683	-0.212439

TYR complex

C	-3.889877	0.216486	0.337102
C	-2.412648	0.007914	0.139958
H	-4.311358	-0.536374	1.005836
H	-4.087811	1.197589	0.769892
C	0.364367	-0.378406	-0.287237
C	-1.889675	-1.265785	-0.103439
C	-1.514670	1.078610	0.167899
C	-0.147750	0.905082	-0.040416
C	-0.527639	-1.460956	-0.314050
H	-2.557381	-2.122024	-0.126748
H	-1.890913	2.078879	0.359556
H	0.547060	1.737044	-0.014947
H	-0.128968	-2.451266	-0.498511
O	1.667267	-0.623169	-0.494690
H	2.195092	0.239055	-0.447482
H	-4.433929	0.156101	-0.608815
Cl	3.162176	1.924964	-0.336305

VAL complex

C	-0.196069	0.546206	0.518256
H	-1.095221	0.135911	0.981251
C	0.957274	-0.420045	0.762124
C	-0.456765	0.722933	-0.972922
H	0.430662	1.118269	-1.475037
H	-1.284309	1.410961	-1.158780
H	-0.709727	-0.248701	-1.401084
H	1.870650	-0.061581	0.278767
H	0.690043	-1.394439	0.348618
H	1.164654	-0.536849	1.828100
H	0.007668	1.514350	0.989159
Cl	-1.378862	-2.787013	-0.698454

Table S12. Cartesian Coordinates (Å) of the ClC Active-Site Models.

WT_Cl2

C	-4.7079855976	-6.2305884944	-3.5418607160
H	-4.5549027064	-5.9785205600	-2.4744750724
H	-5.6489185775	-5.7600763555	-3.8434742898
H	-4.8265136161	-7.3172688450	-3.6260952531
N	-3.6383040337	-5.7925315956	-4.4337208612
H	-2.7626122278	-6.2289682749	-4.1505972758
C	-3.4309704172	-4.3520372997	-4.4285290369
H	-4.3761146217	-3.8490166762	-4.6605443735
H	-2.7209932369	-4.0880610044	-5.2244311891
C	-2.8621478600	-3.8286195932	-3.1192124965
O	-2.0868973941	-4.5084542637	-2.4363153330
N	-3.2316661269	-2.6032310259	-2.7759194592
H	-4.1616625951	-2.2918630909	-3.0953049082
C	-2.7564371872	-1.9911709682	-1.5453224737
H	-1.6622158754	-2.0108209549	-1.5541224723
C	-3.1573478598	-2.7876600146	-0.3197055550
O	-2.3587948323	-3.5343498813	0.2432192227
C	-3.2550216831	-0.5336048336	-1.4472848788
H	-4.3200289692	-0.4945432165	-1.6992202694
H	-2.7151910466	0.0962731280	-2.1595891935
O	-3.0719793144	-0.0528214960	-0.1296096439
H	-2.2864814484	0.5440649162	-0.1341832451
N	-4.4102037530	-2.6176791970	0.0835718092
H	-5.0963700693	-2.2740014833	-0.6046530121
C	-4.9278216335	-3.2998362794	1.2532903415
H	-4.1220944050	-3.8618421073	1.7290478072
H	-5.7581401120	-3.9667778196	1.0036588976
C	-5.4173526932	-2.2178225462	2.1862252926
O	-6.1894168987	-2.4607329171	3.1101524619
N	-4.9474755036	-1.0037830436	1.9453223811
H	-4.2643859889	-0.8240105134	1.2147942541
C	-5.3652463597	0.1080991254	2.7720106865
H	-5.3353118444	-0.2359407666	3.8127933174
C	-6.8648591511	0.3135476990	2.5682393445
O	-7.5978830782	0.4352734871	3.5395334683
C	-4.4436266345	1.3485913032	2.7010689648
H	-4.3275613073	1.6773792190	1.6611240615
C	-3.0486584371	0.9589820461	3.2454019390
H	-2.6612193712	0.1135144577	2.6651368612
H	-3.1710584242	0.5841476103	4.2720600793
C	-5.0692043739	2.4991304177	3.5057366998
H	-4.4342689017	3.3876430640	3.4613175248
H	-5.2008860190	2.2135458159	4.5567548493
H	-6.0526630558	2.7769795418	3.1154956135
C	-2.0007308614	2.0782768060	3.2382712649
H	-1.0282477570	1.6758547468	3.5461268007
H	-2.2570654959	2.8845951466	3.9349428777
H	-1.8777984406	2.5232134371	2.2446547369
N	-7.3417913228	0.3267564216	1.3023996101
C	-8.7770396925	0.5142704064	1.0621005821
H	-9.1062773254	1.4896514763	1.4438664914
C	-9.5254032612	-0.5354371518	1.8652238674

O	-10.4393245933	-0.2265639222	2.6293001247
C	-9.1206062984	-1.9895060972	1.7021931911
H	-8.7114193578	-2.2168893352	0.7125254913
H	-8.3476975701	-2.2268134983	2.4426719725
H	-9.9943487203	-2.6166089242	1.8997752916
C	-8.9240679687	0.4397733793	-0.4639878658
H	-9.8082507334	0.9845993270	-0.8082194040
H	-9.0049774201	-0.5978445322	-0.8050525875
C	-7.5977691511	1.0389599556	-0.9483562969
H	-7.6226024661	2.1309195517	-0.8653774763
H	-7.3579812986	0.7622925926	-1.9785653497
C	-6.5810297082	0.4537930196	0.0376550501
H	-5.6994043216	1.0855398621	0.1558114126
H	-6.2679742492	-0.5280833696	-0.3209747041
C	-1.2971482124	-6.4837475543	0.8080575010
H	-0.4507849179	-5.8067150743	0.7152792632
H	-0.9799045898	-7.5160213972	0.6471785578
H	-1.7319123310	-6.3653067564	1.8012061222
N	-2.2918985148	-6.0755562028	-0.2054948443
H	-1.9384255629	-5.9670167098	-1.1713414688
H	-2.5481315355	-5.0574102372	0.0242554083
H	-3.1289401779	-6.6611921945	-0.2204124082
C	5.6162082280	-1.6710847550	-3.7041200981
H	5.5458313194	-2.6311087978	-3.1666488037
H	5.1043884217	-1.7803185424	-4.6657899477
H	6.6808614219	-1.4819738208	-3.9193929867
N	5.0406381925	-0.5430552705	-3.0076579855
H	4.0461739955	-0.4297836547	-3.1536313204
C	5.5963317209	-0.1725376861	-1.7236036945
H	5.1816664597	0.7796675238	-1.3724988066
H	6.6868788166	-0.0320094055	-1.8157216006
C	5.3126531950	-1.2232215873	-0.6686255745
O	4.6125856792	-2.1984780714	-0.9217288410
N	5.8701817675	-1.0244952659	0.5171719377
H	6.2669162631	-0.1044926447	0.7198529469
C	5.6801910371	-1.9397403981	1.6304333043
H	5.5125456792	-2.9379792163	1.2233166678
C	4.4363674254	-1.5494386193	2.4238676524
O	3.8224785346	-2.3951474166	3.0649722148
C	6.9063371121	-1.8977039890	2.5470730062
H	6.6735233585	-2.4842177967	3.4451835016
H	7.0464021330	-0.8611142338	2.8831520298
C	8.1957843530	-2.4099821781	1.9130973048
H	8.3159018795	-1.9512862898	0.9298683998
H	8.1299469270	-3.4959265430	1.7634244701
C	9.4042621439	-2.1007317909	2.8015153523
H	9.1566303316	-2.3029730871	3.8473158931
H	9.6827947616	-1.0439909395	2.7413315569
N	10.5463285913	-2.9623748658	2.5009866162
H	10.9546900212	-3.4777874766	3.2682667527
C	11.2251924971	-2.9660645751	1.3534432473
N	10.8902588454	-2.1431165203	0.3670898887
H	10.3190100950	-1.2694142471	0.4833743472
H	11.3869388534	-2.2098902829	-0.5107630423
N	12.2418975817	-3.8068168906	1.1901447013
H	12.3160287857	-4.6386345025	1.7584679544
H	12.7494107389	-3.8254870017	0.3179811717

N	4.0768006997	-0.2678057222	2.3749411054
H	4.3536025946	0.2433472972	1.5481264052
C	2.9043706691	0.2531125371	3.0875590467
H	3.1268474631	0.1897278550	4.1587344980
C	1.7237415653	-0.6712249977	2.9001582968
O	1.1334218730	-1.1506323636	3.8654630354
C	2.7201812220	1.7377339592	2.7142902974
H	2.0224466438	2.1786076490	3.4335380594
H	2.2607187710	1.8352340792	1.7270197612
C	4.0566555556	2.5221821588	2.7189622650
H	3.8233318965	3.5926062673	2.6606620763
H	4.6128516176	2.3558017993	3.6481072825
C	4.9539630075	2.1695060844	1.5119153374
O	4.3670352356	2.0129747715	0.4032416376
O	6.1992631721	1.9721888594	1.6805189321
N	1.3687052684	-0.8881144079	1.6400844054
H	1.8185136415	-0.3928646725	0.8844991904
C	0.2586601644	-1.7607819641	1.3412111823
H	0.2812149872	-1.9854094132	0.2724782254
H	-0.6968926083	-1.2837253431	1.5757300551
C	1.3501365506	-2.6879071884	-3.2921792572
H	1.4401006765	-2.2695608482	-4.3066751450
H	1.8699443990	-3.6529854193	-3.2774704652
H	0.2904342376	-2.8940766258	-3.0897703474
N	1.9040321359	-1.8511109471	-2.2419120797
H	2.9164780170	-1.8705669365	-2.2077650016
C	1.3548707425	-0.5233730743	-2.0867979117
H	1.7827075453	-0.0415878707	-1.1993293633
H	0.2751839708	-0.5660378154	-1.9154844711
C	1.6684940337	0.3116865343	-3.3005993788
O	2.4475721971	-0.0939018655	-4.1611305783
N	1.0431182151	1.4751226971	-3.3820998123
H	0.2373371602	1.6128296690	-2.7661423964
C	1.2650723955	2.3872239943	-4.4869674810
H	2.0976536609	1.9914639705	-5.0697468372
C	1.6913770539	3.6703240945	-3.7869557159
O	2.0071379098	4.6793371075	-4.4121540537
N	1.7159993852	3.5848969202	-2.4622325076
H	1.4555855923	2.7347788777	-1.9949161354
C	2.0895544671	4.6850779187	-1.5777512745
H	1.5158047613	5.5711544767	-1.8659998556
C	3.5570880086	5.1365528712	-1.7582524434
O	3.8180912416	6.3056023580	-2.0605453309
C	1.7790184356	4.3311614885	-0.1051788474
H	2.4402018321	3.5151994191	0.2083143850
H	0.7580095158	3.9473646865	-0.0550026566
N	4.5104718109	4.2230129995	-1.5645897773
H	4.3024601883	3.3496944224	-1.0834312107
C	5.9286442421	4.5807440939	-1.7278117723
H	6.1025310797	5.5130851327	-1.1792772476
C	6.9187882385	3.5341414821	-1.2122575974
H	6.7719762709	3.3231416978	-0.1506458258
H	7.9290903956	3.9327698901	-1.3604498011
H	6.8478945849	2.5842373888	-1.7488251477
C	-7.5708275258	5.1747090407	-0.0083516327
H	-8.1218235773	4.5582882630	-0.7282453544
H	-8.0357077152	5.0285217085	0.9740658856

H	-7.7309457498	6.2240376686	-0.2907615043
C	-6.0974471909	4.8335519796	0.0197920786
C	-5.3180207420	5.4245068881	1.0292215867
H	-5.8096328050	6.0307196069	1.7881231352
C	-5.4377665514	4.0697644830	-0.9455334630
H	-6.0033092968	3.6190437461	-1.7577290416
C	-3.9418430269	5.2634982539	1.0822003592
H	-3.3466843838	5.7194803611	1.8678301272
C	-4.0505445057	3.8857972083	-0.9020812527
H	-3.5508472194	3.2917618481	-1.6621739360
C	-3.2945221941	4.4859428831	0.1130240878
O	-1.9433214228	4.3767960604	0.2074404095
H	-1.6171223058	3.5684269948	-0.2553053474
O	8.5608661461	1.3522658572	2.6110999304
H	7.6136130608	1.6099004606	2.4006250357
H	8.9869229926	2.1882838830	2.8557067749
O	9.5843171465	0.2573619308	0.3952705846
H	9.2217874122	0.7235138698	1.2075056545
H	8.9328854338	0.4300660416	-0.3021361912
H	0.3701988677	2.5313119489	-5.1170545018
H	6.1041468164	4.7897916262	-2.7986583650
H	1.9024048619	5.2102248331	0.5410280135
H	0.3592438383	-2.6866105685	1.9293771918
CL	-0.7274523443	1.7487869513	-0.7577929690
CL	-6.3461563079	-2.2525721868	-2.5667202737

PWT_Cl3

C	-5.1269389803	-6.3846819472	-3.1861103227
H	-4.9410397796	-6.0834262712	-2.1369035840
H	-6.0666884856	-5.9109026830	-3.4862701544
H	-5.2675706392	-7.4717341455	-3.2132546233
N	-4.0733473870	-6.0119775339	-4.1256837855
H	-3.1982266847	-6.4491080196	-3.8416517638
C	-3.8409328153	-4.5771211667	-4.1978549176
H	-4.7828750288	-4.0689144375	-4.4315268098
H	-3.1468848026	-4.3664842592	-5.0231362840
C	-3.2298459198	-3.9999694988	-2.9308490934
O	-2.4493480462	-4.6593562055	-2.2340211087
N	-3.5691144071	-2.7523578319	-2.6404476090
H	-4.4990339390	-2.4389578501	-2.9549606245
C	-3.0520453188	-2.0888565763	-1.4541783976
H	-1.9589703106	-2.1256805225	-1.4896048025
C	-3.4353166870	-2.8158334026	-0.1806522878
O	-2.6357534644	-3.5483783141	0.3991697588
C	-3.5288836138	-0.6219110284	-1.4185128681
H	-4.5991972604	-0.5802916422	-1.6481794404
H	-2.9964010405	-0.0362648235	-2.1724122886
O	-3.3041894410	-0.0788231013	-0.1318302645
H	-2.5342636588	0.5370387865	-0.2018608674
N	-4.6743208520	-2.6026933108	0.2443347477
H	-5.3726682047	-2.2850371205	-0.4444390352
C	-5.1736831331	-3.2161020239	1.4591907322
H	-4.3659748294	-3.7687134697	1.9426333070
H	-6.0216536978	-3.8789704615	1.2638287685
C	-5.6203430593	-2.0801194216	2.3484603413
O	-6.3726690991	-2.2623737584	3.3021473374
N	-5.1357368956	-0.8885312440	2.0354739503
H	-4.4710969855	-0.7571182751	1.2775998071
C	-5.5128646287	0.2706592850	2.8153970174
H	-5.4610208790	-0.0204274773	3.8713568787
C	-7.0133879700	0.4936525558	2.6385787394
O	-7.7191473008	0.6771397033	3.6203140570
C	-4.5752023110	1.4907754800	2.6557583576
H	-4.4860021168	1.7661647289	1.5979192234
C	-3.1699654087	1.1064859263	3.1761265267
H	-2.8113370884	0.2300588543	2.6243632932
H	-3.2653827885	0.7820965523	4.2227055347
C	-5.1585634207	2.6901815484	3.4199349763
H	-4.5139542515	3.5658024820	3.3085355293
H	-5.2591532926	2.4608927801	4.4881295116
H	-6.1506455342	2.9622024587	3.0479853654
C	-2.1095358907	2.2101994523	3.0833549844
H	-1.1319029153	1.8077077000	3.3756420120
H	-2.3319436707	3.0502114617	3.7514273811
H	-2.0158029230	2.6080082927	2.0669294010
N	-7.5221872490	0.4528186329	1.3858038656
C	-8.9596263039	0.6548802085	1.1718340473
H	-9.2618261298	1.6539574183	1.5124882947
C	-9.7053764685	-0.3394798322	2.0447863951
O	-10.5939872108	0.0239716257	2.8146863798
C	-9.3300274368	-1.8070450493	1.9448022125
H	-8.9512009018	-2.0909634874	0.9576645630

H	-8.5416989361	-2.0213191690	2.6760238863
H	-10.2087843093	-2.4073461338	2.1961796531
C	-9.1470752405	0.5078144734	-0.3446677400
H	-10.0291152386	1.0531142199	-0.6937281514
H	-9.2569142996	-0.5435498818	-0.6312195319
C	-7.8221705235	1.0542707129	-0.8915246582
H	-7.8228832563	2.1493497752	-0.8636874110
H	-7.6145166712	0.7210892272	-1.9119424204
C	-6.7923039461	0.4978410155	0.0972584354
H	-5.8946925398	1.1146104368	0.1601722600
H	-6.5098372572	-0.5079485468	-0.2177524596
C	-1.6114866566	-6.4853412409	1.0848951213
H	-0.7563839859	-5.8292621547	0.9374165607
H	-1.3160040919	-7.5299645728	0.9680317005
H	-2.0186966584	-6.3098315019	2.0812673030
N	-2.6245339688	-6.1095508555	0.0769612299
H	-2.2938679290	-6.0543305984	-0.9016216807
H	-2.8569910944	-5.0759744563	0.2619468836
H	-3.4718122365	-6.6793426839	0.1113835976
C	5.2677103925	-2.0343850983	-3.8295145921
H	5.2054651568	-2.9625175075	-3.2374770012
H	4.7211008381	-2.1904101868	-4.7653725351
H	6.3262957936	-1.8712728744	-4.0906733667
N	4.7291334574	-0.8608199129	-3.1789461517
H	3.7257341331	-0.7657829937	-3.2726223260
C	5.3237938647	-0.4373636332	-1.9291710603
H	4.9305664858	0.5356676206	-1.6446620546
H	6.4164693091	-0.3442438001	-2.0614451263
C	5.0489213142	-1.4288434139	-0.8161562691
O	4.3257669464	-2.4022542619	-1.0027040683
N	5.6399196986	-1.1818539587	0.3440864290
H	6.2771715827	-0.3893155396	0.4218532650
C	5.4625335544	-2.0369356190	1.5061924955
H	5.2649049807	-3.0557499573	1.1664459801
C	4.2463561340	-1.5845549424	2.3094491205
O	3.6344262895	-2.3857633193	3.0070915805
C	6.7122403266	-1.9722575642	2.3890909794
H	6.4940587485	-2.5111757770	3.3198274260
H	6.8751432843	-0.9240656593	2.6767981187
C	7.9759676303	-2.5393600980	1.7500260232
H	8.0852328370	-2.1423856314	0.7373425478
H	7.8839349344	-3.6293823609	1.6572365141
C	9.2119324410	-2.2089174950	2.5917740098
H	8.9865081849	-2.3598001439	3.6514356276
H	9.5098268326	-1.1674524062	2.4727605143
N	10.3308049569	-3.1055731892	2.3068005742
H	10.7634768429	-3.5724343153	3.0920081787
C	10.9799692768	-3.1789474066	1.1445046093
N	10.6343174545	-2.3999396837	0.1266692663
H	10.3048962202	-1.4220117498	0.3262644113
H	11.1141486843	-2.5189927447	-0.7555053792
N	11.9774048520	-4.0455765827	0.9985760500
H	12.0341530161	-4.8699101764	1.5808646117
H	12.4844850112	-4.0893562144	0.1269457530
N	3.9079919156	-0.3004649012	2.2051830100
H	4.1453543677	0.1443011217	1.3213228615
C	2.7633814354	0.2770004717	2.9194396807

H	3.0111062032	0.1262034651	3.9807240007
C	1.5624580217	-0.6333392364	2.8077769275
O	0.9887341450	-1.0530885904	3.8101607826
C	2.6300576192	1.7940995987	2.7882202408
H	1.7911381030	2.0904035486	3.4271263755
H	2.3778841520	2.1141648964	1.7793371048
C	3.8889881457	2.5255753088	3.3302714483
H	3.6848462509	3.6055301776	3.3107012801
H	4.0760661663	2.2383421928	4.3687328192
C	5.1937701774	2.3391067811	2.5744832893
O	6.2726088429	2.0655192171	3.1045005831
O	5.1914601680	2.5813880007	1.2642853393
N	1.1716427188	-0.9059326372	1.5692963113
H	1.5833040735	-0.4103886306	0.7870742802
C	0.0393214950	-1.7715314214	1.3420048883
H	0.0315497129	-2.0482841775	0.2852596583
H	-0.9023743566	-1.2672207879	1.5765368261
C	1.0249866408	-2.9493303720	-3.2781897971
H	1.1265700009	-2.5879225160	-4.3134056990
H	1.5229196531	-3.9242222779	-3.2104776925
H	-0.0404587605	-3.1219064274	-3.0714719464
N	1.5908341509	-2.0705009191	-2.2715193912
H	2.6014821662	-2.1143809341	-2.2191508507
C	1.0689903751	-0.7266889073	-2.1697041142
H	1.5108806388	-0.2114745218	-1.3185226767
H	-0.0124273003	-0.7497820752	-1.9928760002
C	1.3659932070	0.0410255652	-3.4312225669
O	2.1156678286	-0.4212914344	-4.2892551733
N	0.7590597611	1.2104216334	-3.5555351888
H	-0.0179231149	1.4048878768	-2.9171435797
C	0.9685537744	2.0621852255	-4.7098904381
H	1.7793966054	1.6206766728	-5.2910834655
C	1.4348409884	3.3703212951	-4.0858277349
O	1.7520356163	4.3409588358	-4.7684398741
N	1.4917990330	3.3504040269	-2.7595015745
H	1.3426508440	2.4924562668	-2.2552836125
C	1.9068792921	4.4860243183	-1.9407849372
H	1.3759329866	5.3612999887	-2.3318896457
C	3.3769533230	4.9005343047	-2.1798012857
O	3.6504448837	6.0480525085	-2.5466900128
C	1.5045584994	4.3367287234	-0.4580806039
H	2.0235872068	3.4856781934	-0.0208285875
H	0.4409494892	4.0933866325	-0.4337201858
N	4.3189427614	3.9801352625	-1.9641105322
H	4.0453941483	3.0528907307	-1.6505213574
C	5.7384904637	4.3028125392	-2.1799569960
H	5.9209857416	5.2668280373	-1.6946243378
C	6.7271698708	3.2995099216	-1.6038094316
H	6.6547215560	3.3316185637	-0.5133902693
H	7.7398999476	3.6005350204	-1.8913536713
H	6.5567022087	2.2804921325	-1.9677771421
C	-7.7002891233	5.2330587619	-0.1604027931
H	-8.2850593094	4.5776063973	-0.8165492299
H	-8.1365966826	5.1676585216	0.8435188901
H	-7.8508313936	6.2621474905	-0.5140999262
C	-6.2328302391	4.8663083041	-0.1514851193
C	-5.4216379788	5.4958102817	0.8086788757

H	-5.8886015492	6.1392542031	1.5524863769
C	-5.6056180280	4.0549588104	-1.0993129796
H	-6.1964734767	3.5724343906	-1.8745279516
C	-4.0452578693	5.3289586688	0.8299943882
H	-3.4247895256	5.8153859590	1.5769546675
C	-4.2189633586	3.8642832843	-1.0865002595
H	-3.7438627354	3.2325414744	-1.8313624911
C	-3.4297029720	4.5058867435	-0.1221819583
O	-2.0774520116	4.3913507142	-0.0637784547
H	-1.7807934681	3.5512948019	-0.4939249048
O	9.1736694467	1.2977485464	3.2720171811
H	8.2197194303	1.5118345552	3.2936515701
H	9.5937067075	2.0618668643	3.6951861535
O	10.0682787178	0.2613537337	0.6786576205
H	10.1080798489	0.6272632217	1.5864603608
H	9.1628565618	0.5635131079	0.4228370424
H	4.3248746489	2.3895593716	0.7815161044
H	7.1056606002	1.6236413257	-0.1043542876
O	7.4884497609	1.0526128001	0.5819751590
H	7.1930498233	1.4821604396	1.4153983557
H	1.7088932737	5.2683377178	0.0872543310
H	0.0613869369	2.1945946441	-5.3247717941
H	5.9079603844	4.4323607027	-3.2649494994
H	0.1399028146	-2.6695193173	1.9718630763
CL	-1.0257877193	1.6943563985	-0.9639132908
CL	-6.6833979457	-2.3584744952	-2.3566930377
CL	3.1484457638	1.3611205676	-0.4309786880

PWT_C14

C	-5.2678923326	-6.4613554245	-3.0811645497
H	-5.0494153619	-6.1408898585	-2.0442943089
H	-6.2232258982	-6.0032636434	-3.3555704040
H	-5.3956659040	-7.5505383265	-3.0860490580
N	-4.2521902582	-6.0914138195	-4.0628585009
H	-3.3622147717	-6.5116576978	-3.7996728761
C	-4.0401327047	-4.6550637995	-4.1626994454
H	-4.9957124762	-4.1614616683	-4.3710316845
H	-3.3769445387	-4.4482728115	-5.0138765920
C	-3.3933138902	-4.0527893581	-2.9254743574
O	-2.5813812650	-4.6929103019	-2.2468377909
N	-3.7378648618	-2.8053069107	-2.6407935340
H	-4.6792147163	-2.5063316990	-2.9311546292
C	-3.1888266369	-2.1189594031	-1.4822111560
H	-2.0973321406	-2.1411068883	-1.5545061270
C	-3.5193645869	-2.8323153502	-0.1863990722
O	-2.6914706958	-3.5470138904	0.3756638261
C	-3.6881423739	-0.6591633668	-1.4517488811
H	-4.7662330069	-0.6384978366	-1.6467434038
H	-3.1909139138	-0.0760459217	-2.2311262765
O	-3.4322433223	-0.0922947199	-0.1819452970
H	-2.6707263021	0.5284091203	-0.2858634895
N	-4.7456722544	-2.6279127170	0.2778886274
H	-5.4707388073	-2.3275796455	-0.3890364153
C	-5.1956322269	-3.2299312773	1.5174924658
H	-4.3639977483	-3.7645089488	1.9803766464
H	-6.0408740867	-3.9065748363	1.3610176800
C	-5.6256713858	-2.0868464844	2.4058535850
O	-6.3426778594	-2.2644926979	3.3872166878
N	-5.1668053923	-0.8941392789	2.0600537560
H	-4.5260552533	-0.7659903779	1.2809996595
C	-5.5313795179	0.2714259018	2.8364373703
H	-5.4391470001	-0.0030829551	3.8940236198
C	-7.0397082744	0.4740417692	2.7081713485
O	-7.7137424722	0.6630254545	3.7109330685
C	-4.6134975884	1.4992291469	2.6261399009
H	-4.5606525416	1.7562498335	1.5611649956
C	-3.1884300041	1.1398603699	3.1094244461
H	-2.8399571242	0.2514351423	2.5704012289
H	-3.2466896112	0.8425738938	4.1666880265
C	-5.1865967562	2.7056290311	3.3868324274
H	-4.5528171106	3.5843535620	3.2434058861
H	-5.2542530488	2.4928325287	4.4610329188
H	-6.1912236567	2.9634354775	3.0385511835
C	-2.1407429991	2.2482589688	2.9531315812
H	-1.1529972990	1.8622136571	3.2311865973
H	-2.3507154072	3.1071004867	3.6008063062
H	-2.0779090193	2.6153831197	1.9226963309
N	-7.5904513646	0.4094106646	1.4742775650
C	-9.0367474697	0.5913215414	1.3070082931
H	-9.3397800569	1.5914563051	1.6440395470
C	-9.7398996929	-0.3993576464	2.2186401804
O	-10.6061240550	-0.0356161785	3.0135109239
C	-9.3483707888	-1.8630944329	2.1270955639
H	-9.0048805087	-2.1577211664	1.1302106022
H	-8.5278614821	-2.0545728719	2.8288959810

H	-10.2077537522	-2.4712126805	2.4231611150
C	-9.2738417285	0.4206615294	-0.2002628067
H	-10.1734096725	0.9516104676	-0.5265635001
H	-9.3814597748	-0.6358498668	-0.4683157060
C	-7.9742251118	0.9729617432	-0.7997419793
H	-7.9851332331	2.0682619929	-0.7870969059
H	-7.7979753542	0.6272446592	-1.8219170854
C	-6.9056353569	0.4409398083	0.1607716950
H	-6.0120808880	1.0660696758	0.1833301981
H	-6.6249662749	-0.5672406863	-0.1483144708
C	-1.6081518293	-6.4615816823	1.0661765487
H	-0.7648878344	-5.7997977033	0.8798333714
H	-1.3058242437	-7.5048557535	0.9553283906
H	-1.9812519649	-6.2730951692	2.0734299903
N	-2.6595991822	-6.1121820138	0.0885302241
H	-2.3616352807	-6.0681539329	-0.9006714476
H	-2.8962925245	-5.0786896420	0.2666757518
H	-3.4988839235	-6.6899296190	0.1599886503
C	5.0852491622	-1.9814404192	-4.1434872978
H	5.0779666219	-2.9050337788	-3.5399876792
H	4.5261209617	-2.1718017562	-5.0667138257
H	6.1283291249	-1.7729749880	-4.4260321875
N	4.5131323637	-0.8231050693	-3.4897544553
H	3.5039175567	-0.8178013981	-3.5135979264
C	5.1448471823	-0.3749391759	-2.2670698190
H	4.7470649552	0.5996432856	-1.9655335872
H	6.2225615470	-0.2304302064	-2.4272361449
C	4.9204248085	-1.3537397119	-1.1317403035
O	4.2034107915	-2.3382225437	-1.2799477700
N	5.5476039725	-1.0833230413	0.0040268912
H	6.1757091981	-0.2833597607	0.0315110208
C	5.4205939628	-1.9238943772	1.1831915475
H	5.2253895230	-2.9491134039	0.8618598975
C	4.2270588195	-1.4746590580	2.0214149602
O	3.6492635931	-2.2731141571	2.7506063830
C	6.6988290168	-1.8318606925	2.0217050821
H	6.5247517506	-2.3486041123	2.9720793001
H	6.8629894413	-0.7783241373	2.2883331693
C	7.9469083764	-2.3929058142	1.3475075714
H	8.0178022942	-2.0027015430	0.3302121403
H	7.8604417029	-3.4877204046	1.2807613070
C	9.2067195723	-2.0358996518	2.1417136850
H	9.0197491080	-2.1284281236	3.2169168397
H	9.4882303147	-0.9967858056	1.9358381589
N	10.3262067483	-2.9231440362	1.8308714981
H	10.7950416036	-3.3589624418	2.6127854447
C	10.9361555217	-3.0052655748	0.6480999451
N	10.5463402434	-2.2449262478	-0.3678947186
H	10.0111879785	-1.3057773124	-0.2954623908
H	10.9876403810	-2.3793808048	-1.2677085031
N	11.9386632821	-3.8619609151	0.4799622509
H	11.9844132178	-4.6910404661	1.0558982072
H	12.3500960672	-3.9543639144	-0.4364072865
N	3.8694819896	-0.1962879119	1.9111651374
H	4.3173088005	0.4073196090	1.2183473974
C	2.7428806673	0.3775997171	2.6562721430
H	3.0079410340	0.3036139835	3.7199635335

C	1.5501905491	-0.5484393561	2.5984282415
O	1.0162675884	-0.9607271083	3.6255928249
C	2.4403924976	1.8558444544	2.3840385071
H	1.3735651843	2.0166299200	2.5705458241
H	2.6269067870	2.1082865679	1.3432133033
C	3.2119636009	2.8304186704	3.3275199184
H	3.2947422895	3.8049511698	2.8329907532
H	2.6340796170	2.9644010858	4.2451572829
C	4.5928362639	2.3873184861	3.8035107084
O	4.7898933452	2.0122640884	4.9534254200
O	5.6195830970	2.4384859379	2.9519208255
N	1.1207069675	-0.8431854942	1.3779584273
H	1.6492797434	-0.5414289500	0.5726289849
C	-0.0079282611	-1.7253149647	1.2015948316
H	-0.0535371205	-2.0159377404	0.1495154126
H	-0.9428784835	-1.2241285348	1.4655440761
C	0.8452961552	-2.9564275768	-3.4373209488
H	0.9361077860	-2.6181279608	-4.4811125322
H	1.3443170660	-3.9288770500	-3.3515514956
H	-0.2184668288	-3.1241624847	-3.2151122555
N	1.4228489539	-2.0570139566	-2.4585942810
H	2.4344535395	-2.1069032611	-2.3933709397
C	0.8882133158	-0.7181905363	-2.3574281608
H	1.3647912201	-0.1874405071	-1.5246835393
H	-0.1822344342	-0.7393263711	-2.1245212867
C	1.1324460982	0.0350410309	-3.6388404887
O	1.8580383943	-0.4304494768	-4.5156548402
N	0.5072105664	1.1952618713	-3.7583274393
H	-0.2671356937	1.3767274693	-3.1138176924
C	0.6666129842	2.0330071556	-4.9308029008
H	1.4660328570	1.5950408492	-5.5302308295
C	1.1377330349	3.3553067216	-4.3411693233
O	1.4194061967	4.3198722644	-5.0475562876
N	1.2401959742	3.3548696724	-3.0174309975
H	1.0189832073	2.5306685168	-2.4883270725
C	1.6689233976	4.5068335128	-2.2291454485
H	1.0777290788	5.3771091937	-2.5293517365
C	3.1247401376	4.9353557447	-2.5241561537
O	3.3713347987	6.0807274930	-2.9159694147
C	1.4480796343	4.2256619193	-0.7242280139
H	2.1061105470	3.4051876540	-0.4142457893
H	0.4221030294	3.8751831066	-0.5890425783
N	4.0848529936	4.0293665301	-2.3282790323
H	3.9116753997	3.2006981962	-1.7701610628
C	5.4921033461	4.3657997040	-2.5971380377
H	5.6842954524	5.3380305920	-2.1303973288
C	6.5905699853	3.4051652016	-2.1267693759
H	6.6970729553	3.4092904287	-1.0445329265
H	7.5292264477	3.7567738407	-2.5697164210
H	6.4386611150	2.3693532967	-2.4341133604
C	-7.8803386166	5.1647997110	-0.1305312706
H	-8.4799159525	4.4895397272	-0.7527176344
H	-8.2801694520	5.1136818530	0.8894213706
H	-8.0572213431	6.1850062552	-0.4982834811
C	-6.4090093378	4.8156784057	-0.1669382439
C	-5.5742946444	5.4677622412	0.7572228444
H	-6.0244542468	6.1128335271	1.5101024465

C	-5.8038475791	4.0021798673	-1.1270082870
H	-6.4144706255	3.5021703163	-1.8755934320
C	-4.1959679021	5.3218301628	0.7315420295
H	-3.5565322653	5.8259481515	1.4500654801
C	-4.4151615861	3.8316130536	-1.1612536766
H	-3.9572982841	3.1968763430	-1.9140234511
C	-3.6016416318	4.4971361536	-0.2332956152
O	-2.2485971201	4.4070676635	-0.2220981923
H	-1.9498171101	3.5774736356	-0.6693477732
O	7.4194553260	0.9438149118	4.7858809738
H	6.5151553926	1.2432988818	5.0333576481
H	7.5039481165	1.3088969117	3.8905528279
O	8.1439571563	-1.6998986836	5.2040867546
H	7.2665157439	-2.0901589630	5.3330446762
H	7.9374627324	-0.7416575096	5.0623762275
H	5.3304859982	2.5500421267	1.9962056125
H	1.6414789391	5.1253177344	-0.1248043251
H	0.1196473727	-2.6166660435	1.8370307252
H	5.5733245884	4.5145261925	-3.6899547762
H	-0.2611819283	2.1414266856	-5.5188818280
CL	-1.2407769419	1.7096089110	-1.1723052653
CL	-6.8650621754	-2.4665872952	-2.2591914258
CL	4.7724918068	2.2134538377	0.1435550826
CL	9.2066877209	0.3863621084	-0.5037290062

E148Q_Cl3

C	-5.4169396934	-6.6534290984	-2.5407853166
H	-5.2039146048	-6.2519159066	-1.5309789795
H	-6.3579527517	-6.1996822833	-2.8668936790
H	-5.5703977704	-7.7356883056	-2.4563084115
N	-4.3808214787	-6.3904146595	-3.5351640003
H	-3.5052047629	-6.8120115928	-3.2302206794
C	-4.1315599016	-4.9733059430	-3.7535891630
H	-5.0720646746	-4.4759762382	-4.0149567757
H	-3.4549215550	-4.8552670677	-4.6111707590
C	-3.4827714067	-4.2839548036	-2.5637557731
O	-2.6944117737	-4.8836016589	-1.8231818485
N	-3.7987101541	-3.0088102248	-2.3900893944
H	-4.7340813852	-2.7141817733	-2.7096544602
C	-3.2447195598	-2.2400254903	-1.2869604566
H	-2.1533353709	-2.3007271073	-1.3421263369
C	-3.6067277877	-2.8324847562	0.0603342629
O	-2.8030709983	-3.5167086942	0.6912782916
C	-3.6947637363	-0.7671497785	-1.3841923020
H	-4.7700652395	-0.7263281281	-1.5872294494
H	-3.1756380160	-0.2693514959	-2.2076113927
O	-3.4266863405	-0.1043929107	-0.1629194160
H	-2.6332748420	0.4646384759	-0.2989786977
N	-4.8322930227	-2.5597019445	0.4901637553
H	-5.5418527363	-2.2968704434	-0.2098872377
C	-5.3102801079	-3.0431391523	1.7705249593
H	-4.4983324506	-3.5576462285	2.2876821394
H	-6.1710968853	-3.7091115004	1.6609386063
C	-5.7206434859	-1.8186223125	2.5534185708
O	-6.4521616928	-1.8948120794	3.5371900038
N	-5.2282311626	-0.6710845452	2.1136764003
H	-4.5776918750	-0.6261795745	1.3344864769
C	-5.5714117976	0.5647238344	2.7839246383
H	-5.4995890262	0.3765389093	3.8618557551
C	-7.0727199960	0.7922213055	2.6199746632
O	-7.7522573589	1.0820037629	3.5945633456
C	-4.6194421910	1.7475281211	2.4881569755
H	-4.5451697977	1.9151908818	1.4067244906
C	-3.2116018486	1.3923895117	3.0224513933
H	-2.8764224142	0.4583823282	2.5569594351
H	-3.2943559396	1.1763778210	4.0974891408
C	-5.1716300726	3.0253614224	3.1400491639
H	-4.5150457180	3.8749971204	2.9358919403
H	-5.2596012838	2.9022096988	4.2265822044
H	-6.1648080111	3.2772409993	2.7570279297
C	-2.1341119122	2.4613612451	2.8051939701
H	-1.1611961965	2.0740557934	3.1314515915
H	-2.3351214083	3.3702860004	3.3837320735
H	-2.0446349953	2.7498100376	1.7518453007
N	-7.6119401945	0.6363644727	1.3891459890
C	-9.0513519584	0.8384201295	1.1888704651
H	-9.3323404715	1.8706084820	1.4362481065
C	-9.7888001583	-0.0538833706	2.1721840551
O	-10.6538657454	0.3969708725	2.9224266702
C	-9.4354325931	-1.5298381061	2.2087076206
H	-9.0829744931	-1.9147819099	1.2463270721

H	-8.6338789014	-1.6839061822	2.9406942736
H	-10.3162078980	-2.0889504101	2.5362677239
C	-9.2764864991	0.5465494776	-0.3011738208
H	-10.1606071385	1.0665166958	-0.6820213237
H	-9.4042342140	-0.5262330722	-0.4809630847
C	-7.9591514251	1.0200699840	-0.9284105052
H	-7.9479023892	2.1126561905	-1.0072247342
H	-7.7793781180	0.5866838068	-1.9159397746
C	-6.9120063972	0.5490151337	0.0864783201
H	-6.0073403110	1.1587065777	0.0699136312
H	-6.6462545726	-0.4854751418	-0.1367329030
C	-1.8009296730	-6.3874788079	1.6396899737
H	-0.9412563643	-5.7616005253	1.4102479766
H	-1.5214554820	-7.4427230486	1.6187150369
H	-2.1820922575	-6.1100047010	2.6230884794
N	-2.8329111512	-6.0970128991	0.6228036553
H	-2.5248051329	-6.1445799571	-0.3632049524
H	-3.0480404497	-5.0482009375	0.7103878616
H	-3.6859907788	-6.6484394117	0.7326578444
C	5.0360120602	-2.5383098535	-3.8452062697
H	4.9887871057	-3.4034774695	-3.1635172569
H	4.4711032880	-2.7852410254	-4.7500892747
H	6.0878552403	-2.3992998026	-4.1430686793
N	4.5081211491	-1.3065449414	-3.2998479367
H	3.5029607144	-1.2286552759	-3.3776942848
C	5.1380760925	-0.7715688193	-2.1116428542
H	4.7678283726	0.2380901417	-1.9000366765
H	6.2232165114	-0.6781503392	-2.2747983484
C	4.8771313303	-1.6446421624	-0.9004286829
O	4.1371041640	-2.6204817250	-0.9737631305
N	5.4989802045	-1.2939946960	0.2161716628
H	6.1059358810	-0.4792307380	0.2290617343
C	5.3384386355	-2.0280170634	1.4605825952
H	5.1194528916	-3.0716524458	1.2263144436
C	4.1478863438	-1.4803839563	2.2426569015
O	3.5425120967	-2.1997547533	3.0295022977
C	6.6097193842	-1.8960954844	2.3043254203
H	6.4026110039	-2.3452877835	3.2845858142
H	6.7951285427	-0.8311286491	2.4793313763
C	7.8502536552	-2.5424879446	1.6958293151
H	7.9331904876	-2.2467412158	0.6463828399
H	7.7435211039	-3.6352227792	1.7125349772
C	9.1102669536	-2.1499477812	2.4727589826
H	8.9017391336	-2.2197757891	3.5455166964
H	9.4407224121	-1.1191113357	2.3001048870
N	10.2102150194	-3.0872751546	2.2522852932
H	10.6965994727	-3.4225441549	3.0731322187
C	10.8302756662	-3.2843532260	1.0884919146
N	10.4704486349	-2.6038549914	0.0069357856
H	10.1215991581	-1.6200600586	0.0400467317
H	10.8700737254	-2.8753524736	-0.8812510237
N	11.8125612080	-4.1762904792	1.0061387069
H	11.8797642324	-4.9352089502	1.6695825137
H	12.3406379683	-4.2790319254	0.1527321189
N	3.8238500168	-0.2077090778	2.0200628485
H	4.3407807693	0.3644655267	1.3520646925
C	2.7043283323	0.4545547576	2.6996508194

H	2.9668426089	0.5159231985	3.7619685134
C	1.4893288208	-0.4438588673	2.7054080625
O	0.9344257412	-0.7543203586	3.7569869871
C	2.3476871462	1.8790670221	2.2227351276
H	1.2554429992	1.9579489378	2.2041815952
H	2.6927022841	2.0545650783	1.2051350272
C	2.8355937736	3.0135832663	3.1531188414
H	2.3551837283	3.9455436071	2.8377383135
H	2.4947431949	2.8020856692	4.1741128341
C	4.3408782390	3.2094155331	3.2246091037
O	5.0883316370	2.3514073565	3.7225587697
N	4.8016001559	4.4082332845	2.7935044078
N	1.0653767695	-0.8307304170	1.5089662285
H	1.5913198199	-0.5901492780	0.6820014025
C	-0.0832403608	-1.6970287263	1.3937276619
H	-0.1243888122	-2.0748149720	0.3697377658
H	-1.0088882042	-1.1536453173	1.6002016027
C	0.7637616678	-3.3381633051	-3.1009747939
H	0.8400460724	-3.0853936846	-4.1697353874
H	1.2479041525	-4.3095811759	-2.9473992315
H	-0.2969350955	-3.4677578058	-2.8457648412
N	1.3770426345	-2.3730925091	-2.2069171880
H	2.3879728272	-2.4345961799	-2.1713560096
C	0.8753201870	-1.0179467698	-2.2262203174
H	1.3544347701	-0.4287753126	-1.4351491695
H	-0.1966379923	-0.9961023210	-2.0050751805
C	1.1519103281	-0.3824518311	-3.5636316515
O	1.8746893468	-0.9382093397	-4.3886729122
N	0.5574315188	0.7782397570	-3.7887959973
H	-0.2203162404	1.0277875844	-3.1718165402
C	0.7502119158	1.5092300424	-5.0258949914
H	1.5427270168	1.0029803291	-5.5786073530
C	1.2483271222	2.8650309706	-4.5444564343
O	1.5616411132	3.7589799597	-5.3263762179
N	1.3368502475	2.9745765002	-3.2242498469
H	1.0417260576	2.2238545675	-2.6251504901
C	1.7862069713	4.1786132391	-2.5309994836
H	1.2205719954	5.0369588538	-2.9055440767
C	3.2553864126	4.5450971666	-2.8428749399
O	3.5348953354	5.6467220860	-3.3271272491
C	1.5574579000	4.0306389484	-1.0073307609
H	2.2122848341	3.2368151895	-0.6259287045
H	0.5326755941	3.6910137495	-0.8445874396
N	4.1902295580	3.6360135492	-2.5589096780
H	3.9886951861	2.8645817731	-1.9324851450
C	5.6082631462	3.9141679683	-2.8375435991
H	5.8249354720	4.9166980182	-2.4526673470
C	6.6871186784	2.9720267496	-2.2927902991
H	7.6163628403	3.2281635896	-2.8159696104
H	6.4716999982	1.9152798613	-2.4635271594
H	6.8353295950	3.1190173560	-1.2254643850
C	-7.7649127174	5.2438401865	-0.6160816674
H	-8.3701884848	4.5479990130	-1.2087981067
H	-8.1828810595	5.2627968946	0.3974960515
H	-7.9077810765	6.2444827124	-1.0458338343
C	-6.3025581676	4.8573166526	-0.6042609946
C	-5.4628799177	5.5605146779	0.2769542168

H	-5.9043552739	6.2821045133	0.9621046367
C	-5.7072363711	3.9455317627	-1.4784113575
H	-6.3202906054	3.4013004873	-2.1930117155
C	-4.0899188932	5.3680283895	0.2936722682
H	-3.4490967408	5.9127088155	0.9807924608
C	-4.3240080737	3.7287879123	-1.4684105076
H	-3.8744861231	3.0183036297	-2.1562482897
C	-3.5074978331	4.4434959093	-0.5824334060
O	-2.1554477627	4.3063367474	-0.5323547018
H	-1.8765860899	3.4310123721	-0.8943871286
O	7.6332536504	1.6183727536	3.4288918692
H	7.5561360859	0.8636664152	4.0329065900
H	6.7396114791	2.0662940135	3.5169793605
O	9.8941801234	0.0972186856	-0.1090514758
H	8.9721255630	0.4365115365	0.1342454593
H	10.1438665713	0.5722210896	-0.9166734683
H	5.8009926720	4.4959748532	2.6597910426
H	4.2214426335	4.9745386369	2.1834586313
H	10.3888604808	0.8759663566	1.7002364460
O	10.3776307706	0.8451335369	2.6743905889
H	9.6222478048	1.4049448491	2.9332255604
H	6.8459031822	1.4331092983	0.4381571990
O	7.6083035005	0.8946037890	0.7889826885
H	7.6450107856	1.1329473673	1.7505317408
H	-0.1713621980	1.6063533759	-5.6321820481
H	1.7544697507	4.9828222745	-0.4866702471
H	5.7062438057	3.9701513357	-3.9425593967
H	0.0059633224	-2.5430547748	2.1022021815
CL	-1.1012754722	1.5317025127	-1.2003797123
CL	-6.8866860024	-2.5110950080	-2.0959025832
CL	4.9555104522	2.1081654786	0.1700438768

E148Q_Cl4

C	-5.2640990647	-6.4271445349	-3.0817402968
H	-5.0668558341	-6.1112722768	-2.0393719953
H	-6.2064564606	-5.9557184914	-3.3774023951
H	-5.4054599904	-7.5147369504	-3.0924371605
N	-4.2200659008	-6.0677771964	-4.0377530034
H	-3.3412746967	-6.4957764416	-3.7501928151
C	-3.9908048170	-4.6335433887	-4.1296809124
H	-4.9358007783	-4.1300970260	-4.3611772517
H	-3.3039716782	-4.4326216005	-4.9632748633
C	-3.3692174833	-4.0398444908	-2.8754936037
O	-2.5812706138	-4.6893347623	-2.1777550294
N	-3.7079917876	-2.7893032298	-2.5973757774
H	-4.6336080041	-2.4779997079	-2.9172228362
C	-3.1813024178	-2.1104079578	-1.4241202565
H	-2.0887314571	-2.1376219491	-1.4704175546
C	-3.5517110404	-2.8222686696	-0.1383081476
O	-2.7456373381	-3.5463213316	0.4431640607
C	-3.6766562461	-0.6499705691	-1.4040466861
H	-4.7504405830	-0.6253791071	-1.6241211430
H	-3.1595361433	-0.0662859522	-2.1692758213
O	-3.4435580042	-0.0861398182	-0.1286230242
H	-2.7092850754	0.5695363382	-0.2336016128
N	-4.7871650347	-2.6059205883	0.2953056619
H	-5.4935696510	-2.3071355368	-0.3925013010
C	-5.2743901993	-3.2051325705	1.5221164213
H	-4.4602977344	-3.7488274475	2.0052464931
H	-6.1224556435	-3.8725156156	1.3428052754
C	-5.7149094712	-2.0590117847	2.4013842505
O	-6.4582108963	-2.2307285977	3.3640608980
N	-5.2352368656	-0.8705838123	2.0693614413
H	-4.5758147638	-0.7470167433	1.3046401814
C	-5.6072619648	0.2975094083	2.8383761053
H	-5.5423227344	0.0226641078	3.8979161037
C	-7.1097161069	0.5158757097	2.6725186079
O	-7.8068315520	0.7102930323	3.6583177563
C	-4.6750187938	1.5176548810	2.6470273269
H	-4.6004256942	1.7755744834	1.5836602521
C	-3.2615490025	1.1481335609	3.1552163726
H	-2.9130553513	0.2526482271	2.6283991268
H	-3.3388765028	0.8601626847	4.2140233047
C	-5.2520976377	2.7285049504	3.3977367159
H	-4.6088499378	3.6020664852	3.2652639010
H	-5.3401494874	2.5161009877	4.4706622779
H	-6.2483591267	2.9944022943	3.0319527104
C	-2.2021384143	2.2461477637	3.0039620953
H	-1.2210841247	1.8545219659	3.2973221954
H	-2.4138177840	3.1128397166	3.6407461644
H	-2.1221997500	2.6026871570	1.9710769296
N	-7.6298202970	0.4587942449	1.4250322001
C	-9.0694945766	0.6558752734	1.2217097053
H	-9.3703568459	1.6585413096	1.5530210272
C	-9.8055473594	-0.3288680628	2.1135885439
O	-10.6877455290	0.0425948606	2.8870312930
C	-9.4263165682	-1.7962459977	2.0294114892
H	-9.0620134075	-2.0931950416	1.0406673585

H	-8.6243240267	-1.9963816191	2.7500204494
H	-10.2983598547	-2.3962759872	2.3043949487
C	-9.2706253889	0.4903378346	-0.2916088370
H	-10.1545184762	1.0338359911	-0.6395227299
H	-9.3856489012	-0.5643390399	-0.5638372045
C	-7.9487816595	1.0249812536	-0.8579530291
H	-7.9436614148	2.1203810469	-0.8449284827
H	-7.7520590643	0.6774620512	-1.8758050016
C	-6.9125428668	0.4770764492	0.1283874176
H	-6.0096851680	1.0872462572	0.1720586120
H	-6.6413808582	-0.5363454504	-0.1721385504
C	-1.7100854593	-6.4729536913	1.1555883286
H	-0.8595991395	-5.8131620214	0.9979606204
H	-1.4096445567	-7.5171053286	1.0445038740
H	-2.1102876581	-6.2917831820	2.1537516790
N	-2.7329106412	-6.1112456187	0.1523884894
H	-2.4068949945	-6.0584101162	-0.8285444683
H	-2.9722424891	-5.0757155006	0.3276611092
H	-3.5759487105	-6.6860834929	0.1943825423
C	5.1206534601	-2.0698772257	-3.8742562839
H	5.0676666725	-2.9926702671	-3.2712748293
H	4.5701370761	-2.2410606517	-4.8063109852
H	6.1770966783	-1.9049252561	-4.1406475426
N	4.5817225743	-0.8910893768	-3.2347406389
H	3.5759722749	-0.8176770851	-3.3017724364
C	5.1869937504	-0.4513128107	-1.9957421017
H	4.7875926702	0.5190233394	-1.7135930022
H	6.2758571952	-0.3464584036	-2.1336382119
C	4.9239774367	-1.4294567809	-0.8681580506
O	4.2008440419	-2.4062619102	-1.0361188576
N	5.5250780541	-1.1672418097	0.2835221814
H	6.2597016760	-0.4650571571	0.2883498312
C	5.3597541810	-2.0082356630	1.4576253948
H	5.1604107592	-3.0316603633	1.1310443375
C	4.1501527204	-1.5479706759	2.2663141163
O	3.5459848082	-2.3415189579	2.9793079858
C	6.6173276963	-1.9306652164	2.3282295984
H	6.4055577890	-2.4592349968	3.2667876909
H	6.7983773031	-0.8830779138	2.6043846338
C	7.8761696234	-2.5035443778	1.6846905793
H	7.9752151716	-2.1123300267	0.6704770176
H	7.7854593789	-3.5971937236	1.6075539993
C	9.1191667589	-2.1607588587	2.5110060209
H	8.9031096596	-2.3049372926	3.5740473979
H	9.4403894132	-1.1232197359	2.3941716486
N	10.2369527558	-3.0590405374	2.2268907437
H	10.7460728324	-3.4134837233	3.0251889014
C	10.8756420612	-3.1456684776	1.0597139913
N	10.5193948002	-2.3798141510	0.0355694510
H	9.9765921110	-1.4814229007	0.1149523156
H	10.9097137529	-2.5515117259	-0.8802376363
N	11.8732092867	-4.0124107104	0.9153653423
H	11.9203865540	-4.8347618970	1.4986877347
H	12.3922924103	-4.0435318067	0.0515614138
N	3.8086288107	-0.2658120701	2.1493537439
H	4.1232356646	0.2256088525	1.3182450901
C	2.6695647172	0.3185480973	2.8668620613

H	2.9243504705	0.2084599545	3.9310738204
C	1.4692547408	-0.5950431966	2.7773583826
O	0.9054024846	-1.0033475506	3.7900183392
C	2.4298582110	1.8195192996	2.6762990338
H	1.4723827687	2.0375107872	3.1642655737
H	2.3086363835	2.0812845608	1.6271967382
C	3.4944557833	2.7023860866	3.3689286985
H	3.2234563350	3.7540508884	3.2031240553
H	3.4866698931	2.5254018237	4.4483936423
C	4.9469335427	2.5331348911	2.9321818858
O	5.8534797946	2.3729198892	3.7590766210
N	5.1985336250	2.6462404102	1.6015547180
N	1.0676612031	-0.8834989868	1.5459389222
H	1.5110495167	-0.4320905613	0.7530827534
C	-0.0651790389	-1.7536653712	1.3396443526
H	-0.0817031652	-2.0441028745	0.2863766727
H	-1.0064528485	-1.2491490078	1.5770451752
C	0.9057465033	-2.9860769066	-3.2858862589
H	1.0282004220	-2.6427669279	-4.3253238468
H	1.3979705182	-3.9621317852	-3.1923133038
H	-0.1653883678	-3.1519364307	-3.0985926277
N	1.4539101013	-2.0945912109	-2.2839270563
H	2.4633968779	-2.1423907737	-2.1994597419
C	0.9306858812	-0.7504751319	-2.1938916108
H	1.3956359675	-0.2215154181	-1.3624064178
H	-0.1492828812	-0.7655402585	-2.0001274171
C	1.2148683035	0.0021280862	-3.4674118293
O	1.9575058530	-0.4695031957	-4.3264941327
N	0.6048030953	1.1689193393	-3.6005569135
H	-0.1600070607	1.3802858162	-2.9532898062
C	0.8023097268	2.0067428698	-4.7671621862
H	1.6102580465	1.5584859579	-5.3475128183
C	1.2719872591	3.3232182654	-4.1635119991
O	1.5812756803	4.2858899131	-4.8608734342
N	1.3410440441	3.3197263940	-2.8376157108
H	1.2613795566	2.4540676622	-2.3288379653
C	1.7615867497	4.4660131467	-2.0367458629
H	1.2194645881	5.3328609558	-2.4307175181
C	3.2287047702	4.8799312527	-2.2942366697
O	3.4968578169	6.0232866872	-2.6776884838
C	1.3924031097	4.3291918411	-0.5436012027
H	1.9706716533	3.5198727069	-0.1006702131
H	0.3430974537	4.0306418351	-0.4881885829
N	4.1742113753	3.9637861623	-2.0758415394
H	3.9134307541	3.0491669313	-1.7091593163
C	5.5911751956	4.2860820305	-2.3085750895
H	5.7839407197	5.2526783172	-1.8324942540
C	6.5693858376	3.2657148485	-1.7283117734
H	7.5894285292	3.5505725354	-2.0043417886
H	6.4013223801	2.2439142338	-2.0737562312
H	6.5117372113	3.2724412032	-0.6367832058
C	-7.8302668311	5.2193379743	-0.1781569926
H	-8.4253137799	4.5382779436	-0.7987511086
H	-8.2509684166	5.1928179849	0.8343424136
H	-7.9894626557	6.2336961776	-0.5698987332
C	-6.3621540930	4.8551045519	-0.1781109876
C	-5.5488830424	5.4937332335	0.7737734745

H	-6.0165301748	6.1268438272	1.5263080408
C	-5.7376470542	4.0558942953	-1.1374762103
H	-6.3330209841	3.5665042586	-1.9053829211
C	-4.1700126003	5.3520997246	0.7727307566
H	-3.5448201285	5.8465195548	1.5103722426
C	-4.3488681805	3.8899744038	-1.1475822610
H	-3.8730086225	3.2668752895	-1.8981868158
C	-3.5550817006	4.5464768541	-0.1952546310
O	-2.2028504192	4.4668932946	-0.1670279742
H	-1.9012037076	3.6363811462	-0.6159332008
O	8.2522210991	1.0978186984	3.0112173948
H	7.4800797214	1.6397928392	3.2985432653
H	8.2476019263	1.0976951190	2.0357743622
O	10.9624260003	0.5487543389	2.5651988301
H	10.1638331847	0.8931696196	3.0175746694
H	10.7099823207	0.6751089525	1.6312795877
H	6.1459993020	2.4634311687	1.2973494242
H	4.4688049005	2.5147056018	0.9005976513
H	1.5598748095	5.2828044494	-0.0246993900
H	-0.1099116916	2.1301094151	-5.3763572342
H	0.0417759339	-2.6438056980	1.9796236868
H	5.7500334523	4.4036142722	-3.3963738234
CL	-1.3312672310	1.7592464388	-1.1571779122
CL	-6.8656789675	-2.4770680158	-2.2614862180
CL	3.0230370542	1.3602394637	-0.5429617619
CL	9.0325727480	0.3334751316	-0.1479825989