

fc1

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S U P P L E M E N T A R Y   M A T E R I A L  
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B E L O N G I N G   T O   T H E   P A P E R

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Table S1 - Crystal Data and Details of the Structure Determination  
for: fcl

Crystal Data			
Empirical Formula	C <sub>20</sub> H <sub>2</sub> Cl <sub>2</sub> , C <sub>20</sub> H <sub>19</sub> N O <sub>3</sub>		
Formula Weight	406.29		
Crystal System	Monoclinic		
Space group	P2 <sub>1</sub> /n	(No. 14)	
a, b, c [Angstrom]	8.6530(10)	23.257(2)	10.6200(10)
alpha, beta, gamma [deg]	90	109.410(10)	90
V [Ang**3]	2015.7(4)		
Z	4		
D(obs), D(calc) [g/cm**3]	0.000, 1.339		
F(000)	848		
Mu(CuK $\alpha$ ) [ /mm ]	3.1		
Crystal Size [mm]	0.20 x 0.20 x 0.30		
Data Collection			
Temperature (K)	289		
Radiation [Angstrom]	CuK $\alpha$	1.54178	
Theta Min-Max [Deg]	3.8, 50.4		
Dataset	-1: 8 ; -1: 23 ; -10: 10		
Tot., Uniq. Data, R(int)	2810,	2109,	0.027
Observed data [I > 2.0 sigma(I)]	1549		
Refinement			
Nref, Npar	2109, 265		
R, wR <sub>2</sub> , S	0.0713, 0.2175, 1.04		
w = 1/[\s^2^(Fo^2^)+(0.1511P)^2^+0.5796P] where P=(Fo^2^+2Fc^2^)/3			
Max. and Av. Shift/Error	0.00, 0.00		
Min. and Max. resd. dens. [e/Ang^3]	-0.38, 0.59		

Table S2 - Final Coordinates and Equivalent Isotropic Displacement  
Parameters of the non-Hydrogen atoms  
for: fcl

Atom	x	y	z	U(eq) [Ang <sup>2</sup> ]
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*Cl26	0.7950(8)	0.8922(10)	0.6830(7)	0.314(10)
*Cl27	1.0598(7)	0.9228(3)	0.6056(5)	0.105(2)
C25	0.9906(9)	0.9135(4)	0.7337(8)	0.114(3)
*Cl28	0.7979(11)	0.9400(4)	0.6962(9)	0.206(5)
*Cl29	1.0476(17)	0.8887(10)	0.6256(13)	0.305(9)
O7	0.6724(4)	1.00847(16)	0.1429(4)	0.0766(16)
O16	0.4417(6)	0.81648(19)	0.4209(5)	0.0953(19)
O17	0.4492(5)	0.90883(17)	0.3757(4)	0.0698(17)
N1	0.5056(4)	0.93202(16)	0.0976(4)	0.0469(12)
C2	0.6378(6)	0.9604(2)	0.1746(5)	0.0508(17)
C3	0.7439(6)	0.9320(2)	0.2994(5)	0.060(2)
C4	0.7280(6)	0.8673(2)	0.2977(5)	0.0546(17)
C5	0.5502(6)	0.84466(19)	0.2491(5)	0.0472(17)
C6	0.4509(5)	0.87359(18)	0.1113(5)	0.0431(17)
C8	0.5563(7)	0.7805(2)	0.2153(6)	0.0600(19)
C9	0.5501(6)	0.7816(2)	0.0726(5)	0.0538(19)
C10	0.4879(5)	0.8337(2)	0.0132(5)	0.0452(16)
C11	0.5929(7)	0.7384(3)	-0.0022(7)	0.072(3)
C12	0.5716(7)	0.7495(3)	-0.1348(7)	0.077(3)
C13	0.5068(7)	0.8007(3)	-0.1938(6)	0.070(2)
C14	0.4655(5)	0.8432(2)	-0.1204(5)	0.0541(19)
C15	0.4746(6)	0.8539(2)	0.3566(5)	0.0560(19)
C18	0.3678(10)	0.9220(3)	0.4711(7)	0.103(3)
C19	0.2643(5)	0.8745(2)	0.0865(5)	0.0448(17)
C20	0.1711(6)	0.8248(2)	0.0459(5)	0.0538(17)

Table S2 - Final Coordinates and Equivalent Isotropic Displacement  
Parameters of the non-Hydrogen atoms (continued)  
for: fcl

Atom	x	y	z	U(eq) [Ang <sup>2</sup> ]
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C21	0.0033(6)	0.8253(3)	0.0227(5)	0.064(2)
C22	-0.0733(6)	0.8752(3)	0.0372(6)	0.064(2)
C23	0.0154(6)	0.9241(3)	0.0772(6)	0.065(2)
C24	0.1850(6)	0.9243(2)	0.1031(5)	0.0530(19)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Starred Atom sites have a S.O.F less than 1.0

Table S3 - Hydrogen Atom Positions and Isotropic Displacement Parameters  
for: fcl

Atom	x	y	z	U(iso) [Ang <sup>2</sup> ]
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*H25A	1.05730	0.88600	0.79610	0.1700
*H25B	1.00220	0.95050	0.78280	0.1700
*H25C	1.00620	0.88690	0.80650	0.1700
*H25D	1.06610	0.94580	0.77260	0.1700
H1A	0.44370	0.95100	0.03000	0.0560
H3A	0.71590	0.94710	0.37430	0.0720
H3B	0.85720	0.94200	0.31330	0.0720
H4A	0.78280	0.85300	0.38720	0.0660
H4B	0.78480	0.85170	0.24040	0.0660
H8A	0.65660	0.76270	0.27220	0.0720
H8B	0.46320	0.75990	0.22470	0.0720
H11A	0.63430	0.70330	0.03640	0.0870
H12A	0.60170	0.72170	-0.18530	0.0920
H13A	0.49080	0.80670	-0.28390	0.0850
H14A	0.42290	0.87790	-0.16020	0.0650
H18A	0.36720	0.96280	0.48360	0.1240
H18B	0.42510	0.90380	0.55480	0.1240
H18C	0.25710	0.90810	0.43830	0.1240
H20A	0.22170	0.79090	0.03420	0.0640
H21A	-0.05720	0.79170	-0.00270	0.0760
H22A	-0.18600	0.87570	0.01960	0.0760
H23A	-0.03700	0.95780	0.08760	0.0780
H24A	0.24470	0.95790	0.13140	0.0640

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The Temperature Factor has the Form of  $\text{Exp}(-T)$  Where  
 $T = 8 * (\text{Pi}^{**2}) * U * (\text{Sin}(\text{Theta}) / \text{Lambda})^{**2}$  for Isotropic Atoms

Table S4 - (An)isotropic Displacement Parameters  
for: fcl

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
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Cl26	0.094(4)	0.73(3)	0.105(4)	0.098(9)	0.017(3)	-0.117(8)
Cl27	0.105(4)	0.142(4)	0.066(3)	-0.016(2)	0.025(2)	-0.047(4)
C25	0.091(5)	0.158(7)	0.088(5)	-0.001(5)	0.023(4)	-0.007(5)
Cl28	0.176(8)	0.256(10)	0.138(5)	-0.048(6)	-0.011(5)	0.131(8)
Cl29	0.205(12)	0.42(2)	0.216(11)	-0.161(12)	-0.031(8)	0.162(12)
O7	0.058(2)	0.062(3)	0.090(3)	0.020(2)	-0.002(2)	-0.024(2)
O16	0.130(4)	0.078(3)	0.104(3)	0.016(3)	0.074(3)	-0.015(3)
O17	0.081(3)	0.070(3)	0.071(3)	0.0004(19)	0.042(2)	0.001(2)
N1	0.028(2)	0.051(2)	0.056(2)	0.0109(19)	0.0062(19)	-0.0062(19)
C2	0.038(3)	0.049(3)	0.062(3)	0.007(3)	0.012(3)	-0.007(3)
C3	0.041(3)	0.066(4)	0.064(4)	0.009(3)	0.005(3)	-0.014(3)
C4	0.038(3)	0.061(3)	0.060(3)	0.012(3)	0.010(2)	0.002(2)
C5	0.041(3)	0.045(3)	0.055(3)	0.008(2)	0.015(2)	-0.005(2)
C6	0.029(3)	0.042(3)	0.058(3)	0.008(2)	0.014(2)	-0.006(2)
C8	0.055(3)	0.051(3)	0.073(4)	0.007(3)	0.020(3)	0.003(3)
C9	0.041(3)	0.050(3)	0.070(4)	-0.001(3)	0.018(3)	0.001(2)
C10	0.025(2)	0.057(3)	0.055(3)	0.000(3)	0.015(2)	-0.004(2)
C11	0.053(4)	0.067(4)	0.096(5)	-0.009(3)	0.024(3)	0.006(3)
C12	0.052(4)	0.093(5)	0.091(5)	-0.029(4)	0.032(3)	-0.004(3)
C13	0.051(3)	0.093(5)	0.072(4)	-0.014(4)	0.027(3)	-0.005(3)
C14	0.036(3)	0.064(3)	0.066(4)	0.001(3)	0.022(3)	-0.007(2)
C15	0.053(3)	0.057(4)	0.059(3)	0.007(3)	0.020(3)	-0.011(3)
C18	0.118(6)	0.116(6)	0.097(5)	-0.014(4)	0.065(5)	-0.003(5)
C19	0.033(3)	0.053(3)	0.050(3)	0.005(2)	0.016(2)	-0.004(2)
C20	0.039(3)	0.055(3)	0.069(3)	0.000(3)	0.020(3)	-0.009(2)

Table S4 - (An)isotropic Displacement Parameters (continued)  
for: fcl

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
C21	0.044(3)	0.076(4)	0.074(4)	-0.006(3)	0.024(3)	-0.022(3)
C22	0.033(3)	0.086(4)	0.075(4)	-0.001(3)	0.022(3)	-0.010(3)
C23	0.043(3)	0.075(4)	0.084(4)	-0.005(3)	0.030(3)	0.009(3)
C24	0.040(3)	0.051(3)	0.070(4)	-0.005(3)	0.021(3)	-0.004(2)

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The Temperature Factor has the Form of  $\text{Exp}(-T)$  Where  
 $T = 8 * (\text{Pi}^{**2}) * U * (\text{Sin}(\text{Theta}) / \text{Lambda})^{**2}$  for Isotropic Atoms  
 $T = 2 * (\text{Pi}^{**2}) * \text{Sum}_{ij} (h(i) * h(j) * U(i,j) * \text{Astar}(i) * \text{Astar}(j))$ , for  
Anisotropic Atoms.  $\text{Astar}(i)$  are Reciprocal Axial Lengths and  
 $h(i)$  are the Reflection Indices.

Table S5 - Bond Distances (Angstrom)  
for: fcl

C126	-C25	1.672(13)	C11	-C12	1.382(10)
C127	-C25	1.673(10)	C12	-C13	1.375(10)
C128	-C25	1.696(13)	C13	-C14	1.377(8)
C129	-C25	1.507(18)	C19	-C24	1.387(7)
O7	-C2	1.233(6)	C19	-C20	1.393(7)
O16	-C15	1.197(7)	C20	-C21	1.390(8)
O17	-C18	1.446(9)	C21	-C22	1.370(9)
O17	-C15	1.323(6)	C22	-C23	1.359(9)
N1	-C2	1.338(6)	C23	-C24	1.400(8)
N1	-C6	1.462(6)	C3	-H3A	0.9710
N1	-H1A	0.8611	C3	-H3B	0.9700
C25	-H25D	0.9912	C4	-H4A	0.9692
C25	-H25B	0.9938	C4	-H4B	0.9707
C25	-H25C	0.9640	C8	-H8A	0.9702
C25	-H25A	0.9629	C8	-H8B	0.9705
C2	-C3	1.492(7)	C11	-H11A	0.9301
C3	-C4	1.511(7)	C12	-H12A	0.9308
C4	-C5	1.544(8)	C13	-H13A	0.9307
C5	-C8	1.540(6)	C14	-H14A	0.9286
C5	-C15	1.508(7)	C18	-H18A	0.9584
C5	-C6	1.580(7)	C18	-H18B	0.9603
C6	-C19	1.547(7)	C18	-H18C	0.9600
C6	-C10	1.507(7)	C20	-H20A	0.9300
C8	-C9	1.499(8)	C21	-H21A	0.9293
C9	-C10	1.389(7)	C22	-H22A	0.9300
C9	-C11	1.405(8)	C23	-H23A	0.9302
C10	-C14	1.384(7)	C24	-H24A	0.9299

Table S6 - Bond Angles (Degrees)  
for: fcl

C15	-O17	-C18	117.1(5)	N1	-C6	-C19	108.9(4)
C2	-N1	-C6	129.6(4)	C5	-C6	-C19	112.3(4)
C6	-N1	-H1A	115.29	C10	-C6	-C19	109.9(4)
C2	-N1	-H1A	115.16	C5	-C6	-C10	101.7(4)
C126	-C25	-C127	112.0(6)	N1	-C6	-C5	113.2(4)
C128	-C25	-C129	120.4(8)	C5	-C8	-C9	103.1(4)
C126	-C25	-H25B	109.91	C8	-C9	-C11	129.2(5)
C127	-C25	-H25A	110.55	C10	-C9	-C11	120.1(5)
C126	-C25	-H25A	109.63	C8	-C9	-C10	110.6(4)
C129	-C25	-H25D	105.69	C9	-C10	-C14	120.4(4)
H25A	-C25	-H25B	106.33	C6	-C10	-C9	111.2(4)
H25C	-C25	-H25D	104.77	C6	-C10	-C14	128.4(4)
C127	-C25	-H25B	108.29	C9	-C11	-C12	118.1(6)
C128	-C25	-H25C	106.63	C11	-C12	-C13	121.5(6)
C128	-C25	-H25D	106.43	C12	-C13	-C14	120.4(6)
C129	-C25	-H25C	111.80	C10	-C14	-C13	119.4(5)
O7	-C2	-N1	121.1(5)	O16	-C15	-O17	122.1(5)
N1	-C2	-C3	118.2(4)	O16	-C15	-C5	125.0(5)
O7	-C2	-C3	120.7(5)	O17	-C15	-C5	112.9(4)
C2	-C3	-C4	113.8(4)	C6	-C19	-C20	120.3(4)
C3	-C4	-C5	114.9(4)	C20	-C19	-C24	118.2(5)
C4	-C5	-C15	109.5(4)	C6	-C19	-C24	121.5(4)
C4	-C5	-C6	109.8(4)	C19	-C20	-C21	120.7(5)
C4	-C5	-C8	107.5(4)	C20	-C21	-C22	120.2(6)
C8	-C5	-C15	111.8(4)	C21	-C22	-C23	120.0(5)
C6	-C5	-C15	113.7(4)	C22	-C23	-C24	120.7(6)
C6	-C5	-C8	104.3(4)	C19	-C24	-C23	120.2(5)
N1	-C6	-C10	110.7(4)	C2	-C3	-H3A	108.67

Table S6 - Bond Angles (Degrees) (continued)  
for: fcl

C2	-C3	-H3B	108.75	C14	-C13	-H13A	119.76
C4	-C3	-H3A	108.88	C10	-C14	-H14A	120.29
C4	-C3	-H3B	108.91	C13	-C14	-H14A	120.29
H3A	-C3	-H3B	107.66	O17	-C18	-H18A	109.46
C3	-C4	-H4A	108.49	O17	-C18	-H18B	109.47
C3	-C4	-H4B	108.46	O17	-C18	-H18C	109.52
C5	-C4	-H4A	108.62	H18A	-C18	-H18B	109.46
C5	-C4	-H4B	108.60	H18A	-C18	-H18C	109.45
H4A	-C4	-H4B	107.57	H18B	-C18	-H18C	109.48
C5	-C8	-H8A	111.17	C19	-C20	-H20A	119.66
C5	-C8	-H8B	111.13	C21	-C20	-H20A	119.60
C9	-C8	-H8A	111.17	C20	-C21	-H21A	119.94
C9	-C8	-H8B	111.13	C22	-C21	-H21A	119.86
H8A	-C8	-H8B	109.06	C21	-C22	-H22A	120.14
C9	-C11	-H11A	120.92	C23	-C22	-H22A	119.87
C12	-C11	-H11A	120.95	C22	-C23	-H23A	119.69
C11	-C12	-H12A	119.28	C24	-C23	-H23A	119.62
C13	-C12	-H12A	119.26	C19	-C24	-H24A	119.85
C12	-C13	-H13A	119.81	C23	-C24	-H24A	119.98

Table S7 - Torsion Angles (Degrees)  
for: fc1

C18	-O17	-C15	-O16	-4.6(8)
C18	-O17	-C15	-C5	176.3(5)
C2	-N1	-C6	-C19	135.7(5)
C6	-N1	-C2	-O7	174.5(5)
C2	-N1	-C6	-C5	10.1(7)
C2	-N1	-C6	-C10	-103.3(6)
C6	-N1	-C2	-C3	-4.7(8)
N1	-C2	-C3	-C4	22.4(7)
O7	-C2	-C3	-C4	-156.9(5)
C2	-C3	-C4	-C5	-47.0(6)
C3	-C4	-C5	-C15	-74.4(5)
C3	-C4	-C5	-C8	164.0(4)
C3	-C4	-C5	-C6	51.1(5)
C4	-C5	-C6	-N1	-31.6(5)
C8	-C5	-C6	-C10	-27.8(5)
C4	-C5	-C6	-C19	-155.4(4)
C8	-C5	-C6	-N1	-146.5(4)
C6	-C5	-C15	-O16	126.7(6)
C4	-C5	-C6	-C10	87.2(4)
C8	-C5	-C15	-O16	8.9(8)
C8	-C5	-C15	-O17	-172.1(5)
C6	-C5	-C8	-C9	29.0(5)
C15	-C5	-C8	-C9	152.2(5)
C15	-C5	-C6	-C19	-32.4(5)
C8	-C5	-C6	-C19	89.7(5)
C6	-C5	-C15	-O17	-54.3(6)
C4	-C5	-C15	-O17	68.9(5)
C4	-C5	-C8	-C9	-87.6(5)

Table S7 - Torsion Angles (Degrees) (continued)  
for: fc1

C4	-C5	-C15	-O16	-110.1(6)
C15	-C5	-C6	-N1	91.4(5)
C15	-C5	-C6	-C10	-149.8(4)
C5	-C6	-C10	-C9	16.5(5)
N1	-C6	-C10	-C14	-43.7(7)
C5	-C6	-C19	-C24	103.2(5)
N1	-C6	-C10	-C9	137.1(4)
C19	-C6	-C10	-C14	76.6(6)
N1	-C6	-C19	-C20	156.7(4)
N1	-C6	-C19	-C24	-23.0(6)
C5	-C6	-C19	-C20	-77.2(6)
C5	-C6	-C10	-C14	-164.3(5)
C10	-C6	-C19	-C24	-144.4(5)
C19	-C6	-C10	-C9	-102.6(5)
C10	-C6	-C19	-C20	35.3(6)
C5	-C8	-C9	-C11	162.0(6)
C5	-C8	-C9	-C10	-19.9(6)
C11	-C9	-C10	-C14	0.9(8)
C8	-C9	-C10	-C14	-177.5(5)
C11	-C9	-C10	-C6	-179.9(5)
C8	-C9	-C11	-C12	178.2(6)
C8	-C9	-C10	-C6	1.8(6)
C10	-C9	-C11	-C12	0.2(9)
C6	-C10	-C14	-C13	-179.7(5)
C9	-C10	-C14	-C13	-0.6(7)
C9	-C11	-C12	-C13	-1.5(10)
C11	-C12	-C13	-C14	1.9(10)
C12	-C13	-C14	-C10	-0.8(9)

Table S7 - Torsion Angles (Degrees) (continued)  
for: fc1

C6	-C19	-C20	-C21	-179.7(5)
C6	-C19	-C24	-C23	178.7(5)
C24	-C19	-C20	-C21	0.0(7)
C20	-C19	-C24	-C23	-1.0(8)
C19	-C20	-C21	-C22	1.2(8)
C20	-C21	-C22	-C23	-1.4(9)
C21	-C22	-C23	-C24	0.4(9)
C22	-C23	-C24	-C19	0.8(9)

Table S8 - Contact Distances(Angstrom)  
for: fc1

C126	.C22_a	3.571(10)	O16	.H12A_h	2.9173
C127	.C3	3.491(7)	O16	.H8B	2.5230
C127	.C18_b	3.417(11)	O16	.H18C	2.7060
C127	.O7_c	3.308(7)	O17	.H24A	2.8484
C129	.C11_d	3.33(2)	O17	.H3A	2.4781
C126	.H18B	3.0455	N1	.O17	3.195(6)
C127	.H3B	3.0483	N1	.O7_g	2.863(6)
C127	.H11A_d	3.1419	N1	.H24A	2.4751
C127	.H18C_b	2.8643	N1	.H14A	2.8792
C128	.H24A_e	3.0944	C2	.O17	3.314(7)
C128	.H18A_e	2.9974	C3	.O17	2.970(7)
C129	.H4A	2.9144	C3	.C127	3.491(7)
C129	.H11A_d	2.5516	C8	.C20	3.380(8)
C129	.H18C_b	3.1374	C9	.C20	3.351(8)
O7	.C25_f	3.313(9)	C11	.C129_i	3.33(2)
O7	.N1_g	2.863(6)	C14	.C20	3.575(7)
O7	.C127_f	3.308(7)	C15	.C20	3.533(7)
O17	.C2	3.314(7)	C15	.C24	3.424(7)
O17	.C3	2.970(7)	C18	.C127_j	3.417(11)
O17	.C19	3.060(6)	C19	.O17	3.060(6)
O17	.N1	3.195(6)	C20	.C15	3.533(7)
O17	.C24	3.056(7)	C20	.C14	3.575(7)
O7	.H25D_f	2.3889	C20	.C9	3.351(8)
O7	.H14A_g	2.7925	C20	.C8	3.380(8)
O7	.H25B_f	2.8257	C22	.C25_k	3.560(10)
O7	.H1A_g	2.0108	C22	.C126_k	3.571(10)
O16	.H18B	2.5105	C23	.C25_k	3.591(10)
O16	.H21A_d	2.6426	C24	.C15	3.424(7)

Table S8 - Contact Distances(Angstrom) (continued)  
for: fcl

C24	.O17	3.056(7)	H1A	.C2_g	2.9062
C25	.O7_c	3.313(9)	H1A	.H24A	2.3201
C25	.C22_a	3.560(10)	H3A	.O17	2.4781
C25	.C23_a	3.591(10)	H3A	.C15	2.9719
C2	.H1A_g	2.9062	H3B	.C127	3.0483
C8	.H20A	2.9050	H4A	.C129	2.9144
C9	.H4B	2.7482	H4A	.H8A	2.4916
C9	.H20A	2.7419	H4B	.C10	2.9116
C10	.H20A	2.5861	H4B	.C22_b	2.8678
C10	.H4B	2.9116	H4B	.H8A	2.4245
C10	.H22A_b	2.9654	H4B	.C9	2.7482
C14	.H1A	3.0121	H4B	.H22A_b	2.5035
C14	.H22A_b	2.9825	H8A	.H4B	2.4245
C15	.H3A	2.9719	H8A	.H4A	2.4916
C19	.H25C_k	3.0821	H8B	.H20A	2.4839
C19	.H25A_k	3.0199	H8B	.C20	3.0137
C20	.H25A_k	2.8804	H8B	.O16	2.5230
C20	.H8B	3.0137	H11A	.C129_i	2.5516
C20	.H25C_k	2.8591	H11A	.C127_i	3.1419
C21	.H25C_k	2.7135	H12A	.O16_m	2.9173
C21	.H25A_k	2.9580	H14A	.O7_g	2.7925
C22	.H4B_l	2.8678	H14A	.N1	2.8792
C22	.H25C_k	2.7695	H18A	.C128_n	2.9974
C23	.H25C_k	2.9778	H18B	.O16	2.5105
C24	.H1A	2.6748	H18B	.C126	3.0455
H1A	.O7_g	2.0108	H18C	.O16	2.7060
H1A	.C14	3.0121	H18C	.C127_j	2.8643
H1A	.C24	2.6748	H18C	.C129_j	3.1374

Table S8 - Contact Distances(Angstrom) (continued)  
for: fcl

H20A	.H8B	2.4839	H24A	.N1	2.4751
H20A	.C8	2.9050	H25A	.C21_a	2.9580
H20A	.C9	2.7419	H25A	.C19_a	3.0199
H20A	.C10	2.5861	H25A	.C20_a	2.8804
H21A	.O16_o	2.6426	H25B	.O7_c	2.8257
H22A	.C10_l	2.9654	H25B	.H23A_e	2.5016
H22A	.C14_l	2.9825	H25C	.C23_a	2.9778
H22A	.H4B_l	2.5035	H25C	.C19_a	3.0821
H23A	.H25B_n	2.5016	H25C	.C20_a	2.8591
H24A	.O17	2.8484	H25C	.C21_a	2.7135
H24A	.H1A	2.3201	H25C	.C22_a	2.7695
H24A	.C128_n	3.0944	H25D	.O7_c	2.3889

Table S9 - Hydrogen Bonds (Angstrom, Deg)  
for: fcl

N1	--	H1A	..	O7	0.8611	2.0108	2.863(6)	170.12	3_675	yes
C3	--	H3A	..	O17	0.9710	2.4781	2.970(7)	111.19	.	yes
C24	--	H24A	..	N1	0.9299	2.4751	2.800(7)	100.62	.	yes

Translation of Symmetry Code to Equiv.Pos

a	=	[ 1656.00 ]	=	1+x,y,1+z
b	=	[ 1655.00 ]	=	1+x,y,z
c	=	[ 3776.00 ]	=	2-x,2-y,1-z
d	=	[ 4565.00 ]	=	1/2+x,3/2-y,1/2+z
e	=	[ 3676.00 ]	=	1-x,2-y,1-z
f	=	[ 3776.00 ]	=	2-x,2-y,1-z
g	=	[ 3675.00 ]	=	1-x,2-y,-z
h	=	[ 4465.00 ]	=	-1/2+x,3/2-y,1/2+z
i	=	[ 4464.00 ]	=	-1/2+x,3/2-y,-1/2+z
j	=	[ 1455.00 ]	=	-1+x,y,z
k	=	[ 1454.00 ]	=	-1+x,y,-1+z
l	=	[ 1455.00 ]	=	-1+x,y,z
m	=	[ 4564.00 ]	=	1/2+x,3/2-y,-1/2+z
n	=	[ 3676.00 ]	=	1-x,2-y,1-z
o	=	[ 4464.00 ]	=	-1/2+x,3/2-y,-1/2+z