

No syntax errors found.

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Datablock: ws04

Bond precision:		C-C = 0.0028 Å	Wavelength=1.54184
Cell:	a=8.5079(4)	b=9.6156(4)	c=10.3022(3)
	alpha=83.401(3)	beta=88.993(3)	gamma=79.248(4)
Temperature: 293 K			
	Calculated	Reported	
Volume	822.52(6)	822.51(5)	
Space group	P -1	P -1	
Hall group	-P 1	-P 1	
Moiety formula	C20 H13 Cl2 F O	C20 H13 Cl2 F O	
Sum formula	C20 H13 Cl2 F O	C20 H13 Cl2 F O	
Mr	359.20	359.20	
Dx,g cm-3	1.450	1.450	
Z	2	2	
Mu (mm-1)	3.669	3.669	
F000	368.0	368.0	
F000'	370.40		
h,k,lmax	10,11,12	10,11,12	
Nref	3079	2958	
Tmin,Tmax	0.416,0.618	0.400,1.000	
Tmin'	0.240		
Correction method= # Reported T Limits: Tmin=0.400 Tmax=1.000 AbsCorr = MULTI-SCAN			
Data completeness= 0.961	Theta(max)= 69.442		
R(reflections)= 0.0647(2901)	wR2(reflections)= 0.1756(2958)		
S = 1.641	Npar= 217		

The following ALERTS were generated. Each ALERT has the format

test-name ALERT alert-type alert-level.

Click on the hyperlinks for more details of the test.

Alert level B

[PLAT934 ALERT 3 B](#) Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 5 Check

Alert level C

[PLAT029 ALERT 3 C](#) _diffn_measured_fraction_theta_full value Low . 0.970 Why?[PLAT790 ALERT 4 C](#) Centre of Gravity not Within Unit Cell: Resd. # 1 Note

C20 H13 Cl2 F O

[PLAT911 ALERT 3 C](#) Missing FCF Refl Between Thmin & STh/L= 0.600 90 Report[PLAT918 ALERT 3 C](#) Reflection(s) with I(obs) much Smaller I(calc) . 16 Check[PLAT939 ALERT 3 C](#) Large Value of Not (SHELXL) Weight Optimized S . 35.42 Check[PLAT977 ALERT 2 C](#) Check Negative Difference Density on H1A . -0.50 eA-3**And 2 other PLAT977 Alerts**

More ...

Alert level G

[PLAT199 ALERT 1 G](#) Reported _cell_measurement_temperature (K) 293 Check[PLAT200 ALERT 1 G](#) Reported _diffn_ambient_temperature (K) 293 Check[PLAT343 ALERT 2 G](#) Unusual sp3 Angle Range in Main Residue for C14 Check[PLAT398 ALERT 2 G](#) Deviating C-O-C Angle From 120 for O1 . 62.1 Degree[PLAT793 ALERT 4 G](#) Model has Chirality at C6 (Centro SPGR) S Verify[PLAT793 ALERT 4 G](#) Model has Chirality at C14 (Centro SPGR) R Verify[PLAT912 ALERT 4 G](#) Missing # of FCF Reflections Above STh/L= 0.600 32 Note[PLAT941 ALERT 3 G](#) Average HKL Measurement Multiplicity 3.9 Low[PLAT961 ALERT 5 G](#) Dataset Contains no Negative Intensities Please Check[PLAT978 ALERT 2 G](#) Number C-C Bonds with Positive Residual Density. 0 Info0 **ALERT level A** = Most likely a serious problem - resolve or explain1 **ALERT level B** = A potentially serious problem, consider carefully8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight10 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

6 ALERT type 2 Indicator that the structure model may be wrong or deficient

6 ALERT type 3 Indicator that the structure quality may be low

4 ALERT type 4 Improvement, methodology, query or suggestion

1 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

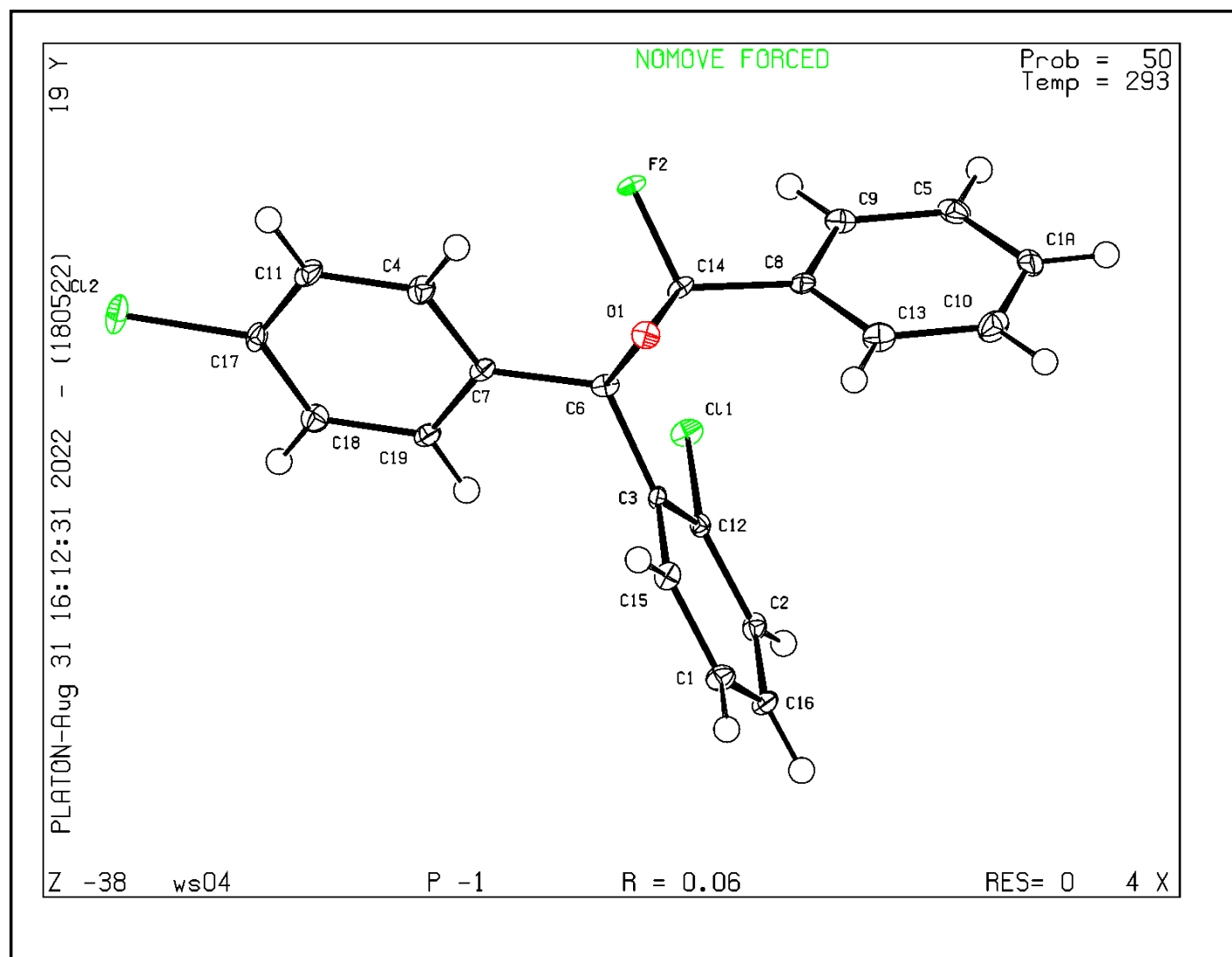
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that [full publication checks](#) are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 18/05/2022; check.def file version of 17/05/2022

Datablock ws04 - ellipsoid plot



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Datablock: ws03-op

Bond precision:		C-C = 0.0040 A	Wavelength=1.54184
Cell:	a=5.79557(11)	b=16.5797(4)	c=17.1963(4)
	alpha=90	beta=90	gamma=90
Temperature: 293 K			
	Calculated	Reported	
Volume	1652.37(6)	1652.38(6)	
Space group	P 21 21 21	P 21 21 21	
Hall group	P 2ac 2ab	P 2ac 2ab	
Moiety formula	C21 H15 F3 O	C21 H15 F3 O	
Sum formula	C21 H15 F3 O	C21 H15 F3 O	
Mr	340.33	340.33	
Dx,g cm-3	1.368	1.368	
Z	4	4	
Mu (mm-1)	0.895	0.895	
F000	704.0	704.0	
F000'	706.51		
h,k,lmax	7,20,20	7,20,20	
Nref	3091[1811]	3071	
Tmin,Tmax	0.910,0.946	0.568,1.000	
Tmin'	0.887		
Correction method= # Reported T Limits: Tmin=0.568 Tmax=1.000 AbsCorr = MULTI-SCAN			
Data completeness= 1.70/0.99	Theta(max)= 69.527		
R(reflections)= 0.0403(2923)	wR2(reflections)= 0.1060(3071)		
S = 1.053	Npar= 226		

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test-name ALERT alert-type alert-level.

Click on the hyperlinks for more details of the test.

Alert level C

[PLAT934 ALERT 3 C](#) Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 1 Check

Alert level G

[PLAT199 ALERT 1 G](#) Reported _cell_measurement_temperature (K) 293 Check
[PLAT200 ALERT 1 G](#) Reported _diffn_ambient_temperature (K) 293 Check
[PLAT343 ALERT 2 G](#) Unusual sp3 Angle Range in Main Residue for C5 Check
[PLAT398 ALERT 2 G](#) Deviating C-O-C Angle From 120 for O2 61.9 Degree
[PLAT767 ALERT 4 G](#) INS Embedded LIST 6 Instruction Should be LIST 4 Please Check
[PLAT791 ALERT 4 G](#) Model has Chirality at C3 (Sohnke SpGr) R Verify
[PLAT791 ALERT 4 G](#) Model has Chirality at C5 (Sohnke SpGr) R Verify
[PLAT912 ALERT 4 G](#) Missing # of FCF Reflections Above STh/L= 0.600 4 Note
[PLAT978 ALERT 2 G](#) Number C-C Bonds with Positive Residual Density. 1 Info

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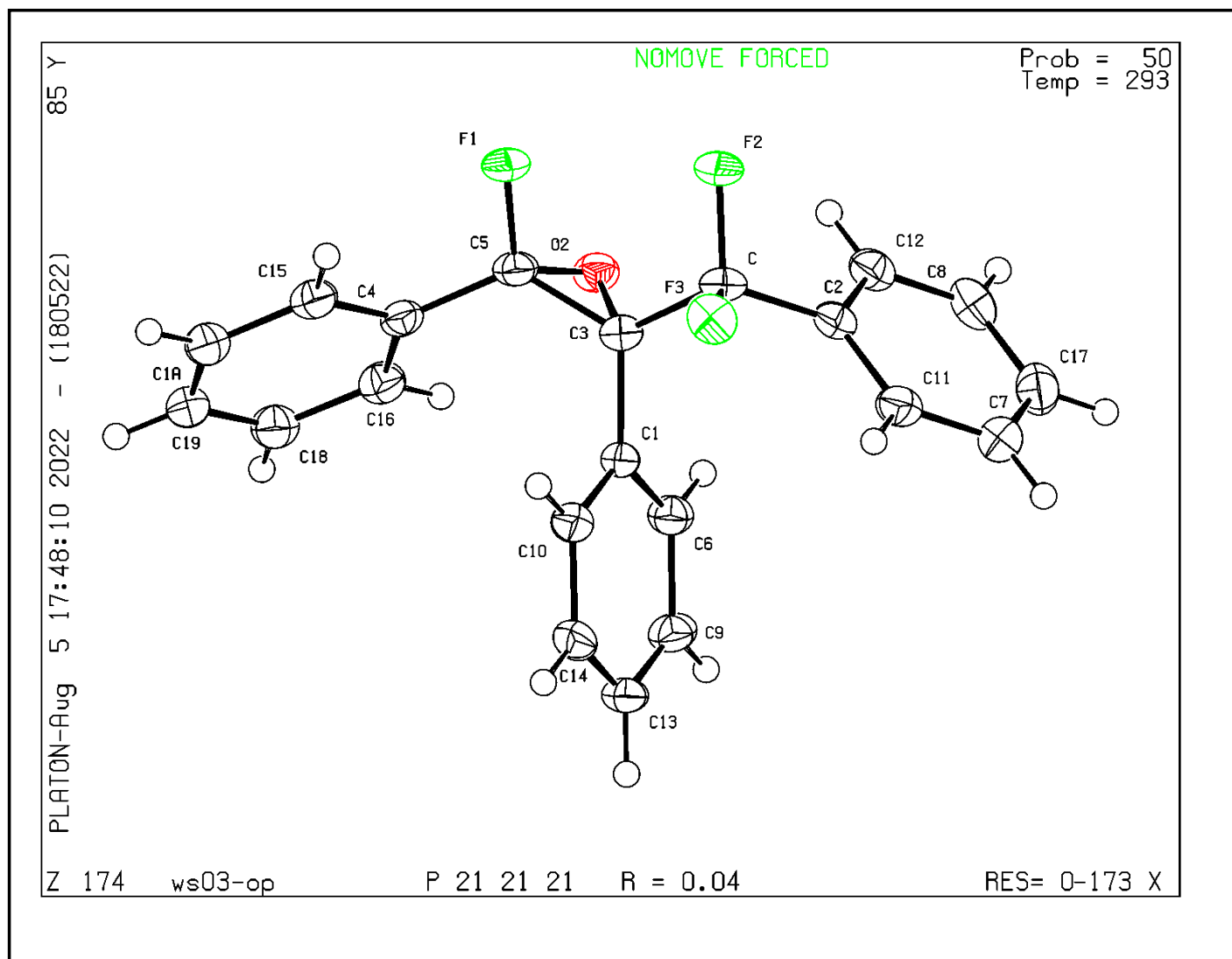
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Datablock ws03-op - ellipsoid plot



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