checkCIF/PLATON report

No syntax errors found. **CIF dictionary** **Interpreting this report**

Datablock: pmorph2

Bond precision: C-C = 0.0092 A Wavelength=0.56087

Cell: a=7.031(4) b=5.924(4) c=7.441(5)
alpha=90 beta=103.563(17) gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	301.3(3)	301.3(3)
Space group	P 21	P 1 21 1
Hall group	P 2yb	P 2yb
Moiety formula	C8 H5 F	C8 H5 F
Sum formula	C8 H5 F	C8 H5 F
Mr	120.12	120.12
Dx,g cm-3	1.324	1.324
Z	2	2
Mu (mm-1)	0.060	0.060
F000	124.0	124.0
F000’	124.03	
h,k,lmax	8,6,8	7,6,7
Nref	1021[566]	489
Tmin,Tmax	0.985,0.994	0.605,0.744
Tmin’	0.985	

Correction method= MULTI-SCAN

Data completeness= 0.86/0.48 Theta(max)= 19.180

R(reflections)= 0.0445(359) wR2(reflections)= 0.0977(489)

S = 1.170 Npar= Npar = 82

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 A
PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full Low ..... 0.496 Note

Author Response: High-pressure dataset, reflections occluded by body of diamond anvil \ cell.

Alert level B

```
REFNR01_ALERT_3_B  Ratio of reflections to parameters is < 6 for a
            non-centrosymmetric structure, where ZMAX < 18
            sine(theta)/lambda                0.5858
            Proportion of unique data used    1.0000
            Ratio reflections to parameters   5.9634
            Crystal system given = monoclinic
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Alert level C

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RADNW01_ALERT_1_C  The radiation wavelength lies outside the expected range
            for the supplied radiation type. Expected range 0.56080-0.56085
            Wavelength given =    0.56087
STRVA01_ALERT_4_C           Flack parameter is too small
           From the CIF: _refine_ls_abs_structure_Flack   -2.000
           From the CIF: _refine_ls_abs_structure_Flack_su    3.000
THETM01_ALERT_3_C  The value of sine(theta_max)/wavelength is less than 0.590
            Calculated sin(theta_max)/wavelength =    0.5858
PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax < 18) ........       6.90 Note
```

Author Response: ...High-pressure dataset, reflections occluded by body of diamond \ anvil cell.

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PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ...............     0.0092 Ang.
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Alert level G

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PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF     Please Do !
PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High .      3.000 Why ?
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C2     -   C3     ...       1.43 Ang.
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   1 ALERT level A = Most likely a serious problem - resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
   5 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   5 ALERT level G = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   1 ALERT type 2 Indicator that the structure model may be wrong or deficient
   5 ALERT type 3 Indicator that the structure quality may be low
   2 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

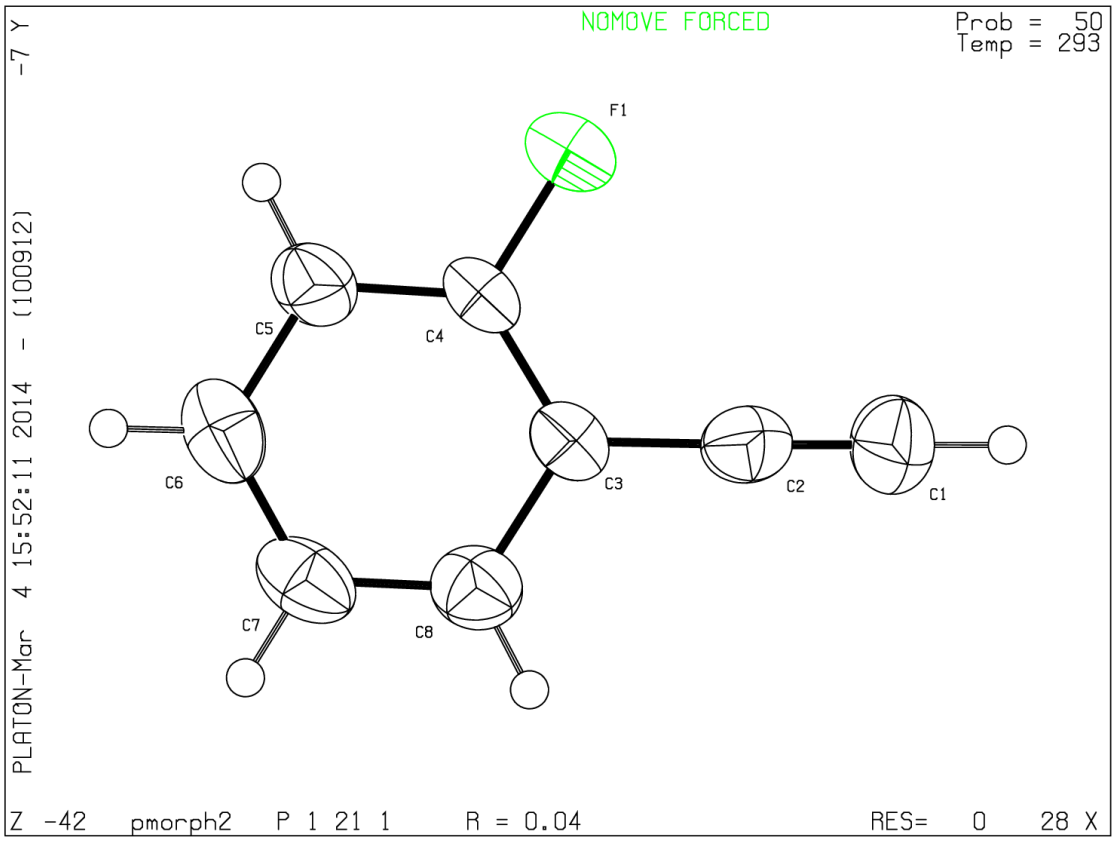
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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*, 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 05/02/2014; check.def file version of 05/02/2014

Datablock pmorph2 - ellipsoid plot