No syntax errors found.
Please wait while processing ....

CIF dictionary
Interpreting this report

Datablock: s1_a

Bond precision: C-C = 0.0030 A Wavelength=0.71073
Cell: a=28.4271(16) b=7.2368(4) c=6.3705(4)
alpha=90 beta=97.766(2) gamma=90
Temperature : 100 K

	Calculated	Reported
Volume	1298.53(13)	1298.53(13)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C17 H15 F O	C17 H15 F O
Sum formula	C17 H15 F O	C17 H15 F O
Mr	254.29	254.29
Dx,g cm-3	1.301	1.301
Z	4	4
Mu (mm-1)	0.089	0.089
F000	536.0	536.0
F000'	536.27	
h,k,lmax	41,10,9	41,10,9
Nref	2112	2105
Tmin,Tmax	0.973,0.996	0.684,0.746
Tmin'	0.968	

Correction method= # Reported T Limits: Tmin=0.684
Tmax=0.746 AbsCorr = MULTI-SCAN
Data completeness= 0.997 Theta(max)= 31.245
R(reflections)= 0.0774(1883) wR2(reflections)= 0.1941(2105)
S = 1.210 Npar= 95

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 C

PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	17.578	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	3.321	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	7	Report

Alert level G

PLAT019_ALERT_1_G	_diffrn_measured_fraction_theta_full/*_max < 1.0	0.997	Report
PLAT128_ALERT_4_G	Alternate Setting for Input Space Group C2/c	I2/a	Note
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	1	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of F1 Constrained at	0.5	Check

And 5 other PLAT300 Alerts

PLAT300_ALERT_4_G	Atom Site Occupancy of O1 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C9 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H9A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H9B Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H9C Constrained at	0.5	Check
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1)	16%	Note
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #	5	Check
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	2	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	4	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	8	Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully

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  3 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 15 ALERT level G = General information/check it is not something unexpected

  1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  2 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
  9 ALERT type 4 Improvement, methodology, query or suggestion
  0 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

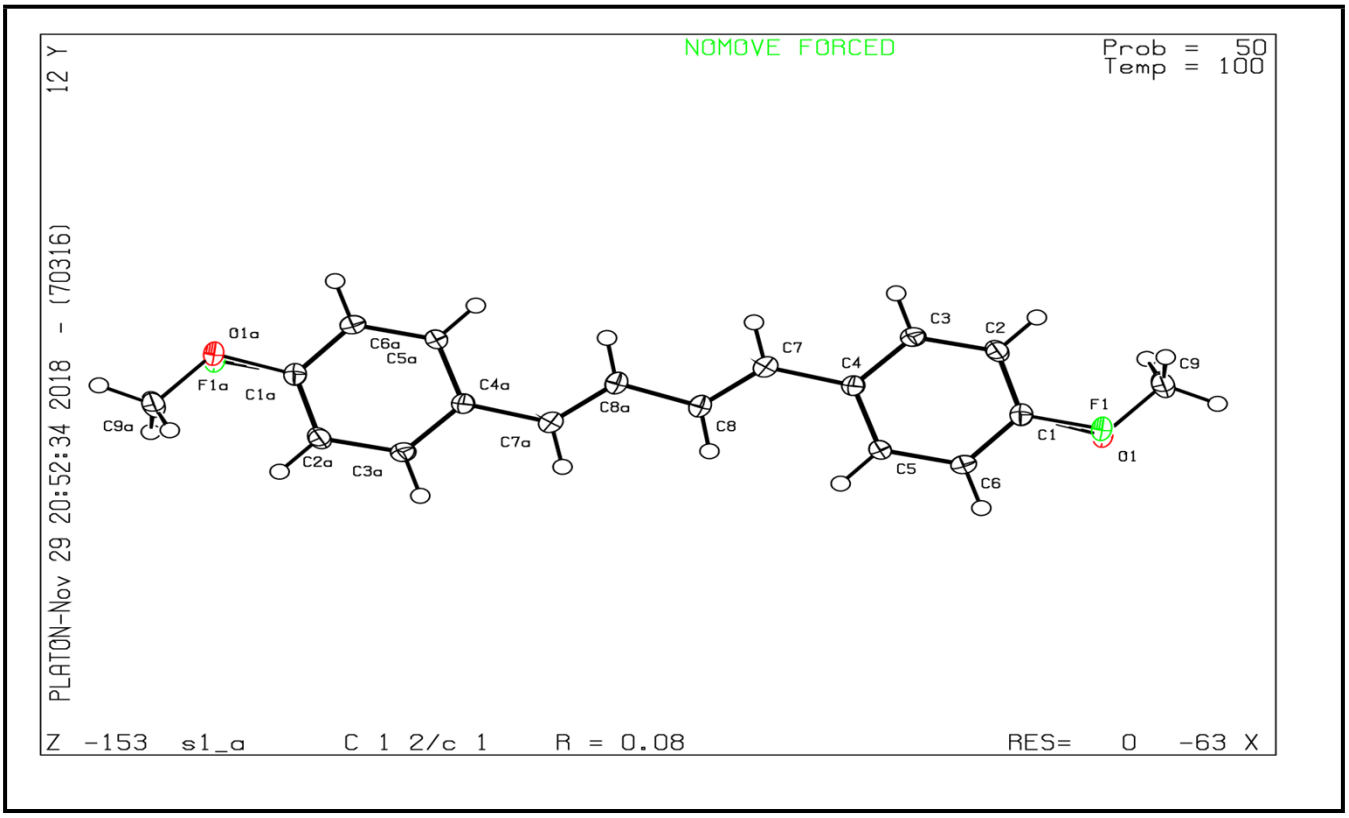
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 19/10/2018; check.def file version of 15/10/2018

Datablock s1_a - ellipsoid plot



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