checkCIF (basic structural check) running

Checking for embedded fcf data in CIF ...
Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait .....

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) 1, 2

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

Structure factor report

Datablock: 1

Bond precision: C-C = 0.0052 A Wavelength=0.71069
Cell: a=10.0433(3) b=11.0189(2) c=16.2612(4)
alpha=95.701(1) beta=101.441(1) gamma=92.611(1)
Temperature: 150 K

	Calculated	Reported
Volume	1751.15(8)	1751.15(8)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C38 H55 O Sm	C38 H55 O Sm
Sum formula	C38 H55 O Sm	C38 H55 O Sm
Mr	678.18	678.17
Dx,g cm-3	1.286	1.286
Z	2	2
Mu (mm-1)	1.702	1.702
F000	706.0	706.0
F000'	705.86	
h,k,lmax	12,13,19	12,13,19
Nref	6646	6598
Tmin,Tmax	0.751,0.873	0.642,0.746
Tmin'	0.665	

Correction method= # Reported T Limits: Tmin=0.642
Tmax=0.746 AbsCorr = MULTI-SCAN
Data completeness= 0.993 Theta(max)= 25.679
R(reflections)= 0.0281(5903) wR2(reflections)= 0.0732(6598)
S = 1.041 Npar= 373

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

PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.1 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for C18 --C21 . 5.7 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for C35 --C36 . 5.6 s.u.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C36 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C37 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C18 Check
And 3 other PLAT242 Alerts

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C27 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C31 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C38 Check

PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C36 - C37 . 1.42 Ang.
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C37 - C38 . 1.41 Ang.
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 8 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 29 Report
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0 Info

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Alert level G
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.001 Degree
PLAT371_ALERT_2_G Long C(sp2)-C(sp1) Bond C2 - C3 . 1.44 Ang.
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 11 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 7 Note

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0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
14 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
4 **ALERT level G** = General information/check it is not something unexpected

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

Datablock: 2

Bond precision: C-C = 0.0116 A Wavelength=0.71069
Cell: a=26.008(2) b=11.2284(9) c=27.4919(19)
alpha=90 beta=108.302(4) gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	7622.3(10)	7622.3(10)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C70 H94 O4 Sm2, 2(C7 H8)	C70 H94 O4 Sm2, 2(C7 H8)
Sum formula	C84 H110 O4 Sm2	C84 H110 O4 Sm2
Mr	1484.44	1484.41
Dx,g cm-3	1.294	1.294
Z	4	4
Mu (mm-1)	1.572	1.572
F000	3080.0	3080.0
F000'	3079.60	
h,k,lmax	31,13,32	30,13,32
Nref	6878	6033
Tmin,Tmax	0.893,0.969	0.668,0.745
Tmin'	0.568	

Correction method= # Reported T Limits: Tmin=0.668
Tmax=0.745 AbsCorr = MULTI-SCAN
Data completeness= 0.877 Theta(max)= 25.208
R(reflections)= 0.0534(5099) wR2(reflections)= 0.1307(6033)
S = 1.189 Npar= 472

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 value Low . 0.877 Why?

Alert level B

PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.599 833 Report

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Alert level C

PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.3 Note
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0116 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 6.532 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 7 Note
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.99A From C10 -2.41 eA-3

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 14 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 84.23 Why ?
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 2 Report
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3) 100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd 2 10.14 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd 3 4.86 Check
PLAT371_ALERT_2_G Long C(sp2)-C(sp1) Bond C1 - C2 . 1.45 Ang.
PLAT371_ALERT_2_G Long C(sp2)-C(sp1) Bond C3 - C4 . 1.43 Ang.
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 96 Note
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 73% Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 11 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 2 Info

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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

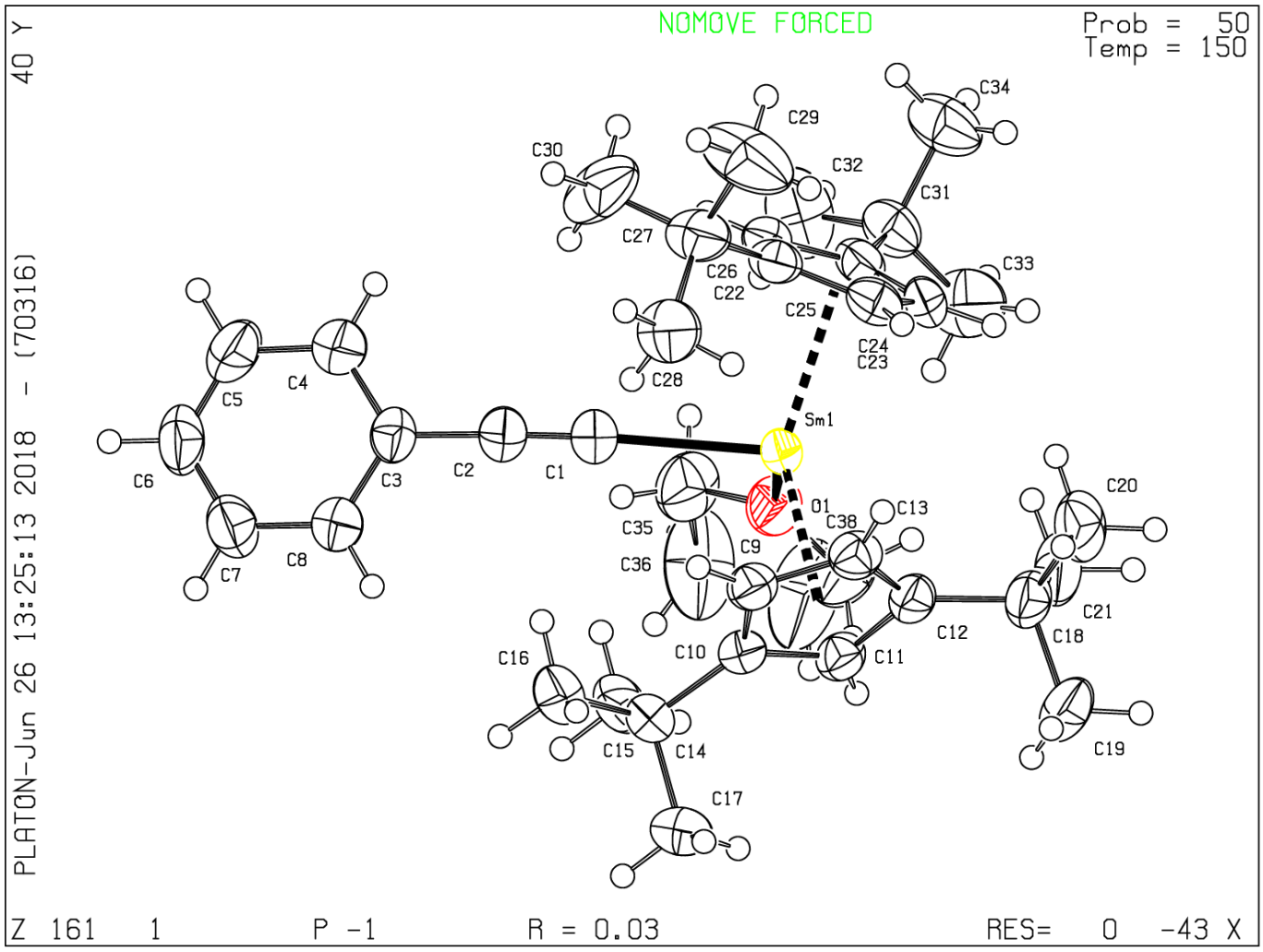
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section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

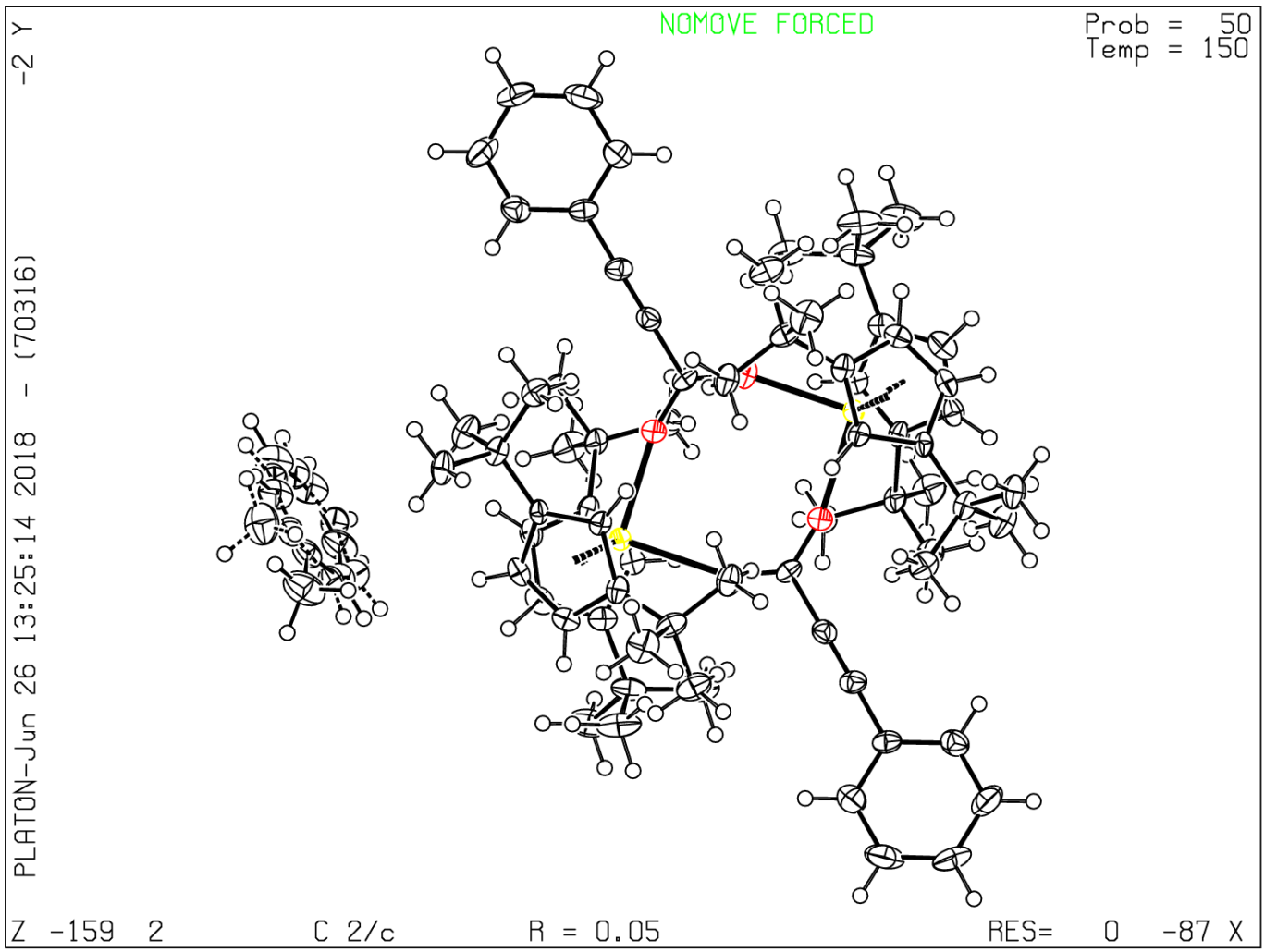
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 23/04/2018; check.def file version of 23/04/2018

Datablock 1 - ellipsoid plot



Datablock 2 - ellipsoid plot



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