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) cu_20210603eutta230oc1_0m

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: cu_20210603eutta230oc1_0m

Bond precision: C-C = 0.0358 A Wavelength=1.54184
Cell: a=16.385(3) b=16.484(3) c=16.295(3)
alpha=90 beta=116.11(3) gamma=90
Temperature: 230 K

	Calculated	Reported
Volume	3952.0(16)	3952.0(15)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C36 H14 Eu2 O13 S10	?
Sum formula	C36 H14 Eu2 O13 S10	C72 H28 Eu4 O26 S20
Mr	1279.01	2557.98
Dx,g cm-3	2.150	2.150
Z	4	2
Mu (mm-1)	28.026	28.026
F000	2480.0	2480.0
F000'	2429.40	
h,k,lmax	19,19,19	19,19,19
Nref	3632	3497
Tmin,Tmax	0.102,0.106	0.285,0.753
Tmin'	0.000	

Correction method= # Reported T Limits: Tmin=0.285 Tmax=0.753
AbsCorr = MULTI-SCAN
Data completeness= 0.963 Theta(max)= 68.511
R(reflections)= 0.1106(2530) wR2(reflections)= 0.2761(3497)
S = 1.083 Npar= 357

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
PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.03583 Ang.

PLAT369_ALERT_2_B Long C(sp2)-C(sp2) Bond C13 - C14 . 1.58 Ang.

Alert level C

PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low . 0.966 Why?
PLAT082_ALERT_2_C High R1 Value ..... 0.11 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..... 0.28 Report
PLAT088_ALERT_3_C Poor Data / Parameter Ratio ..... 9.80 Note
PLAT213_ALERT_2_C Atom O4 has ADP max/min Ratio ..... 3.5 prolat
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O1 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O5 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Eu1 Check
And 5 other PLAT242 Alerts

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C3 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C4 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C6 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C7 Check

PLAT260_ALERT_2_C Large Average Ueq of Residue Including Eu1 0.102 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 14.679 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.831 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 122 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.89A From Eu1 1.90 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.67A From Eu1 -1.80 eA-3
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on Eu1 1.45 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.74A From O7 -0.91 eA-3
And 3 other PLAT976 Alerts

PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.77A From O7 -0.71 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 1.06A From O7 -0.71 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.55A From O7 -0.70 eA-3

PLAT977_ALERT_2_C Check Negative Difference Density on H7 -0.38 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H18 -0.67 eA-3

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 27 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 24 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 2.00 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 231.40 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 4 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 2 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records 2 Report
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records 4 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 3 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 3 Report
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 36% Note
PLAT774_ALERT_1_G Check X-Y Bond in CIF: Eu1 --Eu1 .. 4.46 Ang.
PLAT794_ALERT_5_G Tentative Bond Valency for Eu1 (III) . 3.46 Info
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms .... ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 336 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 13 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 2 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 3.3 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
25 ALERT type 2 Indicator that the structure model may be wrong or deficient
12 ALERT type 3 Indicator that the structure quality may be low
7 ALERT type 4 Improvement, methodology, query or suggestion
3 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

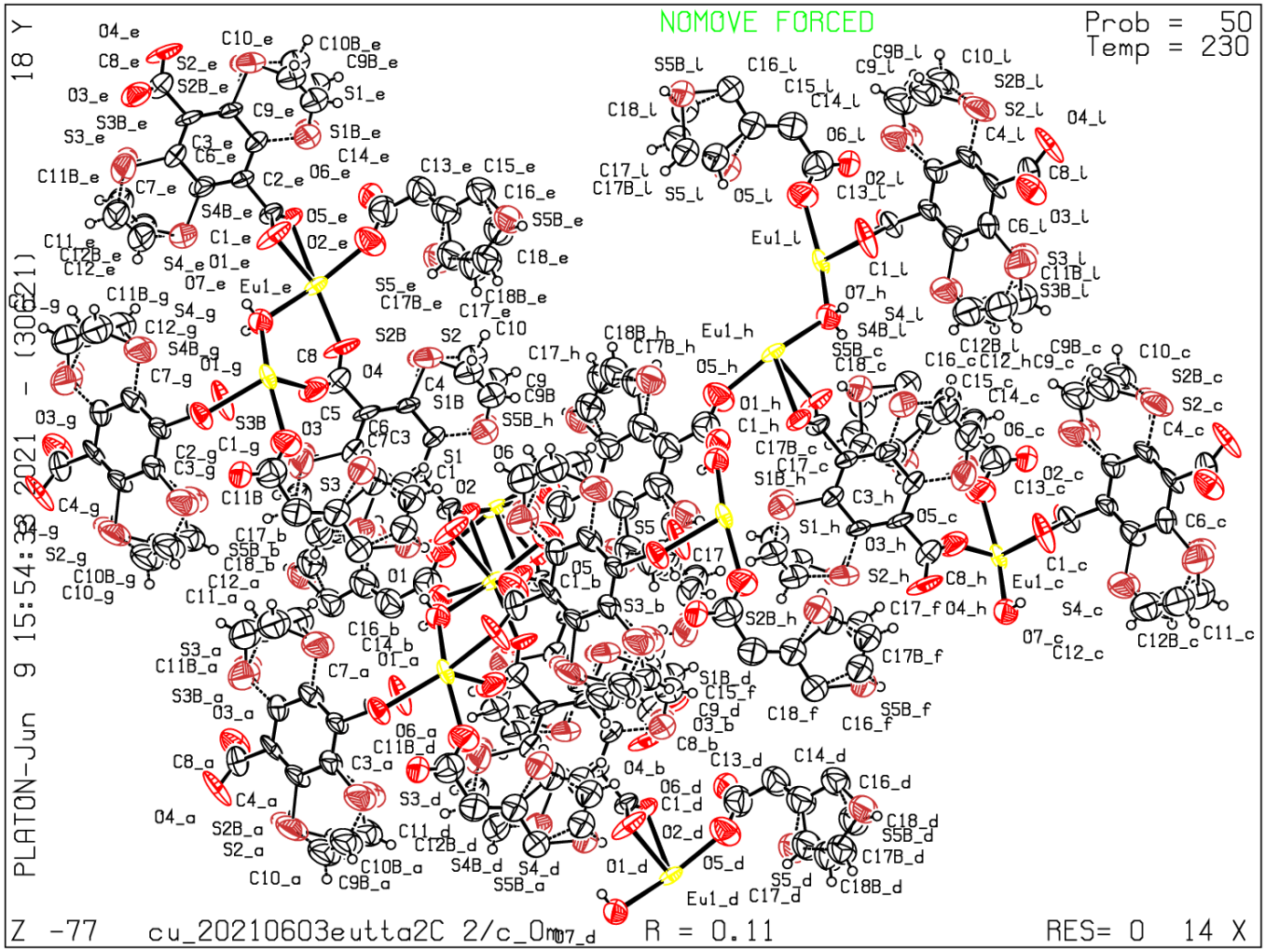
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 03/06/2021; check.def file version of 02/06/2021

Datablock cu_20210603eutta230oc1_0m - ellipsoid plot



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