checkCIF/PLATON report

Structure factors have been supplied for datablock(s) EG1011498082023

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   Interpreting this report

Datablock: EG1011498082023

Bond precision: C-C = 0.0068 A   Wavelength=0.71073

Cell: a=11.6355(7)   b=12.2032(7)   c=14.9256(10)
                 alpha=101.821(3)   beta=104.702(3)   gamma=113.286(3)
Temperature: 273 K

	Calculated	Reported
Volume	1768.4(2)	1768.36(19)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C43 H20 F10 O4 S2	?
Sum formula	C43 H20 F10 O4 S2	C43 H20 F10 O4 S2
Mr	854.71	854.71
Dx,g cm-3	1.605	1.605
Z	2	2
Mu (mm-1)	0.251	0.251
F000	864.0	864.0
F000'	865.12	
h,k,lmax	15,16,19	15,16,19
Nref	8850	8821
Tmin,Tmax	0.956,0.975	0.940,0.970
Tmin'	0.951	

Correction method= # Reported T Limits: Tmin=0.940 Tmax=0.970
AbsCorr = MULTI-SCAN

Data completeness= 0.997   Theta(max)= 28.370

R(reflections)= 0.0819(5089)   wR2(reflections)=
                                                 0.2847(8821)

S = 1.077   Npar= 534

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

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PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ...................    0.28 Report
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ...............  0.00684 Ang.
PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4   Please Check
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...  -13.578 Report
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...   -1.361 Report
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).       6 Note
              1  0  0,  -1  1  0,   0  1  0,   0 -1  1,  -1  0  1,   0  0  1,
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.09Ang From S001          1.54 eA-3
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Alert level G

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PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large    0.16 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)   0.003 Degree
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)     273 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)     273 Check
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C00I      - C00M   .     1.43 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C00P      - C01D   .     1.43 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C00Q      - C010   .     1.41 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C016      - C01A   .     1.41 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact F007      ..F00C   .     2.78 Ang.
                                      2-x,2-y,1-z  =      2_776 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........      79 Note
          S001    S002    F003    F004    F005    F006    F007    F008
          O009    F00A    F00B    F00C    F00D    O00E    O00F    O00G
          C00H    C00I    C00J    C00K    C00L    C00M    C00N    H00N
          C00O    C00P    C00Q    C00R    C00S    C00T    C00U    C00V
          H00V    C00W    C00X    C00Y    H00Y    C00Z    C010    C011
          C012    C013    H01A    H01B    C014    C015    C016    C017
          H017    C018    C019    H019    C01A    C01B    H01C    C01C
          C01D    C01E    C01F    C01G    H01G    C01H    H01D    H01E
          H01F    C01I    C01J    H01J    C01K    H01H    H01I    C01L
          H01K    H01L    H01M    C01M    H01N    C01N    H01O
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .   Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600      21 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....       1 Note
          3 -2  1,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........   8.789 Note
          Predicted wR2: Based on SigI**2  3.24 or SHELX Weight 26.43
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.       0 Info
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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
   7 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

   4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
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8 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
3 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check
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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 15/07/2024; check.def file version of 15/07/2024