checkCIF/PLATON report

Structure factors have been supplied for datablock(s) wky

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: wky

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Bond precision:   C-C = 0.0092 A          Wavelength=0.71073

Cell:             a=9.799(3)     b=25.394(9)          c=18.655(7)
                  alpha=90       beta=91.207(13)      gamma=90
Temperature:      176 K

                 Calculated                 Reported
Volume           4641(3)                    4641(3)
Space group      P 21/c                     P 1 21/c 1
Hall group       -P 2ybc                    -P 2ybc
Moiety formula   C46 H56 O12 [+ solvent]    C46 H56 O12
Sum formula      C46 H56 O12 [+ solvent]    C46 H56 O12
Mr               800.91                     800.90
Dx,g cm-3        1.146                      1.146
Z                4                          4
Mu (mm-1)        0.082                      0.082
F000             1712.0                     1712.0
F000'            1712.93
h,k,lmax                                    12,31,23
Nref                                        9361
Tmin,Tmax        0.984,0.984                0.662,0.745
Tmin'            0.984

Correction method= # Reported T Limits: Tmin=0.662 Tmax=0.745
AbsCorr = ?

Data completeness=                 Theta(max)= 26.330

R(reflections)= 0.1295( 4912)                wR2(reflections)=
                                             0.3101( 9361)
S = 1.062                  Npar= 524
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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

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PLAT031_ALERT_4_B Refined Extinction Parameter Within Range of ...      1.800 Sigma
PLAT230_ALERT_2_B Hirshfeld Test Diff for    O005     --C01P     .        7.1 s.u.
PLAT360_ALERT_2_B Short  C(sp3)-C(sp3) Bond  C01F     - C01M     .       1.33 Ang.
PLAT410_ALERT_2_B Short Intra H...H Contact  H010     ..H01Q     .       1.89 Ang.
                                             x,y,z  =      1_555 Check
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Alert level C

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CRYSC01_ALERT_1_C The word below has not been recognised as a standard
           identifier.
           dull
CRYSC01_ALERT_1_C The word below has not been recognised as a standard
           identifier.
           whiteish
PLAT052_ALERT_1_C Info on Absorption Correction Method   Not Given     Please Do !
PLAT082_ALERT_2_C High R1 Value ..................................       0.13 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ...................       0.31 Report
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.23 Report
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.3 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C01F     --C01M     .        5.1 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C01I     --C01P     .        5.2 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference O00G     --C01C     .       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O00H     --C019     .       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O00H     --C01M     .       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O00I     --C01I     .       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O00O     --C01O     .       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O00R     --C01J     .       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C00Z     --C012     .       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C01E     --C01H     .       0.18 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C01C Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C01E Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C01F Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C01I Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C01K Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C01O Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       O004 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       O00G Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       O00H Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       O00I Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       O00O Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      O001      0.106 Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.00918 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C019     - C01D     .       1.42 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C01B     - C01L     .       1.43 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C01I     - C01P     .       1.37 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      9.034 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      3.289 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      7.151 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.308 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      4.601 Check
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PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.597 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 3 Report
9 19 0, -4 0 14, -1 13 20,

Alert level G

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 8.08 Why ?
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure 201 A**3
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 108 Note

O001	O002	O003	O004	O005	O006	C007	C008
C009	C00A	H00A	C00B	H00B	C00C	C00D	C00E
C00F	O00G	O00H	O00I	C00J	C00K	H00K	O00L
C00M	H00M	C00N	H00N	O00O	C00P	H00P	C00Q
H00Q	O00R	C00S	H00S	C00T	C00U	H00U	C00V
H00V	C00W	H00W	C00X	H00X	C00Y	H00Y	C00Z
H00Z	C010	H010	C011	H011	C012	C014	H01A
H01B	C015	H01C	H01D	C017	H01E	H01F	C018
H01G	H01H	C019	H01I	H01J	C01B	H01K	H01L
C01C	H01M	H01N	C01D	H01O	H01P	C01E	H01Q
H01R	C01F	H01S	H01T	C01G	H01U	H01V	C01H
H01W	H01X	C01I	H01Y	C01J	H01Z	Ha	C01K
H01	Hb	C01L	Hc	C01M	Hd	C01N	He
C01O	Hf	C01P	Hg				

PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed ! Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 2 Note
0 2 0, 0 1 1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 72 Note
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
4 **ALERT level B** = A potentially serious problem, consider carefully
40 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
7 **ALERT level G** = General information/check it is not something unexpected

3 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
10 ALERT type 3 Indicator that the structure quality may be low
13 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 29/11/2023; check.def file version of 14/09/2023

Datablock wky - ellipsoid plot