

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Long-C-C-bond-EDD

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: Long-C-C-bond-EDD

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Bond precision:    C-C = 0.0006 Å                      Wavelength=0.71073

Cell:                      a=9.4181(1)              b=9.0870(1)              c=30.2502(4)  
                            alpha=90              beta=98.5995(8)              gamma=90

Temperature:            90 K

	Calculated	Reported
Volume	2559.78(5)	2559.78(5)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C40 H24	C40 H24
Sum formula	C40 H24	C40 H24
Mr	504.59	504.59
Dx,g cm-3	1.309	1.309
Z	4	4
Mu (mm-1)	0.074	0.074
F000	1056.0	1056.0
F000'	1056.40	
h,k,lmax	20,20,67	20,20,67
Nref	29253	28858
Tmin,Tmax	0.991,0.996	
Tmin'	0.990	

Correction method= Not given

Data completeness= 0.986                      Theta(max)= 52.038

R(reflections)= 0.0284( 19007)              wR2(reflections)= 0.0517( 19007)

S = 1.085                      Npar= 1116

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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.

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### ● Alert level C

PLAT410_ALERT_2_C	Short Intra H...H Contact	H26	..H30	.	1.90	Ang.
			x,y,z	=	1_555	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600			298	Report
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF ....				25	Note
PLAT920_ALERT_1_C	Theta(Max) in CIF and FCF Differ by .....				0.11	Degree

### ● Alert level G

PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF					Please Do !
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C15	--C28			2.04	Ang.
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600			9800	Note
PLAT923_ALERT_1_G	S Values in the CIF and FCF Differ by .....				-0.013	Check
PLAT955_ALERT_1_G	Reported (CIF) and Actual (FCF) Lmax Differ by .				1	Units
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities .....					Please Check

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

3 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  
2 ALERT type 3 Indicator that the structure quality may be low  
1 ALERT type 4 Improvement, methodology, query or suggestion  
2 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 04/06/2020; check.def file version of 02/06/2020

Datablock Long-C-C-bond-EDD - ellipsoid plot

