

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 3a

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: 3a

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Bond precision:      C-C = 0.0143 A

Wavelength=0.71073

Cell:                      a=8.1892 (18)

b=9.5061 (16)

c=11.1371 (19)

alpha=86.021 (14)

beta=71.607 (18)

gamma=70.324 (18)

Temperature:      295 K

	Calculated	Reported
Volume	774.0 (3)	774.0 (3)
Space group	P 1	P 1
Hall group	P 1	P 1
Moiety formula	C31 H20 N2 O4 S, C7 H8	C31 H20 N2 O4 S, C7 H8
Sum formula	C38 H28 N2 O4 S	C38 H28 N2 O4 S
Mr	608.68	608.68
Dx, g cm <sup>-3</sup>	1.306	1.306
Z	1	1
Mu (mm <sup>-1</sup> )	0.149	0.149
F000	318.0	318.0
F000'	318.26	
h, k, lmax	11, 13, 15	11, 13, 15
Nref	8476 [ 4238]	5123
Tmin, Tmax	0.975, 0.993	0.795, 1.000
Tmin'	0.968	

Correction method= # Reported T Limits: Tmin=0.795 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 1.21/0.60

Theta(max)= 29.328

R(reflections)= 0.0661 ( 3682)

wR2(reflections)=  
0.1916 ( 5123)

S = 1.084

Npar= 408

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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 B**

PLAT340_ALERT_3_B	Low Bond Precision on C-C Bonds .....	0.01433	Ang.
PLAT915_ALERT_3_B	No Flack x Check Done: Low Friedel Pair Coverage	35	%

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● **Alert level C**

PLAT230_ALERT_2_C	Hirshfeld Test Diff for N2 --C5 .	5.5	s.u.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C10 --C11 .	0.16	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C15 --C16 .	0.18	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C6S --C7S .	0.22	Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of C17		Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of C30		Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of C13		Check
PLAT243_ALERT_4_C	High 'Solvent' Ueq as Compared to Neighbors of C3S		Check
PLAT243_ALERT_4_C	High 'Solvent' Ueq as Compared to Neighbors of C6S		Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of C2S		Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of C7S		Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 2)	2.9	Note
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including C1S	0.196	Check
PLAT362_ALERT_2_C	Short C(sp3)-C(sp2) Bond C1S - C2S .	1.39	Ang.

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● **Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	6	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	6	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	1	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	1	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1	Report
PLAT192_ALERT_3_G	A Non-default DELU Restraint Value for First Par	0.0050	Report
PLAT192_ALERT_3_G	A Non-default DELU Restraint Value for SecondPar	0.0050	Report
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent) C2S --C7S .	6.7	s.u.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....	3	Note
	H1SA H1SB H1SC		
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	47	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min). 0 0 1,	1	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	611	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File -2 -2 8, -1 1 9, -4 -8 -5, -4 -4 6,	4	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	1.9	Low
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value .....	1.98	Note
	Predicted wR2: Based on SigI**2 9.66 or SHELX Weight 18.43		
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1	Info
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by	7	Check

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
11 ALERT type 2 Indicator that the structure model may be wrong or deficient  
7 ALERT type 3 Indicator that the structure quality may be low  
13 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**

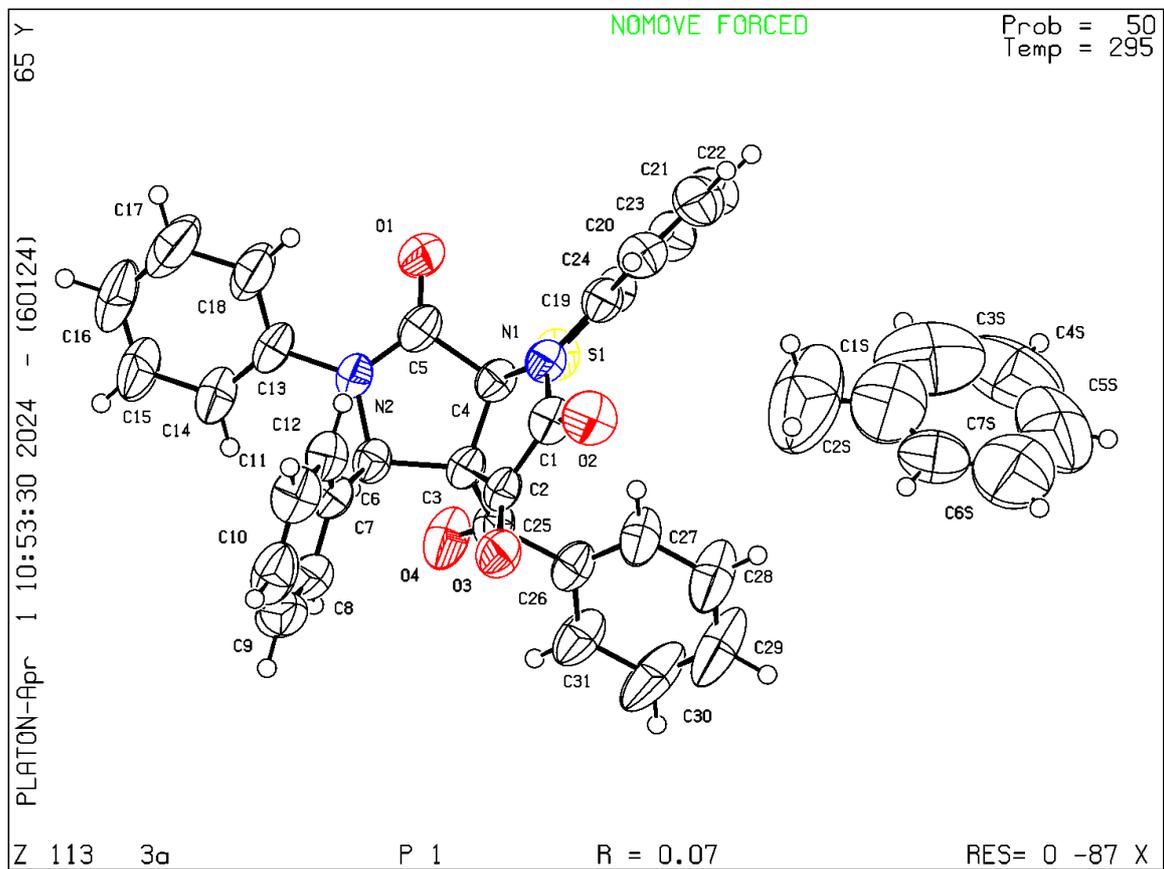
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section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

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**PLATON version of 06/01/2024; check.def file version of 05/01/2024**





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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**

PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C20	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....		2.752	Check

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**Alert level G**

PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		2	Note
	-1 0 1, 0 0 2,			
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		894	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....		2.3	Low
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ.		2	Units
PLAT958_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Lmax Differ.		2	Units
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value .....		2.46	Note
	Predicted wR2: Based on SigI**2 5.14 or SHELX Weight 12.68			
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		6	Info

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2 ALERT type 5 Informative message, check
- 
-

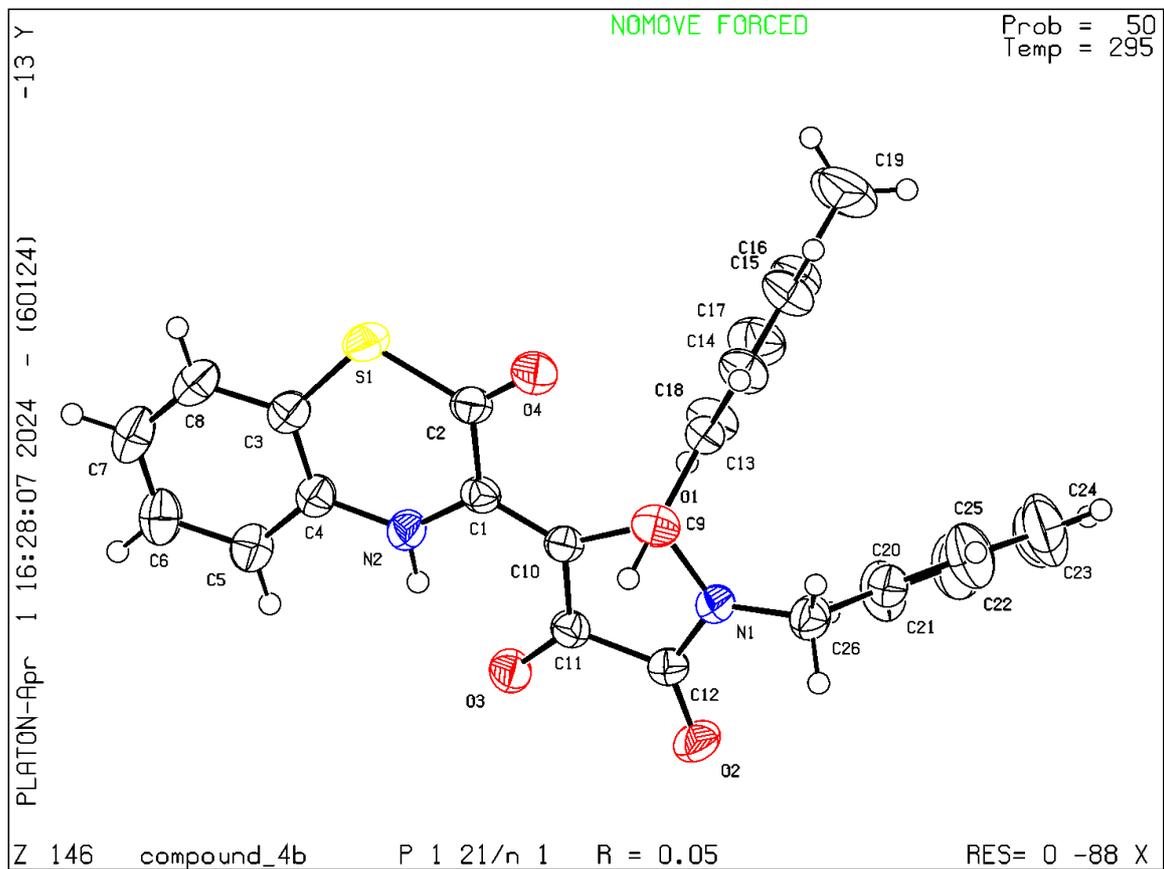
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## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) compound\_6d

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No syntax errors found.      CIF dictionary      Interpreting this report

### Datablock: compound\_6d

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Bond precision:      C-C = 0.0072 Å      Wavelength=0.71073

Cell:                      a=20.406(4)      b=9.309(3)      c=11.069(2)  
                                    alpha=90      beta=93.739(19)      gamma=90

Temperature:              295 K

	Calculated	Reported
Volume	2098.2(9)	2098.2(9)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C23 H15 Br N2 O3 S	C23 H15 Br N2 O3 S
Sum formula	C23 H15 Br N2 O3 S	C23 H15 Br N2 O3 S
Mr	479.33	479.34
Dx, g cm <sup>-3</sup>	1.517	1.517
Z	4	4
Mu (mm <sup>-1</sup> )	2.086	2.086
F000	968.0	968.0
F000'	967.72	
h, k, lmax	28, 12, 15	27, 12, 15
Nref	5758	4934
Tmin, Tmax	0.644, 0.864	0.361, 1.000
Tmin'	0.349	

Correction method= # Reported T Limits: Tmin=0.361 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.857      Theta(max)= 29.353

R(reflections)= 0.0670( 2424)

wR2(reflections)=  
0.2110( 4934)

S = 1.009

Npar= 278

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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 B**

PLAT230\_ALERT\_2\_B Hirshfeld Test Diff for N1 --C5 . 9.0 s.u.

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 **Alert level C**

PLAT026\_ALERT\_3\_C Ratio Observed / Unique Reflections (too) Low .. 49% Check  
PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of C18 Check  
PLAT341\_ALERT\_3\_C Low Bond Precision on C-C Bonds ..... 0.00717 Ang.  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 23.398 Check  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 4.623 Check

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 **Alert level G**

PLAT002\_ALERT\_2\_G Number of Distance or Angle Restraints on AtSite 2 Note  
PLAT172\_ALERT\_4\_G The CIF-Embedded .res File Contains DFIX Records 1 Report  
PLAT860\_ALERT\_3\_G Number of Least-Squares Restraints ..... 1 Note  
PLAT910\_ALERT\_3\_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note  
1 0 0,  
PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 819 Note  
PLAT941\_ALERT\_3\_G Average HKL Measurement Multiplicity ..... 2.2 Low  
PLAT969\_ALERT\_5\_G The 'Henn et al.' R-Factor-gap value ..... 2.70 Note  
Predicted wR2: Based on SigI\*\*2 7.81 or SHELX Weight 21.54  
PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 0 Info

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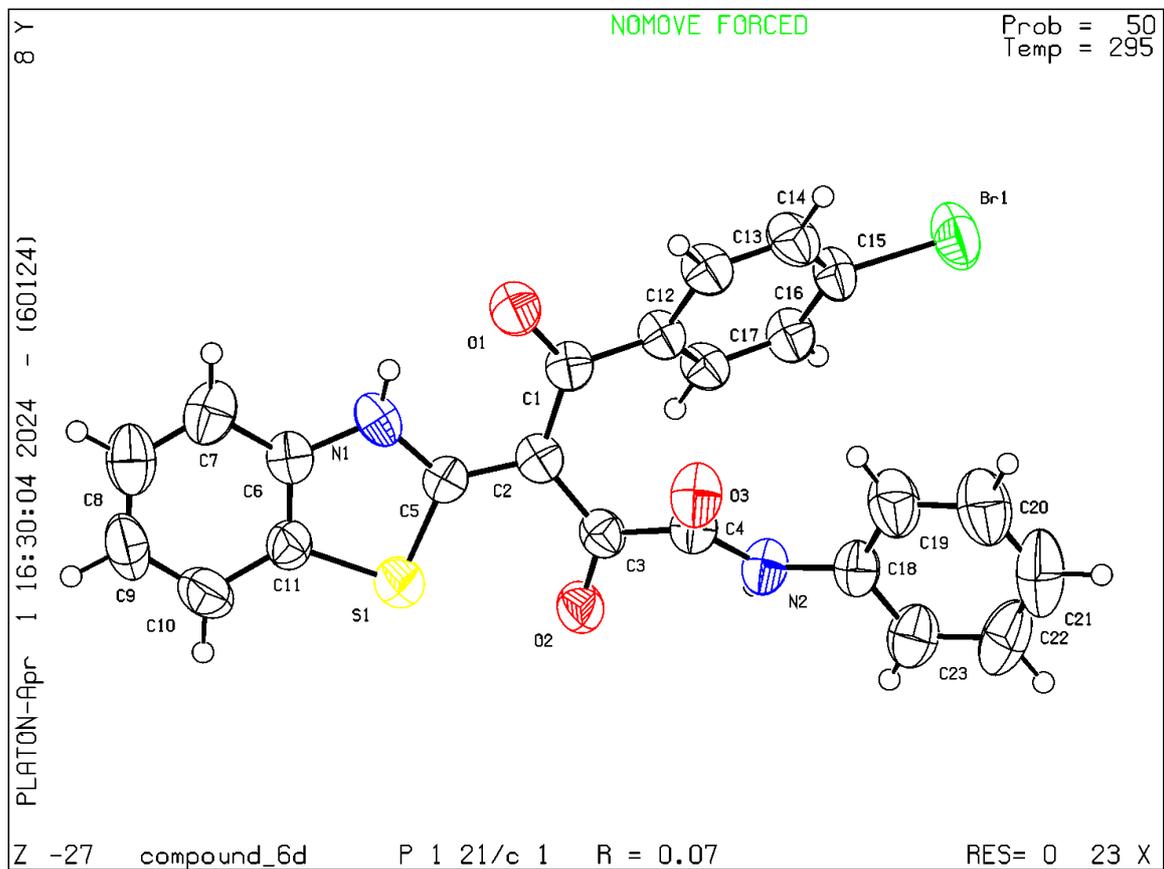
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● **Alert level C**

PLAT230\_ALERT\_2\_C Hirshfeld Test Diff for C25 --C26 . 6.0 s.u.  
PLAT340\_ALERT\_3\_C Low Bond Precision on C-C Bonds ..... 0.00419 Ang.  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 9.117 Check  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 2.211 Check  
PLAT910\_ALERT\_3\_C Missing # of FCF Reflection(s) Below Theta(Min). 7 Note  
1 1 0, 0 2 0, -1 0 1, 1 0 1, -1 1 1, 0 1 1,  
0 2 1,

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● **Alert level G**

PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 1059 Note  
PLAT941\_ALERT\_3\_G Average HKL Measurement Multiplicity ..... 2.6 Low  
PLAT969\_ALERT\_5\_G The 'Henn et al.' R-Factor-gap value ..... 2.29 Note  
Predicted wR2: Based on SigI\*\*2 7.64 or SHELX Weight 17.24  
PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 1 Info

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