



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

Bond precision: C-C = 0.0116 Å

Wavelength=1.54178

Cell: a=12.848 (5) b=16.337 (7) c=16.353 (6)
 alpha=117.71 (2) beta=90.12 (1) gamma=111.57 (1)
Temperature: 100 K

	Calculated	Reported
Volume	2763 (2)	2763 (2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C12 H10 N6, 2 (C6 H2 N3 O7)	?
Sum formula	C24 H14 N12 O14	C24 H14 N12 O14
Mr	694.47	694.47
Dx, g cm ⁻³	1.669	1.670
Z	4	4
Mu (mm ⁻¹)	1.230	1.230
F000	1416.0	1416.0
F000'	1421.62	
h, k, lmax	14, 18, 18	14, 18, 18
Nref	7923	7536
Tmin, Tmax	0.782, 0.832	0.782, 0.811
Tmin'	0.782	

Correction method= # Reported T Limits: Tmin=0.782 Tmax=0.811
AbsCorr = MULTI-SCAN

Data completeness= 0.951 Theta(max)= 58.931

R(reflections)= 0.1049(4795) wR2(reflections)=
0.3302(7536)

S = 1.201 Npar= 901

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

THETM01_ALERT_3_B The value of sine(theta_max)/wavelength is less than 0.575
Calculated sin(theta_max)/wavelength = 0.5556

Author Response: crystals were of poor quality

PLAT029_ALERT_3_B _diffraction_measured_fraction_theta_full value Low . 0.951 Why?

Author Response: the highest resolution used for refinement was a compromise between ac

PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds 0.01157 Ang.

Author Response: crystals were of poor quality, they didn't give diffraction up to high

PLAT430_ALERT_2_B Short Inter D...A Contact O8 ..N10 . 2.82 Ang.
1-x,2-y,2-z = 2_677 Check

Author Response: this is a contact between the picrate oxygen and a tetrazine nitrogen.

PLAT430_ALERT_2_B Short Inter D...A Contact O16 ..N5 . 2.81 Ang.
x,y,z = 1_555 Check

Author Response: this is a contact between the picrate oxygen and a tetrazine nitrogen.



Alert level C

DIFMN02_ALERT_2_C The minimum difference density is < -0.1*ZMAX*0.75
_refine_diff_density_min given = -0.626
Test value = -0.600

DIFMN03_ALERT_1_C The minimum difference density is < -0.1*ZMAX*0.75
The relevant atom site should be identified.

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.

PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) 0.33 Report

PLAT088_ALERT_3_C Poor Data / Parameter Ratio 8.36 Note

PLAT097_ALERT_2_C	Large	Reported Max.	(Positive)	Residual Density	0.77	eA-3
PLAT098_ALERT_2_C	Large	Reported Min.	(Negative)	Residual Density	-0.63	eA-3
PLAT430_ALERT_2_C	Short	Inter D...A Contact	O25	..028	.	2.88 Ang.
				-x,-y,-z =	2_555	Check

Author Response: this is a contact between the picrate oxygen and a tetrazine nitrogen.

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PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 7.371 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.556 389 Report
      -14  7  0, -14  8  0, -14  9  0, -13  9  0,  5  9  0,  6  9  0,
        7  9  0, -13 10  0,  3 10  0,  4 10  0,  5 10  0,  6 10  0,
      -13 11  0,  2 11  0,  3 11  0,  4 11  0,  5 11  0, -13 12  0,
        1 12  0,  2 12  0,  3 12  0,  4 12  0,  0 13  0,  1 13  0,
        2 13  0, -1 14  0,  0 14  0,  1 14  0, -1 15  0,  0-15  1,
      ( 359 More Missing: see the .ckf listing file)
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 1 Check
      8-12  8,

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Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	4 Report
H1 H6 H7 H12		
PLAT432_ALERT_2_G Short Inter X...Y Contact O1	. .C7 . 2.99 Ang.	
	x,y,1+z = 1_556 Check	
PLAT432_ALERT_2_G Short Inter X...Y Contact O1	. .C24 . 3.01 Ang.	
	x,y,z = 1_555 Check	
PLAT432_ALERT_2_G Short Inter X...Y Contact O8	. .C18 . 2.82 Ang.	
	1-x,2-y,2-z = 2_677 Check	
PLAT432_ALERT_2_G Short Inter X...Y Contact O15	. .C6 . 3.00 Ang.	
	x,y,z = 1_555 Check	
PLAT432_ALERT_2_G Short Inter X...Y Contact O17	. .C29 . 2.94 Ang.	
	-1+x,y,-1+z = 1_454 Check	
PLAT432_ALERT_2_G Short Inter X...Y Contact O18	. .C22 . 2.92 Ang.	
	-1+x,y,-1+z = 1_454 Check	
PLAT432_ALERT_2_G Short Inter X...Y Contact O19	. .C14 . 2.96 Ang.	
	-x,1-y,1-z = 2_566 Check	
PLAT432_ALERT_2_G Short Inter X...Y Contact O22	. .C19 . 2.97 Ang.	
	1-x,1-y,1-z = 2_666 Check	
PLAT432_ALERT_2_G Short Inter X...Y Contact O23	. .C3 . 2.97 Ang.	
	x,y,z = 1_555 Check	
PLAT432_ALERT_2_G Short Inter X...Y Contact O26	. .C1 . 2.95 Ang.	
	-x,-y,-z = 2_555 Check	
PLAT790_ALERT_4_G Centre of Gravity not Within Unit-Cell: Resd. #		3 Note
C6 H2 N3 O7		
PLAT790_ALERT_4_G Centre of Gravity not Within Unit-Cell: Resd. #		4 Note
C6 H2 N3 O7		
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters		3 Info
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still		34% Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF		1 Note
-2 0 4,		
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity		4.9 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value		3.710 Note
Predicted wR2: Based on SigI**2 8.90 or SHELX Weight 27.50		
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
5 **ALERT level B** = A potentially serious problem, consider carefully
11 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
19 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
17 ALERT type 2 Indicator that the structure model may be wrong or deficient
11 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
2 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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 26/09/2025; check.def file version of 20/09/2025

duplicate check

No duplication found

