



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) a

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: a

Bond precision: C-C = 0.0202 Å

Wavelength=0.02510

Cell: a=12.093 (2) b=12.5740 (18) c=12.654 (3)
 alpha=108.911 (16) beta=114.21 (2) gamma=94.951 (13)
Temperature: 293 K

	Calculated	Reported
Volume	1605.7 (7)	1605.7 (6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C44 H32 N2 O2 [+ solvent]	C44 H32 N2 O2
Sum formula	C44 H32 N2 O2 [+ solvent]	C44 H32 N2 O2
Mr	620.72	620.75
Dx, g cm ⁻³	1.284	1.284
Z	2	2
Mu (mm ⁻¹)	0.000	0.000
F000	0.0	271.0
F000'	651.90	
h, k, lmax	13, 13, 14	13, 13, 13
Nref	4600	2905
Tmin, Tmax		
Tmin'		

Correction method= Not given

Data completeness= 0.632

Theta(max)= 0.799

R(reflections)= 0.3282(1489)

wR2(reflections)=
0.7582(2905)

S = 1.069

Npar= 132

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 A

ATOM007_ALERT_1_A _atom_site_aniso_label is missing
Unique label identifying the atom site.

Author Response: The quality of the electron diffraction data is sufficient for structure solution, but it is not adequate for the anisotropic refinement of atomic positions.

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.632 Why?

Author Response: The data were collected using three-dimensional electron diffraction technology, thus the collection angles were limited.

PLAT082_ALERT_2_A High R1 Value 0.33 Report

Author Response: The data were collected using three-dimensional electron diffraction technology on only one crystal. Higher R factors are expected due to the strong interaction of electrons.

PLAT084_ALERT_3_A High wR2 Value (i.e. > 0.25) 0.76 Report

Author Response: The data were collected using three-dimensional electron diffraction technology on only one crystal. Higher R factors are expected due to the strong interaction of electrons.

PLAT411_ALERT_2_A Short Inter H...H Contact H3 ..H3 . 1.06 Ang.
-1-x, 2-y, -z = 2_475 Check

Author Response: This abnormally short intermolecular H...H contact is caused by the initial automatic hydrogenation in Olex2, which only calculates intramolecular bonding geometry without considering the steric repulsion between symmetry- related molecules in the unit cell.

PLAT921_ALERT_1_A R1 in CIF and R1 Calcd from FCF Data Differ by . -0.0955 Check

Author Response: The discrepancies in R1 and wR2 are likely associated with the treatment of the empirical extinction correction in the SHELXL refinement and FCF output. The refinement used electron scattering factors together with an EXTI correction. As noted in the IUCr documentation for PLAT921, SHELXL exports extinction-corrected observed intensities to the FCF. This reflection-dependent transformation may lead to differences between the residuals reported for the refinement and those recalculated from the FCF, including differences associated with the weighting scheme for wR2.

PLAT922_ALERT_1_A wR2 in the CIF and FCF Differ by -0.0574 Check

Author Response: The discrepancies in R1 and wR2 are likely associated with the treatment of the empirical extinction correction in the SHELXL refinement and FCF output. The refinement used electron scattering factors together with an EXTI correction. As noted in the IUCr documentation for PLAT921, SHELXL exports extinction-corrected observed intensities to the FCF. This reflection-dependent transformation may lead to differences between the residuals reported for the refinement and those recalculated from the FCF, including differences associated with the weighting scheme for wR2.



Alert level B

THETM01_ALERT_3_B The value of $\sin(\theta_{\max})/\lambda$ is less than 0.575
Calculated $\sin(\theta_{\max})/\lambda = 0.5556$

Author Response: The data were collected using three-dimensional electron diffraction technology on only one crystal and the crystals diffract very weakly on the high angle.

PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) Occ>0.5 48 Report

O00P	O014	N00Z	N006	C00B	C2	C00C	C3
C00G	C00D	C005	C009	C002	C003	C00M	C00N
C00O	C00Q	C00S	C00U	C00V	C00W	C17	C00X
C013	C016	C015	C00Y	C001	C00K	C00I	C00E
C00A	C008	C004	C007	C30	C00J	C31	C00F
C00T	C00L	C00H	C010	C011	C012	C47	C103

Author Response: The quality of the electron diffraction data is sufficient for structure solution, but it is not adequate for the anisotropic refinement of atomic positions.

PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds 0.02023 Ang.

Author Response: The data were collected through three-dimensional electron diffraction technology without accounting for dynamical effects. No action taken.

PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.555 1690 Report
-3 1 0, -2 1 0, -1 1 0, -7 2 0, -6 2 0, -5 2 0,
-4 2 0, -3 2 0, -2 2 0, -1 2 0, -10 3 0, -9 3 0,
-8 3 0, -7 3 0, -6 3 0, -5 3 0, -4 3 0, -3 3 0,
-2 3 0, -12 4 0, -11 4 0, -10 4 0, -9 4 0, -8 4 0,
-7 4 0, -6 4 0, -5 4 0, -4 4 0, -3 4 0, -2 4 0,
(1660 More NOT listed: see .ckf listing file)

Author Response: The data were collected through three-dimensional electron diffraction technology, thus the number of collected diffraction spots was limited.

Alert level C

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.
yellowish

PLAT031_ALERT_4_C Refined Extinction Parameter Within Range of ... 3.087 Sigma
PLAT241_ALERT_2_C High MainResAtom Ueq as Compared to Neighbours N00Z Check
PLAT241_ALERT_2_C High MainResAtom Ueq as Compared to Neighbours C17 Check
PLAT241_ALERT_2_C High MainResAtom Ueq as Compared to Neighbours C016 Check
PLAT241_ALERT_2_C High MainResAtom Ueq as Compared to Neighbours C015 Check
PLAT241_ALERT_2_C High MainResAtom Ueq as Compared to Neighbours C00E Check
PLAT241_ALERT_2_C High MainResAtom Ueq as Compared to Neighbours C30 Check
PLAT241_ALERT_2_C High MainResAtom Ueq as Compared to Neighbours C31 Check
PLAT241_ALERT_2_C High MainResAtom Ueq as Compared to Neighbours C47 Check
PLAT242_ALERT_2_C Low MainResAtom Ueq as Compared to Neighbours C2 Check
PLAT242_ALERT_2_C Low MainResAtom Ueq as Compared to Neighbours C00M Check
PLAT242_ALERT_2_C Low MainResAtom Ueq as Compared to Neighbours C00X Check
PLAT242_ALERT_2_C Low MainResAtom Ueq as Compared to Neighbours C013 Check
PLAT410_ALERT_2_C Short Intra H...H Contact H00E ..H00T . 1.98 Ang.
x,y,z = 1_555 Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor N00Z --H00Z . Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor N006 --H006 . Please Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 156.374 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 16.597 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 10.990 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 5.605 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 3.055 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.279 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.398 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.363 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.850 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.522 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.885 Check
PLAT923_ALERT_1_C S Values in the CIF and FCF Differ by -0.266 Check

● **Alert level G**

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 32 Note

PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H-Atoms 48 Report

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 1 Info

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 2 Report

H00Z H006

PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.70 Report

PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 2 Report

PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 48 Report

PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records 3 Report

PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 1 Report

PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report

PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check

PLAT200_ALERT_1_G Reported _diffn_ambient_temperature (K) 293 Check

PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O014 . 106.7 Degree

PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure 7 A**3

PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 67 Note

O00P O014 N00Z H00Z N006 H006 C00B H00B

C00C C00G H00G C00D C005 C009 C002 C003

H003 C00M C00N C00O C00Q H00Q C00S H00S

C00U H00U C00V H00V C00W H00W C00X C013

C016 H016 C015 H015 C00Y H00Y C001 C00K

C00I H00I C00E H00E C00A C008 H008 C004

C007 C00J H00J C00F C00T H00T C00L H00L

C00H C010 H01A H01B H01C C011 H01D H01E

H01F C012 H012

PLAT768_ALERT_4_G RES Embedded Explicitly Supplied Scattering Data 4 Note

PLAT804_ALERT_5_G Number of ARU-Code Packing Problem(s) in PLATON 10 Info

PLAT860_ALERT_3_G Number of Least-Squares Restraints 124 Note

PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed ! Info

PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 2.0 Low

PLAT948_ALERT_5_G Externally Supplied Scattering Factors RES 4 Note

PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 4.046 Note

Predicted wR2: Based on SigI**2 20.16 or SHELX Weight 61.11 Note

PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by 2 Check

7 **ALERT level A** = Most likely a serious problem - resolve or explain

4 **ALERT level B** = A potentially serious problem, consider carefully

30 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

25 **ALERT level G** = General information/check it is not something unexpected

9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

23 ALERT type 2 Indicator that the structure model may be wrong or deficient

18 ALERT type 3 Indicator that the structure quality may be low

10 ALERT type 4 Improvement, methodology, query or suggestion

6 ALERT type 5 Informative message, check

PLATON version of 23/04/2026; check.def file version of 30/03/2026

No duplication found

(VERSION=230426)
 -16 Y
 NOMOVE FORCED
 Prob = 50%
 Temp = 293K
 PLATON-Sep 5 7:17:26
 Z -43 a P -1 R = 0.33 RES= 0 -15 X