

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) try1

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: try1

Bond precision: C-C = 0.0155 A

Wavelength=0.71073

Cell: a=11.0882(13) b=16.1610(17) c=17.3390(15)
 alpha=84.881(6) beta=78.600(6) gamma=85.512(6)
Temperature: 299 K

	Calculated	Reported
Volume	3027.8(5)	3027.8(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C30 H19 Ce N8 O6, C15 H11 Ce N7 O12 [+ solvent]	C30 H19 Ce N8 O6, C15 H11 Ce N7 O12 [+ solvent]
Sum formula	C45 H30 Ce2 N15 O18 [+ solvent]	C45 H30 Ce2 N15 O18 [+ solvent]
Mr	1349.08	1349.08
Dx, g cm ⁻³	1.480	1.483
Z	2	2
Mu (mm ⁻¹)	1.560	1.560
F000	1330.0	1336.0
F000'	1329.58	
h, k, lmax	13, 19, 20	13, 19, 20
Nref	11188	10745
Tmin, Tmax	0.387, 0.675	0.582, 0.745
Tmin'	0.298	

Correction method= # Reported T Limits: Tmin=0.582 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.960

Theta(max)= 25.423

R(reflections)= 0.0592(7857)

wR2(reflections)=
0.1873(10745)

S = 1.039

Npar= 721

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 C

PLAT029_ALERT_3_C _diffn_measured_fraction_theta_full value Low . 0.973 Why?
PLAT230_ALERT_2_C Hirshfeld Test Diff for O003 --N00N . 5.4 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for C01R --C024 . 6.0 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference C023 --C026 . 0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C025 --C028 . 0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O000 --N00Z . 0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C01L --C024 . 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C01M --C01W . 0.20 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O00D Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O009 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O00H Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O000 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O00V Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C024 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Ce01 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N00J Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Ce02 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N00N Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N00S Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N00Z Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.01545 Ang.
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -4.303 Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 290 Report
-3 1 0, -1 1 0, 1 1 0, 3 1 0, -4 2 0, -3 2 0,
-2 2 0, 0 2 0, -3 3 0, 2 3 0, 1 4 0, -5 5 0,
-4 5 0, 0 5 0, 1 6 0, 2 6 0, -3 8 0, -7 10 0,
-1 16 0, 5-15 1, -1 -8 1, -3 -5 1, -2 -5 1, 0 -5 1,
2 -5 1, -3 -4 1, -2 -4 1, -1 -4 1, 3 -4 1, 5 -4 1,
-2 -3 1, -1 -3 1, 0 -3 1, 1 -3 1, 4 -3 1, -3 -2 1,
0 -2 1, 1 -2 1, 3 -2 1, 4 -2 1, 1 -1 1, 5 -1 1,
-2 0 1, -1 0 1, 1 0 1, 2 0 1, -5 1 1, -4 1 1,
-1 1 1, -4 2 1, -2 2 1, -1 2 1, 0 2 1, 4 2 1,
-1 3 1, 0 3 1, 1 3 1, -3 4 1, 1 4 1, 3 4 1,
1 6 1, 3 6 1, -8 7 1, -7 7 1, 2 9 1, -2 10 1,
-4 11 1, 0 11 1, -6 12 1, 1 13 1, 0 17 1, 0 -6 2,
1 -6 2, -2 -5 2, 0 -5 2, -3 -4 2, 1 -4 2, 4 -3 2,
-5 -2 2, -1 -2 2, 2 -2 2, -4 -1 2, -3 -1 2, -2 -1 2,
0 -1 2, 3 -1 2, 0 0 2, 1 0 2, 2 0 2, -3 1 2,
1 1 2, 0 2 2, 2 2 2, -4 3 2, 1 3 2, -2 4 2,
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF 34 Note
-3 1 0, 0 1 0, 1 1 0, -3 2 0, 0 5 0, 3 -2 1,
0 -1 1, 1 -1 1, 5 -1 1, -1 1 1, -4 2 1, 1 3 1,
1 4 1, 1 -4 2, 0 -1 2, 1 1 2, 0 -3 3, -3 -2 3,
1 -2 3, -2 -1 3, 0 -6 4, 1 -5 4, -4 -1 4, 4 -1 4,
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.04Ang From Ce01 2.10 eA-3

PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	1.07Ang From Ce02	1.62 eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	1.08Ang From Ce02	1.52 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.96Ang From O003	1.05 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.90Ang From O004	1.03 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	1.08Ang From C022	0.64 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H01Z		-0.32 eA-3

Alert level G

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.

CELLZ01_ALERT_1_G ALERT: Large difference may be due to a

symmetry error - see SYMMG tests

From the CIF: _cell_formula_units_Z 2

From the CIF: _chemical_formula_sum C45 H30 Ce2 N15 O18 [+ solvent]

TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	90.00	90.00	0.00
H	60.00	60.00	0.00
Ce	4.00	4.00	0.00
N	30.00	30.00	0.00
O	36.00	36.00	0.00
[+]	2.00	0.00	2.00
solve	2.00	0.00	2.00

PLAT063_ALERT_4_G	Crystal Size Possibly too Large for Beam Size ..	0.75 mm
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	9.68 Why ?
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.006 Degree
PLAT180_ALERT_4_G	Check Cell Rounding: # of Values Ending with 0 =	3 Note
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Ce02 --O003	5.3 s.u.
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C019 Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C022 Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C026 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O00X ..C01Y	2.92 Ang.

x,y,z = 1_555 Check

PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ! Info

PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 110 Note

Ce01	Ce02	O003	O004	O005	O006	N007	O008
O009	O00A	O00B	N00C	O00D	N00E	N00F	N00G
O00H	N00I	N00J	N00K	N00L	N00M	N00N	O00O
N00P	N00Q	C00R	N00S	C00T	O00U	O00V	O00W
O00X	C00Y	H00Y	N00Z	C010	C011	C012	H012
O013	O014	C015	H015	C016	C017	C018	H018
C019	C01A	C01B	C01C	H01C	C01D	C01E	H01E
C01F	O01G	C01H	C01I	C01J	H01J	C01K	H01K
C01L	H01L	C01M	H01M	C01N	H01N	C01O	H01O
C01P	H01P	C01Q	H01Q	C01R	H01R	C01S	H01S
C01T	H01T	C01U	H01U	C01V	H01V	C01W	H01W
C01X	H01X	C01Y	H01Y	C01Z	H01Z	C020	H020
C021	H021	C022	C023	H023	C024	H024	C025
H025	C026	C028	H028	C029	H029		

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). 4 Note

0 1 0, 0 -1 1, 0 0 1, 0 1 1,

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 149 Note

PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 2 Note

1 0 3, -1 5 6,

PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 2.0 Low

PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 2.783 Note
 Predicted wR2: Based on SigI**2 6.73 or SHELX Weight 18.04
 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
 0 **ALERT level B** = A potentially serious problem, consider carefully
 31 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 20 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 29 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
 11 ALERT type 4 Improvement, methodology, query or suggestion
 1 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.

Datablock try1 - ellipsoid plot

