

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) tbdptp_2

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: tbdptp_2

Bond precision:	C-C = 0.0095 A	Wavelength=0.71073	
Cell:	a=40.9140 (15) alpha=90	b=31.3064 (15) beta=90	c=18.6551 (5) gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	23894.8 (16)	23894.8 (16)	
Space group	P c c n	P c c n	
Hall group	-P 2ab 2ac	-P 2ab 2ac	
Moiety formula	C114 H66 F36 O16 P4 Tb2 [+ solvent]	C114 H66 F36 O16 P4 Tb2	
Sum formula	C114 H66 F36 O16 P4 Tb2 [+ solvent]	C114 H66 F36 O16 P4 Tb2	
Mr	2817.41	2817.38	
Dx, g cm ⁻³	1.566	1.566	
Z	8	8	
Mu (mm ⁻¹)	1.345	1.345	
F000	11136.0	11136.0	
F000'	11144.52		
h, k, lmax	59, 45, 26	58, 38, 25	
Nref	37926	29699	
Tmin, Tmax	0.845, 0.914	0.427, 1.000	
Tmin'	0.845		

Correction method= # Reported T Limits: Tmin=0.427 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.783 Theta (max)= 30.949

R(reflections)= 0.0667(20378)

wR2(reflections)=
0.1508(29699)

S = 1.024

Npar= 1549

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

PLAT213_ALERT_2_B Atom F03S	has ADP max/min Ratio	4.1 prolat
PLAT213_ALERT_2_B Atom F044	has ADP max/min Ratio	4.1 prolat
PLAT213_ALERT_2_B Atom F04I	has ADP max/min Ratio	4.2 prolat
PLAT213_ALERT_2_B Atom F04L	has ADP max/min Ratio	5.0 prolat
PLAT213_ALERT_2_B Atom F04S	has ADP max/min Ratio	4.4 prolat
PLAT230_ALERT_2_B Hirshfeld Test Diff for F04I --C04U	.	7.8 s.u.
PLAT331_ALERT_2_B Small Aver Phenyl C-C Dist C01T --C04P	.	1.36 Ang.



Alert level C

PLAT213_ALERT_2_C Atom F01L	has ADP max/min Ratio	3.6 prolat
PLAT213_ALERT_2_C Atom F02K	has ADP max/min Ratio	3.2 prolat
PLAT213_ALERT_2_C Atom F02S	has ADP max/min Ratio	3.8 prolat
PLAT213_ALERT_2_C Atom F035	has ADP max/min Ratio	3.6 prolat
PLAT213_ALERT_2_C Atom F036	has ADP max/min Ratio	3.2 prolat
PLAT213_ALERT_2_C Atom F037	has ADP max/min Ratio	3.9 prolat
PLAT213_ALERT_2_C Atom F03B	has ADP max/min Ratio	3.2 prolat
PLAT213_ALERT_2_C Atom F03F	has ADP max/min Ratio	3.5 prolat
PLAT213_ALERT_2_C Atom F03U	has ADP max/min Ratio	3.3 prolat
PLAT213_ALERT_2_C Atom F04N	has ADP max/min Ratio	3.1 prolat
PLAT213_ALERT_2_C Atom F04Q	has ADP max/min Ratio	3.2 prolat
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range		4.6 Ratio
PLAT220_ALERT_2_C NonSolvent Resd 1 F Ueq(max)/Ueq(min) Range		5.3 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range		4.5 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference F00X --C04E	.	0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F02V --C04H	.	0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F04N --C04U	.	0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F04S --C04E	.	0.17 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of	C03L	Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of	C047	Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of	C04G	Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of	C04P	Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of	C04R	Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of	C04T	Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of	C01T	Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of	C02N	Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of	C02U	Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of	C03D	Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of	C042	Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of	C04C	Check
PLAT331_ALERT_2_C Small Aver Phenyl C-C Dist C02N --C047	.	1.36 Ang.
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds		0.0095 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact H01S ..H02L	.	1.99 Ang.
	x,y,z =	1_555 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance		5.566 Check

PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.576	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	6	Report
	4 1 1, 7 2 1, 0 2 2, 2 4 2, 3 1 2, 4 0 2,		
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.99Ang From Tb01	1.59	eA-3

Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	8	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	98.43	Why ?
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	2	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	2	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0200	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0200	Report
PLAT190_ALERT_3_G	A Non-default RIGU Restraint Value for First Par	0.0020	Report
PLAT190_ALERT_3_G	A Non-default RIGU Restraint Value for SecondPar	0.0020	Report
PLAT190_ALERT_3_G	A Non-default RIGU Restraint Value for First Par	0.0020	Report
PLAT190_ALERT_3_G	A Non-default RIGU Restraint Value for SecondPar	0.0020	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature (K)	293	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C10	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C02D	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C02Z	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C039	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C03R	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C03X	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C049	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C04B	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C04E	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C04H	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C04O	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C04U	Check
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist C011 -C01N .	1.43	Ang.
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist C013 -C01K .	1.43	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F00I ..F00P .	2.81	Ang.
	1-x,-1/2+y,1/2-z =	3_645	Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F01Z ..F037 .	2.81	Ang.
	1-x,-1/2+y,1/2-z =	3_645	Check
PLAT606_ALERT_4_G	Solvent Accessible VOID(S) in Structure	!	Info
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	237	Note

Tb01	Tb02	P003	P004	P005	P006	F007	O008
O009	F00A	O00B	O00C	O00D	O00E	O00F	F00G
O00H	F00I	O00J	O00K	O00L	O00M	O00N	O00O
F00P	O00Q	O00R	F00S	F00T	F00W	F00X	F00Y
F00Z	F010	C011	F012	C013	C014	C015	C016
C017	C018	C019	H019	C01A	C01B	H01B	C01C
F01D	C01E	C01F	H01F	C01G	C01H	H01H	C01I
F01J	C01K	F01L	C01M	C01N	F01O	C01P	C01Q
H01Q	C01R	H01R	C01S	H01S	C01T	C01U	H01U
C01V	H01V	C01W	H01W	C01X	H01X	C01Y	H01Y
F01Z	C020	C021	F022	C023	C024	H024	C025
C026	H026	C027	C028	H028	C029	H029	C02A
C02B	H02B	C02C	C02D	C02E	H02E	C02F	C02G
C02H	H02H	C02I	H02I	C02J	H02J	F02K	C02L
H02L	C02M	H02M	C02N	C02O	H02O	C02P	C02Q
H02Q	C02R	H02R	F02S	C02T	H02T	C02U	F02V
C02W	H02W	C02X	H02X	C02Y	C02Z	C030	H030
C031	C032	H032	C033	H033	C034	H034	F035

F036	F037	C038	H038	C039	C03A	H03A	F03B
C03C	C03D	C03E	H03E	F03F	C03G	H03G	C03H
C03I	H03I	C03J	H03J	C03K	H03K	C03L	H03L
C03M	H03M	C03N	H03N	C03O	H03O	C03P	H03P
C03Q	H03Q	C03R	F03S	C03T	H03T	F03U	F03V
C03W	H03W	C03X	C03Y	H03Y	C03Z	H03Z	C040
H040	C042	H042	C043	H043	F044	C045	H045
C046	H046	C047	H047	C048	C049	C04A	H04A
C04B	C04C	C04D	H04D	C04E	C04F	H04F	C04G
H04G	C04H	F04I	C04J	H04J	C04K	H04K	F04L
C04M	H04M	F04N	C04O	C04P	H04P	F04Q	C04R
H04R	F04S	C04T	H04T	C04U			

PLAT794_ALERT_5_G Tentative Bond Valency for Tb01 (III) . 3.37 Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Tb02 (III) . 3.42 Info
 PLAT860_ALERT_3_G Number of Least-Squares Restraints 78 Note
 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 2 0, 1 1 0, 2 0 0, 1 1 1,
 PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 6819 Note
 PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 6 Note
 2 4 2, 7 2 1, 4 0 2, 0 2 2, 3 1 2, 4 1 1,
 PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 4.2 Low
 PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ 7 Units
 PLAT957_ALERT_1_G Calculated (ThMax) and Actual (FCF) Kmax Differ 7 Units
 PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 2.84 Note
 Predicted wR2: Based on SigI**2 5.31 or SHELX Weight 15.12
 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
 7 **ALERT level B** = A potentially serious problem, consider carefully
 37 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 42 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 55 ALERT type 2 Indicator that the structure model may be wrong or deficient
 14 ALERT type 3 Indicator that the structure quality may be low
 10 ALERT type 4 Improvement, methodology, query or suggestion
 4 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.

