

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Ti2-Bphen

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: Ti2-Bphen

Bond precision: C-C = 0.0076 Å Wavelength=1.54178

Cell: a=28.604 (7) b=21.949 (3) c=21.140 (4)
 alpha=90 beta=92.837 (10) gamma=90

Temperature: 173 K

	Calculated	Reported
Volume	13256 (4)	13256 (5)
Space group	C 2/m	C 1 2/m 1
Hall group	-C 2y	-C 2y
Moiety formula	C136 H136 N4 O8 Ti2 [+ solvent]	2 (C136 H136 N4 O8 Ti2)
Sum formula	C136 H136 N4 O8 Ti2 [+ solvent]	C272 H272 N8 O16 Ti4
Mr	2050.23	4100.56
Dx, g cm ⁻³	1.027	1.027
Z	4	2
Mu (mm ⁻¹)	1.425	1.425
F000	4352.0	4352.0
F000'	4365.13	
h, k, lmax	34, 26, 25	34, 26, 25
Nref	12213	12080
Tmin, Tmax	0.831, 0.867	0.615, 0.753
Tmin'	0.831	

Correction method= # Reported T Limits: Tmin=0.615 Tmax=0.753
AbsCorr = MULTI-SCAN

Data completeness= 0.989 Theta (max)= 67.160

R(reflections)= 0.1097(8670)

wR2(reflections)=
0.3554(12080)

S = 1.411

Npar= 871

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

PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25) 0.36 Report



Alert level C

PLAT082_ALERT_2_C High R1 Value 0.11 Report

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.3 Ratio

PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.00757 Ang.

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.598 132 Report

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1 9 0, 2 0 0, 4 26 0, 22 20 0, 34 0 0, 34 2 0,
-34 0 1, -34 2 1, -22 20 1, -5 1 1, -4 0 1, -4 26 1,
-1 1 1, 2 0 1, 4 26 1, 6 4 1, 22 20 1, 34 0 1,
-34 0 2, -34 2 2, -22 20 2, -6 2 2, 0 0 2, 5 5 2,
7 5 2, 8 2 2, -34 2 3, -11 7 3, -9 13 3, -5 3 3,
-2 26 3, 0 0 3, 0 26 3, 2 0 3, 9 25 3, 23 19 3,
29 13 3, -23 19 4, -18 22 4, -9 3 4, -9 25 4, 0 0 4,
2 0 4, 2 6 4, 3 5 4, -15 23 5, -12 24 5, 6 0 5,
7 25 5, -25 17 6, -19 21 6, -6 4 6, 30 10 6, -33 3 7,
-10 24 7, -4 0 7, 3 25 7, 29 11 7, -17 21 8, 8 24 8,
27 13 8, -32 4 9, -22 18 9, -17 21 9, -6 0 9, 3 1 9,
29 9 9, -32 0 10, -27 13 10, -25 15 10, -24 16 10, -18 20 10,
-4 0 10, -2 0 10, 0 0 10, 1 1 10, 2 0 10, 2 24 10,
-19 19 11, 23 15 11, 24 14 11, 18 18 12, -30 0 13, -30 2 13,
22 14 13, 23 13 13, -29 3 14, -13 19 15, -3 21 15, 1 21 15,
-27 3 16, 25 3 16, 2 0 17, 11 17 17, -25 1 18, -6 18 18,
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PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 2 Check

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.11Ang From C42 -1.70 eA-3

PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.93Ang From C39 . 0.65 eA-3

PLAT977_ALERT_2_C Check Negative Difference Density on H43C . -0.44 eA-3



Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 25 Note

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 69 Report

PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check

Calc: C136 H136 N4 O8 Ti2

Rep.: 2(C136 H136 N4 O8 Ti2)

PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 2 Check

PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.20 Report

PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 18 Report

PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 8 Report

PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0020 Report

PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0020 Report

PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0020 Report

PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0020 Report

PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0020 Report

PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0020	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0020	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0040	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of C5	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C22	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C40	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C47	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C49	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H5A	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H5B	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H5C	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H22A	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H22B	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H22C	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H39A	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H39B	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H39C	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H40A	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H40B	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H40C	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H47A	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H47B	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H47C	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H49A	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H49B	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H49C	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C28	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C41	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C43	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C48	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H28A	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H28B	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H28C	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H31A	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H31B	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H31C	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H41A	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H41B	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H41C	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H42A	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H42B	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H42C	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H43A	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H43B	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H43C	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H48A	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H48B	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H48C	Constrained at	0.5 Check
PLAT301_ALERT_3_G	Main Residue Disorder (Resd 1)	31%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	21%	Note
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist C012 -C012_f .	1.43	Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C3 - C4 .	1.54	Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C21 - C39 .	1.54	Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C31 - C01U .	1.55	Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C32 - C42 .	1.58	Ang.
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H2 ..H5A .	1.99	Ang.
	x,y,z =	1_555	Check

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PLAT412_ALERT_2_G Short Intra XH3 .. XHn      H10      ..H46A      .      1.88 Ang.
x,y,z =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn      H11      ..H15C      .      2.10 Ang.
x,y,z =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn      H11      ..H45B      .      2.08 Ang.
x,y,z =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn      H19      ..H49C      .      1.92 Ang.
x,y,z =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn      H24      ..H41B      .      1.92 Ang.
x,y,z =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn      H24      ..H43B      .      1.72 Ang.
x,y,z =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn      H25      ..H48A      .      2.03 Ang.
x,-y,z =      6_555 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure .....      ! Info
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .....      61 Note
      Ti01      Ti02      O003      O004      O005      O006      O007      O008
      C00A      C00B      C00C      C00D      C00G      C00H      C00I      H00I
      C00K      C00Q      C00U      C00X      C00Y      C00Z      C010      H01A
      H01B      C011      C012      C013      H01C      H01D      C014      C01B
      C01T      H01T      C020      H020      C01Q      H01Q      C01S      H01S
      C01M      H01M      C01D      H01F      C01E      H01E      C01F      C01G
      C01I      H01I      C01J      C01N      H01G      H01H      H01J      C01P
      H01K      H01L      H01N      C01U      C01V
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      22.30 Deg.
      C22      -C21      -C49      6_565      1_555      6_565 .....      #      160 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      22.70 Deg.
      C28      -C01U      -C48      6_555      1_555      6_555 .....      #      254 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      19.70 Deg.
      C41      -C32      -C43      6_555      1_555      6_555 .....      #      326 Check
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group #      21 Check
PLAT822_ALERT_4_G CIF-embedded .res Contains Negative PART Numbers      4 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .....      668 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed      ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .      Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still      42% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).      1 Note
      0      0      1,
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....      1 Note
      -1      1      1,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File      16 Note
      -4      0      1,      7      5      2,      2      6      4,      -5      3      3,      5      5      2,      -11      7      3,
      -4      0      7,      6      4      1,      -6      4      6,      -5      1      1,      8      2      2,      3      5      4,
      1      9      0,      -9      13      3,      -9      3      4,      -6      2      2,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value .....      6.50 Note
      Predicted wR2: Based on SigI**2      5.47 or SHELX Weight      26.16
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.      1 Info

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
 1 **ALERT level B** = A potentially serious problem, consider carefully
 8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 91 **ALERT level G** = General information/check it is not something unexpected
- 3 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
17 ALERT type 3 Indicator that the structure quality may be low
56 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.

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