

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) BM1155s\_100

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: BM1155s\_100

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Bond precision:      C-C = 0.0162 Å      Wavelength=0.71070

Cell:                      a=12.5669(4)                      b=15.5598(5)                      c=22.2169(4)  
                              alpha=92.465(2)                      beta=96.440(2)                      gamma=102.188(2)  
Temperature:              100 K

	Calculated	Reported
Volume	4209.6(2)	4209.6(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C <sub>48</sub> H <sub>90</sub> Hf <sub>6</sub> O <sub>33</sub> , 3(C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> )	?
Sum formula	C <sub>60</sub> H <sub>114</sub> Hf <sub>6</sub> O <sub>39</sub>	C <sub>60</sub> H <sub>114</sub> Hf <sub>6</sub> O <sub>39</sub>
Mr	2530.46	2530.45
Dx, g cm <sup>-3</sup>	1.996	1.996
Z	2	2
Mu (mm <sup>-1</sup> )	7.451	7.451
F000	2436.0	2436.0
F000'	2430.71	
h, k, lmax		15, 19, 27
Nref		17520
Tmin, Tmax	0.272, 0.475	0.340, 1.000
Tmin'	0.217	

Correction method= # Reported T Limits: Tmin=0.340 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness=                      Theta(max)= 26.569

R(reflections)= 0.0501( 12636)	wR2(reflections)= 0.1302( 17520)
S = 1.033	Npar= 964

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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.

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### Alert level A

PLAT973_ALERT_2_A	Check Calcd Positive Resid. Density on	Hf6	2.71 eA-3
PLAT973_ALERT_2_A	Check Calcd Positive Resid. Density on	Hf3	2.34 eA-3
PLAT973_ALERT_2_A	Check Calcd Positive Resid. Density on	Hf2	2.31 eA-3

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### Alert level B

PLAT910_ALERT_3_B	Missing # of FCF Reflection(s) Below Theta(Min).	24	Note
	1 0 0, -1 1 0, 0 1 0, 1 1 0, 0 2 0,	0 -2 1,	
	-1 -1 1, 0 -1 1, 1 -1 1, -1 0 1, 0 0 1,	1 0 1,	
	-1 1 1, 0 1 1, 1 1 1, -1 -1 2, 0 -1 2,	1 -1 2,	
	-1 0 2, 0 0 2, 1 0 2, -1 1 2, 0 1 2,	0 0 3,	
PLAT971_ALERT_2_B	Check Calcd Resid. Dens. 1.10Ang From Hf6	3.36	eA-3
PLAT971_ALERT_2_B	Check Calcd Resid. Dens. 1.15Ang From O27	3.34	eA-3
PLAT971_ALERT_2_B	Check Calcd Resid. Dens. 0.86Ang From Hf1	3.26	eA-3
PLAT971_ALERT_2_B	Check Calcd Resid. Dens. 2.46Ang From C1	3.04	eA-3
PLAT971_ALERT_2_B	Check Calcd Resid. Dens. 1.76Ang From O4	3.03	eA-3
PLAT971_ALERT_2_B	Check Calcd Resid. Dens. 0.88Ang From Hf6	2.79	eA-3
PLAT971_ALERT_2_B	Check Calcd Resid. Dens. 0.91Ang From Hf2	2.77	eA-3
PLAT971_ALERT_2_B	Check Calcd Resid. Dens. 0.94Ang From Hf2	2.77	eA-3
PLAT971_ALERT_2_B	Check Calcd Resid. Dens. 2.47Ang From C5	2.69	eA-3
PLAT971_ALERT_2_B	Check Calcd Resid. Dens. 0.91Ang From Hf4	2.67	eA-3
PLAT971_ALERT_2_B	Check Calcd Resid. Dens. 0.89Ang From Hf5	2.67	eA-3
PLAT971_ALERT_2_B	Check Calcd Resid. Dens. 0.86Ang From Hf3	2.54	eA-3
PLAT971_ALERT_2_B	Check Calcd Resid. Dens. 0.95Ang From Hf5	2.53	eA-3
PLAT971_ALERT_2_B	Check Calcd Resid. Dens. 2.24Ang From C16	2.52	eA-3
PLAT972_ALERT_2_B	Check Calcd Resid. Dens. 0.87Ang From Hf5	-3.48	eA-3
PLAT972_ALERT_2_B	Check Calcd Resid. Dens. 0.78Ang From Hf4	-3.38	eA-3
PLAT972_ALERT_2_B	Check Calcd Resid. Dens. 0.84Ang From Hf6	-3.13	eA-3
PLAT972_ALERT_2_B	Check Calcd Resid. Dens. 0.92Ang From Hf1	-2.86	eA-3
PLAT972_ALERT_2_B	Check Calcd Resid. Dens. 1.02Ang From O7	-2.75	eA-3
PLAT972_ALERT_2_B	Check Calcd Resid. Dens. 0.78Ang From Hf2	-2.72	eA-3
PLAT972_ALERT_2_B	Check Calcd Resid. Dens. 0.79Ang From Hf2	-2.52	eA-3

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### Alert level C

PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range	6.0	Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range	9.6	Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference C2 --C4	0.17	Ang.
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C2	Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor ....	2.2	Note
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor ....	2.2	Note
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor ....	3.1	Note
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.01622	Ang.
PLAT601_ALERT_2_C	Unit Cell Contains Solvent Accessible VOIDS of .	34	Ang**3
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	3.481	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	22	Report
	-5 -4 10, 3-13 13, 3-12 13, 3-11 13, 3-13 14, 3-12 14,		
	-5-11 14, 3-13 15, 3-14 16, -10 4 19, -11 4 20, -10 4 21,		
	-10 5 21, -5 4 23, -6 5 23, -7 6 23, -5 3 24, -7 4 24,		

-6 4 24, -7 5 24, -5 4 25, -3 5 25,	
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....	5 Note
-1 1 0, 0 -1 1, -1 0 1, 0 1 1, 0 0 2,	
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 2.45Ang From O2	2.50 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.88Ang From Hf6	2.48 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.06Ang From Hf4	2.38 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.84Ang From Hf2	2.34 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.03Ang From Hf5	2.33 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.89Ang From Hf2	2.29 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.88Ang From Hf4	2.29 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.93Ang From Hf3	2.26 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.96Ang From Hf3	-2.49 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.93Ang From Hf4	-2.49 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.15Ang From C25	-2.44 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.74Ang From Hf3	-2.38 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.89Ang From O19	-2.36 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.70Ang From O37	-2.36 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.14Ang From O2	-2.28 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.59Ang From Hf3	-2.26 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.86Ang From Hf5	-2.18 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.90Ang From Hf1	-2.16 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.93Ang From Hf6	-2.10 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.20Ang From O7	-2.08 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.47Ang From C23	-2.07 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.22Ang From O3	-2.02 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.68Ang From O20	-1.98 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.72Ang From Hf5	-1.97 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.23Ang From Hf4	-1.81 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.25Ang From Hf3	-1.75 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H3C .	-0.31 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H4B .	-0.75 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H11C .	-0.36 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H16C .	-0.44 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H32 .	-0.60 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H38D .	-0.39 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H51A .	-0.44 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H57A .	-0.40 eA-3

## ● Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite	14 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...	8 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms .....	4 Report
H28 H31 H32 H33	
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large	43.91 Why ?
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)	0.002 Degree
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records	7 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records	2 Report
PLAT300_ALERT_4_G Atom Site Occupancy of H32 Constrained at	0.9 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H33 Constrained at	0.1 Check
PLAT303_ALERT_2_G Full Occupancy Atom H2 with # Connections	2.00 Check
PLAT309_ALERT_2_G Single Bonded Oxygen (C-O > 1.3 Ang) .....	033 Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .	1.11 Ratio
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #	2 Note
C4 H8 O2	
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #	4 Note
C4 H8 O2	

PLAT794_ALERT_5_G	Tentative Bond Valency for Hf1	(IV)	.	4.03	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Hf2	(IV)	.	4.07	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Hf3	(IV)	.	4.04	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Hf5	(IV)	.	4.05	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Hf6	(IV)	.	4.00	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....			58	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .				Please Do !
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600			23	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....			2.2	Low
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged				Please Check
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..			53.1	Degree
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.			0	Info

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3 **ALERT level A** = Most likely a serious problem - resolve or explain  
22 **ALERT level B** = A potentially serious problem, consider carefully  
46 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
26 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
71 ALERT type 2 Indicator that the structure model may be wrong or deficient  
8 ALERT type 3 Indicator that the structure quality may be low  
9 ALERT type 4 Improvement, methodology, query or suggestion  
7 ALERT type 5 Informative message, check

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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.

PLATON version of 14/11/2023; check.def file version of 14/09/2023

Datablock BM1155s\_100 - ellipsoid plot

