

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: 1a

Bond precision:	C-C = 0.0115 A	Wavelength=0.71073	
Cell:	a=17.91800	b=21.64100	c=90
	alpha=118.6900	beta=90	gamma=
Temperature:	195 K		
	Calculated	Reported	
Volume	4621.723	4622	
Space group	P 21/c	P2(1)/c	
Hall group	-P 2ybc	?	
Moiety formula	C42 H69 Lu N2 O S Si2	?	
Sum formula	C42 H69 Lu N2 O S Si2	C42 H69 Lu N2 O S Si2	
Mr	881.21	881.21	
Dx, g cm-3	1.266	1.266	
Z	4	4	
Mu (mm-1)	2.263	2.263	
F000	1832.0	1832.0	
F000'	1831.71		
h, k, lmax	16, 22, 26	16, 22, 26	
Nref	9131	9092	
Tmin, Tmax	0.783, 0.873	0.789, 0.876	
Tmin'	0.780		

Correction method= NONE

Data completeness= 0.996 Theta(max)= 26.050

R(reflections)= 0.0541(6974) wR2(reflections)= 0.1290(9092)

S = 1.050 Npar= Npar = 438

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

PLAT094_ALERT_2_B Ratio of Maximum / Minimum Residual Density

4.61 Why ?

🟢 Alert level C

ABSTY03_ALERT_1_C The _exptl_absorpt_correction_type has been given as none.

However values have been given for Tmin and Tmax. Remove these if an absorption correction has not been applied.

From the CIF: _exptl_absorpt_correction_T_min 0.789

From the CIF: _exptl_absorpt_correction_T_max 0.876

PLAT057_ALERT_3_C	Correction for Absorption Required	RT(exp) ...	1.11
PLAT141_ALERT_4_C	su on a - Axis Small or Missing		0.00000 Ang.
PLAT142_ALERT_4_C	su on b - Axis Small or Missing		0.00000 Ang.
PLAT143_ALERT_4_C	su on c - Axis Small or Missing		0.00000 Ang.
PLAT145_ALERT_4_C	su on beta	Small or Missing	0.0000 Degree
PLAT151_ALERT_1_C	No su (esd) Given on Volume		Please Do !
PLAT220_ALERT_2_C	Large Non-Solvent C	Ueq(max)/Ueq(min) Range	4.5 Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	01 -- C39 ..	6.4 su
PLAT241_ALERT_2_C	High	Ueq as Compared to Neighbors for	 C39 Check
PLAT241_ALERT_2_C	High	Ueq as Compared to Neighbors for	 C42 Check
PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for	 Si1 Check
PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for	 Si2 Check
PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for	 01 Check
PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for	 C24 Check
PLAT342_ALERT_3_C	Low Bond Precision on	C-C Bonds	 0.0115 Ang.
PLAT360_ALERT_2_C	Short C(sp3)-C(sp3) Bond	C41 - C42 ...	1.37 Ang.
PLAT601_ALERT_2_C	Structure Contains Solvent Accessible VOIDS of	.	34 Ang3

🟡 Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	1 Why ?
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in the CIF	Please Do !
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	? Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large.	7.24 Why ?
PLAT128_ALERT_4_G	Alternate Setting for Input Space-Group	P21/c P21/n Note
PLAT343_ALERT_2_G	Check sp3	Angle Range in Main Residue for .. C1
PLAT343_ALERT_2_G	Check sp3	Angle Range in Main Residue for .. C5
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	 6 Note

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

1 ALERT level B = A potentially serious problem, consider carefully

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

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

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

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

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

5 ALERT type 4 Improvement, methodology, query or suggestion

1 ALERT type 5 Informative message, check

Datablock: 1b

Bond precision: C-C = 0.0171 A

Wavelength=0.71073

Cell: a=36.82000 b=11.15600 c=90
 alpha=90 beta=120 gamma=
 Temperature: 193 K

	Calculated	Reported
Volume	13098.051	13098
Space group	R 3 m	R3m
Hall group	R 3 -2"	?
Moiety formula	C46 H77 N2 O2 S Si2 Y	?
Sum formula	C46 H77 N2 O2 S Si2 Y	C46 H77 N2 O2 S Si2 Y
Mr	867.26	867.25
Dx, g cm-3	0.990	0.990
Z	9	9
Mu (mm-1)	1.109	1.109
F000	4194.0	4194.0
F000'	4172.50	
h, k, lmax	43, 43, 13	43, 43, 13
Nref	5419[2720]	4754
Tmin, Tmax	0.856, 0.905	0.860, 0.907
Tmin'	0.856	

Correction method= NONE

Data completeness= 1.75/0.88 Theta(max)= 25.040

R(reflections)= 0.0697(3134) wR2(reflections)= 0.2100(4754)

S = 1.062 Npar= Npar = 273

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

PLAT601_ALERT_2_A Structure Contains Solvent Accessible VOIDS of . 912 Ang3

Alert level B

SYMMS02_ALERT_1_B The unit-cell lengths a and c should be equal for a rhombohedral cell

Cell 36.8200 36.8200 11.1560

Angles 90.0000 90.0000 120.0000

SYMMS02_ALERT_1_B Cell angles alpha and gamma should be equal for a rhombohedral cell

Cell 36.8200 36.8200 11.1560

Angles 90.0000 90.0000 120.0000

SYMMS02_ALERT_1_B All angles should not be 90 for a rhombohedral cell

Cell 36.8200 36.8200 11.1560

Angles 90.0000 90.0000 120.0000

PLAT049_ALERT_1_B Calculated Density less than 1.0 gcm-3 0.9895

PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds 0.0171 Ang.

● Alert level C

ABSTY03_ALERT_1_C The _exptl_absorpt_correction_type has been given as none.
However values have been given for Tmin and Tmax. Remove
these if an absorption correction has not been applied.
From the CIF: _exptl_absorpt_correction_T_min 0.860
From the CIF: _exptl_absorpt_correction_T_max 0.907

PLAT090_ALERT_3_C	Poor Data / Parameter Ratio (Zmax > 18)	9.96	Note
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.53	Why ?
PLAT141_ALERT_4_C	su on a - Axis Small or Missing	0.00000	Ang.
PLAT143_ALERT_4_C	su on c - Axis Small or Missing	0.00000	Ang.
PLAT151_ALERT_1_C	No su (esd) Given on Volume		Please Do !
PLAT213_ALERT_2_C	Atom C28 has ADP max/min Ratio	3.4	prolat
PLAT220_ALERT_2_C	Large Non-Solvent C Ueq(max)/Ueq(min) Range	5.2	Ratio
PLAT222_ALERT_3_C	Large Non-Solvent H Uiso(max)/Uiso(min) ..	6.5	Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for Si1 -- C2 ..	5.5	su
PLAT230_ALERT_2_C	Hirshfeld Test Diff for Si2 -- C5 ..	5.5	su
PLAT234_ALERT_4_C	Large Hirshfeld Difference Si1 -- C3 ..	0.20	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C9 -- C10 ..	0.23	Ang.
PLAT241_ALERT_2_C	High Ueq as Compared to Neighbors for	C9	Check
PLAT242_ALERT_2_C	Low Ueq as Compared to Neighbors for	Si2	Check
PLAT242_ALERT_2_C	Low Ueq as Compared to Neighbors for	01	Check
PLAT242_ALERT_2_C	Low Ueq as Compared to Neighbors for	C1	Check
PLAT242_ALERT_2_C	Low Ueq as Compared to Neighbors for	C19	Check
PLAT722_ALERT_1_C	Angle Calc 114.00, Rep 112.60 Dev...	1.40	Degree
	C27B -C28B -H28C 1.555 1.555 1.555 #	199	
PLAT722_ALERT_1_C	Angle Calc 111.00, Rep 112.60 Dev...	1.60	Degree
	01 -C28B -H28D 1.555 1.555 1.555 #	200	

● Alert level G

PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in the CIF	Please Do !
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	? Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large.	0.11 Why ?
PLAT104_ALERT_1_G	The Reported Crystal System is Inconsistent with	R3m Check
PLAT301_ALERT_3_G	Main Residue Disorder Percentage =	11 Note
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #	152 Check
	C28 -O1 -C28B 1.555 1.555 1.555	2.00 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #	159 Check
	C26 -C25 -C26B 1.555 1.555 1.555	20.00 Deg.

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7 **ALERT level G** = General information/check it is not something unexpected
- 10 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
12 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
6 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check
-

Datablock: le

Bond precision: C-C = 0.0073 A

Wavelength=0.71073

Cell: a=12.007(2) b=20.514(4) c=19.104(4)
 alpha=90 beta=90.26(3) gamma=90
 Temperature: 195 K

	Calculated	Reported
Volume	4705.5(16)	4705.5(16)
Space group	P 21/n	P2(1)/n
Hall group	-P 2yn	?
Moiety formula	C40 H75 Lu N2 O S Si3	?
Sum formula	C40 H75 Lu N2 O S Si3	C40 H75 Lu N2 O S Si3
Mr	891.33	891.32
Dx, g cm-3	1.258	1.258
Z	4	4
Mu (mm-1)	2.248	2.248
F000	1864.0	1864.0
F000'	1864.00	
h, k, lmax	14, 25, 23	14, 25, 23
Nref	9303	9274
Tmin, Tmax	0.754, 0.854	0.759, 0.859
Tmin'	0.739	

Correction method= NONE

Data completeness= 0.997 Theta(max)= 26.050

R(reflections)= 0.0422(7476) wR2(reflections)= 0.0875(9274)

S = 1.040 Npar= Npar = 450

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

ABSTY03_ALERT_1_C The _exptl_absorpt_correction_type has been given as none.

However values have been given for Tmin and Tmax. Remove these if an absorption correction has not been applied.

From the CIF: _exptl_absorpt_correction_T_min 0.759

From the CIF: _exptl_absorpt_correction_T_max 0.859

PLAT057_ALERT_3_C	Correction for Absorption Required	RT(exp) ...	1.13
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density		2.28 Why ?
PLAT220_ALERT_2_C	Large Non-Solvent C	Ueq(max)/Ueq(min) Range	3.5 Ratio
PLAT241_ALERT_2_C	High	Ueq as Compared to Neighbors for	C37 Check
PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for	Si1 Check
PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for	Si3 Check
PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for	C19 Check
PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for	C22 Check



Alert level G

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF Please Do !

PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
 PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Lu1 -- C5 .. 6.3 su
 PLAT343_ALERT_2_G Check sp3 Angle Range in Main Residue for .. C5

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

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

Datablock: 2

Bond precision: C-C = 0.0055 A Wavelength=0.71073

Cell: a=11.8843(4) b=12.5062(4) c=19.4482(7)
 alpha=78.546(1) beta=81.900(1) gamma=62.267(1)
 Temperature: 197 K

	Calculated	Reported
Volume	2503.61(15)	2503.61(15)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C48 H74 Lu N2 O P Si2	?
Sum formula	C48 H74 Lu N2 O P Si2	C48 H74 Lu N2 O P Si2
Mr	957.21	957.21
Dx, g cm-3	1.270	1.270
Z	2	2
Mu (mm-1)	2.085	2.085
F000	996.0	996.0
F000'	995.83	
h, k, lmax	14, 15, 24	14, 15, 24
Nref	9904	9653
Tmin, Tmax	0.754, 0.846	0.759, 0.851
Tmin'	0.739	

Correction method= NONE

Data completeness= 0.975 Theta(max)= 26.050

R(reflections)= 0.0274(9026) wR2(reflections)= 0.0662(9653)

S = 1.047 Npar= Npar = 510

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

ABSTY03_ALERT_1_C The _exptl_absorpt_correction_type has been given as none.
However values have been given for Tmin and Tmax. Remove
these if an absorption correction has not been applied.
From the CIF: _exptl_absorpt_correction_T_min 0.759
From the CIF: _exptl_absorpt_correction_T_max 0.851
PLAT029_ALERT_3_C _diffn_measured_fraction_theta_full Low 0.975 Note
PLAT057_ALERT_3_C Correction for Absorption Required RT(exp) ... 1.12
PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) Range 3.5 Ratio
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for Si2 Check
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of . 42 Ang3

● Alert level G

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF Please Do !
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal 0.00100 Degree
PLAT343_ALERT_2_G Check sp3 Angle Range in Main Residue for .. C5

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

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

Datablock: 3

Bond precision: C-C = 0.0128 A Wavelength=0.71073

Cell: a=14.63100 b=22.30500 c=90
 alpha=90 beta=90 gamma=

Temperature: 193 K

	Calculated	Reported
Volume	4671.947	4672
Space group	P 21 21 21	P2(1)2(1)2(
Hall group	P 2ac 2ab	?
Moiety formula	C44 H66 Lu N2 O P Si2	?
Sum formula	C44 H66 Lu N2 O P Si2	C44 H66 Lu N2 O P Si2
Mr	901.11	901.11
Dx, g cm-3	1.281	1.281
Z	4	4
Mu (mm-1)	2.230	2.230
F000	1864.0	1864.0
F000'	1863.63	
h, k, lmax	17, 17, 26	17, 17, 26
Nref	8276[4599]	8262
Tmin, Tmax	0.829, 0.875	0.791, 0.878
Tmin'	0.782	

Correction method= NONE

Data completeness= 1.80/1.00 Theta(max)= 25.050

R(reflections)= 0.0494(6490) wR2(reflections)= 0.1060(8262)

S = 1.015 Npar= Npar = 439

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

PLAT230_ALERT_2_B	Hirshfeld Test Diff for	Si1	--	C2	..	12.1	su
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	Si1	--	C3	..	18.0	su
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	Si1	--	C4	..	13.1	su
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	Si2	--	C6	..	12.1	su
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	Si2	--	C7	..	9.0	su
PLAT232_ALERT_2_B	Hirshfeld Test Diff (M-X)	Lu1	--	C5	..	15.9	su
PLAT242_ALERT_2_B	Low	Ueq as Compared to Neighbors for				Si1	Check

🟡 Alert level C

ABSTY03_ALERT_1_C The _exptl_absorpt_correction_type has been given as none.

However values have been given for Tmin and Tmax. Remove these if an absorption correction has not been applied.

From the CIF: _exptl_absorpt_correction_T_min 0.791

From the CIF: _exptl_absorpt_correction_T_max 0.878

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density		2.47	Why ?
PLAT141_ALERT_4_C	su on a - Axis Small or Missing		0.00000	Ang.
PLAT142_ALERT_4_C	su on b - Axis Small or Missing		0.00000	Ang.
PLAT143_ALERT_4_C	su on c - Axis Small or Missing		0.00000	Ang.
PLAT151_ALERT_1_C	No su (esd) Given on Volume			Please Do !
PLAT213_ALERT_2_C	Atom C5	has ADP max/min Ratio		3.1 prolat
PLAT220_ALERT_2_C	Large Non-Solvent C	Ueq(max)/Ueq(min) Range		5.5 Ratio

PLAT222_ALERT_3_C	Large Non-Solvent	H	Uiso(max)/Uiso(min)	..	5.0	Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	Si2	--	C5	..	5.6 su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Lu1	--	C1	..	5.6 su
PLAT234_ALERT_4_C	Large Hirshfeld Difference	Si2	--	C8	..	0.21 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	O1	--	C12	..	0.20 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C34	--	C35	..	0.20 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C43	--	C44	..	0.17 Ang.
PLAT241_ALERT_2_C	High	Ueq as Compared to Neighbors for				C5 Check
PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for				Lu1 Check
PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for				Si2 Check
PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for				O1 Check
PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for				C19 Check
PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for				C43 Check
PLAT342_ALERT_3_C	Low Bond Precision on	C-C Bonds				0.0128 Ang.

● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	8	Note
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in the CIF		Please Do !
PLAT301_ALERT_3_G	Main Residue Disorder	8	Note
PLAT343_ALERT_2_G	Check sp3 Angle Range in Main Residue for ..		C5
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	5	Note
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #	22	Check
	C9B -O1 -C9 1.555 1.555 1.555	27.00	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #	27	Check
	C12 -O1 -C12B 1.555 1.555 1.555	31.00	Deg.
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	6	Note

-
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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*, 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.









