

R(reflections)= 0.0367( 3874)	wR2(reflections)= 0.0957( 4699)
S = 1.097	Npar= 214

---

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

PLAT242_ALERT_2_C Low	'MainMol' Ueq as Compared to Neighbors of	Si1 Check
PLAT911_ALERT_3_C Missing	FCF Refl Between Thmin & STh/L= 0.600	2 Report

---



#### Alert level G

PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical	? Check
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....	2 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity .....	3.8 Low
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..	56.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.	4 Info

---

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
2 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  
0 ALERT type 4 Improvement, methodology, query or suggestion  
1 ALERT type 5 Informative message, check

---

## Datablock: compound2

---

Bond precision: C-C = 0.0020 A

Wavelength=0.71073

Cell:	a=8.6757(4)	b=8.8740(4)	c=9.0989(4)
	alpha=64.211(3)	beta=75.463(3)	gamma=79.194(3)
Temperature:	180 K		

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
1 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  
0 ALERT type 4 Improvement, methodology, query or suggestion  
2 ALERT type 5 Informative message, check

---

## Datablock: compound3

---

Bond precision: C-C = 0.0028 A Wavelength=0.71073

Cell: a=10.0640(3) b=11.1921(3) c=18.6757(5)  
alpha=72.898(2) beta=89.000(2) gamma=63.346(2)

Temperature: 180 K

|                | Calculated                | Reported                  |
|----------------|---------------------------|---------------------------|
| Volume         | 1780.70(10)               | 1780.70(9)                |
| Space group    | P -1                      | P -1                      |
| Hall group     | -P 1                      | -P 1                      |
| Moiety formula | 2(C13 H15 N9 Si), C4 H8 O | 2(C13 H15 N9 Si), C4 H8 O |
| Sum formula    | C30 H38 N18 O Si2         | C30 H38 N18 O Si2         |
| Mr             | 722.96                    | 722.96                    |
| Dx, g cm-3     | 1.348                     | 1.348                     |
| Z              | 2                         | 2                         |
| Mu (mm-1)      | 0.154                     | 0.154                     |
| F000           | 760.0                     | 760.0                     |
| F000'          | 760.51                    |                           |
| h,k,lmax       | 13,14,24                  | 13,14,24                  |
| Nref           | 8602                      | 8598                      |
| Tmin,Tmax      | 0.937,0.970               | 0.943,0.986               |
| Tmin'          | 0.933                     |                           |

Correction method= # Reported T Limits: Tmin=0.943 Tmax=0.986  
AbsCorr = INTEGRATION

Data completeness= 1.000 Theta(max)= 27.999

R(reflections)= 0.0385( 7536) wR2(reflections)=  
0.1019( 8598)

S = 1.063 Npar= 527

---

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

|                   |                                             |        |   |                   |       |       |        |
|-------------------|---------------------------------------------|--------|---|-------------------|-------|-------|--------|
| PLAT220_ALERT_2_C | NonSolvent                                  | Resd 1 | C | Ueq(max)/Ueq(min) | Range | 3.1   | Ratio  |
| PLAT260_ALERT_2_C | Large Average Ueq of Residue Including      |        |   | O1A               |       | 0.165 | Check  |
| PLAT906_ALERT_3_C | Large K Value in the Analysis of Variance   | .....  |   |                   |       | 2.154 | Check  |
| PLAT911_ALERT_3_C | Missing FCF Refl Between Thmin & STh/L=     |        |   | 0.600             |       | 4     | Report |
| PLAT913_ALERT_3_C | Missing # of Very Strong Reflections in FCF | ....   |   |                   |       | 4     | Note   |

---

### ● Alert level G

|                   |                                                  |               |  |  |  |        |        |
|-------------------|--------------------------------------------------|---------------|--|--|--|--------|--------|
| PLAT002_ALERT_2_G | Number of Distance or Angle Restraints on AtSite |               |  |  |  | 23     | Note   |
| PLAT154_ALERT_1_G | The s.u.'s on the Cell Angles are Equal ..(Note) |               |  |  |  | 0.002  | Degree |
| PLAT171_ALERT_4_G | The CIF-Embedded .res File Contains EADP Records |               |  |  |  | 7      | Report |
| PLAT174_ALERT_4_G | The CIF-Embedded .res File Contains FLAT Records |               |  |  |  | 1      | Report |
| PLAT176_ALERT_4_G | The CIF-Embedded .res File Contains SADI Records |               |  |  |  | 11     | Report |
| PLAT191_ALERT_3_G | A Non-default SADI Restraint Value has been used |               |  |  |  | 0.0010 | Report |
| PLAT191_ALERT_3_G | A Non-default SADI Restraint Value has been used |               |  |  |  | 0.0010 | Report |
| PLAT191_ALERT_3_G | A Non-default SADI Restraint Value has been used |               |  |  |  | 0.0010 | Report |
| PLAT191_ALERT_3_G | A Non-default SADI Restraint Value has been used |               |  |  |  | 0.0010 | Report |
| PLAT191_ALERT_3_G | A Non-default SADI Restraint Value has been used |               |  |  |  | 0.0010 | Report |
| PLAT191_ALERT_3_G | A Non-default SADI Restraint Value has been used |               |  |  |  | 0.0010 | Report |
| PLAT191_ALERT_3_G | A Non-default SADI Restraint Value has been used |               |  |  |  | 0.0010 | Report |
| PLAT191_ALERT_3_G | A Non-default SADI Restraint Value has been used |               |  |  |  | 0.0100 | Report |
| PLAT191_ALERT_3_G | A Non-default SADI Restraint Value has been used |               |  |  |  | 0.0010 | Report |
| PLAT191_ALERT_3_G | A Non-default SADI Restraint Value has been used |               |  |  |  | 0.0010 | Report |
| PLAT191_ALERT_3_G | A Non-default SADI Restraint Value has been used |               |  |  |  | 0.0010 | Report |
| PLAT301_ALERT_3_G | Main Residue Disorder .....                      | (Resd 1 )     |  |  |  | 26%    | Note   |
| PLAT302_ALERT_4_G | Anion/Solvent/Minor-Residue Disorder (Resd 3 )   |               |  |  |  | 100%   | Note   |
| PLAT302_ALERT_4_G | Anion/Solvent/Minor-Residue Disorder (Resd 4 )   |               |  |  |  | 100%   | Note   |
| PLAT304_ALERT_4_G | Non-Integer Number of Atoms in .....             | (Resd 3 )     |  |  |  | 10.02  | Check  |
| PLAT304_ALERT_4_G | Non-Integer Number of Atoms in .....             | (Resd 4 )     |  |  |  | 2.98   | Check  |
| PLAT398_ALERT_2_G | Deviating C-O-C Angle From 120 for O1            |               |  |  |  | 105.8  | Degree |
| PLAT398_ALERT_2_G | Deviating C-O-C Angle From 120 for O1A           |               |  |  |  | 100.8  | Degree |
| PLAT411_ALERT_2_G | Short Inter H...H Contact H11 ..H21A             |               |  |  |  | 2.14   | Ang.   |
|                   |                                                  | 2-x,1-y,1-z = |  |  |  | 2_766  | Check  |
| PLAT432_ALERT_2_G | Short Inter X...Y Contact C11 ..C21A             |               |  |  |  | 3.10   | Ang.   |
|                   |                                                  | 2-x,1-y,1-z = |  |  |  | 2_766  | Check  |
| PLAT860_ALERT_3_G | Number of Least-Squares Restraints .....         |               |  |  |  | 24     | Note   |
| PLAT910_ALERT_3_G | Missing # of FCF Reflection(s) Below Theta(Min). |               |  |  |  | 1      | Note   |
| PLAT941_ALERT_3_G | Average HKL Measurement Multiplicity .....       |               |  |  |  | 3.8    | Low    |
| PLAT967_ALERT_5_G | Note: Two-Theta Cutoff Value in Embedded .res .. |               |  |  |  | 56.0   | Degree |
| PLAT978_ALERT_2_G | Number C-C Bonds with Positive Residual Density. |               |  |  |  | 4      | Info   |
| PLAT992_ALERT_5_G | Repd & Actual _reflns_number_gt Values Differ by |               |  |  |  | 2      | Check  |

---

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

0 **ALERT level B** = A potentially serious problem, consider carefully

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

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

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

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

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

7 ALERT type 4 Improvement, methodology, query or suggestion

2 ALERT type 5 Informative message, check

---

## Datablock: compound4

---

Bond precision: C-C = 0.0029 Å Wavelength=0.71073

Cell: a=15.9611(2) b=21.1674(3) c=22.6832(3)  
alpha=90 beta=97.740(1) gamma=90

Temperature: 180 K

|                        | Calculated              | Reported                |
|------------------------|-------------------------|-------------------------|
| Volume                 | 7593.81(18)             | 7593.81(18)             |
| Space group            | P 21/c                  | P 21/c                  |
| Hall group             | -P 2ybc                 | -P 2ybc                 |
| Moiety formula         | C16 H16 N12 Si, C7 H8 O | C16 H16 N12 Si, C7 H8 O |
| Sum formula            | C23 H24 N12 O Si        | C23 H24 N12 O Si        |
| Mr                     | 512.63                  | 512.63                  |
| Dx, g cm <sup>-3</sup> | 1.345                   | 1.345                   |
| Z                      | 12                      | 12                      |
| Mu (mm <sup>-1</sup> ) | 0.135                   | 0.135                   |
| F000                   | 3216.0                  | 3216.0                  |
| F000'                  | 3217.85                 |                         |
| h, k, lmax             | 20, 27, 28              | 20, 27, 28              |
| Nref                   | 16569                   | 16561                   |
| Tmin, Tmax             | 0.953, 0.973            | 0.952, 0.986            |
| Tmin'                  | 0.941                   |                         |

Correction method= # Reported T Limits: Tmin=0.952 Tmax=0.986  
AbsCorr = INTEGRATION

Data completeness= 1.000 Theta(max)= 26.999

R(reflections)= 0.0407( 14195) wR2(reflections)=  
0.1010( 16561)

S = 1.108 Npar= 1150

---

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

|                                                                    |             |
|--------------------------------------------------------------------|-------------|
| PLAT906_ALERT_3_C Large K Value in the Analysis of Variance .....  | 2.497 Check |
| PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600    | 9 Report    |
| PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF .... | 6 Note      |

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## ● Alert level G

|                   |                                                  |      |        |
|-------------------|--------------------------------------------------|------|--------|
| PLAT168_ALERT_4_G | The CIF-Embedded .res File Contains EXYZ Records | 2    | Report |
| PLAT171_ALERT_4_G | The CIF-Embedded .res File Contains EADP Records | 3    | Report |
| PLAT300_ALERT_4_G | Atom Site Occupancy of O3                        | 0.5  | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C63                       | 0.5  | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C64                       | 0.5  | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C65                       | 0.5  | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C66                       | 0.5  | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C67                       | 0.5  | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C68                       | 0.5  | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C69                       | 0.5  | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H63A                      | 0.5  | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H63B                      | 0.5  | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H63C                      | 0.5  | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H65                       | 0.5  | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H66                       | 0.5  | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H67                       | 0.5  | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H68                       | 0.5  | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H69                       | 0.5  | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of O4                        | 0.5  | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C70                       | 0.5  | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C71                       | 0.5  | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C72                       | 0.5  | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C73                       | 0.5  | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C74                       | 0.5  | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C75                       | 0.5  | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C76                       | 0.5  | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H70A                      | 0.5  | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H70B                      | 0.5  | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H70C                      | 0.5  | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H72                       | 0.5  | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H73                       | 0.5  | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H74                       | 0.5  | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H75                       | 0.5  | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H76                       | 0.5  | Check  |
| PLAT302_ALERT_4_G | Anion/Solvent/Minor-Residue Disorder (Resd 5 )   | 100% | Note   |
| PLAT302_ALERT_4_G | Anion/Solvent/Minor-Residue Disorder (Resd 6 )   | 100% | Note   |
| PLAT302_ALERT_4_G | Anion/Solvent/Minor-Residue Disorder (Resd 7 )   | 100% | Note   |
| PLAT302_ALERT_4_G | Anion/Solvent/Minor-Residue Disorder (Resd 8 )   | 100% | Note   |
| PLAT304_ALERT_4_G | Non-Integer Number of Atoms in ..... (Resd 5 )   | 9.49 | Check  |
| PLAT304_ALERT_4_G | Non-Integer Number of Atoms in ..... (Resd 8 )   | 6.51 | Check  |
| PLAT789_ALERT_4_G | Atoms with Negative _atom_site_disorder_group #  | 32   | Check  |
| PLAT822_ALERT_4_G | CIF-embedded .res Contains Negative PART Numbers | 1    | Check  |
| PLAT933_ALERT_2_G | Number of HKL-OMIT Records in Embedded .res File | 3    | Note   |
| PLAT967_ALERT_5_G | Note: Two-Theta Cutoff Value in Embedded .res .. | 54.0 | Degree |
| PLAT978_ALERT_2_G | Number C-C Bonds with Positive Residual Density. | 6    | Info   |

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

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

2 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  
42 ALERT type 4 Improvement, methodology, query or suggestion  
1 ALERT type 5 Informative message, check

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## checkCIF publication errors

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### Alert level A

PUBL004\_ALERT\_1\_A The contact author's name and address are missing,  
\_publ\_contact\_author\_name and \_publ\_contact\_author\_address.  
PUBL005\_ALERT\_1\_A \_publ\_contact\_author\_email, \_publ\_contact\_author\_fax and  
\_publ\_contact\_author\_phone are all missing.  
At least one of these should be present.  
PUBL006\_ALERT\_1\_A \_publ\_requested\_journal is missing  
e.g. 'Acta Crystallographica Section C'  
PUBL008\_ALERT\_1\_A \_publ\_section\_title is missing. Title of paper.  
PUBL009\_ALERT\_1\_A \_publ\_author\_name is missing. List of author(s) name(s).  
PUBL010\_ALERT\_1\_A \_publ\_author\_address is missing. Author(s) address(es).  
PUBL012\_ALERT\_1\_A \_publ\_section\_abstract is missing.  
Abstract of paper in English.

---

### Alert level G

PUBL017\_ALERT\_1\_G The \_publ\_section\_references section is missing or  
empty.

---

7 **ALERT level A** = Data missing that is essential or data in wrong format  
1 **ALERT level G** = General alerts. Data that may be required is missing

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## Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

## Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PUBL004_GLOBAL
;
PROBLEM: The contact author's name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
```

RESPONSE: ...

;

\_vrf\_PUBL012\_GLOBAL

;

PROBLEM: \_publ\_section\_abstract is missing.

RESPONSE: ...

;

# end Validation Reply Form

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

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### PLATON version of 10/05/2023; check.def file version of 10/05/2023

Datablock compound1 - ellipsoid plot







