checkCIF/PLATON report

Structure factors have been supplied for datablock(s) sk-46_01, sk-54-1_01, sk-54-2s_05

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: sk-54-1_01

```
Bond precision:   C-C = 0.0058 A          Wavelength=0.71073

Cell:               a=9.3792(3)      b=9.3792(3)      c=15.6549(6)
                    alpha=90         beta=90          gamma=120
Temperature:        180 K

                  Calculated                  Reported
Volume            1192.65(9)                  1192.65(9)
Space group       P 3 c 1                     P 3 c 1
Hall group        P 3 -2"c                    P 3 -2"c
Moiety formula    C21 H24 N O6 P3             C21 H24 N O6 P3
Sum formula       C21 H24 N O6 P3             C21 H24 N O6 P3
Mr                479.32                      479.32
Dx,g cm-3         1.335                       1.335
Z                 2                           2
Mu (mm-1)         0.285                       0.285
F000              500.0                       500.0
F000'             500.83
h,k,lmax          12,12,20                    12,12,20
Nref              1934[ 970]                  1932
Tmin,Tmax         0.957,0.964
Tmin'             0.950

Correction method= Not given

Data completeness= 1.99/1.00        Theta(max)= 27.955

R(reflections)= 0.0317( 1651)                wR2(reflections)=
                                             0.0742( 1932)
S = 1.036                  Npar= 99
```

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

```
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00583 Ang.
PLAT354_ALERT_3_C Short  O-H (X0.82,N0.98A)  O1       - H1O      .       0.63 Ang.
PLAT601_ALERT_2_C Unit Cell Contains Solvent Accessible VOIDS of .         39 Ang**3
```

Alert level G

```
PLAT792_ALERT_1_G Model has Chirality at P1          (Polar  SpGr)          S Verify
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..       56.0 Degree
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      4.555 Note
             Predicted wR2: Based on SigI**2  1.63 or SHELX Weight  7.16
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
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
4 **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
2 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: sk-46_01

Bond precision: C-C = 0.0037 A Wavelength=0.71073

Cell:	a=18.2554(5)	b=18.2554(5)	c=11.4177(3)
	alpha=90	beta=90	gamma=120
Temperature:	180 K		

	Calculated	Reported
Volume	3295.3(2)	3295.3(2)
Space group	R 3 c	R 3 c :H
Hall group	R 3 -2"c	R 3 -2"c
Moiety formula	C21 H24 N O6 P3	C21 H24 N O6 P3
Sum formula	C21 H24 N O6 P3	C21 H24 N O6 P3
Mr	479.32	479.32
Dx,g cm-3	1.449	1.449
Z	6	6
Mu (mm-1)	0.310	0.310
F000	1500.0	1500.0
F000'	1502.50	
h,k,lmax	24,24,15	24,24,15
Nref	1778[895]	1748
Tmin,Tmax	0.911,0.955	
Tmin'	0.848	

Correction method= Not given

Data completeness= 1.95/0.98 Theta(max)= 27.993

R(reflections)= 0.0224(1669) wR2(reflections)= 0.0610(1748)

S = 1.055 Npar= 98

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 G

PLAT792_ALERT_1_G Model has Chirality at P1 (Polar SpGr) S Verify
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 56.0 Degree
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 4.795 Note
Predicted wR2: Based on SigI**2 1.27 or SHELX Weight 5.79
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 4 Info

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0 **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

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1 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 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: sk-54-2s_05

Bond precision: C-C = 0.0044 A Wavelength=0.71073

Cell: a=12.1818(3) b=12.1818(3) c=92.431(3)
alpha=90 beta=90 gamma=120
Temperature: 160 K

	Calculated	Reported
Volume	11878.8(7)	11878.8(7)
Space group	R -3	R -3 :H
Hall group	-R 3	-R 3
Moiety formula	C30 H48 N O6 P3 Si3	C30 H48 N O6 P3 Si3
Sum formula	C30 H48 N O6 P3 Si3	C30 H48 N O6 P3 Si3
Mr	695.87	695.87
Dx,g cm-3	1.167	1.167
Z	12	12
Mu (mm-1)	0.278	0.278
F000	4440.0	4440.0
F000'	4448.12	
h,k,lmax	14,14,109	14,14,109
Nref	4693	4686
Tmin,Tmax	0.935,0.959	
Tmin'	0.920	

Correction method= Not given

Data completeness= 0.999 Theta(max)= 24.995

R(reflections)= 0.0376(3464) wR2(reflections)= 0.1066(4686)

S = 1.106 Npar= 265

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	3.5 Ratio
PLAT222_ALERT_3_C	NonSolvent	Resd 1	H	Uiso(max)/Uiso(min)	Range	4.4 Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for		Si1	--C9	.	6.5 s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for		Si1	--C10	.	5.7 s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for		C4	--C5	.	5.7 s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for		Si2	--C19	.	6.4 s.u.

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PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         C4 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Si1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Si2 Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00442 Ang.
PLAT601_ALERT_2_C Unit Cell Contains Solvent Accessible VOIDS of .         74 Ang**3
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.010 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).          6 Note
               -1  1  1,   0  1  2,   0  0  3,  -1  1  4,   0  0  6,   0  0  9,
```

Alert level G

```
PLAT395_ALERT_2_G Deviating  X-O-Y   Angle From 120 for O1       .      134.1 Degree
PLAT395_ALERT_2_G Deviating  X-O-Y   Angle From 120 for O3       .      136.1 Degree
PLAT793_ALERT_4_G Model has Chirality at P1          (Centro SpGr)          R Verify
PLAT793_ALERT_4_G Model has Chirality at P2          (Centro SpGr)          R Verify
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        51% Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          1 Note
               -2  4  3,
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..       50.0 Degree
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      4.310 Note
             Predicted wR2: Based on SigI**2  2.47 or SHELX Weight  9.64
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
```

```
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  13 ALERT type 2 Indicator that the structure model may be wrong or deficient
   5 ALERT type 3 Indicator that the structure quality may be low
   2 ALERT type 4 Improvement, methodology, query or suggestion
   2 ALERT type 5 Informative message, check
```

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checkCIF publication errors

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
```

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.

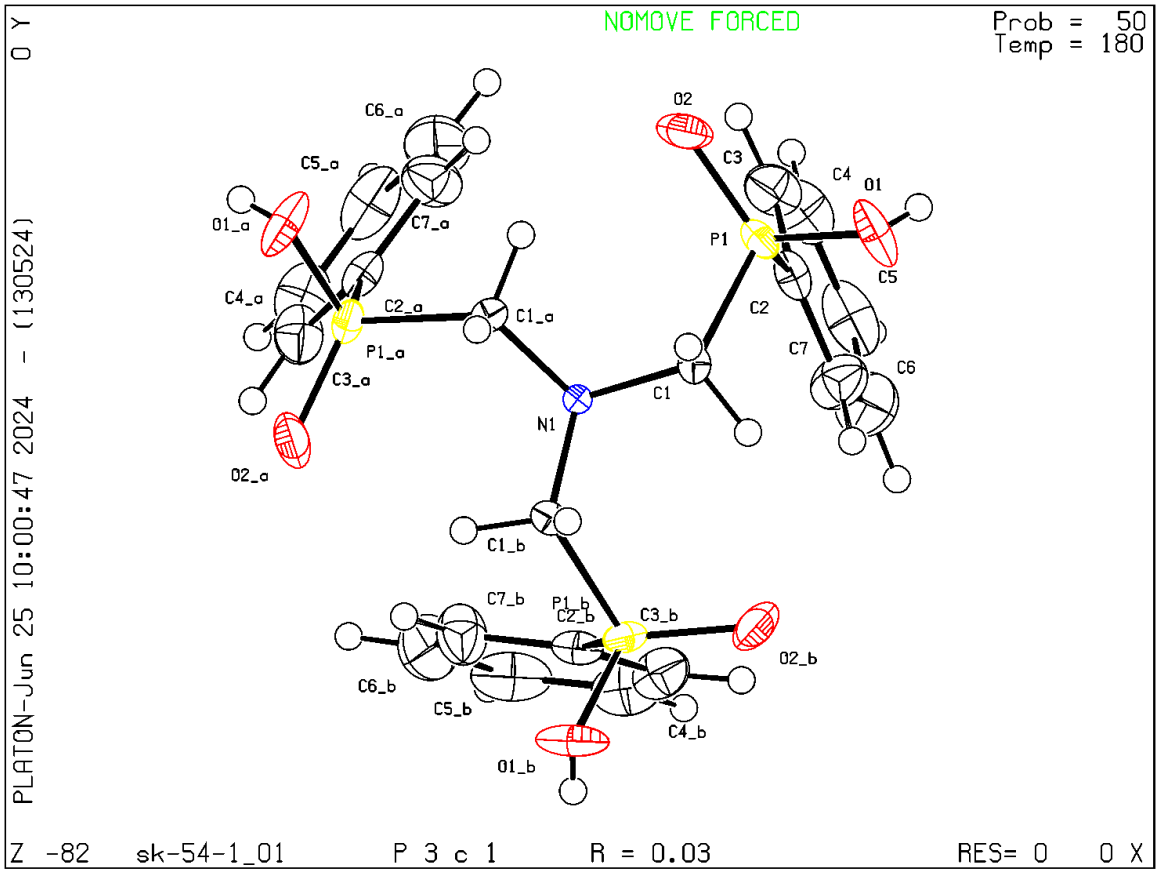
```
# start Validation Reply Form
_vrf_PUBL004_GLOBAL
;
PROBLEM: The contact author's name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
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
```

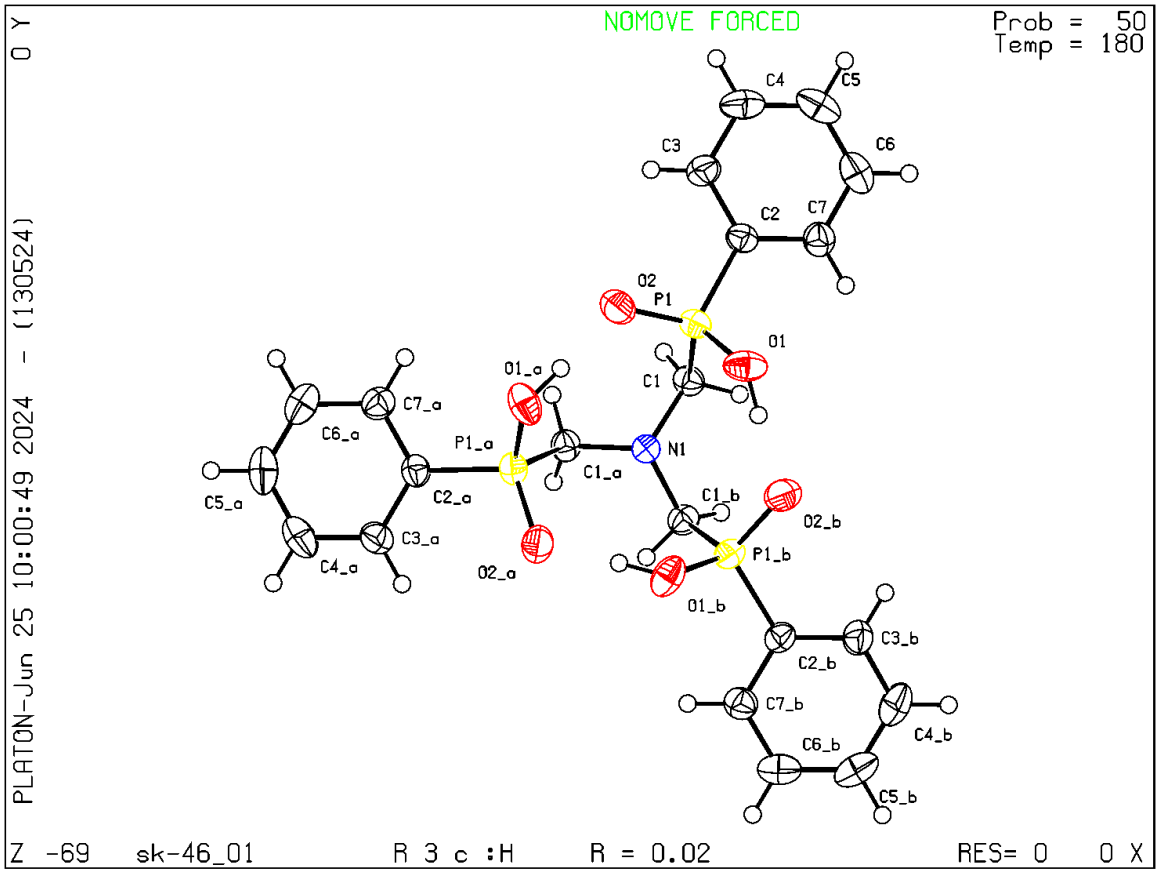
If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you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

PLATON version of 13/05/2024; check.def file version of 04/05/2024

Datablock sk-54-1_01 - ellipsoid plot



Datablock sk-46_01 - ellipsoid plot



Datablock sk-54-2s_05 - ellipsoid plot

