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: MeSipyO3

```
Bond precision:  C-C = 0.0021 A          Wavelength=0.71073

Cell:          a=9.1581(7)       b=9.3250(7)       c=11.4078(9)
               alpha=92.440(6)   beta=109.582(6)   gamma=116.898(6)
Temperature:   200 K
```

	Calculated	Reported
Volume	796.41(13)	796.41(12)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C16 H15 N3 O3 Si	C16 H15 N3 O3 Si
Sum formula	C16 H15 N3 O3 Si	C16 H15 N3 O3 Si
Mr	325.40	325.40
Dx,g cm-3	1.357	1.357
Z	2	2
Mu (mm-1)	0.166	0.166
F000	340.0	340.0
F000’	340.30	
h,k,lmax	12,12,15	12,12,15
Nref	3839	3836
Tmin,Tmax	0.946,0.964	0.958,0.989
Tmin’	0.944	

```
Correction method= # Reported T Limits: Tmin=0.958 Tmax=0.989
AbsCorr = INTEGRATION

Data completeness= 0.999          Theta(max)= 28.000

R(reflections)= 0.0343( 3284)     wR2(reflections)= 0.0925( 3836)

S = 1.066                 Npar= 209
```

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

```
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.006 Degree
PLAT395_ALERT_2_G Deviating  X-O-Y    Angle From 120 for O1             128.0 Degree
PLAT395_ALERT_2_G Deviating  X-O-Y    Angle From 120 for O2             129.5 Degree
PLAT395_ALERT_2_G Deviating  X-O-Y    Angle From 120 for O3             124.9 Degree
```

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 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
0 ALERT type 5 Informative message, check

Datablock: SipyO4

Bond precision: C-C = 0.0035 A Wavelength=0.71073

Cell: a=9.5163(7) b=9.5163(7) c=21.824(2)
alpha=90 beta=90 gamma=90
Temperature: 200 K

	Calculated	Reported
Volume	1976.4(3)	1976.4(3)
Space group	I 41/a	I 41/a
Hall group	-I 4ad	-I 4ad
Moiety formula	C20 H16 N4 O4 Si	C20 H16 N4 O4 Si
Sum formula	C20 H16 N4 O4 Si	C20 H16 N4 O4 Si
Mr	404.46	404.46
Dx,g cm-3	1.359	1.359
Z	4	4
Mu (mm-1)	0.153	0.153
F000	840.0	840.0
F000'	840.69	
h,k,lmax	11,11,25	11,11,25
Nref	873	873
Tmin,Tmax	0.964,0.970	0.946,0.978
Tmin'	0.941	

Correction method= # Reported T Limits: Tmin=0.946 Tmax=0.978
AbsCorr = INTEGRATION

Data completeness= 1.000 Theta(max)= 24.997

R(reflections)= 0.0404(684) wR2(reflections)= 0.1062(873)

S = 1.137 Npar= 66

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
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O1 125.2 Degree

---

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

0 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
0 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Datablock: compound_1

Bond precision: C-C = 0.0047 A Wavelength=0.71073

Cell: a=14.8719(5) b=10.5112(5) c=39.3020(13)
alpha=90 beta=95.404(3) gamma=90
Temperature: 180 K

	Calculated	Reported
Volume	6116.4(4)	6116.4(4)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C21 H19 N4 O4 Pd Si, 2(C H Cl3), Cl	C21 H19 N4 O4 Pd Si, 2(C H Cl3), Cl
Sum formula	C23 H21 Cl7 N4 O4 Pd Si	C23 H21 Cl7 N4 O4 Pd Si
Mr	800.08	800.08
Dx,g cm-3	1.738	1.738
Z	8	8
Mu (mm-1)	1.295	1.295
F000	3184.0	3184.0
F000’	3185.84	
h,k,lmax	17,12,46	17,12,46
Nref	5384	5379
Tmin,Tmax	0.685,0.950	0.656,0.973
Tmin’	0.590	

Correction method= # Reported T Limits: Tmin=0.656 Tmax=0.973
AbsCorr = INTEGRATION

Data completeness= 0.999 Theta(max)= 24.998

R(reflections)= 0.0339(4642) wR2(reflections)= 0.0818(5379)

S = 1.147 Npar= 403

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

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	11	Note
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	29.87	Why ?
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	5	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	4	Report
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100%	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
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 5)	100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... Resd 2	2.75	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... Resd 3	4.82	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... Resd 4	2.25	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... Resd 5	0.17	Check
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O1	129.5	Degree
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O2	131.4	Degree
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O3	128.7	Degree
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O4	129.1	Degree
PLAT794_ALERT_5_G	Tentative Bond Valency for Pd1 (II) .	2.33	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	18	Note

---

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 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
10 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

Datablock: compound_2

Bond precision: C-C = 0.0043 A Wavelength=0.71073

Cell: a=8.7497(4) b=9.2334(5) c=23.5781(13)
alpha=88.255(4) beta=89.283(4) gamma=68.654(4)
Temperature: 200 K

	Calculated	Reported
Volume	1773.36(17)	1773.36(17)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C16 H15 Cl Cu N3 O3 Si	C16 H15 Cl Cu N3 O3 Si
Sum formula	C16 H15 Cl Cu N3 O3 Si	C16 H15 Cl Cu N3 O3 Si
Mr	424.40	424.39
Dx,g cm-3	1.590	1.590
Z	4	4
Mu (mm-1)	1.470	1.470
F000	864.0	864.0
F000’	866.44	
h,k,lmax	11,12,31	11,12,31
Nref	8572	8555
Tmin,Tmax	0.710,0.863	0.769,0.909
Tmin’	0.686	

Correction method= # Reported T Limits: Tmin=0.769 Tmax=0.909
AbsCorr = INTEGRATION

Data completeness= 0.998 Theta(max)= 27.999

R(reflections)= 0.0350(7263) wR2(reflections)= 0.0900(8555)

S = 1.073 Npar= 453

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

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.78	Report
PLAT241_ALERT_2_C	High ’MainMol’ Ueq as Compared to Neighbors of	O1	Check
PLAT241_ALERT_2_C	High ’MainMol’ Ueq as Compared to Neighbors of	O2	Check
PLAT242_ALERT_2_C	Low ’MainMol’ Ueq as Compared to Neighbors of	Si1	Check

---

Alert level G

PLAT154_ALERT_1_G	The s.u.’s on the Cell Angles are Equal ..(Note)	0.004	Degree
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Cu1 --Cl1 .	7.0	s.u.
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O1	140.4	Degree
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O2	139.4	Degree
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O3	142.1	Degree
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O4	138.0	Degree
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O5	136.6	Degree
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O6	141.2	Degree
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	10	Note

---

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

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

1 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
0 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Datablock: compound_3

Bond precision: C-C = 0.0027 A Wavelength=0.71073

Cell: a=18.3774(5) b=18.3774(5) c=26.4847(8)
alpha=90 beta=90 gamma=90
Temperature: 200 K

	Calculated	Reported
Volume	8944.7(6)	8944.6(6)
Space group	I 41/a	I 41/a
Hall group	-I 4ad	-I 4ad
Moiety formula	C21 H19 Cl Cu N4 O4 Si	C21 H19 Cl Cu N4 O4 Si
Sum formula	C21 H19 Cl Cu N4 O4 Si	C21 H19 Cl Cu N4 O4 Si
Mr	518.49	518.48
Dx,g cm-3	1.540	1.540
Z	16	16
Mu (mm-1)	1.186	1.186
F000	4240.0	4240.0
F000’	4250.13	
h,k,lmax	24,24,34	24,24,34
Nref	5397	5409
Tmin,Tmax	0.708,0.837	0.854,0.948
Tmin’	0.694	

Correction method= # Reported T Limits: Tmin=0.854 Tmax=0.948
AbsCorr = INTEGRATION

Data completeness= 1.002 Theta(max)= 27.997

R(reflections)= 0.0278(4692) wR2(reflections)= 0.0712(5409)

S = 1.081 Npar= 290

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
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of . 35 Ang**3

Alert level G

```
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       6.87 Why ?
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu1      --Si1       .        8.0 s.u.
PLAT395_ALERT_2_G Deviating  X-O-Y    Angle From 120 for O1            132.6 Degree
PLAT395_ALERT_2_G Deviating  X-O-Y    Angle From 120 for O2            130.0 Degree
PLAT395_ALERT_2_G Deviating  X-O-Y    Angle From 120 for O3            128.6 Degree
PLAT395_ALERT_2_G Deviating  X-O-Y    Angle From 120 for O4            130.3 Degree
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1       (II)      .       2.18 Info
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          2 Note
```

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
1 **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

0 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
0 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: compound_3_CHCl3

Bond precision: C-C = 0.0052 A Wavelength=0.71073

Cell: a=9.2616(4) b=15.6201(7) c=9.2773(5)
alpha=90 beta=93.049(4) gamma=90
Temperature: 200 K

	Calculated	Reported
Volume	1340.22(11)	1340.22(11)
Space group	P 21	P 21
Hall group	P 2yb	P 2yb
Moiety formula	C21 H19 Cl Cu N4 O4 Si, C H Cl3	C21 H19 Cl Cu N4 O4 Si, C H Cl3
Sum formula	C22 H20 Cl4 Cu N4 O4 Si	C22 H20 Cl4 Cu N4 O4 Si
Mr	637.86	637.85
Dx,g cm-3	1.581	1.581
Z	2	2
Mu (mm-1)	1.295	1.295
F000	646.0	646.0
F000’	648.17	
h,k,lmax	12,20,12	12,20,12
Nref	6454[3344]	6449
Tmin,Tmax	0.685,0.879	0.666,0.869
Tmin’	0.629	

Correction method= # Reported T Limits: Tmin=0.666 Tmax=0.869
AbsCorr = INTEGRATION

Data completeness= 1.93/1.00 Theta(max)= 27.997

R(reflections)= 0.0269(6105) wR2(reflections)= 0.0639(6449)

S = 1.060 Npar= 326

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

PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C22 Check

---

Alert level G

PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu1 --N3 . 5.1 s.u.
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O1 130.1 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O2 130.8 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O3 131.0 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O4 130.3 Degree
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1 (II) . 2.17 Info

---

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

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

Datablock: compound_4

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

Cell: a=11.2079(5) b=13.1431(6) c=15.1242(7)
  alpha=78.113(4) beta=87.403(4) gamma=89.899(4)
Temperature: 200 K

	Calculated	Reported
Volume	2177.81(17)	2177.81(17)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C25 H21 Cl N5 O5 Pd Si, 4(C H Cl3), Cl	C25 H21 Cl N5 O5 Pd Si, 4(C H Cl3), Cl
Sum formula	C29 H25 Cl14 N5 O5 Pd Si	C29 H25 Cl14 N5 O5 Pd Si
Mr	1154.33	1154.33
Dx,g cm-3	1.760	1.760
Z	2	2
Mu (mm-1)	1.357	1.357
F000	1144.0	1144.0
F000’	1146.60	
h,k,lmax	14,16,19	14,16,19
Nref	9512	9502
Tmin,Tmax	0.672,0.873	0.694,0.891
Tmin’	0.659	

Correction method= # Reported T Limits: Tmin=0.694 Tmax=0.891
AbsCorr = INTEGRATION

Data completeness= 0.999 Theta(max)= 26.999

R(reflections)= 0.0230(8590) wR2(reflections)= 0.0577(9502)

S = 1.059 Npar= 562

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

PLAT244_ALERT_4_C	Low	’Solvent’ Ueq as Compared to Neighbors of	C28 Check

---

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	8	Note
PLAT154_ALERT_1_G	The s.u.’s on the Cell Angles are Equal ..(Note)	0.004	Degree
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	2	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	4	Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Pd1 --Cl1 .	22.0	s.u.
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	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
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... Resd 2	3.49	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... Resd 3	3.20	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... Resd 6	1.51	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... Resd 7	1.80	Check
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O1	128.0	Degree
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O2	127.2	Degree
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O3	126.6	Degree

```
PLAT395_ALERT_2_G Deviating  X-O-Y    Angle From 120 for O4            127.1 Degree
PLAT395_ALERT_2_G Deviating  X-O-Y    Angle From 120 for O5            131.7 Degree
PLAT794_ALERT_5_G Tentative Bond Valency for Pd1       (II)      .      2.33 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       12 Note
```

---

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

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   7 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
  11 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check

Datablock: compound_5_2CHCl3

Bond precision: C-C = 0.0132 A Wavelength=0.71073

Cell: a=22.458(2) b=11.8102(7) c=17.4818(18)
       alpha=90 beta=111.330(7) gamma=90
Temperature: 200 K

	Calculated	Reported
Volume	4319.2(7)	4319.1(7)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C30 H26 Cl4 N6 O6 Pd2 Si, 2(C H Cl3)	C30 H26 Cl4 N6 O6 Pd2 Si, 2(C H Cl3)
Sum formula	C32 H28 Cl10 N6 O6 Pd2 Si	C32 H28 Cl10 N6 O6 Pd2 Si
Mr	1187.99	1187.99
Dx,g cm-3	1.827	1.827
Z	4	4
Mu (mm-1)	1.529	1.529
F000	2344.0	2344.0
F000’	2342.91	
h,k,lmax	26,14,20	26,14,20
Nref	3800	3789
Tmin,Tmax	0.863,0.970	0.926,0.990
Tmin’	0.832	

Correction method= # Reported T Limits: Tmin=0.926 Tmax=0.990
AbsCorr = INTEGRATION

Data completeness= 0.997 Theta(max)= 24.999

R(reflections)= 0.0474(2903) wR2(reflections)= 0.1166(16169)

S = 1.034 Npar= 289

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

PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01317 Ang.

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 8 Note
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 2 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 3 Report
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3) 100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd 2 3.30 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd 3 1.70 Check
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O1 127.8 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O2 124.5 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O3 136.7 Degree
PLAT794_ALERT_5_G Tentative Bond Valency for Pd1 (II) . 2.13 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 9 Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed .. ! Info
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 17 Note

---

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

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

Datablock: compound_5_6CHCl3

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

Cell: a=12.1698(6) b=12.1951(7) c=13.1643(8)
alpha=107.904(4) beta=103.147(4) gamma=114.671(4)
Temperature: 200 K

	Calculated	Reported
Volume	1539.81(19)	1539.81(19)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C30 H26 Cl4 N6 O6 Pd2 Si, 6(C H Cl3)	C30 H26 Cl4 N6 O6 Pd2 Si, 6(C H Cl3)
Sum formula	C36 H32 Cl22 N6 O6 Pd2 Si	C36 H32 Cl22 N6 O6 Pd2 Si
Mr	1665.47	1665.46
Dx,g cm-3	1.796	1.796
Z	1	1
Mu (mm-1)	1.604	1.604
F000	818.0	818.0
F000’	819.53	
h,k,lmax	15,15,16	15,15,16
Nref	6736	6728
Tmin,Tmax	0.687,0.786	0.712,0.848
Tmin’	0.663	

Correction method= # Reported T Limits: Tmin=0.712 Tmax=0.848
AbsCorr = INTEGRATION

Data completeness= 0.999 Theta(max)= 26.999

R(reflections)= 0.0331(5683) wR2(reflections)= 0.0776(6728)

S = 1.055 Npar= 410

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

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	20	Note
PLAT154_ALERT_1_G	The s.u.’s on the Cell Angles are Equal ..(Note)	0.004	Degree
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	6	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	6	Report
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100%	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
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
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... Resd 2	3.15	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... Resd 3	2.59	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... Resd 4	4.42	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... Resd 5	1.84	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... Resd 6	2.41	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... Resd 7	0.58	Check
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O1	124.0	Degree
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O2	128.2	Degree
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O3	134.2	Degree
PLAT794_ALERT_5_G	Tentative Bond Valency for Pd1 (II) .	2.12	Info

```
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        66 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          1 Note
```

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

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

Datablock: compound_5_8CHCl3

Bond precision: C-C = 0.0042 A Wavelength=0.71073

Cell: a=12.3681(5) b=13.1356(4) c=22.2337(9)
       alpha=90 beta=95.990(3) gamma=90
Temperature: 200 K

	Calculated	Reported
Volume	3592.4(2)	3592.4(2)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C30 H26 Cl4 N6 O6 Pd2 Si, 8(C H Cl3)	C30 H26 Cl4 N6 O6 Pd2 Si, 8(C H Cl3)
Sum formula	C38 H34 Cl28 N6 O6 Pd2 Si	C38 H34 Cl28 N6 O6 Pd2 Si
Mr	1904.44	1904.20
Dx,g cm-3	1.761	1.760
Z	2	2
Mu (mm-1)	1.603	1.603
F000	1868.2	1868.0
F000’	1873.10	
h,k,lmax	15,16,28	15,16,28
Nref	7837	7828
Tmin,Tmax	0.687,0.786	0.541,0.742
Tmin’	0.612	

Correction method= # Reported T Limits: Tmin=0.541 Tmax=0.742
AbsCorr = INTEGRATION

Data completeness= 0.999 Theta(max)= 26.999

R(reflections)= 0.0299(6609) wR2(reflections)= 0.0699(7828)

S = 1.033 Npar= 539

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

PLAT352_ALERT_3_C Short N-H (X0.87,N1.01A) N3 - H3N . 0.72 Ang.

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 28 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 12 Report
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 3 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 9 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 3 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 3 Report
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 100% 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
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
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 9) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 10) 100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd 2 2.78 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd 3 3.76 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd 4 3.10 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd 5 1.46 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd 6 2.27 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd 7 1.28 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd 8 2.22 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd 9 1.90 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd 10 1.24 Check
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O1 126.4 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O2 124.6 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O3 135.8 Degree
PLAT794_ALERT_5_G Tentative Bond Valency for Pd1 (II) . 2.13 Info
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms .... ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 166 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 1 Note

---

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 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
22 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

Datablock: compound_6

Bond precision: C-C = 0.0078 A Wavelength=0.71073

Cell: a=9.1063(8) b=11.0475(6) c=17.1744(17)
alpha=90 beta=104.705(7) gamma=90
Temperature: 200 K

	Calculated	Reported
Volume	1671.2(2)	1671.2(2)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C30 H26 Cl4 Cu2 N6 O6 Si	C30 H26 Cl4 Cu2 N6 O6 Si
Sum formula	C30 H26 Cl4 Cu2 N6 O6 Si	C30 H26 Cl4 Cu2 N6 O6 Si
Mr	863.56	863.54
Dx,g cm-3	1.716	1.716
Z	2	2
Mu (mm-1)	1.682	1.682
F000	872.0	872.0
F000’	874.88	
h,k,lmax	10,13,20	10,13,20
Nref	2942	2933
Tmin,Tmax	0.886,0.951	0.815,0.927
Tmin’	0.777	

Correction method= # Reported T Limits: Tmin=0.815 Tmax=0.927
AbsCorr = INTEGRATION

Data completeness= 0.997 Theta(max)= 24.998

R(reflections)= 0.0441(1727) wR2(reflections)= 0.0907(2933)

S = 0.924 Npar= 226

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

PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds .... 0.00775 Ang.
PLAT352_ALERT_3_C Short N-H (X0.87,N1.01A) N3 - H3N . 0.74 Ang.

Alert level G

PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O1 122.1 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O3 138.6 Degree
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 9 Note

---

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

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   3 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
   0 ALERT type 5 Informative message, check
```

---

checkCIF publication errors

Alert level G

```
PUBL017_ALERT_1_G The _publ_section_references section is missing or
            empty.
```

```
   0 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
```

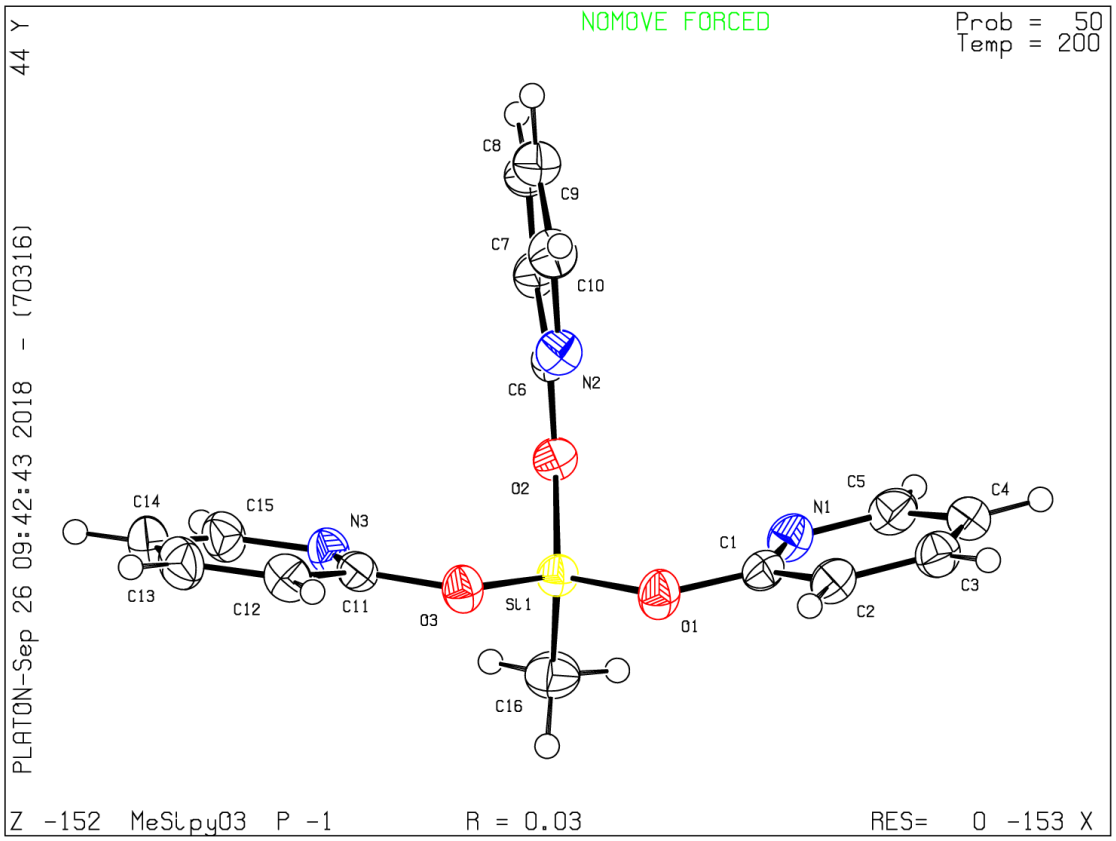
Publication of your CIF

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.

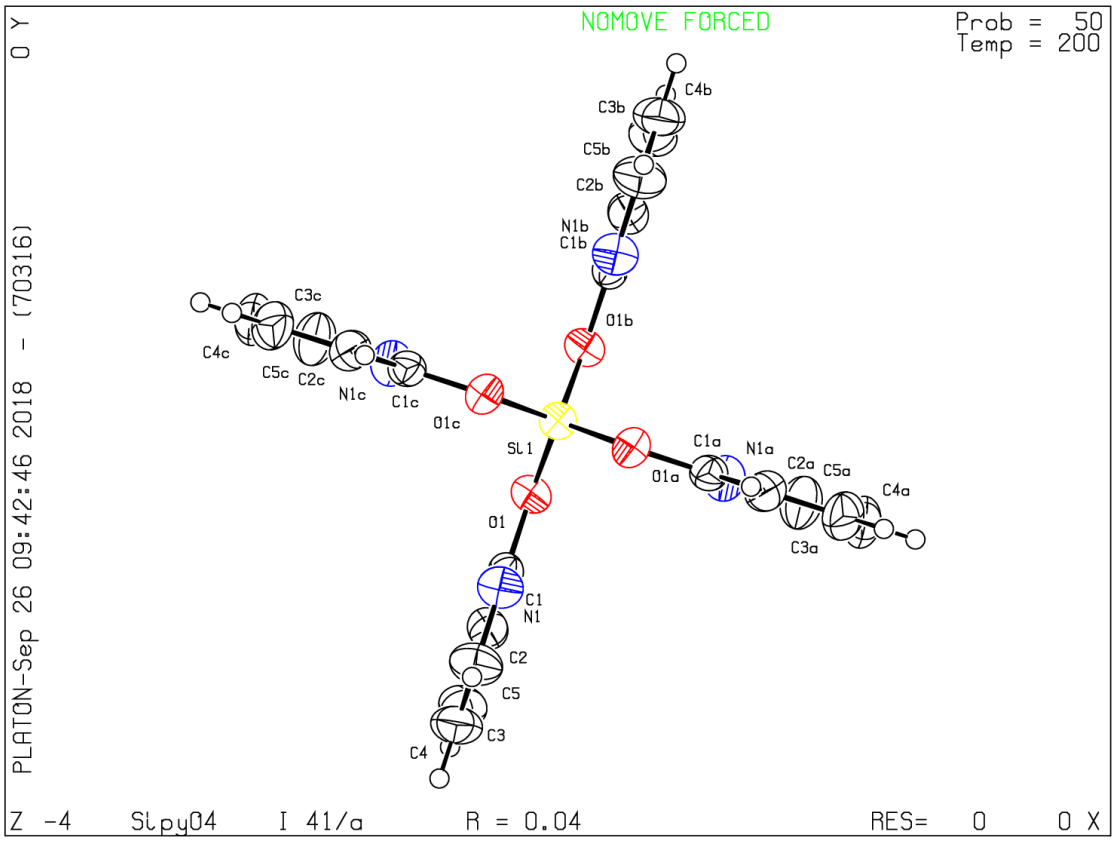
If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you 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 20/08/2018; check.def file version of 20/08/2018

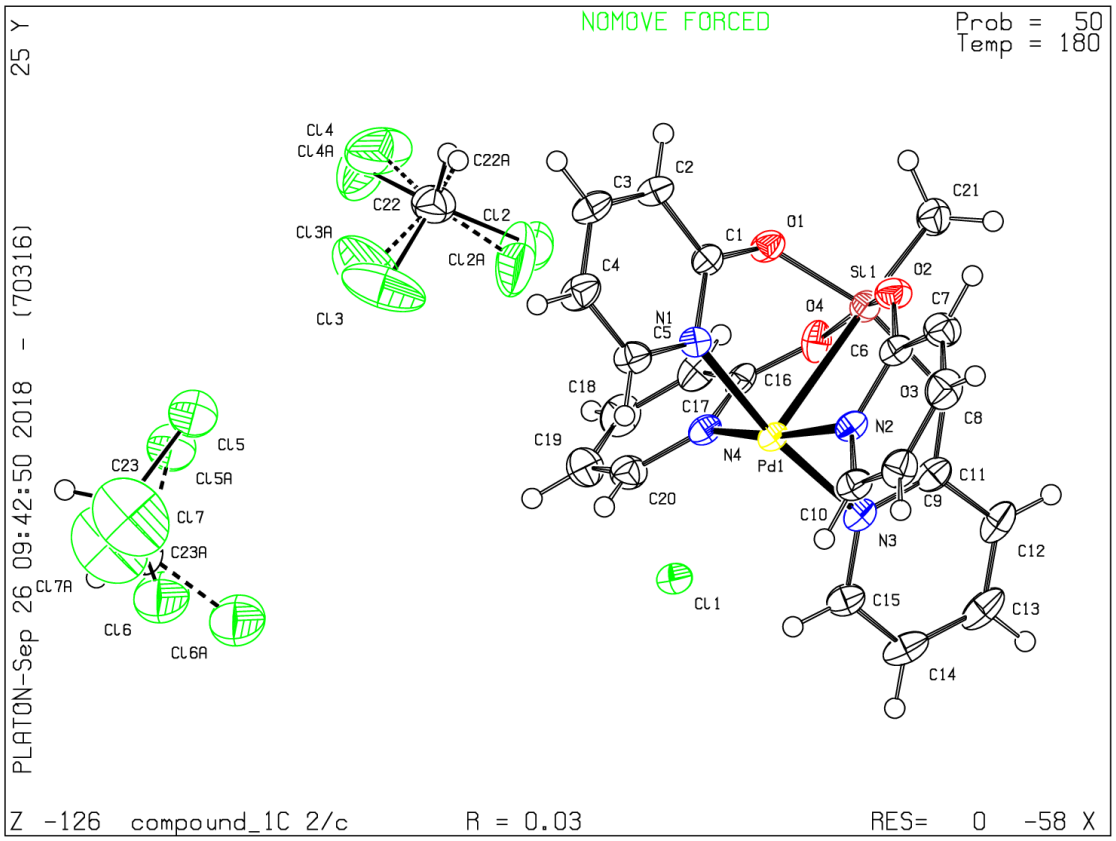
Datablock MeSipyO3 - ellipsoid plot



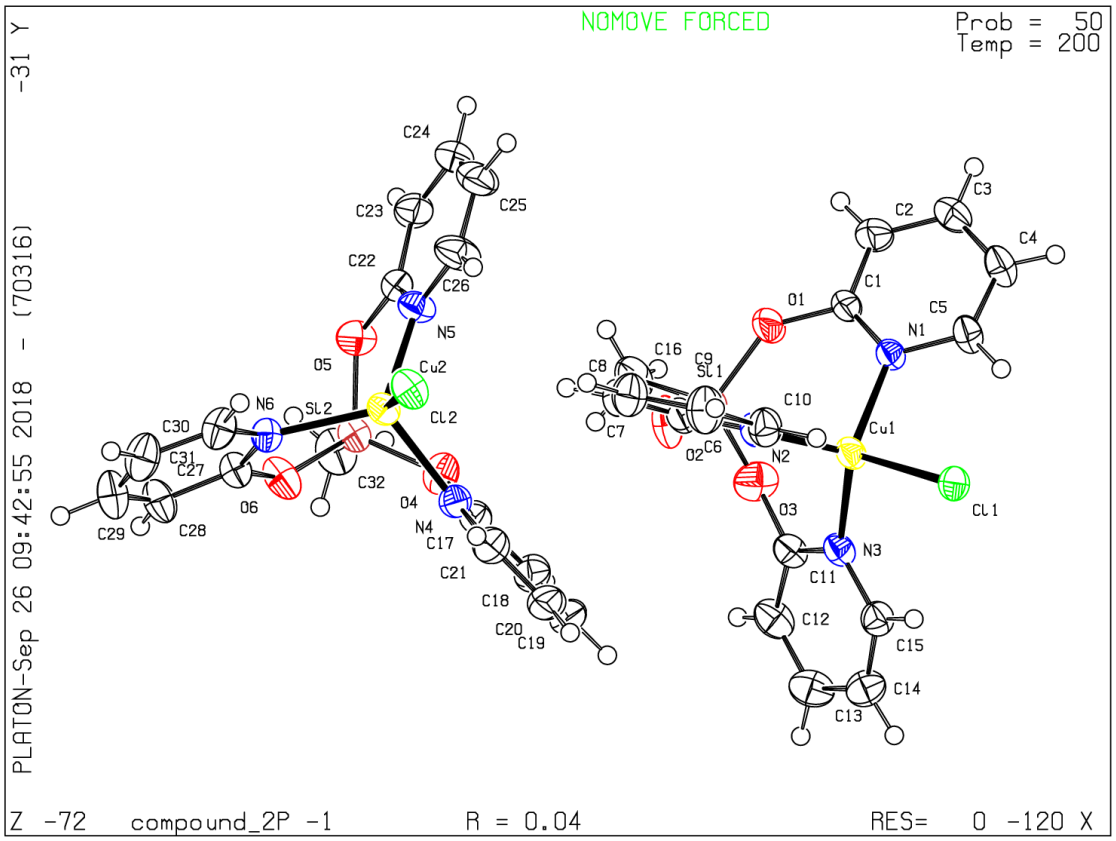
Datablock SipyO4 - ellipsoid plot



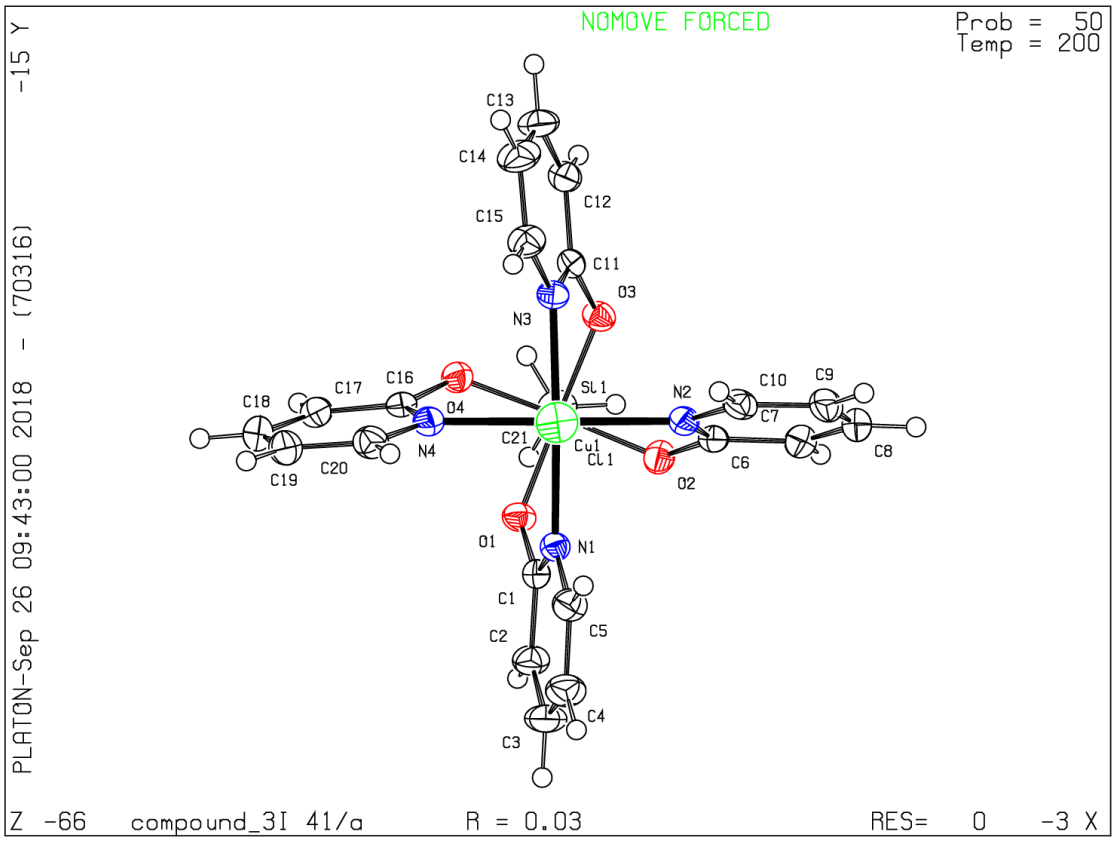
Datablock compound_1 - ellipsoid plot



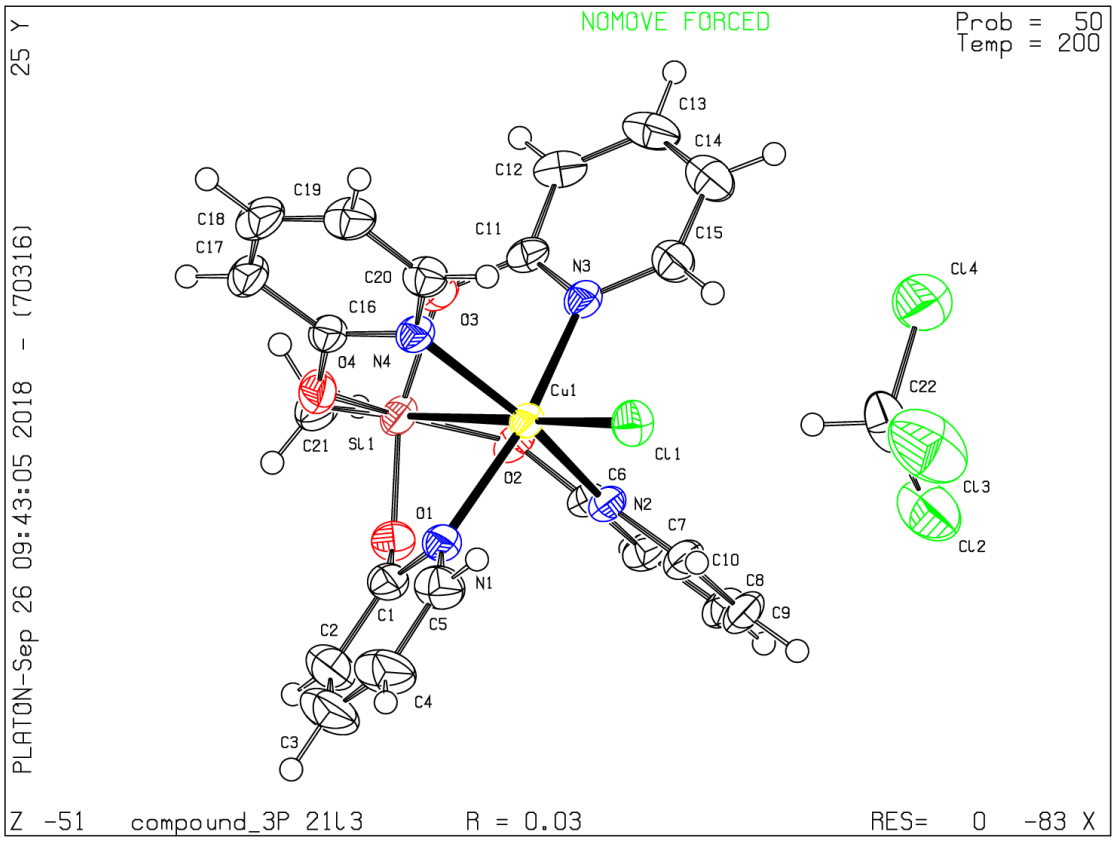
Datablock compound_2 - ellipsoid plot



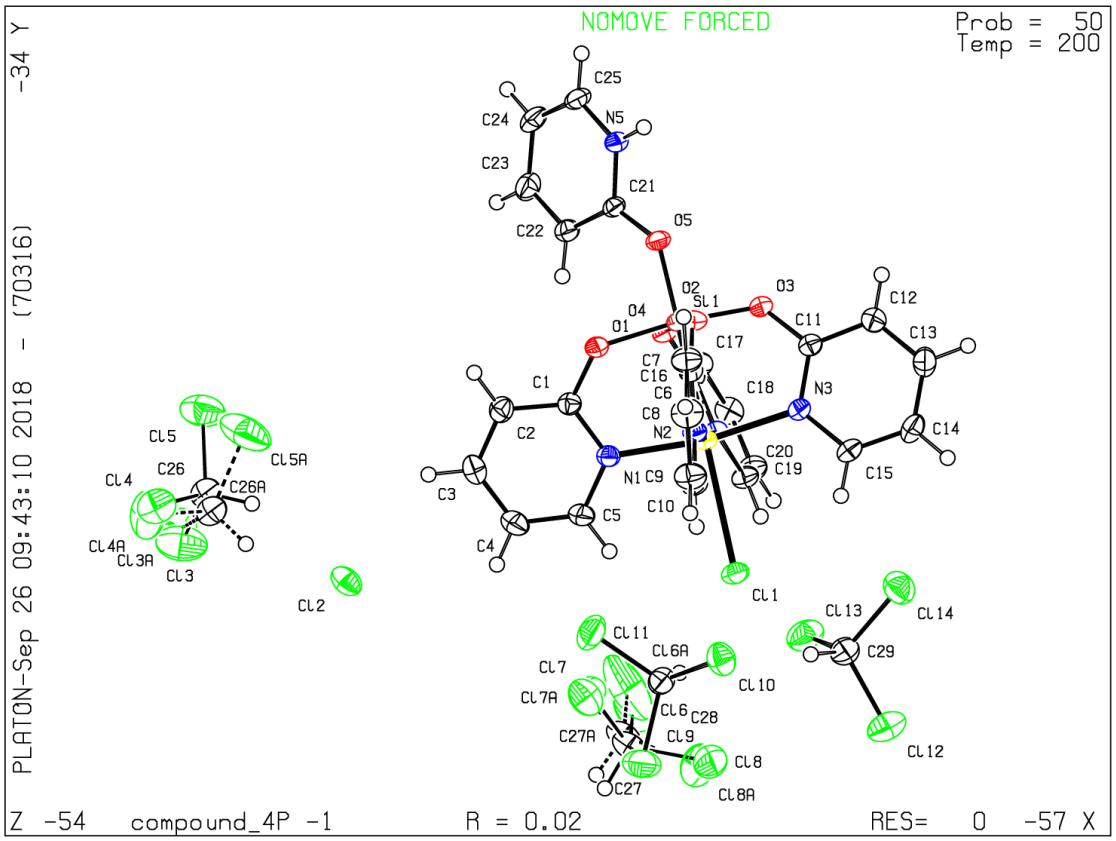
Datablock compound_3 - ellipsoid plot



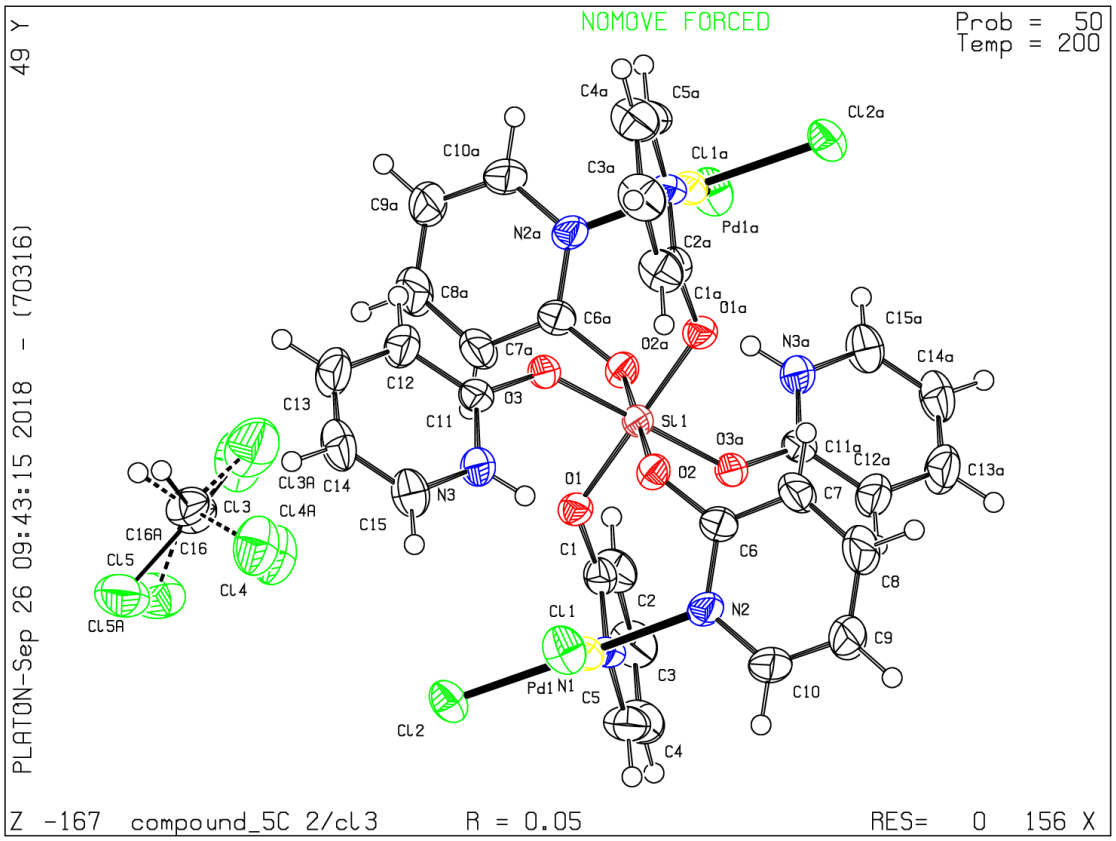
Datablock compound_3_CHCl3 - ellipsoid plot



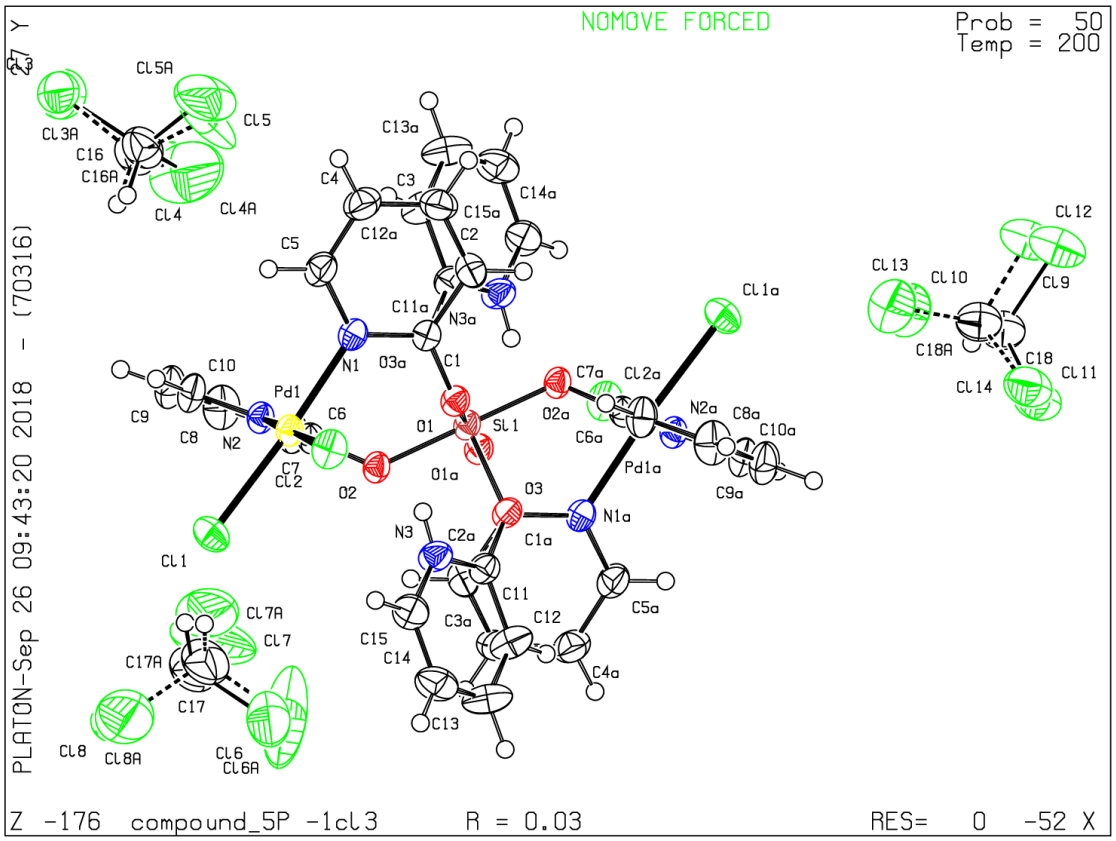
Datablock compound_4 - ellipsoid plot



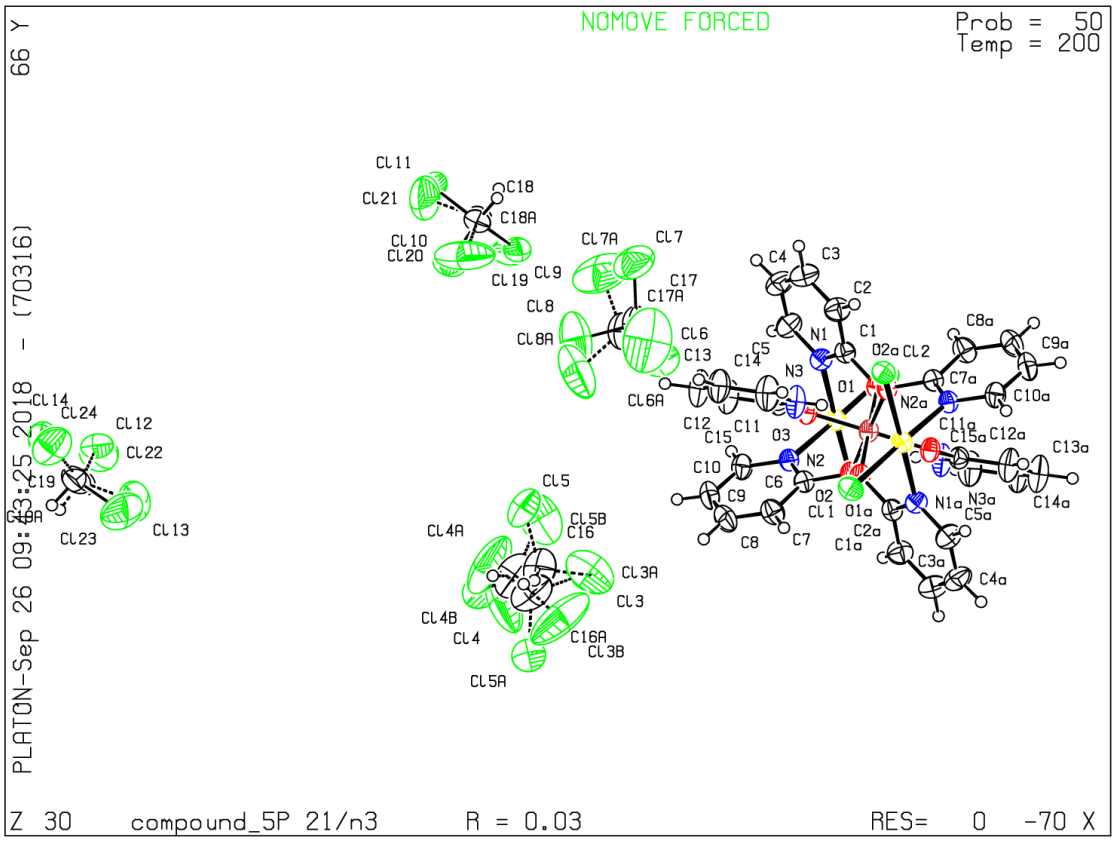
Datablock compound_5_2CHCl3 - ellipsoid plot



Datablock compound_5_6CHCl3 - ellipsoid plot



Datablock compound_5_8CHCl3 - ellipsoid plot



Datablock compound_6 - ellipsoid plot