

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) H3Ad

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: H3Ad

Bond precision: C-C = 0.0020 Å Wavelength=0.71073

Cell: a=13.0156(4) b=13.4914(3) c=14.0146(3)
 alpha=91.216(2) beta=106.490(2) gamma=116.398(3)
Temperature: 180 K

	Calculated	Reported
Volume	2082.30(11)	2082.30(10)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C54 H63 N3	C54 H63 N3
Sum formula	C54 H63 N3	C54 H63 N3
Mr	754.07	754.07
Dx, g cm ⁻³	1.203	1.203
Z	2	2
Mu (mm ⁻¹)	0.069	0.069
F000	816.0	816.0
F000'	816.27	
h, k, lmax	17, 18, 19	17, 18, 19
Nref	11469	10198
Tmin, Tmax	0.984, 0.988	0.580, 1.000
Tmin'	0.983	

Correction method= # Reported T Limits: Tmin=0.580 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.889 Theta(max)= 29.372

R(reflections)= 0.0454(7937)	wR2(reflections)=
S = 1.038	0.1202(10198)
Npar= 526	

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

PLAT420_ALERT_2_C	D-H Bond Without Acceptor	N1	--H1	.	Please Check
PLAT420_ALERT_2_C	D-H Bond Without Acceptor	N2	--H2	.	Please Check
PLAT420_ALERT_2_C	D-H Bond Without Acceptor	N3	--H3	.	Please Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance				3.246 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600			38 Report



Alert level G

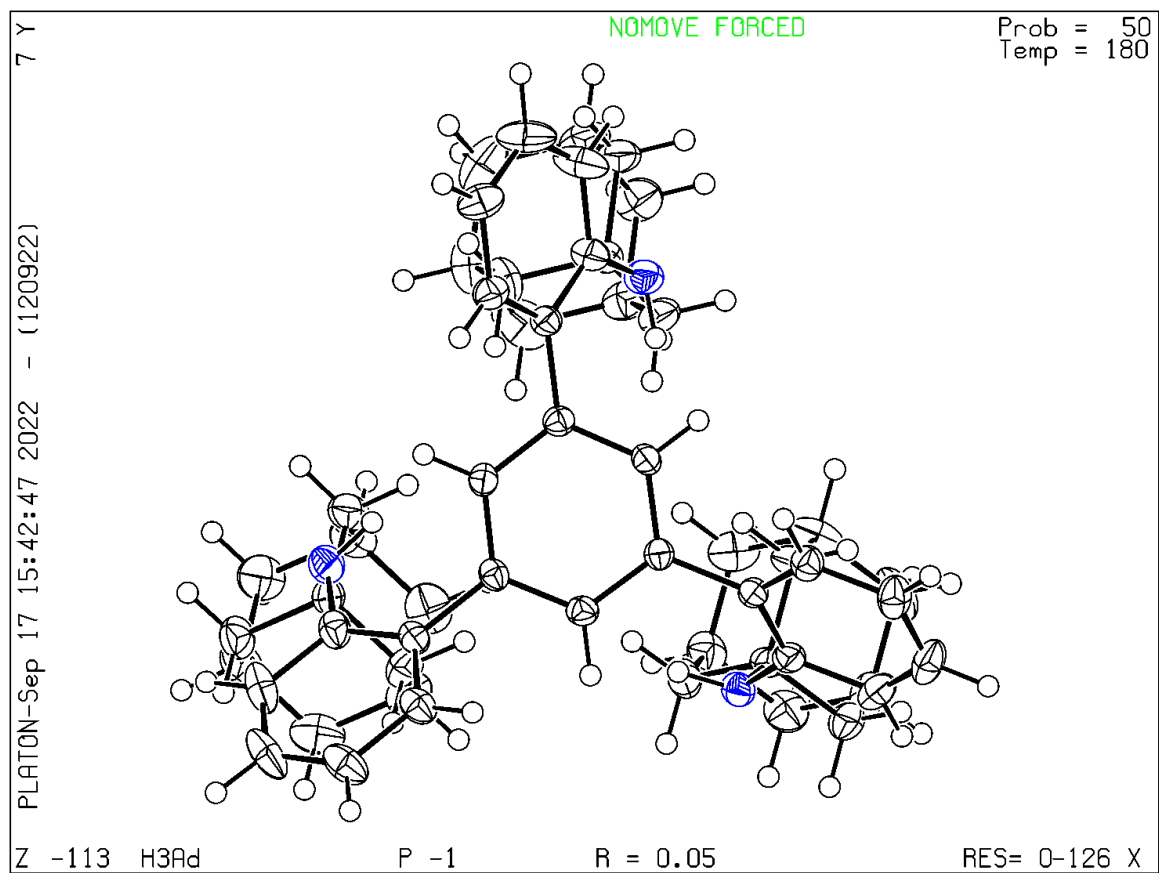
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary				Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).				4 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600			1230 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File				2 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity				2.3 Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.				24 Info
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by				3 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
7 **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
4 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
-

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.



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) AdU_sq

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: AdU_sq

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

Cell: a=11.6503(2) b=14.5422(2) c=15.3316(3)
 alpha=94.225(1) beta=105.144(2) gamma=90.410(1)
Temperature: 180 K

	Calculated	Reported
Volume	2499.54(8)	2499.53(8)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C54 H60 N3 U [+ solvent]	C54 H60 N3 U, 1.8[C4H10O]
Sum formula	C54 H60 N3 U [+ solvent]	C54 H60 N3 U
Mr	989.08	989.08
Dx, g cm ⁻³	1.314	1.314
Z	2	2
Mu (mm ⁻¹)	3.282	3.282
F000	994.0	994.0
F000'	975.05	
h, k, lmax	16, 20, 21	16, 20, 21
Nref	14854	13156
Tmin, Tmax	0.226, 0.374	0.441, 1.000
Tmin'	0.128	

Correction method= # Reported T Limits: Tmin=0.441 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.886 Theta(max)= 30.198

R(reflections)= 0.0316(11339)	wR2(reflections)=
S = 1.035	0.0754(13156)
Npar= 531	

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	2.05	Report
PLAT410_ALERT_2_C	Short Intra H...H Contact H9 ..H34A .	1.94	Ang.
	x,y,z =	1_555	Check
PLAT410_ALERT_2_C	Short Intra H...H Contact H15 ..H54A .	1.95	Ang.
	x,y,z =	1_555	Check
PLAT410_ALERT_2_C	Short Intra H...H Contact H21 ..H44A .	1.95	Ang.
	x,y,z =	1_555	Check
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).	6	Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	11	Report
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.87Ang From U1	2.43	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.77Ang From U1	2.21	eA-3
PLAT973_ALERT_2_C	Check Calcd Positive Resid. Density on U1	1.13	eA-3



Alert level G

FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and _chemical_formula_moiety. This is
usually due to the moiety formula being in the wrong format.
Atom count from _chemical_formula_sum: C54 H60 N3 U1
Atom count from _chemical_formula_moiety:C61.2 H78 N3 O1.8 U1

PLAT164_ALERT_4_G	Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.	2	Note
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) U1 --C5 .	5.1	s.u.
PLAT606_ALERT_4_G	Solvent Accessible VOID(S) in Structure	!	Info
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	1679	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	1	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	10	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.9	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0	Info

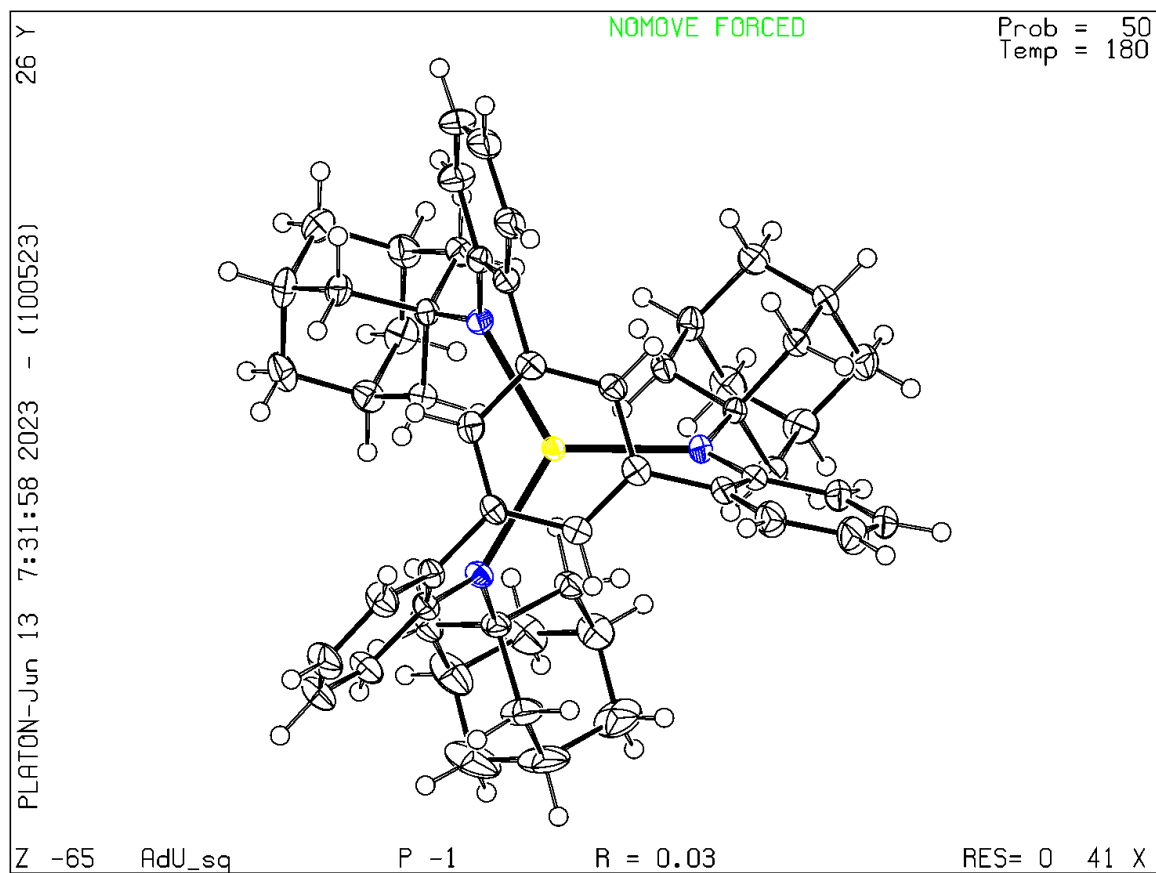
- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
9 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
10 **ALERT level G** = General information/check it is not something unexpected

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

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.



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Kcrypt_AdU_THF_sq

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: Kcrypt_AdU_THF_sq

Bond precision: C-C = 0.0060 Å Wavelength=0.71073

Cell: a=12.9095(2) b=23.2609(3) c=25.3412(4)
 alpha=105.030(1) beta=90.328(1) gamma=100.678(1)
Temperature: 180 K

	Calculated	Reported
Volume	7210.44(19)	7210.43(19)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C54 H60 N3 U), 2(C18 H36 K N2 O6), C4 H8 O [+ solvent]	2(C54 H60 N3 U), 2(C18 H36 K N2 O6), C4 H8 O, 2.43[C4H8O]
Sum formula	C148 H200 K2 N10 O13 U2 [+ solvent]	C148 H200 K2 N10 O13 U2
Mr	2881.44	2881.43
Dx, g cm ⁻³	1.327	1.327
Z	2	2
Mu (mm ⁻¹)	2.362	2.362
F000	2968.0	2968.0
F000'	2931.24	
h, k, lmax	17, 32, 35	17, 31, 34
Nref	40471	36454
Tmin, Tmax	0.359, 0.389	0.258, 1.000
Tmin'	0.332	

Correction method= # Reported T Limits: Tmin=0.258 Tmax=1.000
AbsCorr = MULTII-SCAN

Data completeness= 0.901

Theta(max)= 29.579

R(reflections)= 0.0398(27338)

wR2(reflections)=
0.1045(36454)

S = 1.026

Npar= 1576

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

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min).

16 Note

Author Response: Several low-order reflections might have been 'Omitted' from the (final) least-squares refinement



Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without a literature citation. This should be contained in the _exptl_absorpt_process_details field.

Absorption correction given as multi-scan

PLAT220_ALERT_2_C	NonSolvent	Resd 1	C	Ueq(max)/Ueq(min)	Range	3.6	Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C13	--C14	.	.	5.7	s.u.
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including				O13	0.106	Check
PLAT410_ALERT_2_C	Short Intra H...H Contact	H15	..H38A	.	.	1.95	Ang.
			x,y,z =			1_555	Check
PLAT410_ALERT_2_C	Short Intra H...H Contact	H21	..H46B	.	.	1.95	Ang.
			x,y,z =			1_555	Check
PLAT410_ALERT_2_C	Short Intra H...H Contact	H11D	..H93	.	.	1.93	Ang.
			x,y,z =			1_555	Check
PLAT410_ALERT_2_C	Short Intra H...H Contact	H81	..H99B	.	.	1.91	Ang.
			x,y,z =			1_555	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=			0.600		43	Report
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	1.49Ang	From N7			1.68	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	1.00Ang	From U2			1.64	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	1.00Ang	From U1			1.58	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	1.12Ang	From C78			1.57	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	1.02Ang	From U2			1.54	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	0.89Ang	From U2			1.53	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	1.17Ang	From N7			-1.64	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	1.62Ang	From U2			-1.57	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	1.50Ang	From C27			-1.51	eA-3



Alert level G

FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the _chemical_formula_sum and _chemical_formula_moiety. This is usually due to the moiety formula being in the wrong format.

Atom count from _chemical_formula_sum: C148 H200 K2 N10 O13 U2

Atom count from _chemical_formula_moiety:C157.7199 H219.44 K2 N10 O15.

PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.001 Degree

PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O13 108.5 Degree

PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure	! Info
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #	5 Note
C4 H8 O	
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	3909 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF	1 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File	43 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity	2.9 Low
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
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
11 **ALERT level G** = General information/check it is not something unexpected

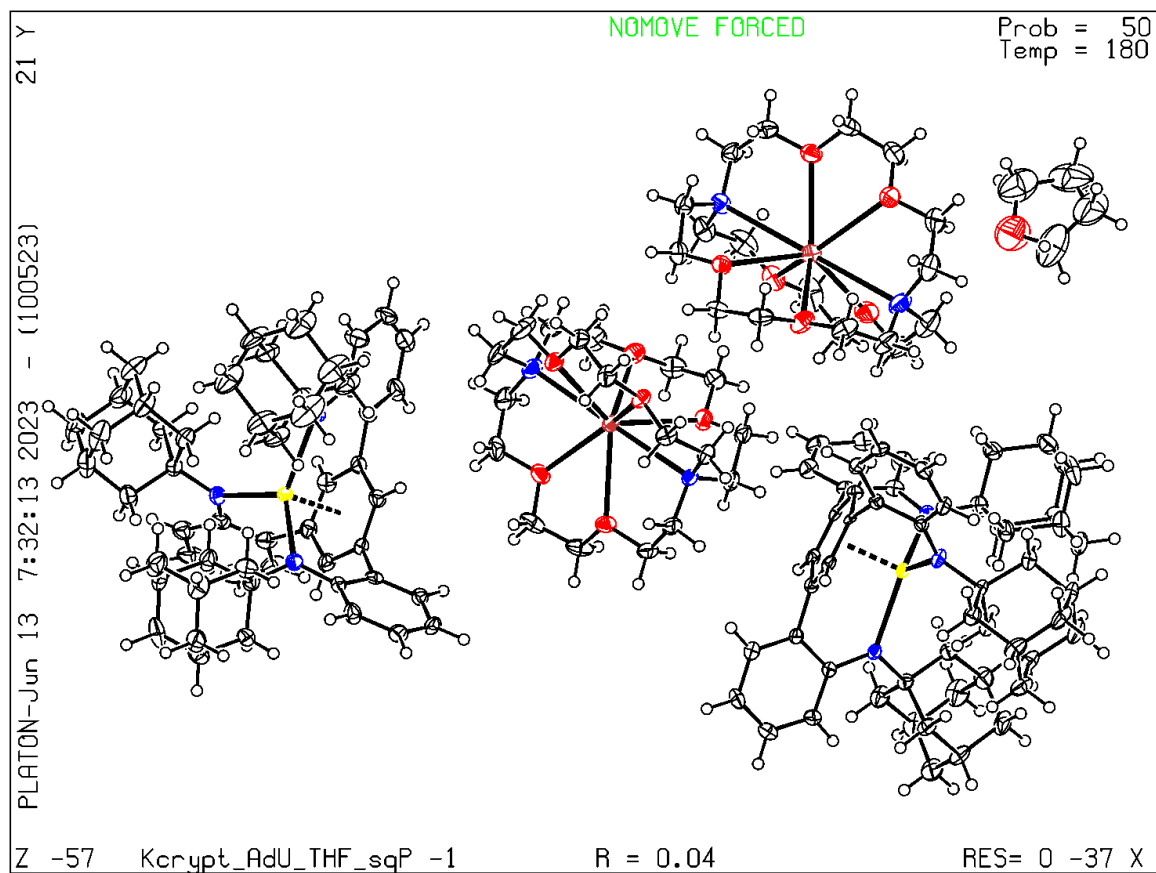
4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
19 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative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

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



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	2.72	Report
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C55	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	2	Report
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.92Ang From U1	2.08	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 1.08Ang From U1	1.95	eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 1.08Ang From N2 .	0.45	eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.64Ang From O1 .	-0.50	eA-3



Alert level G

FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and _chemical_formula_moiety. This is
usually due to the moiety formula being in the wrong format.
Atom count from _chemical_formula_sum: C61 H68 N3 O1 U1
Atom count from _chemical_formula_moiety:C63.5 H74 N3 O1 U1

PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure	206	A**3
PLAT794_ALERT_5_G	Tentative Bond Valency for U1 (IV) .	4.16	Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min) .	4	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	1	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	4	Info

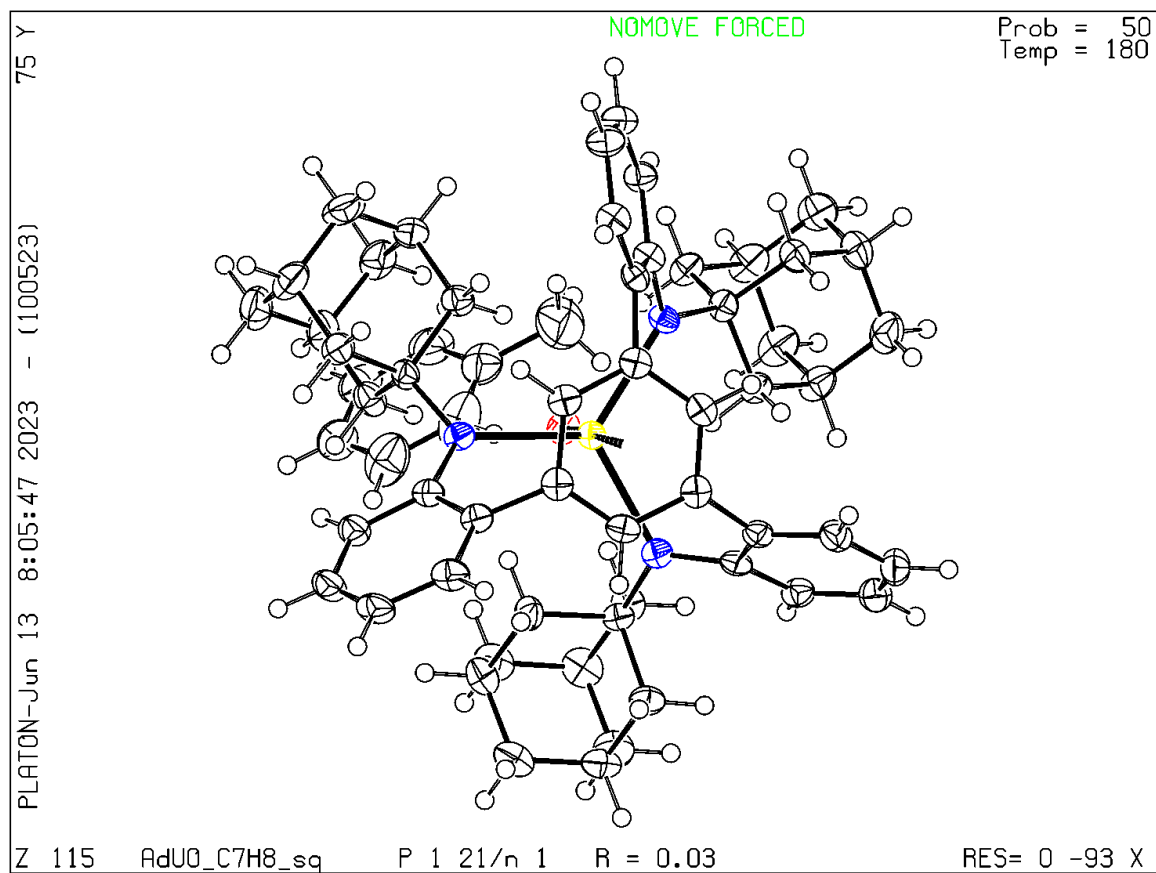
0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
7 **ALERT level G** = General information/check it is not something unexpected

2 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
2 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

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.



```
R(reflections)= 0.0251( 8956)      wR2(reflections)=
S = 1.044                        0.0583( 10717)
Npar= 532
```

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

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.

Absorption correction given as multi-scan

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	3.16	Report
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).	5	Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	2	Report
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.86Ang From U1	1.82	eA-3



Alert level G

PLAT794_ALERT_5_G	Tentative Bond Valency for U1 (IV) .	4.22	Info
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	899	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	3	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.0	Low
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ.	2	Units
PLAT958_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Lmax Differ.	2	Units
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	12	Info

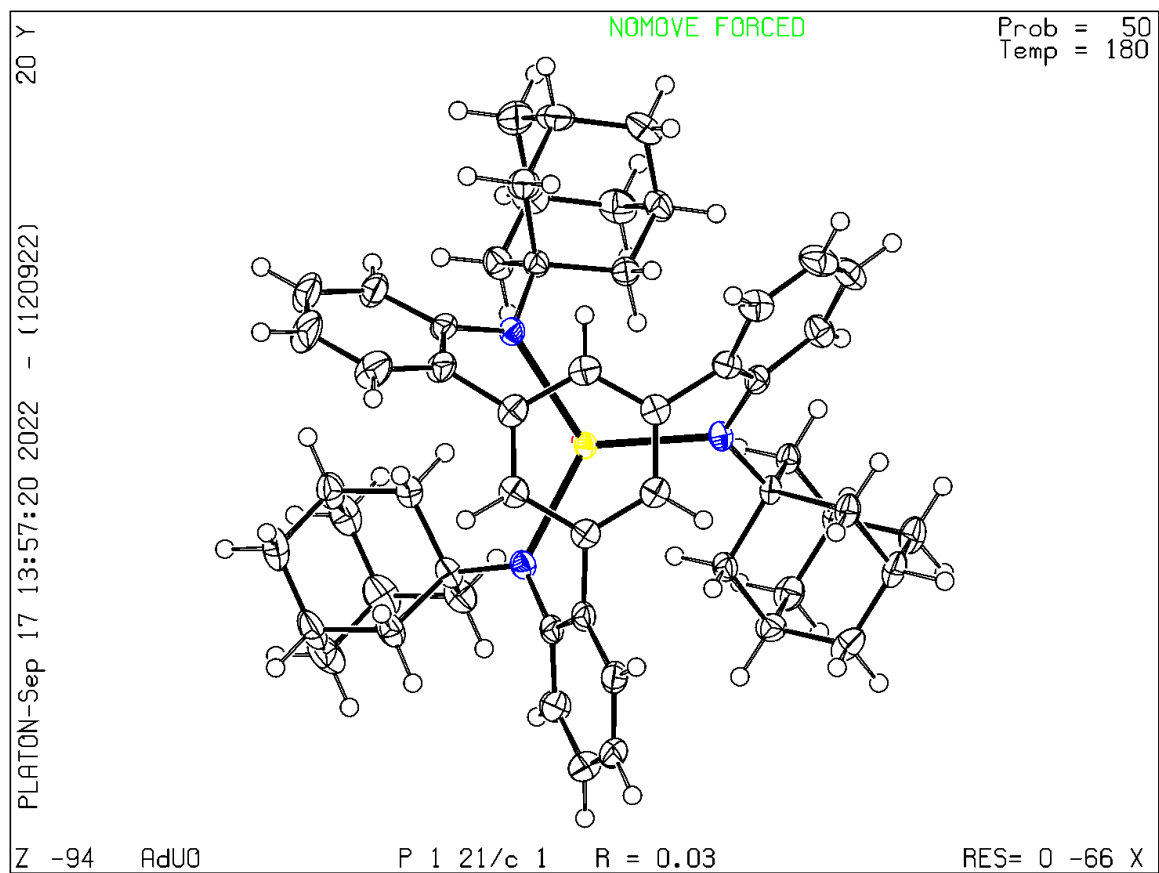
0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
8 **ALERT level G** = General information/check it is not something unexpected

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

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.



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Kcrypt_AdUO

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: Kcrypt_AdUO

Bond precision:	C-C = 0.0071 Å	Wavelength=0.71073
Cell:	a=17.4587(4)	b=17.4587(4) c=18.5858(6)
	alpha=90	beta=90 gamma=120
Temperature:	180 K	
	Calculated	Reported
Volume	4906.1(3)	4906.1(3)
Space group	R 3	R 3
Hall group	R 3	R 3
Moiety formula	C54 H60 N3 O U, C18 H36 K N2 O6	C54 H60 N3 O1 U1, C18 H36 K1 N2 O6
Sum formula	C72 H96 K N5 O7 U	C72 H96 K N5 O7 U
Mr	1420.67	1420.66
Dx, g cm ⁻³	1.443	1.443
Z	3	3
Mu (mm ⁻¹)	2.603	2.603
F000	2190.0	2190.0
F000'	2162.44	
h, k, lmax	24, 24, 25	22, 23, 24
Nref	6102 [3051]	4511
Tmin, Tmax	0.855, 0.925	0.811, 1.000
Tmin'	0.522	

Correction method= # Reported T Limits: Tmin=0.811 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.48/0.74 Theta(max)= 29.528

R(reflections)= 0.0205(4511)	wR2(reflections)= 0.0448(4511)
S = 1.036	Npar= 259

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

CRYSC01_ALERT_1_C The word below has not been recognised as a standard identifier.

greenish

PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT915_ALERT_3_C	No Flack x Check Done: Low Friedel Pair Coverage	58 %
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.93Ang From O1	1.90 eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.82Ang From U1	1.83 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.89Ang From O1 .	0.41 eA-3



Alert level G

PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.12 Ratio
PLAT794_ALERT_5_G	Tentative Bond Valency for U1 (IV) .	3.47 Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min) .	1 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	304 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	2 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	2.3 Low
PLAT950_ALERT_5_G	Calculated (ThMax) and CIF-Reported Hmax Differ	2 Units
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities	Please Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1 Info

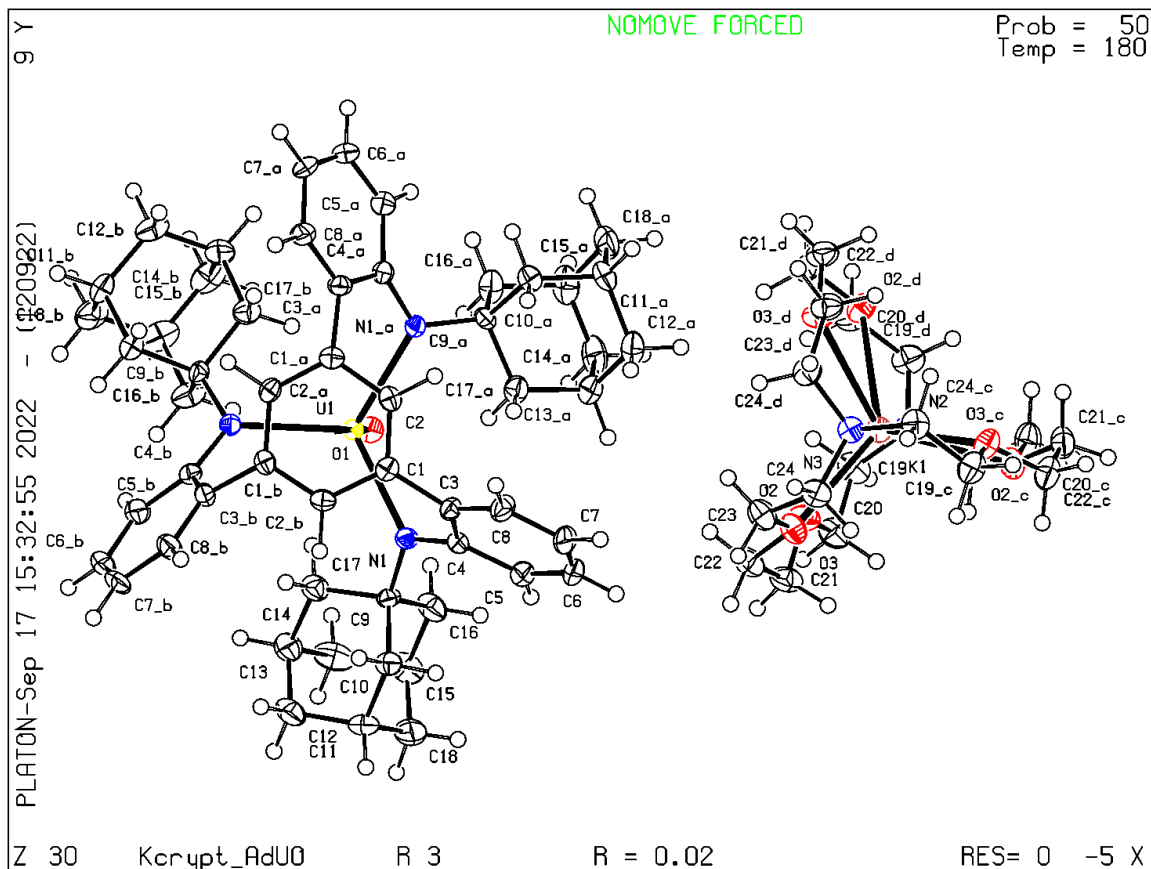
- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
10 **ALERT level G** = General information/check it is not something unexpected

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

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.



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Cpstar2Co_AdUO_THF

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: Cpstar2Co_AdUO_THF

Bond precision: C-C = 0.0183 Å Wavelength=0.71073

Cell: a=13.3624 (5) b=26.7946 (8) c=18.4675 (7)
 alpha=90 beta=90.015 (3) gamma=90

Temperature: 180 K

	Calculated	Reported
Volume	6612.1 (4)	6612.1 (4)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C54 H60 N3 O U, C20 H30 Co, C4 H8 O	C54 H60 N3 O U, C20 H30 Co, C4 H8 O
Sum formula	C78 H98 Co N3 O2 U	C78 H98 Co N3 O2 U
Mr	1406.55	1406.55
Dx, g cm ⁻³	1.413	1.413
Z	4	4
Mu (mm ⁻¹)	2.746	2.746
F000	2888.0	2888.0
F000'	2851.70	
h, k, lmax	15, 31, 21	15, 31, 21
Nref	11662	11650
Tmin, Tmax	0.848, 0.872	0.799, 1.000
Tmin'	0.662	

Correction method= # Reported T Limits: Tmin=0.799 Tmax=1.000
AbsCorr = MULTII-SCAN

Data completeness= 0.999

Theta(max)= 25.026

R(reflections)= 0.0765 (8587)

wR2(reflections)=
0.1769 (11650)

S = 1.104

Npar= 775

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

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.92Ang From U1

4.03 eA-3

Author Response: This error is due to residual density near heavy metal (U) or incomplete absorption correction. The specific structural parameter might not be precise; however, we believe the key finding (atom connection) of the structure is shown unambiguously.

 Alert level B

PLAT973_ALERT_2_B Check Calcd Positive Resid. Density on

U1

1.82 eA-3

Author Response: Near heavy metal or incomplete absorption correction

 Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.

Absorption correction given as multi-scan

RINTA01_ALERT_3_C The value of Rint is greater than 0.12

Rint given 0.133

PLAT020_ALERT_3_C	The Value of Rint is Greater Than 0.12	0.133	Report
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.79	Report
PLAT214_ALERT_2_C	Atom C74 (Anion/Solvent) ADP max/min Ratio	4.6	prolat
PLAT221_ALERT_2_C	Solv./Anion Resd 2 C Ueq(max)/Ueq(min) Range	5.3	Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference C5 --C6	0.16	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C29 --C30	0.16	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C41 --C42	0.17	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C46 --C50	0.17	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C49 --C53	0.24	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C50 --C53	0.22	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C58 --C59	0.17	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C66 --C67	0.18	Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C52	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C45	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C51	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	Co1	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C65	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C66	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C67	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C68	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C69	Check
PLAT243_ALERT_4_C	High 'Solvent' Ueq as Compared to Neighbors of	C75	Check
PLAT243_ALERT_4_C	High 'Solvent' Ueq as Compared to Neighbors of	C78	Check

PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of	C77	Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of	C79	Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor	2.6	Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including Co1	0.107	Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including O2	0.185	Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds	0.0183	Ang.
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C75 - C79 .	1.42	Ang.
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C77 - C78 .	1.38	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	6.266	Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).	8	Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.595	4	Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.82Ang From U1	1.80	eA-3

Author Response: This error is due to residual density near heavy metal (U) or incomplete absorption correction. The specific structural parameter might not be precise; however, we believe the key finding (atom connection) of the structure is shown unambiguously.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 2.38Ang From O1	1.67	eA-3
--	------	------

Author Response: This error is due to residual density near heavy metal (U) or incomplete absorption correction. The specific structural parameter might not be precise; however, we believe the key finding (atom connection) of the structure is shown unambiguously.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.93Ang From C14	-2.07	eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.76Ang From U1	-1.80	eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.79Ang From U1	-1.67	eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H79A .	-0.32	eA-3



Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite	6	Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...	2	Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large	73.90	Why ?
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records	1	Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records	1	Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records	1	Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par	0.0010	Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar	0.0010	Report
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety	C73	Check
PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O2 .	103.6	Degree
PLAT794_ALERT_5_G Tentative Bond Valency for U1 (IV) .	3.54	Info
PLAT794_ALERT_5_G Tentative Bond Valency for Co1 (III) .	3.42	Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints	16	Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .	Please	Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still	48%	Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File	4	Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity	4.6	Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.	0	Info

1 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
43 **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

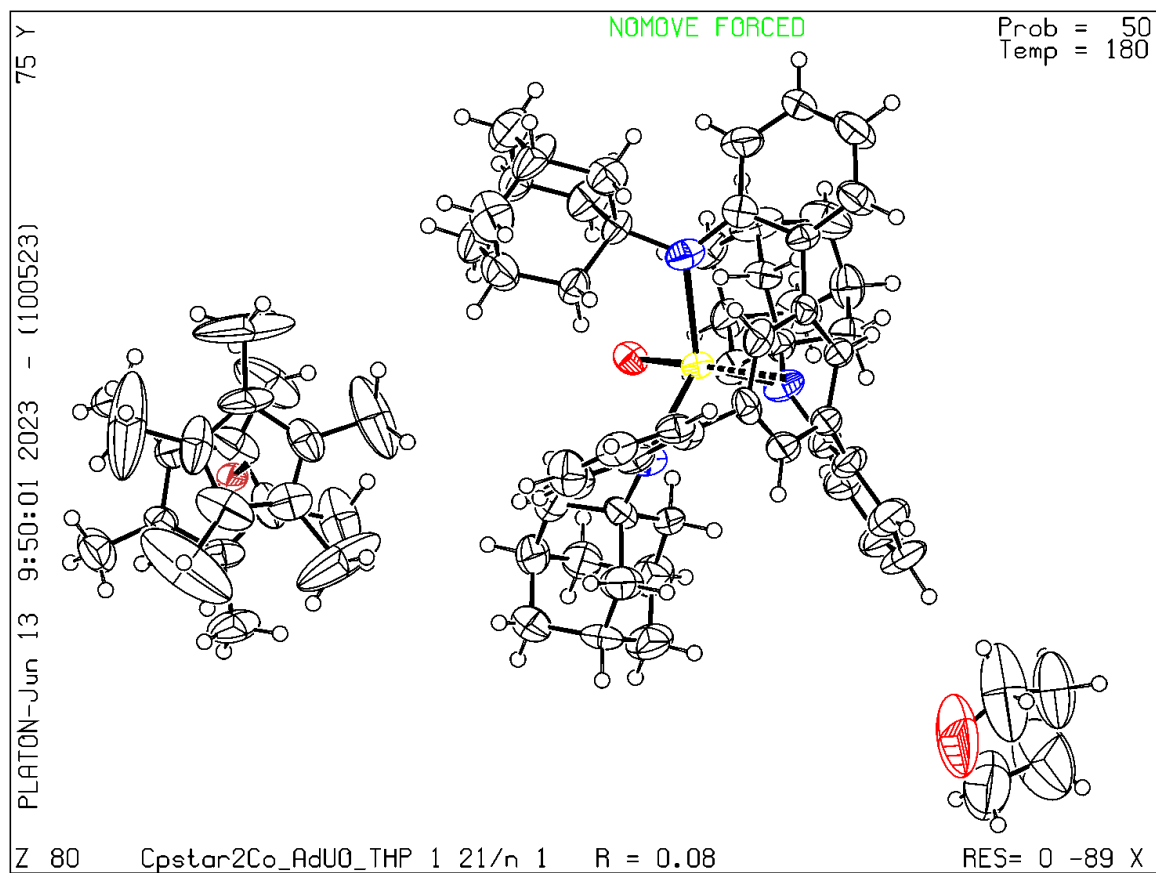
2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
32 ALERT type 2 Indicator that the structure model may be wrong or deficient
11 ALERT type 3 Indicator that the structure quality may be low
16 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative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

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



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) AdUO_SbF6_2CH2Cl2

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: AdUO_SbF6_2CH2Cl2

Bond precision: C-C = 0.0057 Å Wavelength=0.71073

Cell: a=13.4938 (4) b=14.1867 (4) c=15.4238 (4)
 alpha=66.506 (3) beta=82.626 (2) gamma=78.965 (2)
Temperature: 180 K

	Calculated	Reported
Volume	2653.34 (14)	2653.34 (14)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C54 H60 N3 O U, F6 Sb, 2 (C H2 Cl2)	C54 H60 N3 O U, F6 Sb, 2 (C H2 Cl2)
Sum formula	C56 H64 Cl4 F6 N3 O Sb U	C56 H64 Cl4 F6 N3 O Sb U
Mr	1410.69	1410.68
Dx, g cm ⁻³	1.766	1.766
Z	2	2
Mu (mm ⁻¹)	3.823	3.823
F000	1388.0	1388.0
F000'	1369.31	
h, k, lmax	16, 17, 19	16, 17, 19
Nref	10828	10820
Tmin, Tmax	0.415, 0.466	0.397, 1.000
Tmin'	0.208	

Correction method= # Reported T Limits: Tmin=0.397 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 26.372

R(reflections)= 0.0280 (9872)	wR2(reflections)= 0.0664 (10820)
S = 1.053	Npar= 704

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

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.

Absorption correction given as multi-scan

PLAT243_ALERT_4_C	High 'Solvent' Ueq as Compared to Neighbors of	C55	Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	Sb1	Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.4	Note
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including Sb1	0.102	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	4	Report
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.76Ang From F4	2.04	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.72Ang From Sb1	-2.13	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.58Ang From Sb1	-1.54	eA-3



Alert level G

PLAT233_ALERT_4_G	Hirshfeld (M-X Solvent) Sb1 --F4 .	22.9	s.u.
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	86%	Note
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	3	Note
PLAT794_ALERT_5_G	Tentative Bond Valency for U1 (IV) .	4.54	Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !	
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	4	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	2	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.0	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1	Info

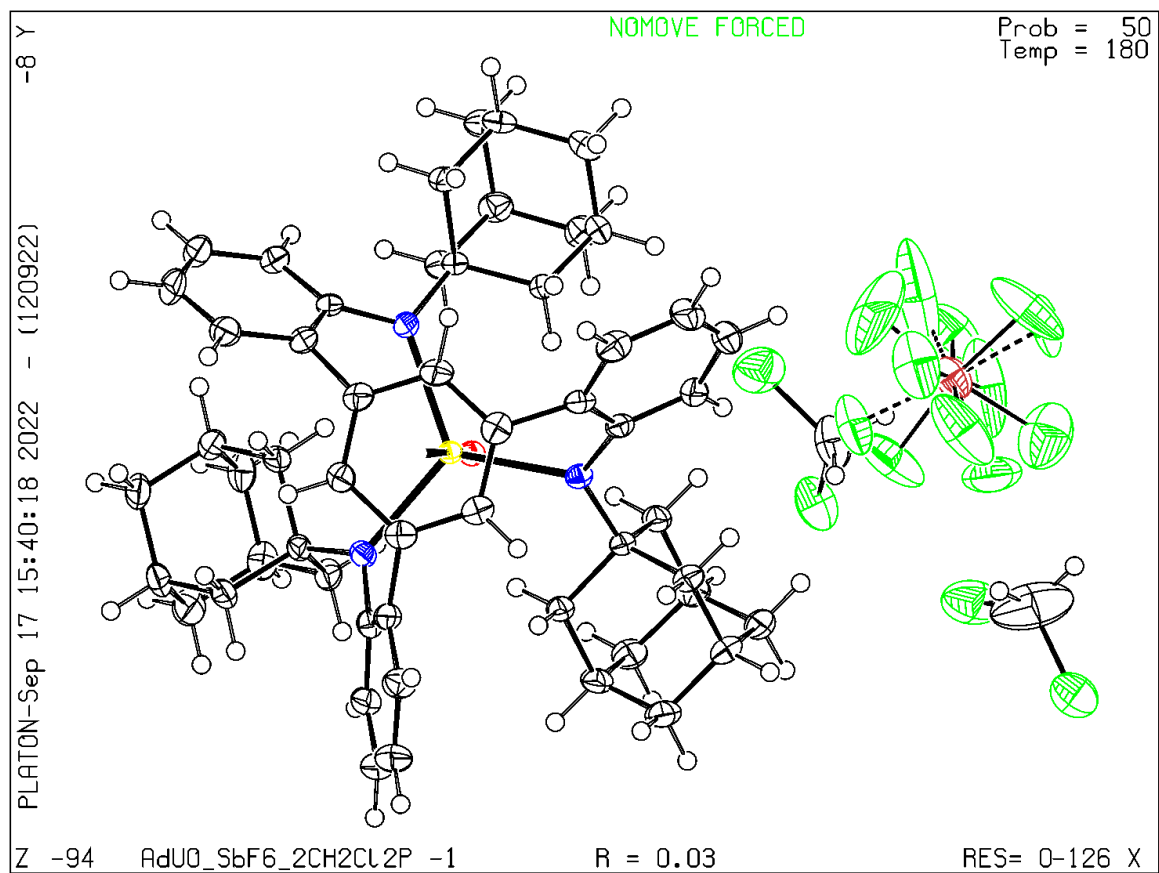
0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
9 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
9 **ALERT level G** = General information/check it is not something unexpected

2 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
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

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.



```
R(reflections)= 0.0289( 9164)
S = 1.042
Npar= 532
```

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 5.94 Report

Author Response: High residual density near heavy metal or incomplete absorption correction

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 2.16Ang From C46 3.48 eA-3

Author Response: Near heavy metal or incomplete absorption correction



Alert level C

PLAT057_ALERT_3_C Correction for Absorption Required RT(exp) ... 1.12 Do !
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.997 Check



Alert level G

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 6.29 Why ?
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 1027 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 3.0 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 7 Info

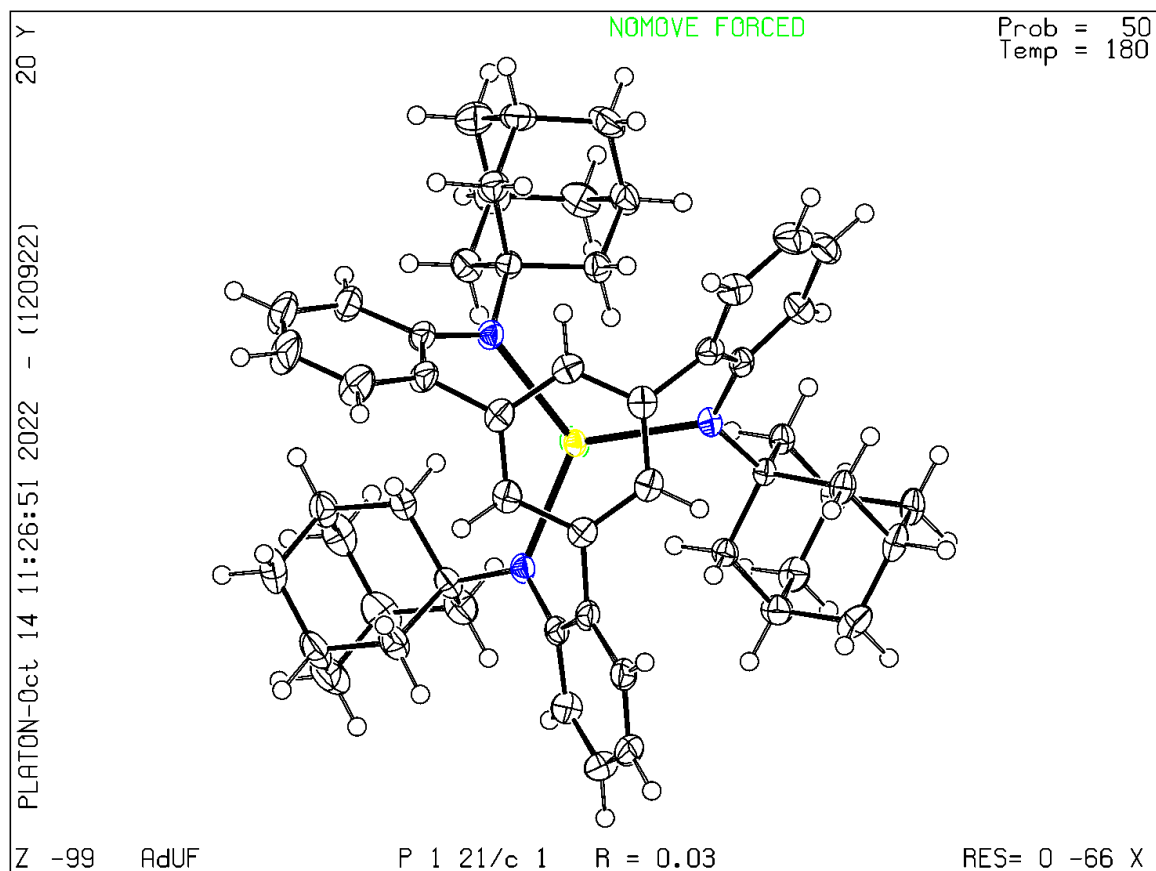
- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
7 **ALERT level G** = General information/check it is not something unexpected

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

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.



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

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.

Absorption correction given as multi-scan

PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.854	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	34	Report
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 1.00Ang From U1	1.70	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.79Ang From U1	1.65	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.65Ang From U1	-1.67	eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.81Ang From N3	0.65	eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 1.04Ang From N2	0.59	eA-3



Alert level G

PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	12.02	Why ?
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) U1 --I1	9.2	s.u.
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary		Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	1031	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	5	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.1	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1	Info

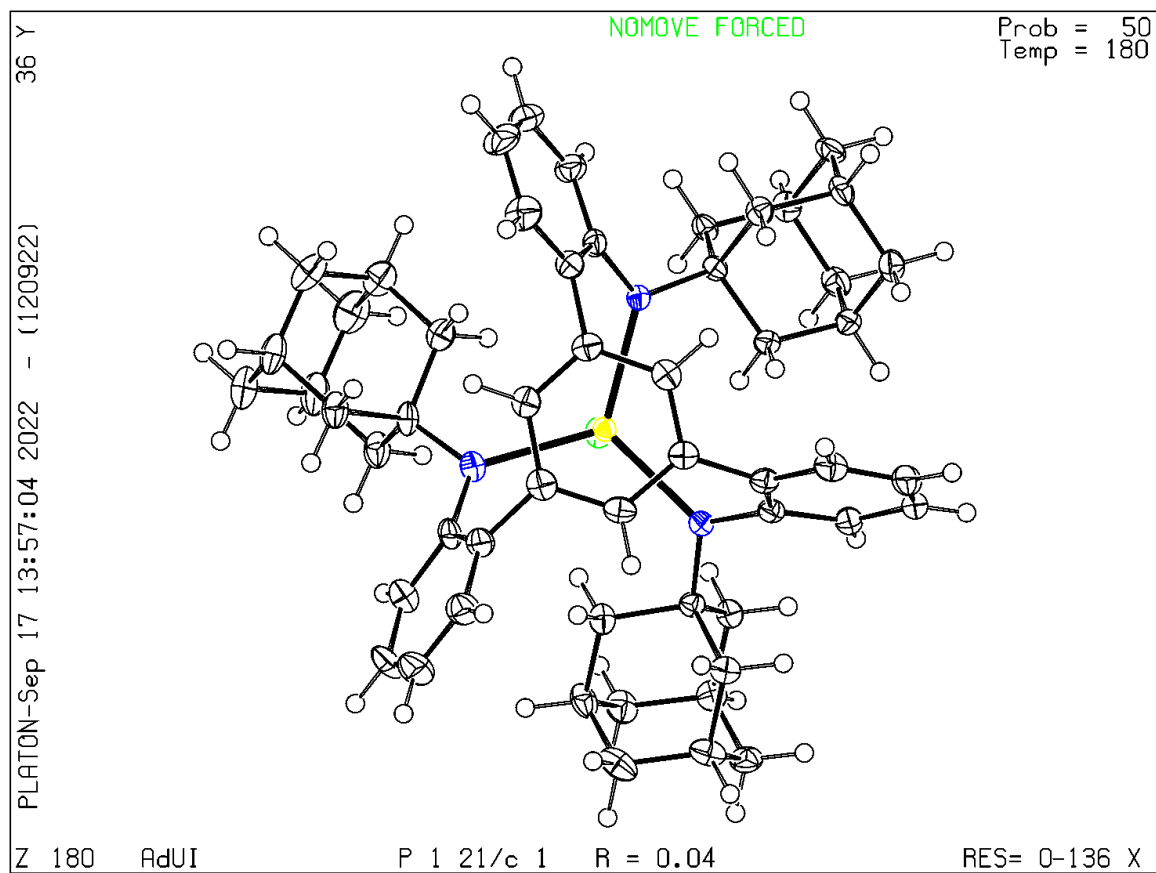
0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
8 **ALERT level G** = General information/check it is not something unexpected

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

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.



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	2.525 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).	6 Note



Alert level G

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	1005 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File	1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity	4.5 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.	21 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
1 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

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.

Datablock XPhos - ellipsoid plot

