
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)	0.004 Degree
PLAT432_ALERT_2_G	Short Inter X...Y Contact O2 ..C6 .	2.95 Ang.
	1-x,1-y,1-z =	2_666 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C6 ..C6 .	3.13 Ang.
	1-x,1-y,1-z =	2_666 Check
PLAT767_ALERT_4_G	INS Embedded LIST 6 Instruction Should be LIST 4	Please Check
PLAT793_ALERT_4_G	Model has Chirality at C7 (Centro SPGR)	S Verify
PLAT793_ALERT_4_G	Model has Chirality at C8 (Centro SPGR)	S Verify
PLAT793_ALERT_4_G	Model has Chirality at C9 (Centro SPGR)	R Verify
PLAT793_ALERT_4_G	Model has Chirality at C12 (Centro SPGR)	S Verify
PLAT793_ALERT_4_G	Model has Chirality at C13 (Centro SPGR)	R Verify
PLAT793_ALERT_4_G	Model has Chirality at C14 (Centro SPGR)	R Verify
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	10 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	4.6 Low
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities	Please Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	14 Info

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

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

Datablock: 2

Bond precision: C-C = 0.0050 A

Wavelength=0.71073

Cell: a=6.80779 (8) b=11.83139 (14) c=14.71857 (16)

alpha=80.4699 (6) beta=85.6414 (6) gamma=81.8897 (6)

Temperature: 296 K

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

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & Sth/L= 0.600 7 Report

Alert level G

PLAT793_ALERT_4_G Model has Chirality at C7 (Centro SPGR) R Verify
PLAT793_ALERT_4_G Model has Chirality at C8 (Centro SPGR) R Verify
PLAT793_ALERT_4_G Model has Chirality at C9 (Centro SPGR) S Verify
PLAT793_ALERT_4_G Model has Chirality at C12 (Centro SPGR) R Verify
PLAT793_ALERT_4_G Model has Chirality at C13 (Centro SPGR) S Verify
PLAT793_ALERT_4_G Model has Chirality at C14 (Centro SPGR) S Verify
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 7 Note
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 52.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 7 Info

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11 **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
1 ALERT type 3 Indicator that the structure quality may be low
6 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check
-

Datablock: 4

Bond precision: C-C = 0.0057 A

Wavelength=0.71073

Cell: a=25.8153(6) b=7.0635(2) c=27.1652(7)

alpha=90 beta=97.5487(12) gamma=90

Temperature: 296 K

PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 2 Note
 PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 2.8 Low
 PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 3 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
 12 **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
 3 ALERT type 3 Indicator that the structure quality may be low
 7 ALERT type 4 Improvement, methodology, query or suggestion
 0 ALERT type 5 Informative message, check

Datablock: 5

Bond precision: C-C = 0.0067 A Wavelength=0.71073

Cell: a=26.208(2) b=7.1272(7) c=27.046(3)
 alpha=90 beta=97.866(5) gamma=90

Temperature: 305 K

	Calculated	Reported
Volume	5004.4(8)	5004.3(8)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C48 H40 Br4 Hg2 N8 O8	?
Sum formula	C48 H40 Br4 Hg2 N8 O8	C48 H40 Br4 Hg2 N8 O8
Mr	1577.66	1577.70
Dx, g cm ⁻³	2.094	2.094
Z	4	4
Mu (mm ⁻¹)	9.383	9.383
F000	2992.0	2992.0
F000'	2970.78	
h, k, lmax	34, 9, 36	34, 9, 36
Nref	6320	6265
Tmin, Tmax	0.121, 0.391	0.366, 0.746
Tmin'	0.052	

Correction method= # Reported T Limits: Tmin=0.366 Tmax=0.746
 AbsCorr = MULTI_SCAN

Data completeness= 0.991 Theta(max)= 28.445

R(reflections)= 0.0397(4327)

wR2(reflections)=
0.0904(6265)

S = 1.025

Npar= 298

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

PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	5.07	Why ?
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	1	Report
PLAT793_ALERT_4_G	Model has Chirality at C8 (Centro SPGR)	R	Verify
PLAT793_ALERT_4_G	Model has Chirality at C9 (Centro SPGR)	S	Verify
PLAT793_ALERT_4_G	Model has Chirality at C15 (Centro SPGR)	S	Verify
PLAT793_ALERT_4_G	Model has Chirality at C16 (Centro SPGR)	R	Verify
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	55	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.9	Low
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged		Please Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	2	Info

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 - 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
 - 11 **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
 - 1 ALERT type 3 Indicator that the structure quality may be low
 - 6 ALERT type 4 Improvement, methodology, query or suggestion
 - 0 ALERT type 5 Informative message, check
-

Datablock: 6

Bond precision: C-C = 0.0053 A

Wavelength=0.71073

Cell: a=26.7552(5)

b=7.2351(1)

c=27.0340(5)

alpha=90

beta=98.0783(9)

gamma=90

Temperature: 305 K

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

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

Datablock: 7

Bond precision: C-C = 0.0045 A Wavelength=0.71073
Cell: a=18.4293(3) b=13.6689(2) c=9.8057(2)
alpha=90 beta=90.3635(9) gamma=90
Temperature: 296 K

	Calculated	Reported
Volume	2470.09(7)	2470.09(7)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C24 H18 Cl2 Hg N4 O3, H2 O	?
Sum formula	C24 H20 Cl2 Hg N4 O4	C24 H20 Cl2 Hg N4 O4
Mr	699.93	699.93
Dx, g cm ⁻³	1.882	1.882
Z	4	4
Mu (mm ⁻¹)	6.486	6.486
F000	1352.0	1352.0
F000'	1344.42	
h, k, lmax	24, 18, 13	24, 18, 13
Nref	6169	6145
Tmin, Tmax	0.164, 0.273	0.286, 0.746
Tmin'	0.124	

Correction method= # Reported T Limits: Tmin=0.286 Tmax=0.746
AbsCorr = MULTI_SCAN

Data completeness= 0.996 Theta(max)= 28.352

R(reflections)= 0.0285(5187)

wR2(reflections)=
0.0722(6145)

S = 1.048

Npar= 324

	Calculated	Reported
Volume	2543.7(4)	2543.7(4)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	2(C24 H18 Br2 Hg N4 O3), 0.375(O4), 2(H0.50 O0.25)	?
Sum formula	C48 H37 Br4 Hg2 N8 O8	C24 H20 Br2 Hg N4 O4
Mr	1574.64	788.85
Dx, g cm ⁻³	2.056	2.060
Z	2	4
Mu (mm ⁻¹)	9.230	9.230
F000	1490.0	1496.0
F000'	1479.40	
h, k, lmax	22, 17, 12	22, 17, 12
Nref	5040	4984
Tmin, Tmax	0.182, 0.158	0.437, 0.746
Tmin'	0.137	

Correction method= # Reported T Limits: Tmin=0.437 Tmax=0.746
AbsCorr = MULTI_SCAN

Data completeness= 0.989 Theta(max)= 26.054

R(reflections)= 0.0535(3771) wR2(reflections)=
0.1506(4984)
S = 1.044 Npar= 321

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

PLAT041_ALERT_1_C	Calc. and Reported SumFormula	Strings Differ	Please Check
PLAT043_ALERT_1_C	Calculated and Reported Mol. Weight	Differ by ..	3.06 Check
PLAT068_ALERT_1_C	Reported F000	Differs from Calcd (or Missing)...	Please Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq	as Compared to Neighbors of	02 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq	as Compared to Neighbors of	C13 Check
PLAT334_ALERT_2_C	Small Aver. Benzene C-C Dist	C7 -C12	1.37 Ang.
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.01536 Ang.
PLAT414_ALERT_2_C	Short Intra D-H..H-X	H3A ..H17A	1.96 Ang.
		x, y, z =	1_555 Check
PLAT430_ALERT_2_C	Short Inter D...A Contact	O4 ..O4	2.85 Ang.
		-1-x, 2-y, -z =	3_475 Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	3.209 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	12 Report

● Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum: C24 H20 Br2 Hg1 N4 O4
Atom count from the _atom_site data: C24 H18.5 Br2 Hg1 N4 O4
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
From the CIF: _cell_formula_units_Z 4
From the CIF: _chemical_formula_sum C24 H20 Br2 Hg N4 O4
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	96.00	96.00	0.00
H	80.00	74.00	6.00
Br	8.00	8.00	0.00
Hg	4.00	4.00	0.00
N	16.00	16.00	0.00
O	16.00	16.00	0.00

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension		1	Info
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms		4	Report
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...		0.500	Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large		13.76	Why ?
PLAT300_ALERT_4_G	Atom Site Occupancy of O4	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O4'	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H4'A	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H4'B	Constrained at	0.25	Check
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
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)		04	Check
PLAT415_ALERT_2_G	Short Inter D-H..H-X	H15A ..H4'B	0.78	Ang.
		x, 3/2-y, 1/2+z =	4_576	Check
PLAT415_ALERT_2_G	Short Inter D-H..H-X	H17A ..H4'A	2.08	Ang.
		-1-x, 2-y, -z =	3_475	Check
PLAT415_ALERT_2_G	Short Inter D-H..H-X	H18A ..H4'A	1.47	Ang.
		-1-x, 2-y, -z =	3_475	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O4' ..C15	2.47	Ang.
		x, 3/2-y, -1/2+z =	4_575	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O4' ..C17	2.72	Ang.
		-1-x, 2-y, -z =	3_475	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O4' ..C18	2.76	Ang.
		-1-x, 2-y, -z =	3_475	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		2	Note
PLAT870_ALERT_4_G	ALERTS Related to Twinning Effects Suppressed ..		!	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
PLAT931_ALERT_5_G	CIFcalcFCF Twin Law (1 0 0)	Est.d BASF	0.17	Check
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		1	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		1.0	Low
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged		Please	Check

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

16 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
8 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check

Datablock: 9

Bond precision: C-C = 0.0091 A Wavelength=0.71073
Cell: a=18.052(3) b=14.386(3) c=10.1560(18)
alpha=90 beta=91.810(7) gamma=90
Temperature: 296 K

	Calculated	Reported
Volume	2636.2(8)	2636.3(8)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C24 H18 Hg I2 N4 O3, H2 O	?
Sum formula	C24 H20 Hg I2 N4 O4	C24 H20 Hg I2 N4 O4
Mr	882.83	882.83
Dx, g cm ⁻³	2.224	2.224
Z	4	4
Mu (mm ⁻¹)	8.217	8.217
F000	1640.0	1640.0
F000'	1627.71	
h, k, lmax	24, 19, 13	24, 19, 13
Nref	6583	6571
Tmin, Tmax	0.106, 0.193	0.385, 0.746
Tmin'	0.068	

Correction method= # Reported T Limits: Tmin=0.385 Tmax=0.746
AbsCorr = MULTI_SCAN

Data completeness= 0.998 Theta(max)= 28.350

R(reflections)= 0.0396(5056) wR2(reflections)=
0.1008(6571)
S = 1.034 Npar= 316

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
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● **Alert level C**

PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	O2	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C22	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C13	Check
PLAT260_ALERT_2_C	Large	Average Ueq of Residue Including	O4	0.145 Check
PLAT342_ALERT_3_C	Low	Bond Precision on C-C Bonds		0.00914 Ang.
PLAT414_ALERT_2_C	Short	Intra D-H..H-X H3A ..H17A .		1.94 Ang.
		x,y,z =	1_555	Check
PLAT906_ALERT_3_C	Large	K Value in the Analysis of Variance		2.570 Check
PLAT971_ALERT_2_C	Check	Calcd Resid. Dens. 0.89Ang From I2		1.68 eA-3
PLAT976_ALERT_2_C	Check	Calcd Resid. Dens. 0.59Ang From O4 .		-0.45 eA-3
PLAT977_ALERT_2_C	Check	Negative Difference Density on H4C .		-0.37 eA-3
PLAT977_ALERT_2_C	Check	Negative Difference Density on H4D .		-0.33 eA-3

● **Alert level G**

PLAT004_ALERT_5_G	Polymeric	Structure Found with Maximum Dimension	1	Info
PLAT007_ALERT_5_G	Number of	Unrefined Donor-H Atoms	4	Report
PLAT232_ALERT_2_G	Hirshfeld	Test Diff (M-X) Hg --I2 .	6.3	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	12	Note
PLAT941_ALERT_3_G	Average	HKL Measurement Multiplicity	4.0	Low
PLAT965_ALERT_2_G	The SHELXL	WEIGHT Optimisation has not Converged		Please Check
PLAT978_ALERT_2_G	Number	C-C Bonds with Positive Residual Density.	1	Info

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4 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

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 19/02/2022; check.def file version of 19/02/2022

Datablock 1 - ellipsoid plot

















