

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1, 2, 3, 4, 5, 6, 7, 8, 9

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: 1

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Bond precision:      C-C = 0.0021 Å      Wavelength=0.71073

Cell:                  a=8.7814 (14)                  b=10.5498 (16)                  c=10.9631 (16)  
                         alpha=85.121 (4)                  beta=74.166 (4)                  gamma=81.889 (4)  
Temperature:          100 K

	Calculated	Reported
Volume	966.2 (3)	966.2 (3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C44 H32 Cl2 Hg N8 O8	?
Sum formula	C44 H32 Cl2 Hg N8 O8	C44 H32 Cl2 Hg N8 O8
Mr	1072.27	1072.26
Dx, g cm <sup>-3</sup>	1.843	1.843
Z	1	1
Mu (mm <sup>-1</sup> )	4.192	4.192
F000	530.0	530.0
F000'	528.15	
h, k, lmax	11, 14, 14	11, 14, 14
Nref	4826	4816
Tmin, Tmax	0.380, 0.432	0.508, 0.746
Tmin'	0.180	

Correction method= # Reported T Limits: Tmin=0.508 Tmax=0.746  
AbsCorr = MULTI\_SCAN

Data completeness= 0.998      Theta(max)= 28.364

R(reflections)= 0.0142 ( 4815)	wR2(reflections)= 0.0368 ( 4816)
S = 1.088	Npar= 286

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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.

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### ● 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

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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

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## Datablock: 2

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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		

	Calculated	Reported
Volume	1155.78 (2)	1155.78 (2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C22 H16 Br2 Hg N4 O4	?
Sum formula	C22 H16 Br2 Hg N4 O4	C22 H16 Br2 Hg N4 O4
Mr	760.78	760.80
Dx, g cm <sup>-3</sup>	2.186	2.186
Z	2	2
Mu (mm <sup>-1</sup> )	10.153	10.153
F000	716.0	716.0
F000'	710.71	
h, k, lmax	9, 15, 19	9, 15, 19
Nref	5741	5727
Tmin, Tmax	0.024, 0.362	0.320, 0.746
Tmin'	0.012	

Correction method= # Reported T Limits: Tmin=0.320 Tmax=0.746  
AbsCorr = MULTI\_SCAN

Data completeness= 0.998                      Theta(max)= 28.297

R(reflections)= 0.0289( 5182)                      wR2(reflections)=  
0.0714( 5727)  
S = 1.070                      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 C

PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.89Ang From Hg	-2.06 eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.86Ang From Br1	-1.53 eA-3



#### Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1 Info
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.0006 Degree
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Hg --Br1 .	9.2 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Hg --Br2 .	14.5 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Hg --N4_a .	6.4 s.u.
PLAT804_ALERT_5_G	Number of ARU-Code Packing Problem(s) in PLATON	2 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	13 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	3.7 Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	3 Info

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

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

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## Datablock: 3

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Bond precision: C-C = 0.0051 A Wavelength=0.71073  
 Cell: a=9.7275(5) b=11.5101(8) c=12.4521(7)  
 alpha=106.3362(18) beta=98.0437(13) gamma=114.9454(11)  
 Temperature: 100 K

	Calculated	Reported
Volume	1158.30(12)	1158.30(12)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C22 H16 Hg I2 N4 O4	?
Sum formula	C22 H16 Hg I2 N4 O4	C22 H16 Hg I2 N4 O4
Mr	854.78	854.78
Dx, g cm-3	2.451	2.451
Z	2	2
Mu (mm-1)	9.347	9.347
F000	788.0	788.0
F000'	781.86	
h, k, lmax	11, 14, 15	11, 14, 15
Nref	4546	4540
Tmin, Tmax	0.048, 0.154	0.411, 0.746
Tmin'	0.017	

Correction method= # Reported T Limits: Tmin=0.411 Tmax=0.746  
 AbsCorr = MULTI\_SCAN

Data completeness= 0.999 Theta(max)= 25.998

R(reflections)= 0.0158( 4481) wR2(reflections)=  
 0.0397( 4540)  
 S = 1.029 Npar= 298

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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.

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 **Alert level C**

PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 7 Report

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 **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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- 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  
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
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## Datablock: 4

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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

PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Hg	--C11	.	9.8 s.u.
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 C11		(Centro SPGR)		S Verify
PLAT793_ALERT_4_G	Model has Chirality at C14		(Centro SPGR)		R Verify
PLAT793_ALERT_4_G	Model has Chirality at C15		(Centro SPGR)		S Verify
PLAT793_ALERT_4_G	Model has Chirality at C18		(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			7 Note

PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	2	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	2.8	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	3	Info

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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

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## Datablock: 5

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Bond precision:    C-C = 0.0067 Å                      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 <sup>-3</sup>	2.094	2.094
Z	4	4
Mu (mm <sup>-1</sup> )	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

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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.

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### 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 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  
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

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## Datablock: 6

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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

	Calculated	Reported
Volume	5181.22 (15)	5181.22 (15)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C48 H40 Hg2 I4 N8 O8	?
Sum formula	C48 H40 Hg2 I4 N8 O8	C48 H40 Hg2 I4 N8 O8
Mr	1765.66	1765.66
Dx, g cm <sup>-3</sup>	2.263	2.264
Z	4	4
Mu (mm <sup>-1</sup> )	8.362	8.362
F000	3280.0	3280.0
F000'	3255.42	
h, k, l <sub>max</sub>	35, 9, 36	35, 9, 36
Nref	6465	6439
Tmin, Tmax	0.102, 0.188	0.383, 0.746
Tmin'	0.065	

Correction method= # Reported T Limits: Tmin=0.383 Tmax=0.746  
AbsCorr = MULTI\_SCAN

Data completeness= 0.996                      Theta(max)= 28.339

R(reflections)= 0.0294 ( 5625)                      wR2(reflections)=  
0.0706 ( 6439)  
S = 1.033                      Npar= 317

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                      2 Report



#### Alert level G

PLAT083\_ALERT\_2\_G SHELXL Second Parameter in WGHT Unusually Large 13.85 Why ?  
 PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) Hg --I2 . 6.0 s.u.  
 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 24 Note  
 PLAT941\_ALERT\_3\_G Average HKL Measurement Multiplicity ..... 3.8 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



**test-name\_ALERT\_alert-type\_alert-level.**  
Click on the hyperlinks for more details of the test.

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PLAT414_ALERT_2_C Short Intra D-H..H-X      H3A      ..H17A      .          1.96 Ang.  
x,y,z =          1.555 Check
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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 --N1 .	7.0	s.u.
PLAT300_ALERT_4_G	Atom Site Occupancy of O4 Constrained at	0.6	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O4' Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O4" Constrained at	0.2	Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2 )	100%	Note
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?) .....	O4'	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?) .....	O4"	Check
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	24	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	6	Info

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

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|                 |                |                    |              |  |
|-----------------|----------------|--------------------|--------------|--|
| Bond precision: | C-C = 0.0154 Å | Wavelength=0.71073 |              |  |
| Cell:           | a=18.2680 (16) | b=13.9475 (11)     | c=9.9861 (8) |  |
|                 | alpha=90       | beta=91.326 (4)    | gamma=90     |  |
| Temperature:    | 296 K          |                    |              |  |

|                        | 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),<br>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 <sup>-3</sup> | 2.056                                                 | 2.060                |
| Z                      | 2                                                     | 4                    |
| Mu (mm <sup>-1</sup> ) | 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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 28 **ALERT level G** = General information/check it is not something unexpected

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

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## Datablock: 9

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Bond precision: C-C = 0.0091 Å 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 <sup>-3</sup> | 2.224                     | 2.224               |
| Z                      | 4                         | 4                   |
| Mu (mm <sup>-1</sup> ) | 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

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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.

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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   |

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### ● 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.

















