

Structure factors have been supplied for datablock(s) 4-IPy2\_HI, Buen-3-IPy2\_Br2, N-BuenI-3-IPy\_I, N\_Ace\_3-BrPy\_I, N\_Et\_3-BrPy\_I, N\_Et\_3-ClPy\_I, N\_Et\_3-IPy\_I, N\_PropI\_3-IPy\_I

No syntax errors found. CIF dictionary Interpreting this report

Bond precision:	C-C = 0.0106 A	Wavelength=0.71073		
Cell:	a=6.3486 (3)	b=10.4216 (5)	c=14.7025 (7)	
	alpha=90	beta=96.626 (4)	gamma=90	
Temperature:	293 K			

	Calculated	Reported
Volume	966.26(8)	966.26(8)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C7 H9 Cl N, I	I, C7 H9 Cl N
Sum formula	C7 H9 Cl I N	C7 H9 Cl I N
Mr	269.50	269.50
Dx, g cm <sup>-3</sup>	1.853	1.853
Z	4	4
Mu (mm <sup>-1</sup> )	3.524	3.524
F000	512.0	512.0
F000'	510.83	
h, k, lmax	7, 12, 18	7, 12, 18
Nref	1891	1878
Tmin, Tmax	0.844, 0.900	0.849, 1.000
Tmin'	0.589	

Data completeness= 0.993                      Theta (max)= 25.998

```
R(reflections)= 0.0563( 1514)      wR2(reflections)=
S = 1.097                          0.1390( 1878)
Npar= 92
```

---

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

PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C6	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	N1	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C2	Check
PLAT342_ALERT_3_C	Low	Bond Precision on C-C Bonds .....	0.0106	Ang.
PLAT360_ALERT_2_C	Short	C(sp3)-C(sp3) Bond C6 - C7	1.41	Ang.
PLAT910_ALERT_3_C	Missing #	of FCF Reflection(s) Below Theta(Min).	10	Note
PLAT911_ALERT_3_C	Missing	FCF Refl Between Thmin & STh/L= 0.600	3	Report
PLAT918_ALERT_3_C	Reflection(s)	with I(obs) much Smaller I(calc)	6	Check
PLAT939_ALERT_3_C	Large Value	of Not (SHELXL) Weight Optimized S	12.66	Check
PLAT972_ALERT_2_C	Check	Calcd Resid. Dens. 1.04A From I1	-2.35	eA-3
PLAT977_ALERT_2_C	Check	Negative Difference Density on H6B	-0.31	eA-3

---

### ● Alert level G

PLAT042_ALERT_1_G	Calc. and Reported Moiety Formula Strings Differ	Please	Check
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature .....	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature .....	293	Check
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary	Please	Do !
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF ....	2	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	3	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	3.5	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  
11 **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

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

## Datablock: N\_Et\_3-BrPy\_I

---

Bond precision:	C-C = 0.0088 A	Wavelength=0.71073
Cell:	a=6.8018(4)	b=10.2748(5) c=13.8404(8)
	alpha=90	beta=99.623(5) gamma=90
Temperature:	293 K	

PLAT042_ALERT_1_G	Calc. and Reported Moiety Formula Strings Differ	Please	Check
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature ..... (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature ..... (K)	293	Check
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	1	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	3.2	Low
PLAT960_ALERT_3_G	Number of Intensities with I < - 2*sig(I) ...	1	Check

---

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

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

---

## Datablock: N\_Et\_3-IPy\_I

---

Bond precision: C-C = 0.0040 Å

Wavelength=0.71073

Cell: a=7.8812(1) b=12.1185(2) c=10.2971(2)  
 alpha=90 beta=91.892(2) gamma=90  
 Temperature: 170 K

	Calculated	Reported
Volume	982.92(3)	982.92(3)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C7 H9 I N, I	C7 H9 I N, I
Sum formula	C7 H9 I2 N	C7 H9 I2 N
Mr	360.95	360.95
Dx, g cm <sup>-3</sup>	2.439	2.439
Z	4	4
Mu (mm <sup>-1</sup> )	6.334	6.334
F000	656.0	656.0
F000'	652.44	
h, k, lmax	11, 17, 14	11, 17, 14
Nref	2862	2860
Tmin, Tmax	0.428, 0.468	0.480, 1.000
Tmin'	0.396	

Correction method= # Reported T Limits: Tmin=0.480 Tmax=1.000  
 AbsCorr = MULTI-SCAN

Data completeness= 0.999

Theta(max)= 29.996

R(reflections)= 0.0233( 2708)

wR2(reflections)=  
0.0519( 2860)

S = 1.089

Npar= 93

---

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

PLAT434\_ALERT\_2\_B Short Inter HL..HL Contact I1      ..I2      3.47 Ang.  
x,y,z =      1\_555 Check



#### Alert level C

PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & Sth/L=      0.600      2 Report



#### Alert level G

PLAT910\_ALERT\_3\_G Missing # of FCF Reflection(s) Below Theta(Min).      1 Note  
PLAT933\_ALERT\_2\_G Number of OMIT Records in Embedded .res File ...      2 Note  
PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density.      2 Info

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

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

## Datablock: N\_Ace\_3-BrPy\_I

---

Bond precision:      C-C = 0.0078 A

Wavelength=0.71073

Cell:      a=8.8788(6)      b=7.0447(4)      c=17.4511(9)  
            alpha=90      beta=95.905(5)      gamma=90

Temperature:      293 K

	Calculated	Reported
Volume	1085.75(11)	1085.75(11)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C8 H9 Br N O, I	I, C8 H9 Br N O
Sum formula	C8 H9 Br I N O	C8 H9 Br I N O
Mr	341.96	341.97
Dx, g cm <sup>-3</sup>	2.092	2.092
Z	4	4
Mu (mm <sup>-1</sup> )	6.587	6.587
F000	640.0	640.0
F000'	637.27	
h, k, lmax	10, 8, 21	10, 8, 21
Nref	2135	2116
Tmin, Tmax	0.558, 0.590	0.244, 1.000
Tmin'	0.547	

Correction method= # Reported T Limits: Tmin=0.244 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.991                      Theta(max)= 25.999

R(reflections)= 0.0354( 1509)                      wR2(reflections)=  
S = 0.939                      Npar= 118                      0.0792( 2116)

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

PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range	6.4 Ratio
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance .....	4.402 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).	7 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600	8 Report



#### Alert level G

PLAT042_ALERT_1_G Calc. and Reported Moiety Formula Strings Differ	Please Check
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)	293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K)	293 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....	C8 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # I	2 Note
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	4 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....	1 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...	2 Note

PLAT941\_ALERT\_3\_G Average HKL Measurement Multiplicity ..... 2.6 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  
 4 **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  
 2 ALERT type 2 Indicator that the structure model may be wrong or deficient  
 6 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

---

## Datablock: 4-IPy2\_HI

---

Bond precision: C-C = 0.0085 A Wavelength=0.71073

Cell: a=6.8903(4) b=17.6755(10) c=11.3564(8)  
 alpha=90 beta=100.199(7) gamma=90

Temperature: 170 K

	Calculated	Reported
Volume	1361.24(15)	1361.24(15)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	2(C5 H4.50 I N), I	C10 H9 I2 N2, I
Sum formula	C10 H9 I3 N2	C10 H9 I3 N2
Mr	537.89	537.89
Dx, g cm <sup>-3</sup>	2.625	2.625
Z	4	4
Mu (mm <sup>-1</sup> )	6.861	6.861
F000	968.0	968.0
F000'	962.67	
h, k, lmax	8, 21, 13	8, 21, 13
Nref	2395	2392
Tmin, Tmax	0.727, 0.934	0.617, 1.000
Tmin'	0.656	

Correction method= # Reported T Limits: Tmin=0.617 Tmax=1.000  
 AbsCorr = MULTII-SCAN

Data completeness= 0.999 Theta(max)= 24.994

R(reflections)= 0.0311( 1979)

wR2(reflections)=  
0.0721( 2392)

S = 1.057

Npar= 136

The following ALERTS were generated. Each ALERT has the format

**test-name\_ALERT\_alert-type\_alert-level.**

Click on the hyperlinks for more details of the test.



### Alert level C

PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds .....	0.0085 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance .....	3.296 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.594	2 Report



### Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms .....	2 Report
PLAT042_ALERT_1_G Calc. and Reported Moiety Formula Strings Differ	Please Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1 Constrained at	0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2 Constrained at	0.5 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 1 )	11.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 2 )	11.50 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact I1 ..I3	3.50 Ang.
x,y,z =	1_555 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact I2 ..I3	3.53 Ang.
-2+x,y,1+z =	1_356 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #	2 Note
C5 H4.50 I N	
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #	3 Note
I	
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still	61% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).	2 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...	2 Note
PLAT954_ALERT_1_G Reported (CIF) and Actual (FCF) Kmax Differ by .	1 Units
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.	0 Info

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
15 **ALERT level G** = General information/check it is not something unexpected
- 2 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  
5 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: N\_PropI\_3-IPy\_I

Bond precision: C-C = 0.0116 A

Wavelength=0.71073



Cell: a=7.2177(2) b=30.4077(11) c=11.6116(4)  
 alpha=90 beta=93.483(3) gamma=90  
 Temperature: 293 K

	Calculated	Reported
Volume	2543.73(15)	2543.73(15)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C8 H10 I2 N, I	?
Sum formula	C8 H10 I3 N	C8 H10 I3 N
Mr	500.87	500.87
Dx, g cm <sup>-3</sup>	2.616	2.616
Z	8	8
Mu (mm <sup>-1</sup> )	7.330	7.330
F000	1792.0	1792.0
F000'	1781.33	
h, k, lmax	9, 40, 15	9, 40, 15
Nref	6443	106756
Tmin, Tmax	0.839, 0.864	0.521, 1.000
Tmin'	0.447	

Correction method= # Reported T Limits: Tmin=0.521 Tmax=1.000  
 AbsCorr = MULTI-SCAN

Data completeness= 16.569 Theta(max)= 28.498

R(reflections)= 0.0414( 75158) wR2(reflections)=  
 0.0893(106756)  
 S = 0.970 Npar= 218

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

PLAT434\_ALERT\_2\_B Short Inter HL..HL Contact I1 ..I5 3.49 Ang.  
 x, y, z = 1\_555 Check  
 PLAT910\_ALERT\_3\_B Missing # of FCF Reflection(s) Below Theta(Min). 25 Note



#### Alert level C

PLAT342\_ALERT\_3\_C Low Bond Precision on C-C Bonds ..... 0.01158 Ang.  
 PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 4.329 Check



#### Alert level G

PLAT199_ALERT_1_G	Reported _cell_measurement_temperature .....	(K)	293	Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature .....	(K)	293	Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact I3	..I6	3.56	Ang.
	x,y,z =		1_555	Check
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #		4	Note
	I			
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 !
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	2	Note
PLAT931_ALERT_5_G	CIFcalcFCF Twin Law	[ 1 0 0] Est.d BASF	0.16	Check
PLAT931_ALERT_5_G	CIFcalcFCF Twin Law	[ 1 0 0] Est.d BASF	0.16	Check
PLAT931_ALERT_5_G	CIFcalcFCF Twin Law	[ 1 0 0] Est.d BASF	0.16	Check
PLAT931_ALERT_5_G	CIFcalcFCF Twin Law	[ 1 0 0] Est.d BASF	0.16	Check
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...		10	Note
PLAT960_ALERT_3_G	Number of Intensities with I < - 2*sig(I) ...		10	Check

- 
- 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  
13 **ALERT level G** = General information/check it is not something unexpected
- 3 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  
4 ALERT type 3 Indicator that the structure quality may be low  
3 ALERT type 4 Improvement, methodology, query or suggestion  
4 ALERT type 5 Informative message, check
- 

## Datablock: Buen-3-IPy2\_Br2

---

Bond precision:	C-C = 0.0052 A	Wavelength=0.71073
Cell:	a=7.7257(13)	b=11.5890(18)
	alpha=90	beta=93.698(16)
		gamma=90
Temperature:	295 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
3 ALERT level G = General information/check it is not something unexpected

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

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

---

## Datablock: N-BuenI-3-IPy\_I

---

Bond precision: C-C = 0.0206 Å Wavelength=0.71073  
Cell: a=34.8020(14) b=10.3728(4) c=7.3369(3)  
alpha=90 beta=90 gamma=90  
Temperature: 170 K

|                        | Calculated     | Reported       |
|------------------------|----------------|----------------|
| Volume                 | 2648.58(18)    | 2648.58(18)    |
| Space group            | P n a 21       | P n a 21       |
| Hall group             | P 2c -2n       | P 2c -2n       |
| Moiety formula         | C9 H10 I2 N, I | C9 H10 I2 N, I |
| Sum formula            | C9 H10 I3 N    | C9 H10 I3 N    |
| Mr                     | 512.88         | 512.88         |
| Dx, g cm <sup>-3</sup> | 2.572          | 2.572          |
| Z                      | 8              | 8              |
| Mu (mm <sup>-1</sup> ) | 7.044          | 7.044          |
| F000                   | 1840.0         | 1840.0         |
| F000'                  | 1829.34        |                |
| h, k, lmax             | 42, 12, 9      | 42, 12, 9      |
| Nref                   | 5193[ 2810]    | 5018           |
| Tmin, Tmax             | 0.388, 0.494   | 0.211, 1.000   |
| Tmin'                  | 0.359          |                |

Correction method= # Reported T Limits: Tmin=0.211 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 1.79/0.97 Theta(max)= 25.998

R(reflections)= 0.0443( 4629) wR2(reflections)=  
0.1049( 5018)  
S = 1.059 Npar= 235

---

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

PLAT342\_ALERT\_3\_B Low Bond Precision on C-C Bonds ..... 0.02057 Ang.  
PLAT434\_ALERT\_2\_B Short Inter HL..HL Contact I1 ..I3 3.39 Ang.  
x,y,z = 1\_555 Check

---

### 🟢 Alert level C

PLAT910\_ALERT\_3\_C Missing # of FCF Reflection(s) Below Theta(Min). 7 Note  
PLAT977\_ALERT\_2\_C Check Negative Difference Density on H4 -0.32 eA-3

---

### 🟠 Alert level G

PLAT083\_ALERT\_2\_G SHELXL Second Parameter in WGHT Unusually Large 21.18 Why ?  
PLAT434\_ALERT\_2\_G Short Inter HL..HL Contact I4 ..I6 3.57 Ang.  
x,y,z = 1\_555 Check  
PLAT933\_ALERT\_2\_G Number of OMIT Records in Embedded .res File ... 3 Note  
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  
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  
4 **ALERT level G** = General information/check it is not something unexpected

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

---

## Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT241_N_Et_3-ClPy_I
;
PROBLEM: High 'MainMol' Ueq as Compared to Neighbors of C6 Check
RESPONSE: ...
;
_vrf_PLAT242_N_Et_3-ClPy_I
;
PROBLEM: Low 'MainMol' Ueq as Compared to Neighbors of N1 Check
RESPONSE: ...
;
_vrf_PLAT342_N_Et_3-ClPy_I
;
PROBLEM: Low Bond Precision on C-C Bonds ..... 0.0106 Ang.
RESPONSE: ...
;
_vrf_PLAT360_N_Et_3-ClPy_I
;
PROBLEM: Short C(sp3)-C(sp3) Bond C6 - C7 . 1.41 Ang.
RESPONSE: ...
;
```

```

_vrf_PLAT910_N_Et_3-ClPy_I
;
PROBLEM: Missing # of FCF Reflection(s) Below Theta(Min).      10 Note
RESPONSE: ...
;
_vrf_PLAT911_N_Et_3-ClPy_I
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L=      0.600      3 Report
RESPONSE: ...
;
_vrf_PLAT918_N_Et_3-ClPy_I
;
PROBLEM: Reflection(s) with I(obs) much Smaller I(calc) .      6 Check
RESPONSE: ...
;
_vrf_PLAT939_N_Et_3-ClPy_I
;
PROBLEM: Large Value of Not (SHELXL) Weight Optimized S .      12.66 Check
RESPONSE: ...
;
_vrf_PLAT972_N_Et_3-ClPy_I
;
PROBLEM: Check Calcd Resid. Dens.  1.04A      From I1      -2.35 eA-3
RESPONSE: ...
;
_vrf_PLAT977_N_Et_3-ClPy_I
;
PROBLEM: Check Negative Difference Density on H6B      -0.31 eA-3
RESPONSE: ...
;
_vrf_PLAT342_N_Et_3-BrPy_I
;
PROBLEM: Low Bond Precision on  C-C Bonds .....      0.0088 Ang.
RESPONSE: ...
;
_vrf_PLAT910_N_Et_3-BrPy_I
;
PROBLEM: Missing # of FCF Reflection(s) Below Theta(Min).      10 Note
RESPONSE: ...
;
_vrf_PLAT971_N_Et_3-BrPy_I
;
PROBLEM: Check Calcd Resid. Dens.  1.11A      From I1      1.84 eA-3
RESPONSE: ...
;
_vrf_PLAT972_N_Et_3-BrPy_I
;
PROBLEM: Check Calcd Resid. Dens.  0.87A      From I1      -1.80 eA-3
RESPONSE: ...
;
_vrf_PLAT911_N_Et_3-IPy_I
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L=      0.600      2 Report
RESPONSE: ...
;
_vrf_PLAT222_N_Ace_3-BrPy_I
;

```

```

PROBLEM: NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 6.4 Ratio
RESPONSE: ...
;
_vrf_PLAT906_N_Ace_3-BrPy_I
;
PROBLEM: Large K Value in the Analysis of Variance ..... 4.402 Check
RESPONSE: ...
;
_vrf_PLAT910_N_Ace_3-BrPy_I
;
PROBLEM: Missing # of FCF Reflection(s) Below Theta(Min). 7 Note
RESPONSE: ...
;
_vrf_PLAT911_N_Ace_3-BrPy_I
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L= 0.600 8 Report
RESPONSE: ...
;
_vrf_PLAT342_4-IPy2_HI
;
PROBLEM: Low Bond Precision on C-C Bonds ..... 0.0085 Ang.
RESPONSE: ...
;
_vrf_PLAT906_4-IPy2_HI
;
PROBLEM: Large K Value in the Analysis of Variance ..... 3.296 Check
RESPONSE: ...
;
_vrf_PLAT911_4-IPy2_HI
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L= 0.594 2 Report
RESPONSE: ...
;
_vrf_PLAT342_N_PropI_3-IPy_I
;
PROBLEM: Low Bond Precision on C-C Bonds ..... 0.01158 Ang.
RESPONSE: ...
;
_vrf_PLAT906_N_PropI_3-IPy_I
;
PROBLEM: Large K Value in the Analysis of Variance ..... 4.329 Check
RESPONSE: ...
;
_vrf_PLAT911_Buen-3-IPy2_Br2
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L= 0.600 2 Report
RESPONSE: ...
;
_vrf_PLAT910_N-BuenI-3-IPy_I
;
PROBLEM: Missing # of FCF Reflection(s) Below Theta(Min). 7 Note
RESPONSE: ...
;
_vrf_PLAT977_N-BuenI-3-IPy_I
;

```

PROBLEM: Check Negative Difference Density on H4

-0.32 eA-3

RESPONSE: ...

;

# end Validation Reply Form

---

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 13/07/2021; check.def file version of 13/07/2021**

















