

# checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found.      CIF dictionary      Interpreting this report

## Datablock: 3

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Bond precision:    C-C = 0.0039 A                      Wavelength=1.54184

Cell:              a=6.94004(12)      b=11.60676(13)      c=22.9171(3)  
                    alpha=90              beta=98.1622(15)      gamma=90

Temperature:      293 K

	Calculated	Reported
Volume	1827.30(5)	1827.30(5)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C17 H13 N4, C F3 O3 S	C17 H13 N4, C F3 O3 S
Sum formula	C18 H13 F3 N4 O3 S	C18 H13 F3 N4 O3 S
Mr	422.39	422.38
Dx,g cm-3	1.535	1.535
Z	4	4
Mu (mm-1)	2.122	2.122
F000	864.0	864.0
F000'	868.44	
h,k,lmax	8,14,28	8,14,28
Nref	3675	3588
Tmin,Tmax	0.832,0.863	0.751,0.890
Tmin'	0.603	

Correction method= ANALYTICAL

Data completeness= 0.976                      Theta(max)= 73.200

R(reflections)= 0.0573( 3071)              wR2(reflections)= 0.1804( 3588)

S = 1.123                                      Npar= 267

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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

PLAT244_ALERT_4_C Low	'Solvent' Ueq as Compared to Neighbors of	S1
PLAT244_ALERT_4_C Low	'Solvent' Ueq as Compared to Neighbors of	C1T
PLAT250_ALERT_2_C Large	U3/U1 Ratio for Average U(i,j) Tensor ....	2.4

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## ● Alert level G

PLAT005\_ALERT\_5\_G No \_iucr\_refine\_instructions\_details in the CIF ?  
PLAT199\_ALERT\_1\_G Check the Reported \_cell\_measurement\_temperature 293 K  
PLAT200\_ALERT\_1\_G Check the Reported \_diffn\_ambient\_temperature 293 K

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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  
3 **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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
1 ALERT type 2 Indicator that the structure model may be wrong or deficient  
0 ALERT type 3 Indicator that the structure quality may be low  
2 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 = 0.0112 Å                      Wavelength=1.54184

Cell:                      a=21.8972(10)              b=15.3474(3)              c=15.1806(7)  
                            alpha=90                      beta=130.218(8)              gamma=90

Temperature:              180 K

	Calculated	Reported
Volume	3895.6(5)	3895.6(3)
Space group	C c	Cc
Hall group	C -2yc	C -2yc
Moiety formula	C17 H14 N4, 2(C1 O4)	C17 H14 N4, 2(C1 O4)
Sum formula	C17 H14 Cl2 N4 O8	C17 H14 Cl2 N4 O8
Mr	473.22	473.22
Dx, g cm <sup>-3</sup>	1.614	1.614
Z	8	8
Mu (mm <sup>-1</sup> )	3.520	3.520
F000	1936.0	1936.0
F000'	1948.17	
h, k, lmax	27, 19, 18	27, 18, 18
Nref	3925[ 7841]	6067
Tmin, Tmax	0.607, 0.682	0.621, 0.776
Tmin'	0.525	

Correction method= ANALYTICAL

Data completeness= 1.55/0.77                      Theta(max)= 73.420

R(reflections)= 0.0637( 5830)                      wR2(reflections)= 0.1761( 6067)

S = 1.025

Npar= 562

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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 B**

PLAT340\_ALERT\_3\_B Low Bond Precision on C-C Bonds ..... 0.0112 Ang

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**Alert level C**

PLAT202\_ALERT\_3\_C Isotropic non-H Atoms in Anion/Solvent ..... 4  
PLAT234\_ALERT\_4\_C Large Hirshfeld Difference C14B -- C15B .. 0.16 Ang.  
PLAT244\_ALERT\_4\_C Low 'Solvent' Ueq as Compared to Neighbors of C11R  
PLAT731\_ALERT\_1\_C Bond Calc 1.438(11), Rep 1.438(5) ..... 2 su-Ra  
O4Q -CL1Q 1.555 1.555 # 19

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**Alert level G**

PLAT002\_ALERT\_2\_G Number of Distance or Angle Restraints on AtSite 14  
PLAT005\_ALERT\_5\_G No \_iucr\_refine\_instructions\_details in the CIF ?  
PLAT072\_ALERT\_2\_G SHELXL First Parameter in WGHT Unusually Large. 0.13  
PLAT152\_ALERT\_1\_G The Supplied and Calc. Volume s.l. Differ by ... 2 Units  
PLAT302\_ALERT\_4\_G Note: Anion/Solvent Disorder ..... 20 Perc.  
PLAT720\_ALERT\_4\_G Number of Unusual/Non-Standard Labels ..... 9  
PLAT779\_ALERT\_4\_G Suspect or Irrelevant (Bond) Angle in CIF .... # 7  
O3RB -CL1R -O3RA 1.555 1.555 1.555 41.40 Deg.  
PLAT850\_ALERT\_4\_G Check Flack Parameter Exact Value 0.00 and su .. 0.02  
PLAT860\_ALERT\_3\_G Note: Number of Least-Squares Restraints ..... 11

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

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## Datablock: 5

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Bond precision: C-C = 0.0047 A

Wavelength=1.54180

Cell: a=7.4188(5) b=10.2066(10) c=12.4306(8)  
alpha=111.463(8) beta=94.292(6) gamma=93.597(7)

Temperature: 180 K

	Calculated	Reported
Volume	869.40(13)	869.40(12)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C17 H14 Cl Li N4 O5	C17 H14 Cl Li N4 O5
Sum formula	C17 H14 Cl Li N4 O5	C17 H14 Cl Li N4 O5
Mr	396.71	396.71
Dx,g cm-3	1.515	1.515
Z	2	2
Mu (mm-1)	2.299	2.299
F000	408.0	408.0
F000'	410.01	
h,k,lmax	9,12,15	9,12,15
Nref	3516	3365
Tmin,Tmax	0.689,0.875	0.758,0.880
Tmin'	0.572	

Correction method= ANALYTICAL

Data completeness= 0.957

Theta(max)= 73.590

R(reflections)= 0.0546( 2976)

wR2(reflections)= 0.1552( 3365)

S = 1.050

Npar= 296

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

PLAT230_ALERT_2_C	Hirshfeld Test Diff for	N15	--	C14	..	5.5	su
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C19	--	C20	..	6.3	su
PLAT242_ALERT_2_C	Check Low	Ueq	as Compared to Neighbors for			C127	
PLAT340_ALERT_3_C	Low Bond Precision on	C-C Bonds	.....			0.0047	Ang



#### Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	12
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained Atom Sites ....	9
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in the CIF	?
PLAT301_ALERT_3_G	Note: Main Residue Disorder .....	14 Perc.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....	2
PLAT860_ALERT_3_G	Note: Number of Least-Squares Restraints .....	33

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



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**Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	2
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in the CIF	?
PLAT302_ALERT_4_G	Note: Anion/Solvent Disorder .....	20 Perc.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....	10
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF .... #	101
	O8SB -CL2S -O8SA    1.555    1.555    1.555	31.30 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF .... #	104
	O7SB -CL2S -O7SA    1.555    1.555    1.555	29.40 Deg.
PLAT860_ALERT_3_G	Note: Number of Least-Squares Restraints .....	1

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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  
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

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## Datablock: 7

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Bond precision: C-C = 0.0067 A

Wavelength=1.54184

Cell: a=10.0614(1) b=15.2720(2) c=19.2585(3)  
alpha=90 beta=114.150(1) gamma=90  
Temperature: 180 K

	Calculated	Reported
Volume	2700.22(6)	2700.22(6)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C23 H20 F6 N4 O7 S2 Zn	C23 H20 F6 N4 O7 S2 Zn
Sum formula	C23 H20 F6 N4 O7 S2 Zn	C23 H20 F6 N4 O7 S2 Zn
Mr	707.96	707.92
Dx, g cm <sup>-3</sup>	1.742	1.741
Z	4	4
Mu (mm <sup>-1</sup> )	3.573	3.573
F000	1432.0	1432.0
F000'	1433.53	
h,k,lmax	12,18,23	12,18,23
Nref	5423	5294
Tmin,Tmax	0.491,0.572	0.583,0.719
Tmin'	0.370	

Correction method= ANALYTICAL

Data completeness= 0.976

Theta(max)= 73.310

R(reflections)= 0.0616( 4879)

wR2(reflections)= 0.1633( 5294)

S = 1.028

Npar= 372

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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 B

PLAT201\_ALERT\_2\_B Isotropic non-H Atoms in Main Residue(s) ..... 7

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#### Alert level C

PLAT241\_ALERT\_2\_C Check High Ueq as Compared to Neighbors for 04T  
PLAT241\_ALERT\_2\_C Check High Ueq as Compared to Neighbors for 05T  
PLAT341\_ALERT\_3\_C Low Bond Precision on C-C Bonds ..... 0.0067 Ang

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#### Alert level G

PLAT002\_ALERT\_2\_G Number of Distance or Angle Restraints on AtSite 3  
PLAT005\_ALERT\_5\_G No \_iucr\_refine\_instructions\_details in the CIF ?  
PLAT083\_ALERT\_2\_G SHELXL Second Parameter in WGHT Unusually Large. 8.13  
PLAT242\_ALERT\_2\_G Check Low Ueq as Compared to Neighbors for S2TA  
PLAT242\_ALERT\_2\_G Check Low Ueq as Compared to Neighbors for S2TB  
PLAT301\_ALERT\_3\_G Note: Main Residue Disorder ..... 16 Perc.  
PLAT434\_ALERT\_2\_G Short Inter HL..HL Contact F1T .. F5TB . 2.77 Ang.  
PLAT720\_ALERT\_4\_G Number of Unusual/Non-Standard Labels ..... 28  
PLAT793\_ALERT\_4\_G The Model has Chirality at S2TA (Verify) .... S  
PLAT811\_ALERT\_5\_G No ADDSYM Analysis: Too Many Excluded Atoms .... !  
PLAT860\_ALERT\_3\_G Note: Number of Least-Squares Restraints ..... 2

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

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

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## Datablock: 8

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Bond precision: C-C = 0.0048 A

Wavelength=1.54180

Cell: a=12.7973(4) b=13.0890(3) c=22.9289(7)  
alpha=76.931(2) beta=86.061(2) gamma=84.064(2)

Temperature: 180 K

	Calculated	Reported
Volume	3717.07(19)	3717.06(18)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C34 H24 N8 Zn, 2(C F3 O3 S), 0.13(H2 O)	1(C34 H24 N8 Zn), 2(C F3 O3 S), 0.13(H2 O)
Sum formula	C36 H24.25 F6 N8 O6.13 S2 Zn	C36 H24.25 F6 N8 O6.12 S2 Zn
Mr	910.41	910.37
Dx,g cm-3	1.627	1.627
Z	4	4
Mu (mm-1)	2.767	2.767
F000	1845.0	1845.0
F000'	1847.67	
h,k,lmax	15,16,28	15,16,28
Nref	14935	14506
Tmin,Tmax	0.750,0.900	0.524,0.900
Tmin'	0.423	

Correction method= ANALYTICAL

Data completeness= 0.971                      Theta(max)= 73.290

R(reflections)= 0.0484( 12329)              wR2(reflections)= 0.1312( 14506)

S = 1.013                                      Npar= 1225

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	?
PLAT077_ALERT_4_C	Unitcell contains non-integer number of atoms	..	?
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	....	2.11
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C19A -- C20A ..	5.8 su
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C31A -- C32A ..	0.18 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	S9B -- C0AA ..	0.18 Ang.
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of		S1
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of		C5B
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of		S17
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of		C1D
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of		S25
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of		C1C
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	....	2.2
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	....	2.5
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	....	3.0
PLAT601_ALERT_2_C	Structure Contains Solvent Accessible VOIDS of	.	46 A**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: C36 H24.25 F6 N8 O6.12 S2 Z

Atom count from \_chemical\_formula\_moiety:C36 H24.26 F6 N8 O6.13 S2 Z

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite				50
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained Atom Sites ....				18
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in the CIF				?
PLAT007_ALERT_5_G	Note: Number of Unrefined D-H Atoms .....				2
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ				?
PLAT093_ALERT_1_G	No su's on H-positions, refinement reported as .			mixed	
PLAT154_ALERT_1_G	The su's on the Cell Angles are Equal .....			0.00200 Deg.	
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent) S9B -- O10B ..			6.8 su	
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent) S9B -- O11A ..			6.0 su	
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent) S9B -- O12B ..			21.9 su	
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of			C0AA	
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of			S9A	
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of			C1E	
PLAT301_ALERT_3_G	Note: Main Residue Disorder .....			24 Perc.	
PLAT302_ALERT_4_G	Note: Anion/Solvent Disorder .....			26 Perc.	
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....			1	
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C32B -- C31B .			1.86 Ang.	
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms ....			!	
PLAT860_ALERT_3_G	Note: Number of Least-Squares Restraints .....			290	

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5 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  
2 ALERT type 3 Indicator that the structure quality may be low  
17 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 = 0.0112 A

Wavelength=1.54184

Cell: a=9.9524(4) b=13.0566(5) c=14.5815(6)  
alpha=91.029(3) beta=90.220(3) gamma=92.195(3)

Temperature: 180 K

	Calculated	Reported
Volume	1893.07(13)	1893.07(14)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C34 H24 Cl2 N8 Y, I3, C H2 Cl2	C34 H24 Cl2 N8 Y, I3, C H2 Cl2
Sum formula	C35 H26 Cl4 I3 N8 Y	C35 H26 Cl4 I3 N8 Y
Mr	1170.05	1170.05
Dx,g cm-3	2.053	2.053
Z	2	2
Mu (mm-1)	24.289	24.289
F000	1116.0	1116.0
F000'	1119.19	
h,k,lmax	12,16,18	12,16,18
Nref	7615	7379
Tmin,Tmax	0.201,0.346	0.097,0.422
Tmin'	0.006	

Correction method= ANALYTICAL

Data completeness= 0.969                      Theta(max)= 73.400


R(reflections)= 0.0573( 6770)              wR2(reflections)= 0.1689( 7379)


S = 1.119                                      Npar= 463

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 ..... 0.0112 Ang

 **Alert level G**  
 PLAT005\_ALERT\_5\_G No \_iucr\_refine\_instructions\_details in the CIF ?  
 PLAT083\_ALERT\_2\_G SHELXL Second Parameter in WGHT Unusually Large. 9.22  
 PLAT154\_ALERT\_1\_G The su's on the Cell Angles are Equal ..... 0.00300 Deg.  
 PLAT720\_ALERT\_4\_G Number of Unusual/Non-Standard Labels ..... 2

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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*, 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.

