
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 C01U --C01W . 6.0 s.u.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.376 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 59 Report

-2	1	0,	-1	1	0,	-10	3	0,	-10	4	0,	-10	5	0,	-5	6	0,
-2	11	0,	-7	14	0,	2	-7	1,	10	-4	1,	10	-3	1,	-10	4	1,
-3	6	1,	10	-5	2,	10	-4	2,	2	-2	2,	0	-1	2,	-1	0	2,
-1	1	2,	-2	6	2,	-2	-3	3,	0	-1	3,	2	-1	4,	-1	1	4,
3	1	4,	-10	4	4,	0	5	4,	10	-3	5,	-2	-2	5,	-1	-1	5,
3	0	5,	-2	2	5,	-7	-12	6,	0	2	6,	-6	14	6,	0	-1	7,
-2	0	7,	-3	1	7,	-2	1	8,	-2	0	9,	-10	2	9,	-10	-1	10,
-3	0	10,	-2	3	10,	-1	-1	11,	0	-1	12,	0	-2	13,	-3	-1	13,
3	8	17,	3	7	18,	3	-13	19,	3	6	19,	3	-12	20,	2	6	20,
3	-11	21,	-4	2	21,	-3	5	22,	-4	-8	23,	-3	-2	25,			



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: C11 H10 Cl.09 N1 O1
Atom count from _chemical_formula_moiety: C10.98 H7.02 N1.26

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: C11 H10 Cl.09 N1 O1
Atom count from the _atom_site data: C11.09090 H7.090909 N1.272727

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.

CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
symmetry error - see SYMMG tests
From the CIF: _cell_formula_units_Z 11
From the CIF: _chemical_formula_sum C11 H10 Cl0.09 N O
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	121.00	122.00	-1.00
H	110.00	78.00	32.00
Cl	0.99	0.00	0.99
N	11.00	14.00	-3.00
O	11.00	0.00	11.00

PLAT041_ALERT_1_G Calc. and Reported SumFormula Strings Differ Please Check
Calc: C11.09 H7.09 N1.27
Rep.: C11 H10 Cl0.09 N O

PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
Calc: C61 H39 N7
Rep.: 0.18(C61 H39 N7)

PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.182 Check

PLAT051_ALERT_1_G Mu(calc) and Mu(cif) Ratio Differs from 1.0 by . 40.08 %

PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.11 Report

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

PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C00A -C00J . 1.44 Ang.

PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ! Info

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PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 107 Note
      N003   N004   N005   N006   N007   C008   C009   C00A
      C00B   C00C   C00D   C00E   C00F   C00G   C00H   C00I
      C00J   C00K   C00L   C00M   H00M   C00N   C00O   C00P
      C00Q   C00R   C00S   C00T   H00T   C00U   H00U   C00V
      C00X   H00X   C00Y   H00Y   C00Z   H00Z   C010   H010
      C011   C012   H012   C013   C014   C015   C016   H016
      C017   H017   C018   H018   C019   H019   C01A   H01A
      C01B   H01B   C01C   H01C   C01D   H01D   C01E   H01E
      C01F   C01G   H01G   C01H   H01H   C01I   H01I   C01J
      C01K   H01K   N01L   C01M   H01F   H01J   H01L   C01N
      C01O   H01O   C01P   C01Q   H01M   H01N   H01P   C01R
      H01Q   H01R   H01S   C01S   H01T   C01T   H01U   C01U
      H01V   C01V   H01W   C01W   H01X   N01X   C01Z   C02I
      H02A   H02B   H02C

PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed      ! Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600      590 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File      33 Note
      -3  0 10,    0  5  4,   -5  6  0,   -2 11  0,   -2 -2  5,    2 -7  1,
      2 -2  2,   -2  6  2,   -1  0  2,    2 -1  4,    0 -1  7,    0  2  6,
      -2 -3  3,   -2  0  7,   -1  1  2,   -3 -1 13,   -1 -1  5,    0 -1 12,
      0 -1  3,   -2  2  5,   -1  1  0,   -3  1  7,   -1 -1 11,   -2  0  9,
      -1  1  4,   -2  3 10,   -3  6  1,    0 -1  2,   -2  1  8,    0 -2 13,
      -2  1  0,    3  0  5,    3  1  4,

PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 3.4 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 3.168 Note
      Predicted wR2: Based on SigI**2 5.26 or SHELX Weight 17.76
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.      0 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by      2 Check

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

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

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Validation response form

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

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# start Validation Reply Form
_vrf_PLAT230_exp_10189_auto
;
PROBLEM: Hirshfeld Test Diff for      C01U      --C01W      .      6.0 s.u.
RESPONSE: ...
;
_vrf_PLAT906_exp_10189_auto
;
PROBLEM: Large K Value in the Analysis of Variance ..... 2.376 Check
RESPONSE: ...

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;
_vrf_PLAT911_exp_10189_auto
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L=      0.600      59 Report
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 22/08/2024; check.def file version of 21/08/2024

