

PLAT242_ALERT_2_A	Check	Low	Ueq as Compared to Neighbors for	Mo6A
PLAT242_ALERT_2_A	Check	Low	Ueq as Compared to Neighbors for	C131
PLAT242_ALERT_2_A	Check	Low	Ueq as Compared to Neighbors for	C133
PLAT242_ALERT_2_A	Check	Low	Ueq as Compared to Neighbors for	A12
PLAT242_ALERT_2_A	Check	Low	Ueq as Compared to Neighbors for	C210
PLAT242_ALERT_2_A	Check	Low	Ueq as Compared to Neighbors for	C230
PLAT242_ALERT_2_A	Check	Low	Ueq as Compared to Neighbors for	C232
PLAT234_ALERT_4_A	Large	Hirshfeld	Difference F2 -- C111 ..	0.33 Ang.
PLAT234_ALERT_4_A	Large	Hirshfeld	Difference F25 -- C133 ..	0.31 Ang.
PLAT234_ALERT_4_A	Large	Hirshfeld	Difference F62 -- C233 ..	0.35 Ang.
PLAT234_ALERT_4_A	Large	Hirshfeld	Difference C230 -- C233 ..	0.36 Ang.

Alert level B

PLAT230_ALERT_2_B	Hirshfeld	Test	Diff for F19 -- C131 ..	8.71 su
PLAT230_ALERT_2_B	Hirshfeld	Test	Diff for F65 -- C241 ..	7.66 su
PLAT232_ALERT_2_B	Hirshfeld	Test	Diff (M-X) Mo6A -- C37A ..	11.56 su
PLAT241_ALERT_2_B	Check	High	Ueq as Compared to Neighbors for	C5
PLAT241_ALERT_2_B	Check	High	Ueq as Compared to Neighbors for	O204
PLAT242_ALERT_2_B	Check	Low	Ueq as Compared to Neighbors for	Mo1
PLAT242_ALERT_2_B	Check	Low	Ueq as Compared to Neighbors for	Mo5B
PLAT242_ALERT_2_B	Check	Low	Ueq as Compared to Neighbors for	Mo6B
PLAT242_ALERT_2_B	Check	Low	Ueq as Compared to Neighbors for	All
PLAT242_ALERT_2_B	Check	Low	Ueq as Compared to Neighbors for	C110
PLAT242_ALERT_2_B	Check	Low	Ueq as Compared to Neighbors for	C113
PLAT242_ALERT_2_B	Check	Low	Ueq as Compared to Neighbors for	C122
PLAT242_ALERT_2_B	Check	Low	Ueq as Compared to Neighbors for	C132
PLAT242_ALERT_2_B	Check	Low	Ueq as Compared to Neighbors for	C220
PLAT242_ALERT_2_B	Check	Low	Ueq as Compared to Neighbors for	C222
PLAT242_ALERT_2_B	Check	Low	Ueq as Compared to Neighbors for	C223
PLAT242_ALERT_2_B	Check	Low	Ueq as Compared to Neighbors for	C241
PLAT242_ALERT_2_B	Check	Low	Ueq as Compared to Neighbors for	C242
PLAT234_ALERT_4_B	Large	Hirshfeld	Difference F3 -- C111 ..	0.25 Ang.
PLAT234_ALERT_4_B	Large	Hirshfeld	Difference F20 -- C131 ..	0.28 Ang.
PLAT234_ALERT_4_B	Large	Hirshfeld	Difference F24 -- C132 ..	0.29 Ang.
PLAT234_ALERT_4_B	Large	Hirshfeld	Difference F30 -- C141 ..	0.27 Ang.
PLAT234_ALERT_4_B	Large	Hirshfeld	Difference F39 -- C211 ..	0.28 Ang.

Alert level C

RFACR01_ALERT_3_C The value of the weighted R factor is > 0.25
 Weighted R factor given 0.265

PLAT084_ALERT_2_C	High	R2 Value	0.26
PLAT213_ALERT_2_C	Atom	P5B	has ADP max/min Ratio	3.20 prola
PLAT213_ALERT_2_C	Atom	F4	has ADP max/min Ratio	3.60 prola
PLAT213_ALERT_2_C	Atom	F22	has ADP max/min Ratio	3.10 oblat
PLAT213_ALERT_2_C	Atom	F44	has ADP max/min Ratio	3.10 prola
PLAT213_ALERT_2_C	Atom	F61	has ADP max/min Ratio	3.10 prola
PLAT213_ALERT_2_C	Atom	F67	has ADP max/min Ratio	3.20 prola
PLAT220_ALERT_2_C	Large	Non-Solvent	C Ueq(max)/Ueq(min) ...	3.45 Ratio
PLAT220_ALERT_2_C	Large	Non-Solvent	O Ueq(max)/Ueq(min) ...	3.92 Ratio
PLAT220_ALERT_2_C	Large	Non-Solvent	C Ueq(max)/Ueq(min) ...	3.18 Ratio
PLAT222_ALERT_3_C	Large	Non-Solvent	H Ueq(max)/Ueq(min) ...	3.46 Ratio
PLAT230_ALERT_2_C	Hirshfeld	Test	Diff for F27 -- C133 ..	5.11 su
PLAT230_ALERT_2_C	Hirshfeld	Test	Diff for F56 -- C231 ..	6.49 su
PLAT230_ALERT_2_C	Hirshfeld	Test	Diff for C210 -- C212 ..	5.14 su
PLAT232_ALERT_2_C	Hirshfeld	Test	Diff (M-X) Mo5A -- C29A ..	7.66 su
PLAT232_ALERT_2_C	Hirshfeld	Test	Diff (M-X) Mo5A -- C30A ..	5.77 su
PLAT232_ALERT_2_C	Hirshfeld	Test	Diff (M-X) Mo6A -- P6A ..	6.14 su
PLAT232_ALERT_2_C	Hirshfeld	Test	Diff (M-X) Mo6A -- C36A ..	8.86 su
PLAT232_ALERT_2_C	Hirshfeld	Test	Diff (M-X) Mo6A -- C38A ..	7.48 su

PLAT241_ALERT_2_C	Check High	Ueq as Compared to Neighbors for	P2
PLAT241_ALERT_2_C	Check High	Ueq as Compared to Neighbors for	C2
PLAT241_ALERT_2_C	Check High	Ueq as Compared to Neighbors for	C4
PLAT241_ALERT_2_C	Check High	Ueq as Compared to Neighbors for	C7
PLAT241_ALERT_2_C	Check High	Ueq as Compared to Neighbors for	C8
PLAT241_ALERT_2_C	Check High	Ueq as Compared to Neighbors for	C15
PLAT241_ALERT_2_C	Check High	Ueq as Compared to Neighbors for	O101
PLAT241_ALERT_2_C	Check High	Ueq as Compared to Neighbors for	O102
PLAT241_ALERT_2_C	Check High	Ueq as Compared to Neighbors for	O103
PLAT241_ALERT_2_C	Check High	Ueq as Compared to Neighbors for	C111
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for	In1
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for	Mo2
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for	Mo5A
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for	C40A
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for	C112
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for	C120
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for	C121
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for	C123
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for	C130
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for	C140
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for	C143
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for	C212
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for	C213
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for	C221
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for	C240
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for	C243
PLAT313_ALERT_2_C	Oxygen with three covalent bonds (rare)		O14A
PLAT313_ALERT_2_C	Oxygen with three covalent bonds (rare)		O14B
PLAT313_ALERT_2_C	Oxygen with three covalent bonds (rare)		O16A
PLAT313_ALERT_2_C	Oxygen with three covalent bonds (rare)		O16B
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds (x 1000) Ang ..		19
PLAT431_ALERT_2_C	Short Inter HL..A Contact F23 .. O14B ..		2.84 Ang.
PLAT431_ALERT_2_C	Short Inter HL..A Contact F38 .. O14A ..		2.87 Ang.
PLAT432_ALERT_2_C	Short Inter X..Y Contact F59 .. C36B ..		2.87 Ang.
PLAT141_ALERT_4_C	su on a - Axis Small or Missing (x 100000)		30 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference Mo5A -- C31A ..		0.16 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference Mo5A -- C32A ..		0.16 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference Mo5A -- C33A ..		0.16 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference Mo5A -- C39A ..		0.18 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference Mo5A -- C40A ..		0.16 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference Mo6A -- C34A ..		0.18 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference O5 -- C25 ..		0.17 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference O9A -- C39A ..		0.21 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C1 -- C2 ..		0.23 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C1 -- C5 ..		0.23 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C2 -- C3 ..		0.18 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C15 -- C16 ..		0.16 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C17 -- C18 ..		0.15 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C20 -- C21 ..		0.16 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference F10 -- C121 ..		0.19 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference F32 -- C142 ..		0.19 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C110 -- C112 ..		0.19 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C120 -- C123 ..		0.15 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C130 -- C131 ..		0.17 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C140 -- C141 ..		0.18 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference F37 -- C211 ..		0.22 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference F40 -- C212 ..		0.22 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference F59 -- C232 ..		0.23 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference F66 -- C241 ..		0.18 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference F67 -- C242 ..		0.23 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C210 -- C211 ..		0.25 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C220 -- C222 ..		0.16 Ang.

● **Alert level G**

PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large..	0.19
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.	9.06
PLAT301_ALERT_3_G Note: Main Residue Disorder	23.00 Perc.
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints	475
PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus.	P2
PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus.	P4
PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus.	<P5B
PLAT605_ALERT_4_G Structure Contains Solvent Accessible VOIDS of .	144.00 A**3
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels	2
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms	!

14 **ALERT level A** = In general: serious problem

23 **ALERT level B** = Potentially serious problem

83 **ALERT level C** = Check and explain

10 **ALERT level G** = General alerts; check

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

81 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

43 ALERT type 4 Improvement, methodology, query or suggestion

1 ALERT type 5 Informative message, check

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.

PLATON version of 13/08/2009; check.def file version of 12/08/2009

Datablock sw204V - ellipsoid plot

