

## 5. APPLICATIONS

Table A5.7.2.2 (cont.).

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Test name	Type	Purpose
PLAT320	2	Hybridization problem on C in main residue(s)
PLAT321	2	Hybridization problem on C in solvent/ion
PLAT322	2	Hybridization problem on non-C in main residue(s)
PLAT323	2	Hybridization problem on non-C in solvent/ion
PLAT324	2	Check for possibly missing H on coordinating X—N—X in main residue
PLAT325	2	Check for possibly missing H on coordinating X—N—X in solvent/anion
PLAT326	2	Check for possibly missing hydrogen atom on carbon with $sp^3$ -like geometry in the main residue
PLAT327	2	Check for possibly missing hydrogen atom on carbon with $sp^3$ -like geometry in the solvent/anion
PLAT328	2	Check for possibly missing H on potentially $sp^3$ P
PLAT330	2	Check average phenyl C—C
PLAT331	2	Check average phenyl C—C
PLAT332	2	Check phenyl C—C range
PLAT333	2	Check average in multiply substituted benzene C—C
PLAT334	2	Check average in multiply substituted benzene C—C
PLAT335	2	Check multiply substituted benzene C—C range
PLAT338	2	Check average torsion angle in cyclohexane ring
PLAT340	3	Check bond precision for C—C in light-atom structures [ $Z(\max) < 20$ ]
PLAT341	3	Check bond precision for C—C in structures [ $19 < Z(\max) < 40$ ]
PLAT342	3	Check bond precision for C—C in structures [ $Z(\max) > 39$ ]
PLAT350	3	Test for short C—H (ångstrom difference) XRAY: 0.96
PLAT351	3	Test for long C—H (ångstrom difference) XRAY: 0.96
PLAT352	3	Test for short N—H (ångstrom difference) XRAY: 0.87
PLAT353	3	Test for long N—H (ångstrom difference) XRAY: 0.87
PLAT354	3	Test for short O—H (ångstrom difference) XRAY: 0.82
PLAT355	3	Test for long O—H (ångstrom difference) XRAY: 0.82
PLAT360	2	Test for short C4—C4 (ångstrom difference) XRAY: 1.54
PLAT361	2	Test for long C4—C4 (ångstrom difference) XRAY: 1.54
PLAT362	2	Test for short C4—C3 (ångstrom difference) XRAY: 1.52
PLAT363	2	Test for long C4—C3 (ångstrom difference) XRAY: 1.52
PLAT364	2	Test for short C4—C2 (ångstrom difference) XRAY: 1.46
PLAT365	2	Test for long C4—C2 (ångstrom difference) XRAY: 1.46
PLAT366	2	Test for short C?—C? (ångstrom difference) XRAY: 1.50
PLAT367	2	Test for long C?—C? (ångstrom difference) XRAY: 1.50
PLAT368	2	Test for short C3—C3 (ångstrom difference) XRAY: 1.34
PLAT369	2	Test for long C3—C3 (ångstrom difference) XRAY: 1.34
PLAT370	2	Test for short C3—C2 (ångstrom difference) XRAY: 1.31
PLAT371	2	Test for long C3—C2 (ångstrom difference) XRAY: 1.31
PLAT372	2	Test for short C2—C2 (ångstrom difference) XRAY: 1.25
PLAT373	2	Test for long C2—C2 (ångstrom difference) XRAY: 1.25
PLAT374	2	Test for long N—N bond ( $> 1.45$ Å)
PLAT380	4	Test for incorrectly oriented methyl moiety
PLAT390	3	Test methyl moiety X—C—H bond angle
PLAT391	3	Test methyl moiety H—C—H bond angle
PLAT395	2	Test X—O—Y angle
PLAT396	2	Test Si—O—Si angle
PLAT410	2	Test for short non-bonding intra H···H contacts
PLAT411	2	Test for short non-bonding inter H···H contacts
PLAT412	2	Test for short non-bonding intra H···H contacts (involving XH3)
PLAT413	2	Test for short non-bonding inter H···H contacts (involving XH3)
PLAT414	2	Test for short non-bonding intra D—H···H—X contacts
PLAT415	2	Test for short non-bonding inter D—H···H—X contacts
PLAT416	2	Test for short non-bonding intra D—H···H—D contacts
PLAT417	2	Test for short non-bonding inter D—H···H—D contacts
PLAT420	2	Test for D—H without acceptor
PLAT430	2	Test for short non-bonding inter D···A contacts
PLAT431	2	Test for short non-bonding inter HL···A contacts (HL = halogen)
PLAT432	2	Test for short non-bonding inter X···Y contacts
PLAT433	4	Test for short non-bonding minor···minor inter X···Y contacts
PLAT480	4	Test for too large H···A
PLAT481	4	Test for too large D···A
PLAT482	4	Test for too small D—H···A angle
PLAT601	2	Test for solvent accessible voids
PLAT602	4	Test for too large solvent accessible voids
PLAT603	4	Test for too large unit cell for void search
PLAT604	4	Test for too many voids
PLAT701	1	Test for consistency of bonds and coordinates in CIF
PLAT702	1	Test for consistency of angles and coordinates in CIF
PLAT703	1	Test for consistency of torsions and coordinates in CIF
PLAT704	1	Test for consistency of contact distances and coordinates in CIF
PLAT705	1	Test for consistency of H-bond D—H distances and coordinates in CIF
PLAT706	1	Test for consistency of H-bond H···A distances and coordinates in CIF
PLAT707	1	Test for consistency of H-bond D···A distances and coordinates in CIF
PLAT708	1	Test for consistency of H-bond D—H···A angles and coordinates in CIF
PLAT710	4	Test for linear torsions in CIF
PLAT711	1	Test for label problem for bonds in CIF
PLAT712	1	Test for label problem for angles in CIF
PLAT713	1	Test for label problem for torsions in CIF
PLAT714	1	Test for label problem for contact distances in CIF
PLAT715	1	Test for label problem for H-bond D—H distances in CIF
PLAT716	1	Test for label problem for H-bond H···A distances in CIF
PLAT717	1	Test for label problem for H-bond D···A distances in CIF

Test name	Type	Purpose
PLAT718	1	Test for label problem for H-bond D—H···A angles in CIF
PLAT720	4	Test for unusual labels
PLAT721	1	Test for consistency of bonds and coordinates in CIF
PLAT722	1	Test for consistency of angles and coordinates in CIF
PLAT723	1	Test for consistency of torsions and coordinates in CIF
PLAT724	1	Test for consistency of contact distances and coordinates in CIF
PLAT725	1	Test for consistency of H-bond D—H distances and coordinates in CIF
PLAT726	1	Test for consistency of H-bond H···A distances and coordinates in CIF
PLAT727	1	Test for consistency of H-bond D···A distances and coordinates in CIF
PLAT728	1	Test for consistency of H-bond D—H···A angles and coordinates in CIF
PLAT731	1	Test for consistency of bond s.u.'s and coordinate s.u.'s in CIF
PLAT732	1	Test for consistency of angle s.u.'s and coordinate s.u.'s in CIF
PLAT733	1	Test for consistency of torsion s.u.'s and coordinate s.u.'s in CIF
PLAT734	1	Test for consistency of contact distance s.u.'s and coordinate s.u.'s in CIF
PLAT735	1	Test for consistency of H-bond D—H distance s.u.'s and coordinate s.u.'s in CIF
PLAT736	1	Test for consistency of H-bond H···A distance s.u.'s and coordinate s.u.'s in CIF
PLAT737	1	Test for consistency of H-bond D···A distance s.u.'s and coordinate s.u.'s in CIF
PLAT738	1	Test for consistency of H-bond D—H···A angle s.u.'s and coordinate s.u.'s in CIF
PLAT741	1	Test for missing bond s.u. in CIF
PLAT742	1	Test for missing angle s.u. in CIF
PLAT743	1	Test for missing torsion s.u. in CIF
PLAT744	1	Test for missing contact distance s.u. in CIF
PLAT745	1	Test for missing H-bond D—H distance s.u. in CIF
PLAT746	1	Test for missing H-bond H···A distance s.u. in CIF
PLAT747	1	Test for missing H-bond D···A distance s.u. in CIF
PLAT748	1	Test for missing H-bond D—H···A angle s.u. in CIF
PLAT751	4	Test for senseless bond s.u. in CIF
PLAT752	4	Test for senseless angle s.u. in CIF
PLAT753	4	Test for senseless torsion s.u. in CIF
PLAT754	4	Test for senseless contact distance s.u. in CIF
PLAT755	4	Test for senseless H-bond D—H distance s.u. in CIF
PLAT756	4	Test for senseless H-bond H···A distance s.u. in CIF
PLAT757	4	Test for senseless H-bond D···A distance s.u. in CIF
PLAT758	4	Test for senseless H-bond D—H···A angle s.u. in CIF
PLAT761	1	Test for the presence of at least one X—H in the CIF
PLAT762	1	Test for at least one X—Y—H or H—Y—H entry in the CIF
PLAT763	1	Test for missing bonds in CIF
PLAT764	4	Test for overcomplete bonds in CIF
PLAT770	2	Test for suspect C—H bonds in CIF (not caught otherwise)
PLAT771	2	Test for suspect N—H bonds in CIF (not caught otherwise)
PLAT772	2	Test for suspect O—H bonds in CIF (not caught otherwise)
PLAT773	2	Test for suspect C—C bonds in CIF (not caught otherwise)
PLAT779	2	Test for suspect angle in CIF (not caught otherwise)
PLAT780	2	Test whether coordinates form a connected set
PLAT790	4	Test whether c.g. residue in unit-cell box
PLAT798	4	Test for alphanumeric label on coordinate record
PLAT799	4	Test for alphanumeric label on displacement-parameter record
PLAT801	4	Test for missing, incomplete or out-of-order cell data
PLAT802	1	Test for input lines longer than 80 characters
PLAT803	1	Test for loop problem in CIF-read
PLAT804	4	Test for ARU-pack problem in PLATON
PLAT805	4	Test for insufficient coordinate data
PLAT806	4	Test for insufficient $U_{ij}$ data
PLAT810	4	Test for out-of-memory problem
PLAT850	4	Test for BASF/TWIN problem in SHELXL

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