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*Australian Journal of Chemistry –
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Department of Chemistry
University of Western Australia
35 Stirling Highway
Crawley
Western Australia 6009
Australia

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_publ_contact_author_email          bws@crystal.uwa.edu.au
_publ_contact_author_fax            (+61)_08_9380_1118
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'Skelton, Brian W.' .
; Department of Chemistry,
University of Western Australia,
35 Stirling Highway,
Crawley,
WA 6009,
Australia.
;

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text
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  Sheldrick, G M. (1996). SADABS. Program for Empirical Absorption
  Correction
  of Area Detector Data. University of Gottingen, Germany.

  Siemens (1995). SMART and SAINT. Area-Detector Control and Integration
  Software. Siemens Analytical X-ray Systems Inc., Madison, Wisconsin,
  USA.

  Hall, S.R., King, G.S.D., and Stewart., J.M. (1995).
  The Xtal 3.5 User's Manual. University of Western Australia, Lamb:
  Perth.
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1/2-x,-y,1/2+z 1/2+x,1/2-y,-z 1/2-x,+y,-z

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3. Information for the "methods" section

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4. Supplementary data for validation and tables

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O	?	0	48	.008	.006	'Int Tables Vol IV Tables 2.2B and 2.3.1'

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O22'	.801(3)	.341(3)	.5739(11)	.034(7)	Uiso	?	?	.238(17)	?
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C23'	.670(2)	.506(2)	.5710(7)	.018(6)	Uiso	?	?	.238(17)	?
C24'	.5457(16)	.4516(17)	.5617(5)	.012(6)	Uiso	?	?	.238(17)	?
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C25'	.428(3)	.509(3)	.5508(11)	.031(8)	Uiso	?	?	.238(17)	?
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O25'	.421(3)	.625(3)	.5749(12)	.044(8)	Uiso	?	?	.238(17)	?
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H15	.79840	.84954	.68454	.04400	Uiso	?	?	1.00000	?
H16a	.63871	.88745	.74270	.04200	Uiso	?	?	1.00000	?
H16b	.62799	.74443	.74890	.04200	Uiso	?	?	1.00000	?
H17a	.86741	.75531	.76342	.04500	Uiso	?	?	1.00000	?
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H181c	.57846	.85060	.82193	.07500	Uiso	?	?	1.00000	?
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H24	.65452	.59754	.56401	.05500	Uiso	?	?	.762(17)	?
H25	.40019	.48430	.55871	.04400	Uiso	?	?	.762(17)	?
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H26b	.51648	.62373	.49052	.06900	Uiso	?	?	1.00000	?
H27a	.50245	.38961	.48813	.06500	Uiso	?	?	1.00000	?
H27b	.35737	.41069	.47367	.06500	Uiso	?	?	1.00000	?
H28	.46605	.38787	.41085	.05500	Uiso	?	?	1.00000	?
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H24'	.55203	.36035	.56148	.06000	Uiso	?	?	.238(17)	?
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C12	.044(3)	.041(3)	.013(2)	.007(2)	.003(2)	-.003(2)
O12	.051(2)	.051(2)	.033(2)	.0025(19)	.0049(17)	.0047(18)
C13	.046(3)	.040(3)	.026(3)	-.003(2)	-.004(2)	.003(2)
C14	.039(3)	.050(3)	.015(3)	.003(2)	.004(2)	.001(2)
C15	.039(3)	.043(3)	.021(3)	-.003(2)	-.003(2)	.004(2)
O15	.064(2)	.047(2)	.036(2)	.000(2)	-.0211(19)	.0027(16)
C16	.041(2)	.038(3)	.027(3)	.001(2)	-.002(2)	-.005(2)
C17	.046(3)	.043(3)	.025(3)	-.009(2)	-.000(2)	.002(2)
C18	.061(3)	.036(3)	.018(3)	-.010(2)	-.002(2)	-.001(2)
C181	.091(5)	.047(3)	.021(3)	-.003(3)	.008(3)	-.001(2)
O21	.043(4)	.044(5)	.022(3)	.005(4)	.000(2)	.005(3)

C22	.058(6)	.056(10)	.006(4)	.022(7)	.003(3)	.004(5)
O22	.071(4)	.054(5)	.031(3)	-.006(4)	-.002(3)	.001(3)
C23	.064(6)	.070(6)	.010(4)	-.010(5)	.005(3)	.005(3)
C24	.056(6)	.052(5)	.016(4)	.002(5)	.007(3)	-.003(3)
C25	.047(5)	.051(6)	.022(4)	.002(5)	.009(3)	-.002(4)
O25	.045(4)	.073(6)	.032(3)	.025(4)	.002(2)	-.008(4)
C26	.048(3)	.090(4)	.027(3)	.017(3)	-.004(2)	-.006(3)
C27	.050(3)	.084(4)	.019(3)	-.001(3)	.005(2)	.002(3)
C28	.044(3)	.071(4)	.025(3)	-.003(3)	.001(2)	-.003(3)
C281	.090(5)	.106(5)	.032(4)	.026(5)	.003(4)	.007(4)

5. Molecular Geometry

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C12	O12	.	.	1.193(6)	?
C12	C13	.	.	1.480(7)	?
C13	C14	.	.	1.311(7)	?
C13	H13	.	.	.950	?
C14	C15	.	.	1.487(7)	?
C14	H14	.	.	.958	?
C15	O15	.	.	1.442(6)	?
C15	C16	.	.	1.539(7)	?
C15	H15	.	.	.975	?
C16	C17	.	.	1.523(7)	?
C16	H16a	.	.	.954	?
C16	H16b	.	.	.964	?
C17	C18	.	.	1.536(7)	?
C17	H17a	.	.	.969	?
C17	H17b	.	.	.950	?
C18	C181	.	.	1.500(8)	?
C18	H18	.	.	.967	?
C181	H181a	.	.	.934	?
C181	H181b	.	.	.957	?
C181	H181c	.	.	.968	?
O21	C22	.	.	1.311(17)	?
O21	C28	.	'8 656'	1.479(10)	?
C22	O22	.	.	1.26(2)	?
C22	C23	.	.	1.465(13)	?
C22	C23'	.	.	1.65(3)	?
C23	C24	.	.	1.251(13)	?
C23	H23	.	.	.964	?
C24	C25	.	.	1.515(13)	?
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C25	O25	.	.	1.435(15)	?
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C25	H25	.	.	.977	?

C26 C27 . . 1.516(9) ?
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 C26 H26a . . .969 ?
 C26 H26b . . .990 ?
 C27 C28 . . 1.526(7) ?
 C27 H27a . . .991 ?
 C27 H27b . . .975 ?
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 O21' C22' . . 1.44(5) ?
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 C16 C17 C18 . . . 113.9(4) ?
 C16 C17 H17a . . . 107.9 ?

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H17a	C17	H17b	.	.	.	107.9	?
C17	C18	C181	.	.	.	114.1(4)	?
C17	C18	H18	.	.	.	107.0	?
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C181	C18	H18	.	.	.	108.0	?
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C18	C181	H181a	.	.	.	111.7	?
C18	C181	H181b	.	.	.	109.7	?
C18	C181	H181c	.	.	.	108.2	?
H181a	C181	H181b	.	.	.	110.3	?
H181a	C181	H181c	.	.	.	109.3	?
H181b	C181	H181c	.	.	.	107.4	?
C22	O21	C28	.	.	'8 656'	119.5(9)	?
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O21	C22	C23	.	.	.	119.4(13)	?
O22	C22	C23	.	.	.	118.2(12)	?
C22	C23	C24	.	.	.	123.2(11)	?
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C23	C24	C25	.	.	.	124.8(9)	?
C23	C24	H24	.	.	.	118.6	?
C25	C24	H24	.	.	.	116.6	?
C24	C25	O25	.	.	.	111.1(8)	?
C24	C25	C26	.	.	.	109.1(6)	?
C24	C25	H25	.	.	.	108.8	?
O25	C25	C26	.	.	.	110.7(8)	?
O25	C25	H25	.	.	.	109.5	?
C26	C25	H25	.	.	.	107.4	?
C25	C26	H26a	.	.	.	108.3	?
C25	C26	H26b	.	.	.	106.1	?
C27	C26	C25'	.	.	.	99.0(11)	?
C27	C26	H26a	.	.	.	111.1	?
C27	C26	H26b	.	.	.	109.8	?
C25'	C26	H26a	.	.	.	108.4	?
C25'	C26	H26b	.	.	.	123.7	?
H26a	C26	H26b	.	.	.	104.7	?
C26	C27	C28	.	.	.	114.6(5)	?
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H27a	C27	H27b	.	.	.	104.2	?
C27	C28	C281	.	.	.	114.7(5)	?
C27	C28	H28	.	.	.	104.7(5)	?
C27	C28	O21	.	.	'8 656'	107.9(4)	?
C27	C28	O21'	.	.	'8 656'	109.0(13)	?
C281	C28	H28	.	.	.	108.1	?
C281	C28	O21	.	.	'8 656'	108.1(6)	?
C281	C28	O21'	.	.	'8 656'	89.6(12)	?
H28	C28	O21	.	.	'8 656'	113.6(6)	?
H28	C28	O21'	.	.	'8 656'	130.5(13)	?
C28	C281	H281a	.	.	.	108.9	?
C28	C281	H281b	.	.	.	111.7	?

```

C28 C281 H281c . . . 108.9 ?
H281a C281 H281b . . . 109.7 ?
H281a C281 H281c . . . 107.0 ?
H281b C281 H281c . . . 110.5 ?
C22' O21' C28 . . '8 656' 113(3) ?
O21' C22' O22' . . . 116(4) ?
O21' C22' C23' . . . 116(3) ?
O22' C22' C23' . . . 127(4) ?
C22' C23' C24' . . . 128(3) ?
C22' C23' H23' . . . 120 ?
C24' C23' H23' . . . 112 ?
C23' C24' C25' . . . 129(2) ?
C23' C24' H24' . . . 110.8 ?
C25' C24' H24' . . . 119.8 ?
C26 C25' C24' . . . 108(2) ?
C26 C25' H25' . . . 130 ?
C26 C25' O25' . . . 97(2) ?
C24' C25' O25' . . . 108(2) ?
C24' C25' H25' . . . 104 ?
O25' C25' H25' . . . 108 ?

```

```

loop_
_geom_torsion_atom_site_label_1
_geom_torsion_atom_site_label_2
_geom_torsion_atom_site_label_3
_geom_torsion_atom_site_label_4
_geom_torsion_site_symmetry_1
_geom_torsion_site_symmetry_2
_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
_geom_torsion
_geom_torsion_publ_flag          #<< enter YES for value to be
published
  ? ? ? ? ? ? ? ? ? ?

```

```

loop_
_geom_hbond_atom_site_label_D
_geom_hbond_atom_site_label_H
_geom_hbond_atom_site_label_A
_geom_hbond_site_symmetry_D
_geom_hbond_site_symmetry_H
_geom_hbond_site_symmetry_A
_geom_hbond_distance_DH
_geom_hbond_distance_HA
_geom_hbond_distance_DA
_geom_hbond_angle_DHA
_geom_hbond_publ_flag          #<< enter YES for value to be
published
  ? ? ? ? ? ? ? ? ? ?

```

```

#-----
#
# Special items requested by author for inclusion in paper
#-----
#-----

```

```

loop_
  _publ_manuscript_incl_extra_item
  _publ_manuscript_incl_extra_defn
    ? ?

#-----
----
#       Items which are non-mandatory for Acta C submissions
#-----
----

_atom_sites_solution_primary           ?
_atom_sites_solution_secondary         ?
_atom_sites_solution_hydrogens        ?

_geom_special_details                  ?

_cell_special_details
;   ?
;

_exptl_special_details
;   ?
;

_diffrn_special_details
;   ?
;

_chemical_compound_source              ?
_chemical_name_systematic              ?
_chemical_name_common                  ?
_chemical_formula_analytical           ?
_chemical_formula_structural           ?

_exptl_crystal_F_000                  1344

loop_
  _diffrn_standard_refl_index_h
  _diffrn_standard_refl_index_k
  _diffrn_standard_refl_index_l
    ? ? ?
loop_
  _diffrn_attenuator_code
  _diffrn_attenuator_scale
    ? ?

_reflns_limit_h_min                    0
_reflns_limit_h_max                    11
_reflns_limit_k_min                    0
_reflns_limit_k_max                    12
_reflns_limit_l_min                    0
_reflns_limit_l_max                    33
_reflns_number_observed                 ?
_reflns_d_resolution_high               .848

```

