

```
#=====
data_global
#=====
```

```
_audit_creation_method      'Jana2006 Version : 23/10/2008'
```

1. PROCESSING SUMMARY (IUCr Office Use Only)

```
_journal_date_recd_electronic      ?
_journal_date_to_coeditor          ?
_journal_date_from_coeditor        ?
_journal_date_accepted              ?
_journal_date_printers_first        ?
_journal_date_printers_final        ?
_journal_date_proofs_out            ?
_journal_date_proofs_in            ?
_journal_coeditor_name              ?
_journal_coeditor_code              ?
_journal_coeditor_notes
; ?
;
_journal_techeditor_code            ?
_journal_paper_category              ?
_journal_techeditor_notes
; ?
;
_journal_coden_ASTM                 ?
_journal_name_full                  'Acta Crystallographica Section C'
_journal_year                       ?
_journal_volume                     ?
_journal_issue                      ?
_journal_page_first                 ?
_journal_page_last                  ?
_journal_suppl_publ_number          ?
_journal_suppl_publ_pages           ?
```

```
#=====
```

2. SUBMISSION DETAILS

```
_publ_contact_author_name          'T Baikie'
_publ_contact_author_address
; School of Materials Science and Engineering,
Nanyang Technological University,
50 Nanyang Avenue,
Singapore, 639798
;
_publ_contact_author_email          'tbaikie@ntu.edu.sg'
_publ_contact_author_fax            ?
_publ_contact_author_phone          ?
```

_publ_requested_journal 'American Mineralogist'
_publ_requested_category ?

_publ_contact_letter
; ?
;

#=====

3. TITLE AND AUTHOR LIST

_publ_section_title
; A Multi-Domain Brazilian Apatite Gem: Implications for Technological Materials
;

_publ_section_title_footnote
; ?
;

loop_

_publ_author_name
_publ_author_address

'Tom Baikie'

; Division of Materials Science & Engineering,
Nanyang Technological University, Singapore

;

'Martin Schreyer'

;Institute of Chemical Engineering Sciences (ICES),
Agency for Science, Technology and Research (A*Star), 1 Pesek Road,
Jurong Island, 627833, Singapore

;

'Chui Ling Wong'

;Division of Materials Science & Engineering,
Nanyang Technological University, Singapore

;

'Stevin S. Pramana'

;Division of Materials Science & Engineering,
Nanyang Technological University, Singapore

;

'Wim T. Klooster'

;Division of Materials Science & Engineering,
Nanyang Technological University, Singapore

;

'Cristiano Ferraris'

;Laboratoire de Mineralogie, USM 201, Museum National d'histoire naturelle,
CP 52, 61 Rue Buffon, 75005, Paris, France

;

'Garry J. McIntyre'

;The Bragg Institute, Australian Nuclear Science and Technology Organisation,
Lucas Heights, NSW 2234, Australia

;

'T. J. White'

;Electron Microscopy Unit, Australian National University,
Research School of Biology, GPO Box 475 Canberra, ACT 2601 Australia

;

```
#=====
data_(I)
#=====
```

4. CHEMICAL DATA

```
_chemical_name_systematic
; ?
;
_chemical_name_common      ?
_chemical_formula_moiety    ?
_chemical_formula_structural ?
_chemical_formula_analytical ?
_chemical_formula_iupac     ?
_chemical_formula_sum       'Ca5 F0.73 O12.27 P3'
_chemical_formula_weight    503.50
_chemical_melting_point     'not measured'
```

```
#=====
```

6. CRYSTAL DATA

```
_symmetry_cell_setting      hexagonal
_symmetry_space_group_name_H-M 'P 63/m'
_symmetry_space_group_name_Hall '-P 6c'
_symmetry_Int_Tables_number 176
loop_
  _symmetry_equiv_pos_site_id
  _symmetry_equiv_pos_as_xyz
1  x,y,z
2  -y,x-y,z
3  -x+y,-x,z
4  -x,-y,z+1/2
5  y,-x+y,z+1/2
6  x-y,x,z+1/2
7  -x,-y,-z
8  y,-x+y,-z
9  x-y,x,-z
10 x,y,-z+1/2
11 -y,x-y,-z+1/2
12 -x+y,-x,-z+1/2
_cell_length_a              9.3687(2)
_cell_length_b              9.3687(2)
_cell_length_c              6.8739(1)
_cell_angle_alpha           90
_cell_angle_beta            90
_cell_angle_gamma           120
_cell_volume                 522.51(3)
_cell_formula_units_Z       2

_cell_measurement_reflns_used      8078
_cell_measurement_theta_min       2.51
_cell_measurement_theta_max       30.51
```

```

_cell_measurement_temperature      100
_cell_special_details
; ?
;

_exptl_crystal_density_diffn      3.200
_exptl_crystal_density_meas       'not measured'
_exptl_crystal_density_method     'not measured'
_exptl_crystal_F_000              499.5

_exptl_absorpt_coefficient_mu      3.106
_exptl_crystal_description         'regular'
_exptl_crystal_size_max            0.1
_exptl_crystal_size_mid            0.1
_exptl_crystal_size_min            0.1
_exptl_crystal_size_rad            ?
_exptl_crystal_colour              'blue under sunlight'
_exptl_absorpt_correction_type     'multi-scan'
_exptl_absorpt_process_details
;'R.H. Blessing, Acta Crystallogr., Sect A 1995, 51, 33-38. '
;

_exptl_absorpt_correction_T_min    0.4226
_exptl_absorpt_correction_T_max    1

#=====

```

6. EXPERIMENTAL DATA

```

_exptl_special_details             ?

_diffn_ambient_temperature         100
_diffn_radiation_type              'Mo K\alpha'
_diffn_radiation_source            'X-ray tube'
_diffn_radiation_wavelength        0.71069
_diffn_radiation_monochromator      graphite
_diffn_measurement_device           'three-circle diffractometer'
_diffn_measurement_device_type      'Bruker CCD'
_diffn_detector_area_resol_mean     ?
_diffn_measurement_method           \w/2\q

_diffn_reflns_number               8078
_diffn_reflns_theta_min             2.51
_diffn_reflns_theta_max             30.51
_diffn_reflns_theta_full            30
_diffn_measured_fraction_theta_max  0.94
_diffn_measured_fraction_theta_full 0.98
_diffn_reflns_av_R_equivalents     0.0296
_diffn_reflns_av_sigmaI/netI       0.0107
_diffn_reflns_limit_h_min           -12
_diffn_reflns_limit_h_max           11
_diffn_reflns_limit_k_min           -11
_diffn_reflns_limit_k_max           12
_diffn_reflns_limit_l_min           -9
_diffn_reflns_limit_l_max           9

```

```

_diffrn_reflms_reduction_process      ?
_diffrn_standards_number              ?
_diffrn_standards_interval_count      ?
_diffrn_standards_interval_time       ?
_diffrn_standards_decay_%             ?
loop_
_diffrn_standard_refl_index_h
_diffrn_standard_refl_index_k
_diffrn_standard_refl_index_l
? ? ?

```

```
#=====
```

7. REFINEMENT DATA

```

_refine_special_details
; ?
;

_reflms_number_total      551
_reflms_number_gt         542
_reflms_threshold_expression 'I>3\s(I)'

_refine_ls_structure_factor_coef      Fsqr
_refine_ls_R_factor_gt                0.0198
_refine_ls_wR_factor_gt               0.0642
_refine_ls_R_factor_all               0.0200
_refine_ls_wR_factor_ref              0.0643
_refine_ls_goodness_of_fit_ref        1.56
_refine_ls_goodness_of_fit_gt         1.57
_refine_ls_restrained_S_gt            ?
_refine_ls_restrained_S_all           ?
_refine_ls_number_reflms              551
_refine_ls_number_parameters           40
_refine_ls_number_restraints           0
_refine_ls_number_constraints          0
_refine_ls_weighting_scheme            sigma
_refine_ls_weighting_details           'w=1/(\s^2^(I)+0.0004I^2^)'
_refine_ls_hydrogen_treatment         ?
_refine_ls_shift/su_max                0.0050
_refine_ls_shift/su_mean               0.0021
_refine_diff_density_max               0.44
_refine_diff_density_min               -0.24
_refine_ls_extinction_method
'B-C type 1 Gaussian isotropic (Becker & Coppens, 1974)'
_refine_ls_extinction_coef             10400(500)
_refine_ls_abs_structure_details       ?
_refine_ls_abs_structure_Flack         ?
_refine_ls_abs_structure_Rogers        ?

loop_
_atom_type_symbol
_atom_type_scatter_dispersion_real

```

_atom_type_scatter_dispersion_imag
_atom_type_scatter_source
Ca 0.2262 0.3064
'International Tables Vol C tables 4.2.6.8 and 6.1.1.1'
P 0.1023 0.0942
'International Tables Vol C tables 4.2.6.8 and 6.1.1.1'
O 0.0106 0.0060
'International Tables Vol C tables 4.2.6.8 and 6.1.1.1'
F 0.0171 0.0103
'International Tables Vol C tables 4.2.6.8 and 6.1.1.1'

_computing_data_collection ?
 _computing_cell_refinement ?
 _computing_data_reduction ?
 _computing_structure_solution ?
_computing_structure_refinement
'Jana2006 (Petricek, Dusek & Palatinus, 2006)'
 _computing_molecular_graphics ?
_computing_publication_material
'Jana2006 (Petricek, Dusek & Palatinus, 2006)'

#=====

8. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

loop_
 _atom_site_label
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_adp_type
 _atom_site_U_iso_or_equiv
 _atom_site_symmetry_multiplicity
 _atom_site_occupancy
 _atom_site_calc_flag
 _atom_site_refinement_flags
 _atom_site_disorder_assembly
 _atom_site_disorder_group
 Ca1 Ca 0.333333 0.666667 0.00111(5) Uani 0.00774(16) 4 1 d . . .
 Ca2 Ca 0.24293(4) -0.00716(4) 0.25 Uani 0.00725(18) 6 1 d . . .
 P1 P 0.39852(6) 0.36890(6) 0.25 Uani 0.0057(2) 6 1 d . . .
 O1 O 0.32624(17) 0.48413(15) 0.25 Uani 0.0081(5) 6 1 d . . .
 O2 O 0.58796(17) 0.46605(16) 0.25 Uani 0.0109(5) 6 1 d . . .
 O3 O 0.34215(12) 0.25649(10) 0.07012(12) Uani 0.0129(4) 12 1 d . . .
 F F 0 0 0.25 Uiso 0.0101(8) 2 0.730(10) d . . .
 O4 O 0 0 0.305 Uiso 0.0101(8) 4 0.135(5) d . . .

loop_
 _atom_site_aniso_label
 _atom_site_aniso_type_symbol
 _atom_site_aniso_U_11
 _atom_site_aniso_U_22
 _atom_site_aniso_U_33

_atom_site_aniso_U_12
 _atom_site_aniso_U_13
 _atom_site_aniso_U_23
 Ca1 Ca 0.0091(2) 0.0091(2) 0.0051(2) 0.00453(10) 0 0
 Ca2 Ca 0.0080(2) 0.0066(2) 0.0070(2) 0.00355(16) 0 0
 P1 P 0.0066(3) 0.0058(3) 0.0056(2) 0.00381(19) 0 0
 O1 O 0.0099(6) 0.0072(6) 0.0092(5) 0.0057(5) 0 0
 O2 O 0.0069(6) 0.0084(6) 0.0172(6) 0.0037(5) 0 0
 O3 O 0.0216(5) 0.0110(5) 0.0094(4) 0.0106(4) -0.0064(4) -0.0035(3)

#=====

9. MOLECULAR GEOMETRY

loop_
 _geom_bond_atom_site_label_1
 _geom_bond_atom_site_label_2
 _geom_bond_site_symmetry_1
 _geom_bond_site_symmetry_2
 _geom_bond_distance
 _geom_bond_publ_flag
 Ca1 O1 . . 2.3963(11) ?
 Ca1 O1 . 2_665 2.3963(9) ?
 Ca1 O1 . 3_565 2.3963(16) ?
 Ca1 O2 . 4_664 2.4466(13) ?
 Ca1 O2 . 5_564 2.4466(12) ?
 Ca1 O2 . 6_554 2.4466(15) ?
 Ca1 O3 . 7_665 2.7951(11) ?
 Ca1 O3 . 8_565 2.7951(16) ?
 Ca1 O3 . 9_555 2.7951(9) ?
 Ca2 O1 . 3_555 2.6813(17) ?
 Ca2 O2 . 2_655 2.3663(14) ?
 Ca2 O3 . . 2.4896(10) ?
 Ca2 O3 . 5_555 2.3436(10) ?
 Ca2 O3 . 8_555 2.3436(10) ?
 Ca2 O3 . 10_555 2.4896(10) ?
 Ca2 F . . 2.3102(4) ?
 Ca2 O4 . . 2.3409(4) ?
 Ca2 O4 . 10_555 2.3409(4) ?
 P1 O1 . . 1.5346(19) ?
 P1 O2 . . 1.5372(14) ?
 P1 O3 . . 1.5364(9) ?
 P1 O3 . 10_555 1.5364(9) ?
 O1 O1 . 2_665 2.906(2) ?
 O1 O1 . 3_565 2.906(3) ?
 O1 O2 . . 2.541(3) ?
 O1 O3 . . 2.5332(18) ?
 O1 O3 . 6_555 2.9485(13) ?
 O1 O3 . 9_555 2.9485(13) ?
 O1 O3 . 10_555 2.5332(18) ?
 O2 O3 . . 2.4830(12) ?
 O2 O3 . 3_665 2.9349(16) ?

O2 O3 . 10_555 2.4830(12) ?
O2 O3 . 12_665 2.9349(16) ?
O3 O3 . 10_555 2.4730(12) ?
F O4 . . 0.3781 ?
F O4 . 10_555 0.3781 ?
O4 O4 . 7_556 2.6808 ?
O4 O4 . 10_555 0.7561 ?

loop_

_geom_angle_atom_site_label_1
_geom_angle_atom_site_label_2
_geom_angle_atom_site_label_3
_geom_angle_site_symmetry_1
_geom_angle_site_symmetry_2
_geom_angle_site_symmetry_3
_geom_angle
_geom_angle_publ_flag
O1 Ca1 O1 . . 2_665 74.66(5) ?
O1 Ca1 O1 . . 3_565 74.66(6) ?
O1 Ca1 O2 . . 4_664 92.80(4) ?
O1 Ca1 O2 . . 5_564 154.55(6) ?
O1 Ca1 O2 . . 6_554 124.00(4) ?
O1 Ca1 O3 . . 7_665 86.98(4) ?
O1 Ca1 O3 . . 8_565 142.26(4) ?
O1 Ca1 O3 . . 9_555 68.72(3) ?
O1 Ca1 O1 2_665 . 3_565 74.66(4) ?
O1 Ca1 O2 2_665 . 4_664 124.00(5) ?
O1 Ca1 O2 2_665 . 5_564 92.80(4) ?
O1 Ca1 O2 2_665 . 6_554 154.55(7) ?
O1 Ca1 O3 2_665 . 7_665 68.72(4) ?
O1 Ca1 O3 2_665 . 8_565 86.98(6) ?
O1 Ca1 O3 2_665 . 9_555 142.26(4) ?
O1 Ca1 O2 3_565 . 4_664 154.55(4) ?
O1 Ca1 O2 3_565 . 5_564 124.00(6) ?
O1 Ca1 O2 3_565 . 6_554 92.80(5) ?
O1 Ca1 O3 3_565 . 7_665 142.26(4) ?
O1 Ca1 O3 3_565 . 8_565 68.72(4) ?
O1 Ca1 O3 3_565 . 9_555 86.98(4) ?
O2 Ca1 O2 4_664 . 5_564 75.72(5) ?
O2 Ca1 O2 4_664 . 6_554 75.72(6) ?
O2 Ca1 O3 4_664 . 7_665 56.08(3) ?
O2 Ca1 O3 4_664 . 8_565 124.50(4) ?
O2 Ca1 O3 4_664 . 9_555 67.72(4) ?
O2 Ca1 O2 5_564 . 6_554 75.72(4) ?
O2 Ca1 O3 5_564 . 7_665 67.72(5) ?
O2 Ca1 O3 5_564 . 8_565 56.08(5) ?
O2 Ca1 O3 5_564 . 9_555 124.50(3) ?
O2 Ca1 O3 6_554 . 7_665 124.50(4) ?
O2 Ca1 O3 6_554 . 8_565 67.72(5) ?
O2 Ca1 O3 6_554 . 9_555 56.08(4) ?
O3 Ca1 O3 7_665 . 8_565 117.00(3) ?
O3 Ca1 O3 7_665 . 9_555 117.00(4) ?
O3 Ca1 O3 8_565 . 9_555 117.00(4) ?
O1 Ca2 O2 3_555 . 2_655 101.18(7) ?

O1 Ca2 O3 3_555 . . 149.49(2) ?
 O1 Ca2 O3 3_555 . 5_555 71.50(4) ?
 O1 Ca2 O3 3_555 . 8_555 71.50(4) ?
 O1 Ca2 O3 3_555 . 10_555 149.49(2) ?
 O1 Ca2 F 3_555 . . 106.53(5) ?
 O1 Ca2 O4 3_555 . . 106.31(5) ?
 O1 Ca2 O4 3_555 . 10_555 106.31(5) ?
 O2 Ca2 O3 2_655 . . 74.32(5) ?
 O2 Ca2 O3 2_655 . 5_555 86.04(3) ?
 O2 Ca2 O3 2_655 . 8_555 86.04(3) ?
 O2 Ca2 O3 2_655 . 10_555 74.32(5) ?
 O2 Ca2 F 2_655 . . 152.29(6) ?
 O2 Ca2 O4 2_655 . . 150.89(5) ?
 O2 Ca2 O4 2_655 . 10_555 150.89(5) ?
 O3 Ca2 O3 . . 5_555 136.53(4) ?
 O3 Ca2 O3 . . 8_555 78.06(4) ?
 O3 Ca2 O3 . . 10_555 59.56(3) ?
 O3 Ca2 F . . . 81.71(3) ?
 O3 Ca2 O4 . . . 86.44(3) ?
 O3 Ca2 O4 . . 10_555 77.14(3) ?
 O3 Ca2 O3 5_555 . 8_555 139.74(6) ?
 O3 Ca2 O3 5_555 . 10_555 78.06(4) ?
 O3 Ca2 F 5_555 . . 102.59(3) ?
 O3 Ca2 O4 5_555 . . 93.64(3) ?
 O3 Ca2 O4 5_555 . 10_555 111.51(3) ?
 O3 Ca2 O3 8_555 . 10_555 136.53(4) ?
 O3 Ca2 F 8_555 . . 102.59(3) ?
 O3 Ca2 O4 8_555 . . 111.51(3) ?
 O3 Ca2 O4 8_555 . 10_555 93.64(3) ?
 O3 Ca2 F 10_555 . . 81.71(3) ?
 O3 Ca2 O4 10_555 . . 77.14(3) ?
 O3 Ca2 O4 10_555 . 10_555 86.44(3) ?
 F Ca2 O4 . . . 9.2943(18) ?
 F Ca2 O4 . . 10_555 9.2943(18) ?
 O4 Ca2 O4 . . 10_555 18.589(4) ?
 O1 P1 O2 . . . 111.62(8) ?
 O1 P1 O3 . . . 111.15(6) ?
 O1 P1 O3 . . 10_555 111.15(6) ?
 O2 P1 O3 . . . 107.77(6) ?
 O2 P1 O3 . . 10_555 107.77(6) ?
 O3 P1 O3 . . 10_555 107.18(5) ?
 Ca1 O1 Ca1 . . 10_555 91.11(5) ?
 Ca1 O1 Ca2 . . 2_555 101.85(5) ?
 Ca1 O1 P1 . . . 129.61(5) ?
 Ca1 O1 O1 . . 2_665 52.67(3) ?
 Ca1 O1 O1 . . 3_565 52.67(4) ?
 Ca1 O1 O2 . . . 111.36(4) ?
 Ca1 O1 O3 . . . 105.07(2) ?
 Ca1 O1 O3 . . 6_555 126.65(8) ?
 Ca1 O1 O3 . . 9_555 62.05(3) ?
 Ca1 O1 O3 . . 10_555 163.13(6) ?
 Ca1 O1 Ca2 10_555 . 2_555 101.85(5) ?
 Ca1 O1 P1 10_555 . . 129.61(5) ?
 Ca1 O1 O1 10_555 . 2_665 52.67(3) ?

Ca1 O1 O1 10_555 . 3_565 52.67(4) ?
 Ca1 O1 O2 10_555 . . 111.36(4) ?
 Ca1 O1 O3 10_555 . . 163.13(6) ?
 Ca1 O1 O3 10_555 . 6_555 62.05(3) ?
 Ca1 O1 O3 10_555 . 9_555 126.65(8) ?
 Ca1 O1 O3 10_555 . 10_555 105.07(2) ?
 Ca2 O1 P1 2_555 . . 97.38(5) ?
 Ca2 O1 O1 2_555 . 2_665 137.06(8) ?
 Ca2 O1 O1 2_555 . 3_565 77.06(5) ?
 Ca2 O1 O2 2_555 . . 131.60(7) ?
 Ca2 O1 O3 2_555 . . 79.77(4) ?
 Ca2 O1 O3 2_555 . 6_555 48.92(3) ?
 Ca2 O1 O3 2_555 . 9_555 48.92(3) ?
 Ca2 O1 O3 2_555 . 10_555 79.77(4) ?
 P1 O1 O1 . . 2_665 125.57(8) ?
 P1 O1 O1 . . 3_565 174.43(7) ?
 P1 O1 O3 . . 6_555 100.91(5) ?
 P1 O1 O3 . . 9_555 100.91(5) ?
 O1 O1 O1 2_665 . 3_565 60.00(5) ?
 O1 O1 O2 2_665 . . 91.34(6) ?
 O1 O1 O3 2_665 . . 135.41(5) ?
 O1 O1 O3 2_665 . 6_555 114.14(5) ?
 O1 O1 O3 2_665 . 9_555 114.14(5) ?
 O1 O1 O3 2_665 . 10_555 135.41(5) ?
 O1 O1 O2 3_565 . . 151.34(6) ?
 O1 O1 O3 3_565 . . 142.47(5) ?
 O1 O1 O3 3_565 . 6_555 75.50(5) ?
 O1 O1 O3 3_565 . 9_555 75.50(5) ?
 O1 O1 O3 3_565 . 10_555 142.47(5) ?
 O2 O1 O3 . . . 58.60(5) ?
 O2 O1 O3 . . 6_555 121.03(5) ?
 O2 O1 O3 . . 9_555 121.03(5) ?
 O2 O1 O3 . . 10_555 58.60(5) ?
 O3 O1 O3 . . 6_555 109.75(5) ?
 O3 O1 O3 . . 9_555 67.01(4) ?
 O3 O1 O3 . . 10_555 58.43(5) ?
 O3 O1 O3 6_555 . 9_555 96.54(5) ?
 O3 O1 O3 6_555 . 10_555 67.01(4) ?
 O3 O1 O3 9_555 . 10_555 109.75(5) ?
 Ca1 O2 Ca1 4_665 . 7_665 89.74(6) ?
 Ca1 O2 Ca2 4_665 . 3_665 113.77(4) ?
 Ca1 O2 P1 4_665 . . 104.55(5) ?
 Ca1 O2 O1 4_665 . . 125.45(4) ?
 Ca1 O2 O3 4_665 . . 110.22(5) ?
 Ca1 O2 O3 4_665 . 3_665 97.00(6) ?
 Ca1 O2 O3 4_665 . 10_555 69.08(4) ?
 Ca1 O2 O3 4_665 . 12_665 61.80(3) ?
 Ca1 O2 Ca2 7_665 . 3_665 113.77(4) ?
 Ca1 O2 P1 7_665 . . 104.55(5) ?
 Ca1 O2 O1 7_665 . . 125.45(4) ?
 Ca1 O2 O3 7_665 . . 69.08(4) ?
 Ca1 O2 O3 7_665 . 3_665 61.80(3) ?
 Ca1 O2 O3 7_665 . 10_555 110.22(5) ?
 Ca1 O2 O3 7_665 . 12_665 97.00(6) ?

Ca2 O2 P1 3_665 . . 124.58(10) ?
 Ca2 O2 O1 3_665 . . 90.42(7) ?
 Ca2 O2 O3 3_665 . . 135.88(7) ?
 Ca2 O2 O3 3_665 . 3_665 54.76(4) ?
 Ca2 O2 O3 3_665 . 10_555 135.88(7) ?
 Ca2 O2 O3 3_665 . 12_665 54.76(4) ?
 P1 O2 O3 . . 3_665 154.63(3) ?
 P1 O2 O3 . . 12_665 154.63(3) ?
 O1 O2 O3 . . . 60.55(5) ?
 O1 O2 O3 . . 3_665 134.74(6) ?
 O1 O2 O3 . . 10_555 60.55(5) ?
 O1 O2 O3 . . 12_665 134.74(6) ?
 O3 O2 O3 . . 3_665 123.01(3) ?
 O3 O2 O3 . . 10_555 59.73(4) ?
 O3 O2 O3 . . 12_665 164.67(9) ?
 O3 O2 O3 3_665 . 10_555 164.67(9) ?
 O3 O2 O3 3_665 . 12_665 49.83(3) ?
 O3 O2 O3 10_555 . 12_665 123.01(3) ?
 Ca1 O3 Ca2 7_665 . . 99.26(4) ?
 Ca1 O3 Ca2 7_665 . 6_554 99.96(4) ?
 Ca1 O3 P1 7_665 . . 90.44(5) ?
 Ca1 O3 O1 7_665 . . 112.52(4) ?
 Ca1 O3 O1 7_665 . 5_554 49.23(3) ?
 Ca1 O3 O2 7_665 . . 54.85(4) ?
 Ca1 O3 O2 7_665 . 2_655 50.48(3) ?
 Ca1 O3 O3 7_665 . 10_555 100.09(4) ?
 Ca2 O3 Ca2 . . 6_554 117.89(3) ?
 Ca2 O3 P1 . . . 96.33(4) ?
 Ca2 O3 O1 . . . 116.29(4) ?
 Ca2 O3 O1 . . 5_554 93.61(5) ?
 Ca2 O3 O2 . . . 106.01(5) ?
 Ca2 O3 O2 . . 2_655 50.92(3) ?
 Ca2 O3 O3 . . 10_555 60.22(3) ?
 Ca2 O3 P1 6_554 . . 141.62(7) ?
 Ca2 O3 O1 6_554 . . 109.21(5) ?
 Ca2 O3 O1 6_554 . 5_554 59.58(4) ?
 Ca2 O3 O2 6_554 . . 132.93(4) ?
 Ca2 O3 O2 6_554 . 2_655 131.30(5) ?
 Ca2 O3 O3 6_554 . 10_555 159.87(6) ?
 P1 O3 O1 . . 5_554 139.56(6) ?
 P1 O3 O2 . . 2_655 83.16(5) ?
 O1 O3 O1 . . 5_554 148.62(5) ?
 O1 O3 O2 . . . 60.86(6) ?
 O1 O3 O2 . . 2_655 117.54(5) ?
 O1 O3 O3 . . 10_555 60.78(4) ?
 O1 O3 O2 5_554 . . 103.53(5) ?
 O1 O3 O2 5_554 . 2_655 73.19(5) ?
 O1 O3 O3 5_554 . 10_555 138.27(7) ?
 O2 O3 O2 . . 2_655 66.72(6) ?
 O2 O3 O3 . . 10_555 60.13(3) ?
 O2 O3 O3 2_655 . 10_555 65.08(4) ?
 Ca2 F Ca2 . . 2_555 120.000(12) ?
 Ca2 F Ca2 . . 3_555 120.000(17) ?
 Ca2 F O4 . . . 90 ?

Ca2 F O4 . . 10_555 90 ?
Ca2 F Ca2 2_555 . 3_555 120.000(17) ?
Ca2 F O4 2_555 . . 90 ?
Ca2 F O4 2_555 . 10_555 90 ?
Ca2 F O4 3_555 . . 90 ?
Ca2 F O4 3_555 . 10_555 90 ?
O4 F O4 . . 10_555 180.0(5) ?
Ca2 O4 Ca2 . . 2_555 117.444(12) ?
Ca2 O4 Ca2 . . 3_555 117.444(16) ?
Ca2 O4 F . . 80.7057(18) ?
Ca2 O4 O4 . . 7_556 99.2943(18) ?
Ca2 O4 O4 . . 10_555 80.7057(18) ?
Ca2 O4 Ca2 2_555 . 3_555 117.444(16) ?
Ca2 O4 F 2_555 . . 80.706(2) ?
Ca2 O4 O4 2_555 . 7_556 99.294(2) ?
Ca2 O4 O4 2_555 . 10_555 80.706(2) ?
Ca2 O4 F 3_555 . . 80.7057(14) ?
Ca2 O4 O4 3_555 . 7_556 99.2943(14) ?
Ca2 O4 O4 3_555 . 10_555 80.7057(14) ?
F O4 O4 . . 7_556 180.0(5) ?
O4 O4 O4 7_556 . 10_555 180.0(5) ?

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
? ? ? ? ? ? ? ? ?

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
? ? ? ? ? ? ? ? ?

#=====

10. STRUCTURE-FACTOR LIST

```

loop_
_refln_index_h
_refln_index_k
_refln_index_l
_refln_F_squared_calc
_refln_F_squared_meas
_refln_F_squared_sigma
_refln_observed_status
0 1 0 305.34 274.66 2.02 o
-1 2 0 149.98 124.18 0.88 o
0 2 0 709.05 744.39 4.83 o
-2 3 0 246.16 240.66 1.59 o
-1 3 0 2233.10 2222.69 14.38 o
0 3 0 3741.63 4284.56 26.36 o
-3 4 0 3933.24 4429.70 28.90 o
-2 4 0 116.88 122.32 1.07 o
-1 4 0 1803.87 1890.17 12.05 o
0 4 0 715.73 757.46 4.86 o
-4 5 0 4021.05 4187.37 27.08 o
-3 5 0 2268.85 2346.21 15.22 o
-2 5 0 13.81 17.81 0.36 o
-1 5 0 3617.99 3771.25 23.29 o
0 5 0 280.23 269.13 1.96 o
-5 6 0 0.56 5.04 0.36 o
-4 6 0 3979.62 4066.38 28.81 o
-3 6 0 821.05 902.13 6.46 o
-2 6 0 251.59 234.79 1.96 o
-1 6 0 1639.79 1708.85 12.22 o
0 6 0 500.93 521.59 5.32 o
-6 7 0 1746.48 1646.94 19.49 o
-5 7 0 1218.74 1235.12 11.27 o
-4 7 0 22.09 22.13 0.72 o
-3 7 0 738.58 715.95 6.86 o
-2 7 0 3864.82 3876.79 33.75 o
-1 7 0 2205.24 2223.95 21.89 o
0 7 0 107.66 130.68 2.69 o
-7 8 0 4201.03 4162.90 58.96 o
-6 8 0 526.60 538.58 8.70 o
-5 8 0 1293.89 1283.32 17.56 o
-4 8 0 3779.63 3817.13 51.49 o
-3 8 0 424.44 434.75 5.88 o
-2 8 0 66.11 61.46 1.80 o
-1 8 0 325.20 366.52 6.43 o
0 8 0 2717.51 2647.48 38.09 o
-8 9 0 11.51 21.77 1.44 o
-7 9 0 799.40 783.25 13.26 o
-6 9 0 118.19 114.36 3.23 o
-5 9 0 115.44 102.15 3.59 o
-4 9 0 153.58 165.38 4.13 o
-3 9 0 3.47 8.10 1.08 o
-2 9 0 1163.78 1143.97 17.36 o
-1 9 0 243.51 252.87 5.37 o
0 9 0 1198.19 1192.07 21.26 o
-9 10 0 634.80 606.07 11.74 o

```

-8	10	0	353.58	377.00	9.65 o
-7	10	0	141.11	143.23	7.36 o
-6	10	0	898.41	879.80	19.96 o
-5	10	0	1871.61	1859.17	39.59 o
-4	10	0	20.29	21.77	1.98 o
-3	10	0	1708.68	1637.00	35.08 o
-2	10	0	1270.63	1296.41	23.16 o
-1	10	0	307.61	292.59	6.62 o
0	10	0	486.04	470.82	9.63 o
-10	11	0	1852.70	1870.39	58.12 o
-9	11	0	1063.93	1058.78	34.77 o
-8	11	0	359.16	365.49	10.01 o
-7	11	0	1788.25	1824.25	39.29 o
-6	11	0	1463.35	1415.01	31.14 o
-5	11	0	102.23	98.99	4.13 o
-4	11	0	750.64	736.11	17.39 o
-3	11	0	12.20	18.54	2.16 o
-2	11	0	120.83	120.70	4.67 o
-1	11	0	104.52	109.78	3.77 o
0	11	0	16.79	27.35	2.52 o
-10	12	0	1020.24	1003.02	23.34 o
-9	12	0	330.85	345.41	9.84 o
-8	12	0	378.52	371.56	10.37 o
-7	12	0	23.08	25.37	2.52 o
-6	12	0	198.91	190.49	6.46 o
-5	12	0	943.19	953.92	22.12 o
-4	12	0	597.78	604.14	14.96 o
-3	12	0	1591.33	1635.53	35.69 o
-2	12	0	395.96	374.37	10.19 o
-1	12	0	29.06	33.46	2.70 o
0	1	1	139.65	152.36	0.88 o
-1	2	1	400.87	399.83	1.90 o
0	2	1	168.82	193.92	1.06 o
-2	3	1	2651.57	2704.72	12.15 o
-1	3	1	3555.53	3756.76	17.14 o
0	3	1	700.80	817.36	3.79 o
-3	4	1	972.44	981.71	4.44 o
-2	4	1	613.58	575.79	2.61 o
-1	4	1	488.94	591.56	2.81 o
0	4	1	67.10	67.29	0.54 o
-4	5	1	130.10	141.29	0.90 o
-3	5	1	2604.54	2655.18	12.15 o
-2	5	1	2699.32	2801.91	12.70 o
-1	5	1	260.27	262.57	1.43 o
0	5	1	894.41	980.93	4.87 o
-5	6	1	563.04	589.61	3.71 o
-4	6	1	1332.59	1349.87	7.03 o
-3	6	1	2209.37	2215.09	11.39 o
-2	6	1	335.14	346.08	1.96 o
-1	6	1	3486.80	3569.76	19.77 o
0	6	1	19.16	23.75	0.54 o
-6	7	1	544.76	548.46	4.61 o
-5	7	1	651.66	653.82	4.95 o
-4	7	1	102.37	111.08	1.08 o

-3	7	1	3210.30	3196.79	20.15 o
-2	7	1	1465.57	1433.48	10.50 o
-1	7	1	432.19	439.90	3.91 o
0	7	1	4.39	4.68	0.54 o
-7	8	1	4.95	3.42	0.54 o
-6	8	1	198.63	181.99	1.97 o
-5	8	1	6.08	8.82	0.54 o
-4	8	1	1131.18	1122.71	9.61 o
-3	8	1	158.64	156.33	1.79 o
-2	8	1	0.99	3.60	0.54 o
-1	8	1	140.90	143.17	1.79 o
0	8	1	48.92	53.40	1.26 o
-8	9	1	71.92	72.79	1.80 o
-7	9	1	6.87	9.72	0.90 o
-6	9	1	744.46	722.00	8.14 o
-5	9	1	899.15	894.95	8.46 o
-4	9	1	824.41	856.26	9.71 o
-3	9	1	2356.13	2277.15	24.17 o
-2	9	1	668.91	675.34	7.63 o
-1	9	1	128.28	141.28	2.69 o
0	9	1	629.96	607.05	7.64 o
-9	10	1	1.64	7.20	1.08 o
-8	10	1	580.62	596.02	8.90 o
-7	10	1	446.03	417.99	6.60 o
-6	10	1	1017.81	996.16	16.74 o
-5	10	1	599.11	581.21	10.49 o
-4	10	1	10.87	13.32	1.08 o
-3	10	1	848.73	896.01	12.74 o
-2	10	1	474.97	474.03	7.49 o
-1	10	1	329.13	316.28	5.01 o
0	10	1	195.50	184.39	3.77 o
-10	11	1	269.25	281.98	5.91 o
-9	11	1	1939.04	1923.93	29.17 o
-8	11	1	12.01	11.70	1.62 o
-7	11	1	3.30	5.58	1.44 o
-6	11	1	1217.63	1215.07	22.16 o
-5	11	1	918.82	893.41	14.50 o
-4	11	1	475.13	458.51	8.39 o
-3	11	1	249.21	262.32	4.84 o
-2	11	1	61.87	65.09	2.16 o
-1	11	1	2533.25	2510.47	33.50 o
0	11	1	56.23	62.58	2.88 o
-10	12	1	78.42	88.62	4.67 o
-9	12	1	528.26	569.13	11.95 o
-8	12	1	452.53	487.87	10.54 o
-7	12	1	335.81	377.55	8.59 o
-6	12	1	0.05	5.58	1.26 o
-5	12	1	370.85	382.86	7.51 o
-4	12	1	1.91	4.14	1.26 o
-3	12	1	136.15	135.76	3.77 o
-2	12	1	178.09	178.02	4.31 o
-1	12	1	6.59	12.96	2.70 o
0	0	2	2696.93	2678.06	31.56 o
0	1	2	1055.04	992.64	4.43 o

-1	2	2	3192.39	3165.34	15.53 o
0	2	2	2601.46	2586.05	13.73 o
-2	3	2	254.67	338.67	1.95 o
-1	3	2	928.15	1060.54	5.46 o
0	3	2	313.83	398.58	2.13 o
-3	4	2	2286.43	2397.06	11.50 o
-2	4	2	4754.08	4751.28	22.40 o
-1	4	2	1747.29	1761.39	8.58 o
0	4	2	3862.13	3780.31	19.17 o
-4	5	2	14.05	12.95	0.36 o
-3	5	2	140.48	144.13	0.90 o
-2	5	2	2919.99	2853.86	13.54 o
-1	5	2	337.86	351.15	1.96 o
0	5	2	4751.62	4573.92	28.80 o
-5	6	2	1165.57	1159.37	8.15 o
-4	6	2	366.66	398.14	3.02 o
-3	6	2	1026.93	1043.49	7.13 o
-2	6	2	522.84	519.12	3.54 o
-1	6	2	834.59	822.54	5.79 o
0	6	2	914.90	955.83	6.66 o
-6	7	2	773.03	731.04	5.64 o
-5	7	2	4481.90	4392.58	30.83 o
-4	7	2	2218.16	2165.52	16.66 o
-3	7	2	57.36	61.46	0.90 o
-2	7	2	857.35	884.25	6.85 o
-1	7	2	14.93	19.07	0.54 o
0	7	2	1343.61	1291.27	9.92 o
-7	8	2	437.63	433.79	3.92 o
-6	8	2	107.59	112.39	1.62 o
-5	8	2	3688.67	3569.86	27.94 o
-4	8	2	467.67	452.31	3.91 o
-3	8	2	3154.42	3109.00	24.12 o
-2	8	2	1439.02	1437.80	11.99 o
-1	8	2	1796.73	1752.66	15.01 o
0	8	2	4464.27	4366.58	35.47 o
-8	9	2	1769.33	1748.25	19.43 o
-7	9	2	66.76	60.40	1.44 o
-6	9	2	2436.08	2354.32	21.78 o
-5	9	2	593.47	602.98	5.51 o
-4	9	2	582.47	583.05	5.33 o
-3	9	2	1944.70	1957.84	17.91 o
-2	9	2	19.16	21.59	0.90 o
-1	9	2	114.26	114.40	1.98 o
0	9	2	399.30	409.03	5.54 o
-9	10	2	92.70	98.11	2.52 o
-8	10	2	1635.97	1614.21	20.57 o
-7	10	2	67.01	70.29	1.98 o
-6	10	2	34.82	37.41	1.26 o
-5	10	2	889.24	901.47	10.61 o
-4	10	2	124.33	118.87	2.87 o
-3	10	2	12.92	16.74	1.26 o
-2	10	2	213.16	205.80	3.76 o
-1	10	2	2.94	6.84	0.90 o
0	10	2	72.01	83.05	3.06 o

-10	11	2	40.30	48.39	2.16 o
-9	11	2	309.74	310.05	4.83 o
-8	11	2	354.19	334.63	5.72 o
-7	11	2	1.36	3.60	1.08 o
-6	11	2	70.57	73.70	2.70 o
-5	11	2	73.37	79.27	2.88 o
-4	11	2	133.42	140.78	3.41 o
-3	11	2	593.97	572.31	8.90 o
-2	11	2	312.26	318.27	5.55 o
-1	11	2	1813.72	1858.88	28.23 o
0	11	2	22.82	17.27	1.80 o
-10	12	2	12.45	14.76	2.16 o
-9	12	2	601.57	607.10	12.47 o
-8	12	2	1933.48	1942.13	34.42 o
-7	12	2	563.09	536.47	11.23 o
-6	12	2	718.14	717.33	14.22 o
-5	12	2	4.45	8.28	1.62 o
-4	12	2	1509.88	1465.09	22.96 o
-3	12	2	210.60	221.86	4.48 o
-2	12	2	63.40	65.45	3.96 o
0	1	3	87.00	112.89	0.72 o
-1	2	3	1229.20	1364.19	6.41 o
0	2	3	1115.77	1216.41	6.46 o
-2	3	3	3005.85	2963.89	14.37 o
-1	3	3	4835.98	4663.74	23.29 o
0	3	3	510.97	535.90	2.82 o
-3	4	3	846.62	844.54	4.53 o
-2	4	3	22.90	18.70	0.36 o
-1	4	3	1025.86	1047.84	5.53 o
0	4	3	25.84	23.02	0.36 o
-4	5	3	721.61	697.47	4.92 o
-3	5	3	391.95	365.47	2.84 o
-2	5	3	3207.20	3143.06	20.63 o
-1	5	3	591.01	563.85	4.06 o
0	5	3	178.46	171.52	1.61 o
-5	6	3	49.50	57.34	0.90 o
-4	6	3	2881.50	2774.74	20.65 o
-3	6	3	299.74	310.48	2.68 o
-2	6	3	247.46	241.82	2.32 o
-1	6	3	3240.28	3160.84	21.45 o
0	6	3	25.59	26.08	0.54 o
-6	7	3	501.43	486.53	4.27 o
-5	7	3	625.96	620.96	5.31 o
-4	7	3	12.88	14.58	0.54 o
-3	7	3	3907.72	3728.03	28.01 o
-2	7	3	1529.95	1487.04	11.59 o
-1	7	3	14.35	17.81	0.54 o
0	7	3	522.97	509.91	4.62 o
-7	8	3	268.00	251.63	2.68 o
-6	8	3	157.38	158.39	1.97 o
-5	8	3	0.59	1.26	0.36 o
-4	8	3	9.92	11.16	0.54 o
-3	8	3	243.66	248.28	2.51 o
-2	8	3	385.89	373.34	3.39 o

-1	8	3	23.26	25.91	0.72 o
0	8	3	79.97	78.71	1.62 o
-8	9	3	61.86	64.18	1.44 o
-7	9	3	141.82	143.23	2.33 o
-6	9	3	22.30	24.83	0.90 o
-5	9	3	547.66	540.07	5.34 o
-4	9	3	508.63	509.89	5.16 o
-3	9	3	974.57	936.17	9.17 o
-2	9	3	313.98	312.84	4.29 o
-1	9	3	87.33	90.03	1.80 o
0	9	3	692.57	673.89	10.13 o
-9	10	3	145.57	146.50	3.41 o
-8	10	3	661.50	683.99	8.71 o
-7	10	3	105.73	99.16	1.98 o
-6	10	3	514.44	521.50	5.70 o
-5	10	3	455.23	440.90	5.00 o
-4	10	3	3.69	5.76	0.72 o
-3	10	3	1613.94	1616.64	19.19 o
-2	10	3	697.77	702.00	9.06 o
-1	10	3	611.81	591.72	8.37 o
0	10	3	3.74	4.32	0.90 o
-10	11	3	531.89	522.95	10.88 o
-9	11	3	1650.95	1614.86	23.07 o
-8	11	3	11.87	16.38	1.26 o
-7	11	3	88.56	92.01	2.16 o
-6	11	3	426.64	425.11	5.72 o
-5	11	3	1146.98	1148.29	15.51 o
-4	11	3	338.34	341.37	6.08 o
-3	11	3	2.12	4.50	1.08 o
-2	11	3	287.59	303.75	5.73 o
-1	11	3	3263.26	3278.80	56.29 o
-9	12	3	428.08	453.88	9.65 o
-8	12	3	207.76	212.00	5.74 o
-7	12	3	27.45	36.88	2.52 o
-6	12	3	4.72	7.56	1.44 o
-5	12	3	6.70	11.88	1.44 o
-4	12	3	0.32	1.08	1.08 <
-3	12	3	109.66	116.06	5.03 o
0	0	4	5697.91	5547.90	79.56 o
0	1	4	312.35	333.39	1.78 o
-1	2	4	194.51	209.80	1.25 o
0	2	4	49.20	44.56	0.36 o
-2	3	4	1485.67	1520.15	7.84 o
-1	3	4	873.98	849.98	4.71 o
0	3	4	4172.83	3927.88	22.59 o
-3	4	4	126.73	121.21	1.26 o
-2	4	4	0.33	3.96	0.36 o
-1	4	4	232.62	233.22	1.79 o
0	4	4	376.79	373.61	2.85 o
-4	5	4	3595.20	3468.42	24.19 o
-3	5	4	979.14	929.20	6.82 o
-2	5	4	94.27	89.58	1.08 o
-1	5	4	2400.94	2325.77	16.73 o
0	5	4	943.54	907.40	6.84 o

-5	6	4	7.05	10.98	0.54 o
-4	6	4	2441.61	2372.36	17.50 o
-3	6	4	980.64	965.08	7.54 o
-2	6	4	1648.45	1612.07	12.06 o
-1	6	4	2409.24	2303.11	17.22 o
0	6	4	756.66	742.69	6.19 o
-6	7	4	2313.98	2162.50	17.21 o
-5	7	4	6.96	8.28	0.54 o
-4	7	4	67.76	72.43	1.08 o
-3	7	4	656.92	626.38	5.14 o
-2	7	4	1300.57	1287.22	10.12 o
-1	7	4	1299.34	1251.56	10.31 o
0	7	4	0.04	1.80	0.54 o
-7	8	4	3828.83	3670.80	33.38 o
-6	8	4	1204.62	1142.04	10.18 o
-5	8	4	860.63	829.64	7.42 o
-4	8	4	4057.60	3873.31	31.01 o
-3	8	4	459.14	446.00	4.46 o
-2	8	4	5.37	7.20	0.54 o
-1	8	4	220.48	221.68	3.05 o
0	8	4	1780.44	1733.16	17.19 o
-8	9	4	138.35	139.68	2.51 o
-7	9	4	425.48	429.58	4.64 o
-6	9	4	0.65	0.90	0.54 <
-5	9	4	30.75	29.32	0.90 o
-4	9	4	0.13	0.90	0.36 <
-3	9	4	54.70	55.20	1.26 o
-2	9	4	924.29	890.61	9.37 o
-1	9	4	56.74	57.54	1.44 o
0	9	4	728.76	721.36	8.70 o
-9	10	4	265.80	245.45	5.37 o
-8	10	4	86.13	91.66	1.80 o
-7	10	4	182.05	187.66	2.87 o
-6	10	4	488.18	470.06	5.17 o
-5	10	4	554.27	563.53	6.06 o
-4	10	4	95.43	94.87	1.62 o
-3	10	4	905.00	874.36	10.27 o
-2	10	4	874.57	886.96	10.45 o
-1	10	4	456.57	429.08	7.14 o
0	10	4	240.33	235.37	5.92 o
-9	11	4	1271.34	1216.71	27.11 o
-8	11	4	0.88	2.88	1.08 <
-7	11	4	1670.70	1672.93	19.39 o
-6	11	4	1017.65	1002.31	10.78 o
-5	11	4	230.49	229.47	3.59 o
-4	11	4	817.73	818.11	11.18 o
-3	11	4	0.42	0.00	1.08 <
-2	11	4	46.48	51.26	3.24 o
-8	12	4	390.85	402.15	10.37 o
-7	12	4	0.65	0.72	1.26 <
-6	12	4	201.30	198.76	9.15 o
-5	12	4	437.05	452.21	12.15 o
0	1	5	57.66	53.72	0.54 o
-1	2	5	301.75	277.75	1.78 o

0	2	5	214.36	197.48	1.43 o
-2	3	5	1566.18	1561.82	8.76 o
-1	3	5	3097.74	2991.16	16.78 o
0	3	5	129.36	131.83	1.08 o
-3	4	5	530.08	528.60	3.73 o
-2	4	5	480.45	443.39	3.38 o
-1	4	5	257.15	222.96	1.97 o
0	4	5	120.88	116.11	1.26 o
-4	5	5	38.32	38.84	0.72 o
-3	5	5	2009.54	1895.07	12.98 o
-2	5	5	1258.56	1250.09	9.59 o
-1	5	5	95.37	89.08	1.08 o
0	5	5	615.41	578.60	5.15 o
-5	6	5	420.93	416.77	3.75 o
-4	6	5	703.18	703.58	5.31 o
-3	6	5	1589.19	1524.91	11.27 o
-2	6	5	111.02	108.45	1.26 o
-1	6	5	2464.18	2368.06	20.72 o
0	6	5	13.42	13.86	0.72 o
-6	7	5	212.03	203.61	2.69 o
-5	7	5	428.26	404.79	3.92 o
-4	7	5	72.84	69.37	1.08 o
-3	7	5	1646.45	1576.36	13.02 o
-2	7	5	807.40	771.93	7.43 o
-1	7	5	326.54	318.82	3.58 o
0	7	5	26.43	29.68	1.08 o
-7	8	5	9.75	12.60	0.72 o
-6	8	5	114.70	111.17	1.62 o
-5	8	5	5.20	8.10	0.54 o
-4	8	5	875.74	851.69	7.78 o
-3	8	5	67.33	70.47	1.26 o
-2	8	5	29.18	31.30	0.90 o
-1	8	5	138.67	138.96	2.15 o
0	8	5	15.14	16.56	0.90 o
-8	9	5	60.76	68.51	1.80 o
-7	9	5	0.64	2.88	0.54 o
-6	9	5	743.14	727.19	6.57 o
-5	9	5	657.25	651.84	6.22 o
-4	9	5	603.89	600.88	6.05 o
-3	9	5	1770.69	1713.76	16.36 o
-2	9	5	534.97	549.39	6.24 o
-1	9	5	77.68	85.56	1.80 o
0	9	5	354.23	341.86	5.55 o
-9	10	5	1.17	1.80	0.90 <
-8	10	5	369.62	391.50	6.62 o
-7	10	5	412.74	412.27	5.90 o
-6	10	5	722.14	733.74	8.00 o
-5	10	5	410.15	392.42	4.65 o
-4	10	5	6.22	9.36	0.90 o
-3	10	5	434.38	433.72	6.61 o
-2	10	5	256.15	262.71	4.66 o
-1	10	5	167.08	163.69	5.56 o
-8	11	5	12.54	11.34	1.80 o
-7	11	5	0.23	2.34	0.72 o

-6	11	5	1087.90	1114.74	13.60 o
-5	11	5	615.11	607.70	8.01 o
-4	11	5	314.20	317.97	9.13 o
-3	11	5	215.34	237.63	10.58 o
0	0	6	7194.12	6704.87	77.93 o
0	1	6	549.70	550.09	3.37 o
-1	2	6	4116.38	3938.77	24.13 o
0	2	6	256.36	267.07	1.97 o
-2	3	6	257.59	249.04	1.97 o
-1	3	6	23.82	26.26	0.54 o
0	3	6	51.29	48.90	0.72 o
-3	4	6	2800.62	2685.56	17.65 o
-2	4	6	2973.51	2870.79	19.06 o
-1	4	6	17.07	19.79	0.54 o
0	4	6	1731.68	1672.79	11.76 o
-4	5	6	96.06	90.90	1.26 o
-3	5	6	1.41	1.80	0.36 o
-2	5	6	799.32	780.12	6.19 o
-1	5	6	435.94	428.74	4.10 o
0	5	6	1735.02	1669.22	15.61 o
-5	6	6	464.12	449.07	4.46 o
-4	6	6	508.81	501.31	4.28 o
-3	6	6	1394.64	1367.95	11.36 o
-2	6	6	60.96	55.55	1.08 o
-1	6	6	60.37	60.41	1.26 o
0	6	6	1372.02	1314.58	12.44 o
-6	7	6	88.59	87.33	1.62 o
-5	7	6	1122.40	1119.57	9.86 o
-4	7	6	651.55	649.46	5.87 o
-3	7	6	34.23	32.92	0.90 o
-2	7	6	82.53	83.93	1.44 o
-1	7	6	125.31	123.01	1.80 o
0	7	6	220.54	202.04	2.87 o
-7	8	6	53.34	57.19	1.62 o
-6	8	6	3.58	5.94	0.54 o
-5	8	6	2153.28	2104.36	17.27 o
-4	8	6	3.29	5.40	0.54 o
-3	8	6	1306.99	1277.35	12.47 o
-2	8	6	317.68	318.92	3.76 o
-1	8	6	1131.41	1103.05	12.70 o
0	8	6	3223.48	3208.39	38.81 o
-8	9	6	566.48	573.25	8.20 o
-7	9	6	2.25	3.96	0.90 o
-6	9	6	2478.26	2429.49	29.75 o
-5	9	6	189.13	188.19	2.87 o
-4	9	6	685.66	685.51	8.36 o
-3	9	6	1776.66	1712.73	20.22 o
-2	9	6	60.92	62.39	1.98 o
-1	9	6	783.68	790.91	10.83 o
-7	10	6	67.63	67.06	3.06 o
-6	10	6	22.01	23.39	1.26 o
-5	10	6	122.91	123.58	2.51 o
-4	10	6	405.88	417.57	7.87 o
-3	10	6	158.16	168.75	5.92 o

0	1	7	5.86	6.66	0.54 o
-1	2	7	0.49	1.62	0.36 o
0	2	7	8.15	10.26	0.54 o
-2	3	7	1270.68	1281.47	9.99 o
-1	3	7	2144.36	2134.96	17.18 o
0	3	7	79.83	80.87	1.26 o
-3	4	7	438.10	433.78	4.10 o
-2	4	7	166.09	163.62	1.79 o
-1	4	7	10.02	13.32	0.54 o
0	4	7	83.92	84.10	1.44 o
-4	5	7	137.26	134.47	1.80 o
-3	5	7	607.89	601.10	5.51 o
-2	5	7	1028.13	1027.97	9.35 o
-1	5	7	100.45	98.45	1.44 o
0	5	7	20.35	21.41	0.72 o
-5	6	7	212.96	218.57	2.51 o
-4	6	7	741.53	760.17	6.92 o
-3	6	7	603.20	599.63	5.70 o
-2	6	7	85.70	88.24	1.44 o
-1	6	7	1617.22	1608.75	14.32 o
0	6	7	12.28	14.58	0.72 o
-6	7	7	135.50	135.04	2.87 o
-5	7	7	336.78	331.19	4.29 o
-4	7	7	15.62	14.58	0.72 o
-3	7	7	1631.39	1611.97	13.97 o
-2	7	7	699.13	687.74	8.18 o
-1	7	7	136.04	128.75	2.51 o
0	7	7	36.84	40.29	1.44 o
-7	8	7	24.73	34.19	1.98 o
-6	8	7	95.11	102.61	2.52 o
-5	8	7	1.76	1.80	0.72 <
-4	8	7	189.47	191.61	3.41 o
-3	8	7	104.51	112.12	2.52 o
-2	8	7	15.03	14.76	1.08 o
-1	8	7	78.39	76.22	1.98 o
-6	9	7	202.41	194.99	9.33 o
-4	9	7	322.31	345.50	9.49 o
0	0	8	6911.62	6418.86	181.42 o
0	1	8	127.96	139.70	2.51 o
-1	2	8	96.33	102.77	1.98 o
0	2	8	21.42	24.11	0.90 o
-2	3	8	929.31	950.79	9.91 o
-1	3	8	408.90	417.48	4.47 o
0	3	8	1878.81	1903.10	17.19 o
-3	4	8	86.94	86.26	1.44 o
-2	4	8	0.68	0.90	0.54 <
-1	4	8	49.43	48.20	1.26 o
0	4	8	156.35	160.11	2.15 o
-4	5	8	1981.99	1997.18	21.18 o
-3	5	8	334.00	337.11	4.47 o
-2	5	8	42.15	48.56	1.26 o
-1	5	8	900.17	919.65	9.92 o
0	5	8	570.93	589.14	7.66 o
-5	6	8	48.28	50.18	1.62 o

-4	6	8	1173.39	1177.02	16.75 o
-3	6	8	486.59	504.20	7.32 o
-2	6	8	1403.73	1412.61	16.68 o
-1	6	8	1636.11	1653.55	19.23 o
0	6	8	465.79	477.49	7.86 o
-6	7	8	1478.70	1560.56	48.95 o
-5	7	8	53.97	65.82	5.04 o
-3	7	8	293.78	306.98	8.60 o
-2	7	8	372.40	405.83	10.73 o
0	1	9	7.80	8.10	1.44 o
-1	2	9	53.19	60.78	2.88 o
0	2	9	32.06	40.84	1.80 o
-2	3	9	792.71	831.02	10.47 o
-1	3	9	1797.72	1897.52	21.79 o
0	3	9	31.45	35.08	1.80 o
-3	4	9	191.50	214.76	4.84 o
-2	4	9	47.76	56.65	1.98 o
-1	4	9	150.97	164.10	3.05 o
0	4	9	30.37	35.08	1.62 o