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Re-investigation of the crystal structure of enstatite under high-pressure conditions

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Abstract

A synthetic single crystal of pure orthoenstatite ($MgSiO_3$, space group *Pbca*) has been investigated at high pressure for structural determinations by in situ single-crystal X-ray diffraction using a diamond-anvil cell. Ten complete intensity data collections were performed up to 9.36 GPa. This study significantly improved the accuracy of structural parameters in comparison to a previous high-pressure structural study, allowing a more detailed examination of structural behavior of orthoenstatite at high pressures and a comparison to other more recent structural studies performed on orthopyroxenes with different compositions. The structural evolution determined in this work confirms the high-pressure evolution found previously for other orthopyroxenes and removes some ambiguities originating from the less accurate published data on the $MgSiO_3$ structure at high pressure. The structural compression is mostly governed by significant volume decrease of the Mg1 and Mg2 octahedra, affecting in turn the kink of the tetrahedral chains, especially the TB chain of larger SiO_4 tetrahedra. The Mg2 polyhedron undergoes the largest volume variation, 8.7%, due especially to the strong contraction of the longest bond distance (Mg2-O3B), whereas Mg1 polyhedral volume decreases by about 7.4%. The compressional behavior of the tetrahedral sites is quite different from previously published data. The TA and TB tetrahedral volumes decrease by about 2.8 and 1.8%, respectively, and no discontinuities can be observed in the pressure range investigated. Using the data on the pure orthoenstatite as reference, we can confirm the basic influences of element substitutions on the evolution of the crystal structure with pressure.

Keywords: Enstatite, crystal structure, X-ray diffraction, high pressure, diamond-anvil cell

Introduction

As has already been well established by several studies (e.g., Angel 2000; Nestola et al. 2005, 2008a; Gatta et al. 2006; Boffa Ballaran et al. 2009), the determination of accurate and precise unit-cell parameters as a function of pressure by single-crystal X-ray diffraction can be obtained by means of a well-defined experimental protocol (see for example Angel and Finger 2011), used nowadays in several diffraction laboratories. However, it is still extremely difficult to reach comparably high-quality data for crystal-structure measurements at high-pressure conditions. This is evident, for example, by the significant scatter usually observed in the trends of geometrical and structural parameters with pressure. In particular, this problem can become critical for crystal structures built of light atoms, which produce weaker X-ray diffraction from the very small crystals typically measured in diamond-anvil cells (DAC). One example is given by pure orthoenstatite ($Mg_2Si_2O_6$, $Z = 8$), which has 80 atoms in the unit cell and Si as the heaviest atom. An anisotropic crystal structure refinement for orthoenstatite requires no less than 92 parameters to be refined and thus at least 920 unique reflections to obtain an optimal ratio of unique reflections to refined parameters of at least 10:1. For measurements of orthoenstatite in a diamond-anvil cell, using Mo$K\alpha$ radiation, a maximum of 680–700 unique reflections can be accessible, due to access limitations and to the crystal orientation of which typically only 400–450 have an $F_o > 4\sigma(F_o)$. This means that orthoenstatite under pressure can be only isotropically refined (or only Mg and Si sites can be anisotropically refined) affecting the quality and precision of the structural data. Beyond the restriction on the number of accessible unique reflections during a high-pressure measurement, data quality is also affected by the presence of diamond diffraction spots and of diffraction rings from the beryllium backing plates and the steel gasket. However, it has been recently demonstrated that the use of new DACs with diamond-backing plates instead of Be ones allows a significant improvement in data quality and thus the refined crystal structure (Periotto et al. 2011).

Orthoenstatite is a major component of the upper part of the Earth's mantle. Knowledge of the compressional and thermal behavior of orthopyroxene is therefore fundamental for understanding the complex geodynamic processes occurring in the mantle. Pure, synthetic $MgSiO_3$ has already been investigated under high pressure to define its elasticity and structural behavior (Angel and Hugh-Jones 1994; Hugh-Jones and Angel 1994) but these data show large scatter of the structural parameters as a function of pressure when compared to newer data on orthopyroxenes of different compositions (Nestola et al. 2006, 2008b). Therefore, the previous study leaves open the question of the

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detailed compression mechanisms of the pure end-member $MgSiO_3$ and at the same time prevents conclusions to be drawn about the influence of element substitutions on the properties of orthoenstatite.

In a recent analysis of pure orthoenstatite, Angel and Jackson (2002) obtained the best estimate of the equation of state parameters by combining the various results of single-crystal compression data and showing these to be consistent with ultrasonic and Brillouin measurements. However, its high-pressure structural behavior has not been re-analyzed despite the problems mentioned above and their obvious importance. In this work, we report a re-measurement of the pure orthoenstatite structure at high-pressure conditions with the purpose of improving the quality of the crystal structure parameters for the pure orthoenstatite to that obtained in similar recent studies for orthopyroxenes.

The data obtained for the pure $MgSiO_3$ end-member will allow a more reliable comparison of the compression mechanisms among the orthopyroxenes with different compositions, to define the effect of Ca, Al, and Fe substitutions in orthopyroxene at high-pressure conditions. A direct comparison between the results of this work and those obtained previously by Hugh-Jones and Angel (1994) is presented to evaluate the improvement on the structural data quality presently achievable due to the advances in X-ray single-crystal diffraction techniques.

Experimental methods

A colorless synthetic crystal of about $150 \times 100 \times 50$ μm^3 in size was cut from a larger synthetic crystal of orthoenstatite, synthesized as described in Ito (1975) and kindly provided by H. Ohashi. It was selected on the basis of the sharpness of its X-ray diffraction profiles and lack of twins and optical imperfections. The loading was done in an ETH-type DAC equipped with diamond backing plates (Miletich et al. 2000; Periotto et al. 2011), using a stainless steel gasket preindented to 90 μm with a spark-eroded hole of 250 μm in diameter. Ten complete intensity data collections were performed from room pressure up to 9.36 GPa, including two measurements on decompression. The measurements were performed with the crystal in the DAC mounted on a Bruker-AXS four-circle diffractometer equipped with a Smart1000 CCD area detector and a flat graphite monochromator, using Mo$K\alpha$ radiation. The pressure medium used was a 16:3:1 mixture of methanol:ethanol:water, and the pressure was calibrated using the equation of state determined by Angel and Jackson (2002), as done in a previous study of Nestola et al. (2008b). The measurements were made in 16 separate ω-scans with 0.2° steps covering practically all of the available reciprocal space up to 60° in 2θ, using an exposure time of 60 s. The sample-detector distance was 5.5 cm and the generator was operated at 40 kV and 40 mA. The combination of the fine slicing of reciprocal space and a high redundancy offered by the data collection procedure allows the unit-cell volumes to be determined to ~1 part in 4000–8000 and thus pressure to be better than 0.07 GPa. The SMART software was used for the determination of crystal lattice parameters and data collection. Data were integrated with SAINT+ (Bruker-AXS) and corrected for absorption using the ABSORB software (Angel 2004). Weighted structural refinements were done using the SHELX-97 package (Sheldrick 2008). The refinements were performed starting from the room-pressure atomic coordinates of Nestola et al. (2008b). Anisotropic displacement parameters were applied for the cation sites and isotropic for the oxygen sites.

Refinement details, atomic coordinates with equivalent and isotropic atomic displacement parameters, and interatomic distances are reported in Tables 1, 2, and 3, respectively. It is noteworthy that the equation of state calculated from our pressure-volume data, obtained with a CCD diffractometer and reported in Table 1, give a bulk modulus $K_0 = 108(2)$ GPa and its first derivate $K_0' = 7.9(8)$, which are within 1 e.s.d. compared to the more accurate values reported in Angel and Jackson (2002), equal to $K_0 = 105.8(5)$ GPa and $K_0' = 8.5(3)$. For all structures the volumes of coordination polyhedra and their distortion parameters have been calculated by the IVTON program (Balić-Žunić and Vicković 1996). (Lists of structure factors and the CIFs have been deposited[1].)

[1] Deposit item AM-12-071, Structure factors and CIFs. Deposit items are available two ways: For a paper copy contact the Business Office of the Mineralogical Society of America (see inside front cover of recent issue) for price information. For an electronic copy visit the MSA web site at http://www.minsocam.org, go to the *American Mineralogist* Contents, find the table of contents for the specific volume/issue wanted, and then click on the deposit link there.

Table 1. Structure refinement details for $MgSiO_3$

P (GPa)	0.00010(1)	0.22(3)	1.23(4)	2.69(5)	4.19(4)	5.21(7)*	6.57(5)
a (Å)	18.210(3)	18.204(3)	18.158(3)	18.105(3)	18.056(3)	18.019(6)	17.982(3)
b (Å)	8.820(2)	8.810(2)	8.780(2)	8.734(2)	8.692(2)	8.668(3)	8.633(2)
c (Å)	5.1767(4)	5.1731(4)	5.1574(4)	5.1376(4)	5.1192(4)	5.1073(8)	5.0926(4)
V (Å^3)	831.4(2)	829.7(1)	822.2(1)	812.5(1)	803.4(1)	797.7(3)	790.6(1)
Range of *hkl*	$-19 \le h \le 19$	$-19 \le h \le 19$	$-19 \le h \le 19$	$-19 \le h \le 19$	$-19 \le h \le 19$	$-19 \le h \le 19$	$-19 \le h \le 19$
	$-9 \le k \le 9$	$-9 \le k \le 9$	$-9 \le k \le 8$	$-9 \le k \le 8$	$-9 \le k \le 8$	$-9 \le k \le 8$	$-9 \le k \le 8$
	$-6 \le l \le 6$	$-6 \le l \le 6$	$-6 \le l \le 6$	$-6 \le l \le 6$	$-6 \le l \le 6$	$-6 \le l \le 6$	$-6 \le l \le 6$
Unique refl.	603	598	594	584	574	561	549
Observed refl. $F_o > 4\sigma(F_o)$	392	386	383	387	372	366	332
$2\theta_{max}$ (°)	56.53	56.57	56.49	56.57	56.56	56.29	56.48
R_{int}	6.4	7.4	7.2	7.6	8.0	9.8	9.3
R_1	3.9	4.0	3.8	4.5	4.2	5.1	5.0
wR_2	10.1	9.7	9.9	10.8	10.9	12.4	13.7
GooF	1.00	0.99	0.95	0.96	0.97	0.95	0.98
Refined parameters	61	61	61	61	61	61	61

P (GPa)	8.26(6)*	8.65(7)	9.36(5)
a (Å)	17.933(3)	17.916(3)	17.897(3)
b (Å)	8.595(2)	8.590(2)	8.575(2)
c (Å)	5.0766(4)	5.0726(4)	5.0664(4)
V (Å^3)	782.4(1)	780.7(2)	777.5(1)
Range of *hkl*	$-19 \le h \le 19$	$-19 \le h \le 19$	$-19 \le h \le 19$
	$-9 \le k \le 8$	$-9 \le k \le 8$	$-9 \le k \le 8$
	$-6 \le l \le 6$	$-6 \le l \le 6$	$-6 \le l \le 6$
Unique refl.	599	560	560
Observed refl. $F_o > 4\sigma(F_o)$	362	368	368
$2\theta_{max}$ (°)	56.44	56.49	56.57
R_{int}	9.3	8.6	9.0
R_1	4.4	4.6	4.6
wR_2	11.6	11.7	11.4
GooF	0.96	0.96	0.97
Refined parameters	61	61	61

* Data measured during decompression.

TABLE 2. Atomic coordinates and displacement parameters for $MgSiO_3$

P (GPa)		0.00010(1)	0.22(3)	1.23(4)	2.69(5)	4.19(4)	5.21(7)*	6.57(5)	8.26(6)*	8.65(7)	9.36(5)
Mg2	*x*	0.3769(1)	0.3767(1)	0.3771(1)	0.3771(1)	0.3772(1)	0.3774(1)	0.3776(1)	0.3774(1)	0.3774(1)	0.3775(1
	y	0.4868(2)	0.4863(3)	0.4853(2)	0.4843(2)	0.4837(2)	0.4842(3)	0.4831(3)	0.4828(2)	0.4828(2)	0.4824(2)
	z	0.3589(3)	0.3577(2)	0.3555(2)	0.3531(3)	0.3511(3)	0.3503(3)	0.3488(3)	0.3474(3)	0.3474(3)	0.3466(3)
	U_{eq}	0.0096(5)	0.0094(5)	0.0095(5)	0.0089(5)	0.0088(6)	0.0094(6)	0.0090(7)	0.0090(6)	0.0087(6)	0.0090(6)
Mg1	*x*	0.3759(1)	0.3759(1)	0.3758(1)	0.3760(1)	0.3760(1)	0.3761(1)	0.3762(1)	0.3763(1)	0.3763(1)	0.3765(1)
	y	0.6538(2)	0.6538(2)	0.6542(2)	0.6550(2)	0.6556(2)	0.6561(3)	0.6564(3)	0.6571(2)	0.6571(2)	0.6575(2)
	z	0.8659(3)	0.8654(3)	0.8629(3)	0.8608(3)	0.8585(3)	0.8583(3)	0.8566(3)	0.8546(3)	0.8548(3)	0.8544(3)
	U_{eq}	0.0069(5)	0.0069(5)	0.0064(5)	0.0060(5)	0.0069(5)	0.0068(6)	0.0078(7)	0.0065(6)	0.0063(6)	0.0065(6)
TA	*x*	0.27146(9)	0.27160(9)	0.27138(9)	0.27120(9)	0.27123(9)	0.2711(1)	0.2712(1)	0.2711(1)	0.27106(9)	0.2711(1)
	y	0.3420(2)	0.3419(2)	0.3425(2)	0.3428(2)	0.3431(2)	0.3432(2)	0.3436(2)	0.3441(2)	0.3440(2)	0.3443(2)
	z	0.0505(2)	0.0494(2)	0.0474(2)	0.0448(2)	0.0431(3)	0.0422(3)	0.0406(3)	0.0386(2)	0.0386(2)	0.0378(2)
	U_{eq}	0.0065(4)	0.0051(4)	0.0052(4)	0.0049(4)	0.0053(4)	0.0059(5)	0.0073(6)	0.0058(5)	0.0054(5)	0.0057(5)
TB	*x*	0.47368(8)	0.47346(8)	0.47323(8)	0.47305(8)	0.47285(9)	0.4729(1)	0.4727(1)	0.47244(9)	0.47249(9)	0.47243(9)
	y	0.3370(2)	0.3374(2)	0.3371(2)	0.3376(2)	0.3375(2)	0.3375(2)	0.3377(3)	0.3379(2)	0.3376(2)	0.3381(2)
	z	0.7985(2)	0.7989(2)	0.8004(2)	0.8018(2)	0.8025(2)	0.8028(3)	0.8034(3)	0.0050(5)	0.0048(5)	0.0050(5)
	U_{eq}	0.0052(4)	0.0051(4)	0.0049(4)	0.0047(4)	0.0053(4)	0.0056(5)	0.0059(6)	0.0050(5)	0.0048(5)	0.0050(5)
O1A	*x*	0.1832(2)	0.1832(2)	0.1830(2)	0.1828(2)	0.1823(2)	0.1827(2)	0.1821(3)	0.1823(2)	0.1818(2)	0.1821(2)
	y	0.3392(4)	0.3392(4)	0.3397(4)	0.3397(4)	0.3398(4)	0.3404(5)	0.3397(5)	0.3401(5)	0.3400(5)	0.3400(5)
	z	0.0359(5)	0.0354(5)	0.0318(5)	0.0288(5)	0.0265(5)	0.0262(6)	0.0238(6)	0.0219(6)	0.0214(6)	0.0207(6)
	U_{iso}	0.0040(8)	0.0048(8)	0.0053(8)	0.0054(8)	0.0046(8)	0.007(1)	0.005(1)	0.0059(9)	0.0063(9)	0.0046(8)
O2A	*x*	0.3110(2)	0.3105(2)	0.3106(2)	0.3106(2)	0.3102(2)	0.3103(2)	0.3102(3)	0.3094(2)	0.3098(2)	0.3093(2)
	y	0.5022(4)	0.5028(4)	0.5038(4)	0.5049(5)	0.5062(5)	0.5058(5)	0.5069(6)	0.5091(5)	0.5093(5)	0.5091(5)
	z	0.0432(5)	0.0428(5)	0.0404(5)	0.0376(6)	0.0351(6)	0.0340(7)	0.0324(7)	0.0314(6)	0.0312(6)	0.0306(6)
	U_{iso}	0.0080(8)	0.0067(8)	0.0067(8)	0.0073(9)	0.0071(9)	0.008(1)	0.007(1)	0.008(1)	0.007(1)	0.008(1)
O3A	*x*	0.3028(2)	0.3030(2)	0.3030(2)	0.3033(2)	0.3037(2)	0.3034(2)	0.3040(2)	0.3042(2)	0.3043(2)	0.3043(2)
	y	0.2232(4)	0.2242(4)	0.2234(4)	0.2235(5)	0.2230(5)	0.2222(5)	0.2228(6)	0.2223(5)	0.2224(5)	0.2224(5)
	z	0.8299(5)	0.8294(5)	0.8272(5)	0.8252(5)	0.8244(6)	0.8239(6)	0.8230(6)	0.8219(6)	0.8210(6)	0.8211(6)
	U_{iso}	0.0056(8)	0.0056(8)	0.0062(8)	0.0057(8)	0.0060(9)	0.006(1)	0.006(1)	0.0047(9)	0.0044(9)	0.0043(9)
O1B	*x*	0.5626(2)	0.5627(2)	0.5626(2)	0.5624(2)	0.5621(2)	0.5620(2)	0.5623(3)	0.5615(2)	0.5618(2)	0.5619(2)
	y	0.3396(4)	0.3402(4)	0.3391(4)	0.3393(4)	0.3391(4)	0.3386(5)	0.3386(5)	0.3393(5)	0.3384(5)	0.3386(5)
	z	0.7995(5)	0.7998(5)	0.8018(5)	0.8036(6)	0.8053(6)	0.8058(6)	0.8068(7)	0.8089(6)	0.8089(6)	0.8100(6)
	U_{iso}	0.0047(8)	0.0060(8)	0.0059(8)	0.0060(8)	0.0059(8)	0.0055(9)	0.007(1)	0.0068(9)	0.0063(8)	0.0060(8)
O2B	*x*	0.4325(1)	0.4325(2)	0.4324(2)	0.4326(2)	0.4326(2)	0.4328(2)	0.4333(3)	0.4332(2)	0.4332(2)	0.4331(2
	y	0.4820(4)	0.4826(4)	0.4831(4)	0.4831(4)	0.4835(4)	0.4842(5)	0.4843(5)	0.4852(4)	0.4849(4)	0.4855(4)
	z	0.6888(5)	0.6885(5)	0.6875(5)	0.6858(6)	0.6850(6)	0.6840(6)	0.6817(7)	0.6812(6)	0.6814(6)	0.6809(6)
	U_{iso}	0.0075(8)	0.0081(8)	0.0066(8)	0.0075(9)	0.0078(9)	0.007(1)	0.007(1)	0.0079(9)	0.0066(9)	0.0070(9)
O3B	*x*	0.4478(2)	0.4477(2)	0.4474(2)	0.4471(2)	0.4467(2)	0.4467(2)	0.4456(3)	0.4457(2)	0.4457(2)	0.4455(2)
	y	0.1957(4)	0.1954(4)	0.1940(4)	0.1929(4)	0.1922(4)	0.1915(5)	0.1908(5)	0.1895(4)	0.1888(5)	0.1885(4)
	z	0.6037(5)	0.6050(5)	0.6077(5)	0.6103(5)	0.6118(5)	0.6129(6)	0.6148(6)	0.6159(6)	0.6164(6)	0.6171(6)
	U_{iso}	0.0039(8)	0.0049(8)	0.0044(8)	0.0041(8)	0.0040(8)	0.0039(9)	0.004(1)	0.0043(9)	0.0040(8)	0.0039(8)

RESULTS AND DISCUSSION

The structure of orthopyroxene consists of alternating (100) layers of chains of SiO_4 tetrahedra running along the *c* axis and by layers of octahedral Mg1 and Mg2 sites (Cameron and Papike 1981). The tetrahedral sites, forming infinite chains, are labeled A and B. The A-chain is characterized by tetrahedral sites with smaller volume and larger Si-O3-Si angle (O3 is the bridging oxygen), compared to those in the B-chain. The angle that the Si-O bonds make around the bridging oxygen measures the stretching or (oppositely) the kinking of the tetrahedral chain, the smaller angle represents the larger kink. The Mg2 octahedron is larger and more distorted than the Mg1 octahedron.

Beyond the typical geometrical parameters, a further detailed description of the high-pressure structures of enstatite is provided by the crystal-chemical parameters defined by Balić-Žunić and Makovicky (1996) and Makovicky and Balić-Žunić (1998) and evaluated by Balić-Žunić (2007). The geometric parameters used as a measure of polyhedral irregularity are based on the centroid method, where the centroid is defined as the point in the coordination polyhedron having the minimum variance of the distances to the vertices. This method allows the separation of the distortion connected solely to the arrangement of ligands forming the vertices of the polyhedron from that due to the relative position of the central atom to the ligands. The three parameters, which completely describe these distinct aspects of distortion are volume eccentricity, volume asphericity, and volume distortion. The volume eccentricity is the parameter defining the displacement of the central atom from its ligands. The volume asphericity and the volume distortions are parameters connected solely to the arrangement of ligands: the volume asphericity describes the deviation of vertices of a polyhedron from the surface of a best fit sphere to the ligand positions, whereas the volume distortion is measured relative to a regular polyhedron. It compares the volume differences between the distorted polyhedron and the ideal one inscribed in a sphere of the same radius. A sphere was fitted to the six O atoms around the two Mg positions in the structure and the four O atoms around each Si atoms. Note that the asphericity for the tetrahedra is zero by definition since a sphere can always be defined to pass through four non-coplanar points in space.

Mg1 and Mg2 octahedra

The evolution as a function of pressure of Mg1 and Mg2 octahedral volumes is shown in Figure 1 and compared with those calculated from data of Hugh-Jones and Angel (1994). In this and in the following figures we represent our data and those from the latter work as filled and empty symbols, respectively. As already confirmed in previous studies (Hugh-Jones and Angel 1994; Hugh-Jones et al. 1997; Nestola et al. 2006, 2008b), the Mg2 is the most compressible polyhedron in the structure with a volume

TABLE 3. Bond lengths (Å), polyhedral volumes (Å^3), distortion parameters, and O3-O3-O3 (°) angles for $MgSiO_3$

P (GPa)	0.00010(1)	0.22(3)	1.23(4)	2.69(5)	4.19(4)	5.21(7)*	6.57(5)	8.26(6)*	8.65(7)	9.36(5)
Mg1-O1A	2.020(3)	2.018(3)	2.015(3)	2.011(4)	2.000(4)	2.000(4)	1.994(4)	1.989(4)	1.986(4)	1.989(4)
Mg1-O1A	2.146(4)	2.144(4)	2.133(4)	2.117(4)	2.100(4)	2.100(5)	2.080(5)	2.073(4)	2.066(4)	2.064(4)
Mg1-O1B	2.064(4)	2.063(4)	2.059(4)	2.054(4)	2.052(4)	2.047(4)	2.040(5)	2.040(4)	2.035(4)	2.026(4)
Mg1-O1B	2.162(4)	2.163(4)	2.146(4)	2.133(4)	2.120(4)	2.109(5)	2.095(5)	2.094(4)	2.084(4)	2.079(4)
Mg1-O2A	2.006(4)	2.007(4)	1.996(4)	1.987(4)	1.979(4)	1.978(5)	1.970(5)	1.964(4)	1.958(4)	1.965(4)
Mg1-O2B	2.049(4)	2.044(4)	2.032(4)	2.027(4)	2.018(4)	2.014(4)	2.014(5)	1.999(4)	2.000(4)	1.994(4
<Mg1-O>	2.074	2.073	2.064	2.055	2.045	2.041	2.032	2.027	2.021	2.020
V	11.75(6)	11.73(6)	11.58(5)	11.43(6)	11.27(5)	11.22(9)	11.07(6)	11.00(5)	10.90(5)	10.88(5)
eccentricity	0.1274	0.1289	0.1264	0.1204	0.1176	0.1131	0.1051	0.1104	0.1061	0.0976
asphericity	0.0380	0.0370	0.0309	0.0268	0.0224	0.0225	0.0204	0.0144	0.0153	0.0139
volume distortion	0.0113	0.0111	0.0108	0.0106	0.0102	0.0095	0.0099	0.0089	0.0095	0.0090
Mg2-O1A	2.096(4)	2.097(4)	2.093(4)	2.086(4)	2.077(4)	2.071(5)	2.071(5)	2.060(4)	2.055(4)	2.058(4)
Mg2-O1B	2.057(4)	2.054(4)	2.057(4)	2.055(4)	2.053(4)	2.047(5)	2.041(5)	2.042(4)	2.042(4)	2.040(4)
Mg2-O2A	2.032(4)	2.032(3)	2.032(3)	2.027(4)	2.029(4)	2.027(4)	2.027(4)	2.027(4)	2.023(4)	2.027(4)
Mg2-O2B	1.986(3)	1.990(3)	1.984(3)	1.982(4)	1.981(4)	1.975(4)	1.969(4)	1.968(4)	1.967(4)	1.964(4)
Mg2-O3A	2.297(4)	2.294(4)	2.278(4)	2.258(4)	2.238(4)	2.235(5)	2.220(5)	2.201(5)	2.201(5)	2.195(5)
Mg2-O3B	2.450(4)	2.438(4)	2.396(4)	2.358(4)	2.326(4)	2.312(4)	2.274(5)	2.253(4)	2.246(4)	2.232(4)
<Mg2-O>	2.153	2.151	2.140	2.128	2.117	2.111	2.100	2.092	2.089	2.086
V	12.47(6)	12.44(6)	12.26(6)	12.07(6)	11.90(6)	11.81(9)	11.62(6)	11.49(6)	11.44(6)	11.39(5
eccentricity	0.2649	0.2582	0.2364	0.2174	0.2017	0.1998	0.1789	0.1687	0.1672	0.1588
asphericity	0.1568	0.1519	0.1410	0.1305	0.1189	0.1166	0.1077	0.0984	0.0968	0.0937
volume distortion	0.0664	0.0664	0.0653	0.064	0.0625	0.0615	0.0615	0.0599	0.0605	0.0601
TA-O1A	1.609(4)	1.611(4)	1.607(4)	1.604(4)	1.609(4)	1.597(5)	1.604(5)	1.595(4)	1.601(4)	1.596(4)
TA-O2A	1.586(4)	1.585(4)	1.585(4)	1.586(4)	1.583(4)	1.576(5)	1.574(5)	1.576(4)	1.580(4)	1.570(4)
TA-O3A	1.651(4)	1.643(4)	1.648(4)	1.642(4)	1.640(4)	1.637(4)	1.632(4)	1.630(4)	1.632(4)	1.628(4)
TA-O3A	1.658(3)	1.663(3)	1.657(3)	1.658(3)	1.657(3)	1.652(4)	1.657(4)	1.658(4)	1.653(4)	1.655(4)
<SiA-O>	1.626	1.625	1.624	1.623	1.622	1.616	1.617	1.615	1.617	1.612
V	2.18(2)	2.17(2)	2.17(2)	2.16(2)	2.16(2)	2.13(3)	2.14(2)	2.13(2)	2.14(2)	2.12(2
eccentricity	0.0948	0.0961	0.0943	0.0925	0.0925	0.0983	0.0992	0.1016	0.0897	0.1045
volume distortion	0.0113	0.0103	0.0111	0.0113	0.0116	0.0114	0.0120	0.0116	0.0125	0.0119
TB-O1B	1.619(4)	1.624(4)	1.624(4)	1.617(4)	1.612(4)	1.606(5)	1.612(6)	1.598(5)	1.600(5)	1.602(5)
TB-O2B	1.588(4)	1.586(4)	1.591(4)	1.584(4)	1.581(4)	1.582(4)	1.578(5)	1.578(4)	1.577(4)	1.577(4)
TB-O3B	1.671(4)	1.671(4)	1.670(4)	1.669(4)	1.665(4)	1.663(4)	1.664(5)	1.665(4)	1.666(4)	1.668(4)
TB-O3B	1.674(3)	1.676(3)	1.675(3)	1.674(3)	1.672(3)	1.672(4)	1.677(4)	1.669(3)	1.669(3)	1.670(3)
<SiB-O>	1.638	1.640	1.640	1.636	1.632	1.631	1.632	1.628	1.628	1.629
V	2.24(2)	2.25(2)	2.24(2)	2.23(2)	2.22(2)	2.21(3)	2.22(2)	2.20(2)	2.20(2)	2.20(2)
eccentricity	0.1166	0.1164	0.1109	0.1208	0.1207	0.1197	0.1274	0.1288	0.1290	0.1303
volume distortion	0.0067	0.0063	0.0064	0.0063	0.0063	0.0062	0.0057	0.0056	0.0057	0.0055
O3A-O3A-O3A	159.3(2)	160.1(2)	159.4(2)	159.6(2)	159.2(2)	158.6(2)	159.1(3)	158.8(2)	158.8(2)	158.8(2)
O3B-O3B-O3B	139.4(2)	139.2(2)	138.3(2)	137.6(2)	137.1(2)	136.7(2)	136.3(2)	135.4(2)	135.0(2)	134.8(2)

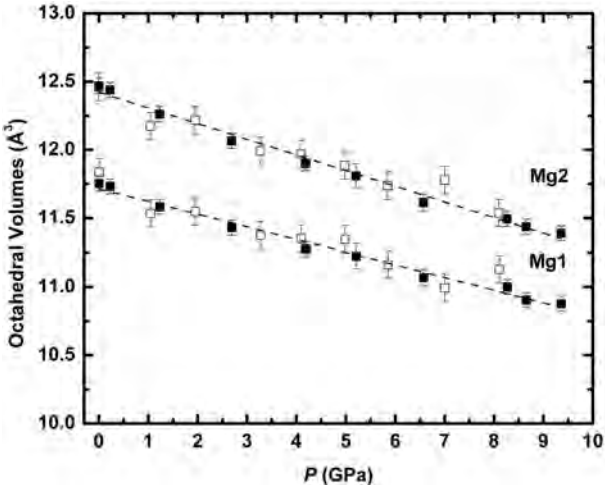

FIGURE 1. Evolution of the Mg coordination polyhedral volumes as a function of pressure. The filled symbols are used for the data of this work, the empty for the Hugh-Jones and Angel (1994) data.

decreasing by about 8.7% up to 9.36 GPa and a linear volume compressibility $\beta_V = 0.0096(6)$ GPa^{-1} (evaluated up to 10 GPa). The Mg1 octahedron shows a slightly smaller reduction with pressure of about 7.4% and a linear volume compressibility corresponding to 0.0082(7) GPa^{-1}. The new data show that the compression of both the Mg1 and Mg2 octahedra (Fig. 1) continues smoothly with increasing pressure. Although the previous data obviously conform to the same trend (Fig. 1), their large scatter would not allow for the same conclusions if they were taken alone. The previous data therefore did not show a convergence of the volumes, which is obvious in the present study, as the polyhedral compressibilities were determined as being identical with β_V for Mg2 being 0.0087(12) GPa^{-1} and β_V = 0.0086(11) GPa^{-1} for Mg1.

An analysis of the Mg-O distances (Table 3) confirms the high-pressure mechanism found for other orthoenstatites with different compositions (Nestola et al. 2006, 2008b). As also observed by Hugh-Jones and Angel (1994) and according to our data, the Mg2-O3B distance undergoes the strongest compression (Fig. 2). It contracts by 8.9%, followed by the Mg2-O3A that shortens by 4.4% (Fig. 3a). The other Mg2-O distances

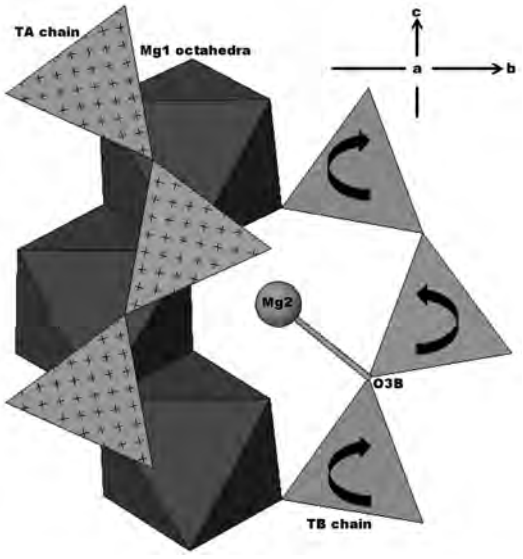

FIGURE 2. Part of the crystal structure of orthoenstatite $MgSiO_3$, showing the relationship between the shorthening of the M2-O3B bond distance and the kinking of the tetrahedral chain. When the tetrahedra rotate, as indicated by arrows, the kinking angle (O3B-O3B-O3B) decreases and the Mg2-O3B bond distance becomes shorter.

show a relatively smaller contraction between 0.2 and 1.8%. In orthopyroxene, the Mg2-O3 bond distances are crucial in determining the high-pressure behavior (Fig. 2). They connect, by means of the bridging O atoms, the Mg2 octahedral sites to the tetrahedral chains and, because it is the bridging oxygen, the O3 position controls the tetrahedral chain kinking (defined by the O3-O3-O3 angle).

In the Mg1 octahedron the longer bonds also undergo the greatest shortening as in the Mg2 site, but while in the case of Mg2 this is to O3 atoms, in Mg1 it is to the O1 atoms. The longest distances $Mg1\text{-}O1A_{long}$ and $Mg1\text{-}O1B_{long}$ (Fig. 3b) show the greatest decrease (3.8%), while the remaining shorter Mg1-O distances all undergo a similar shortening by between 1.5 and 2.7%.

As seen from Figure 3, the increased precision of the present measurement was necessary for a clear conclusion. The present data confirm a practically linear decrease of all Mg-O bond distances, except the Mg2-O3B, which shows a non-linear behavior corresponding to stiffening with pressure. However, the scatter of the previously obtained data did not allow accurate analysis, especially for Mg1-O bonds where the changes in bond lengths are smaller.

The distortion parameters for the Mg sites (Fig. 4) generally decrease with pressure as expected for stable structures (Balić-Žunić 2007) and for the volume eccentricity the more distorted Mg2 site exhibits a much larger decrease (Fig. 4a) as a result of the longest bonds showing the greatest compression. The asphericity, or the deviation of ligands from a common sphere, is also significantly larger in Mg2 than in Mg1 (Fig. 4b) but also shows a more rapid decrease because of the greater compressibility of the longer Mg2-O3 bonds. The volume distortions for Mg1 and Mg2, which measure the discrepancy of volume to an ideal octahedron with the same fitted sphere radius are in both polyhedra the smallest distortion parameter and change the least as a function of pressure (Fig. 4c). However, also here a greater decrease is evident for Mg2 site.

TA and TB tetrahedra

The TA and TB tetrahedral volumes decrease with similar and linear trends by about 3 and 2%, respectively, and no discontinuities are shown in the pressure range investigated (Fig. 5). This is in direct contradiction to the previous conclusions (Hugh-Jones and Angel 1994; Hugh-Jones et al. 1997), which reported for pressures below 4 GPa no significant compression of Si-O bond lengths, whereas above 4 GPa a significant decrease of the Si-O bond lengths was measured, with a consequent considerable decrease of the tetrahedral volumes. Such a two-step evolution with pressure is not confirmed by our data (Fig. 5), which show a uniform tetrahedral volume compression throughout the investigated pressure range. Figure 5 shows also that the previous data

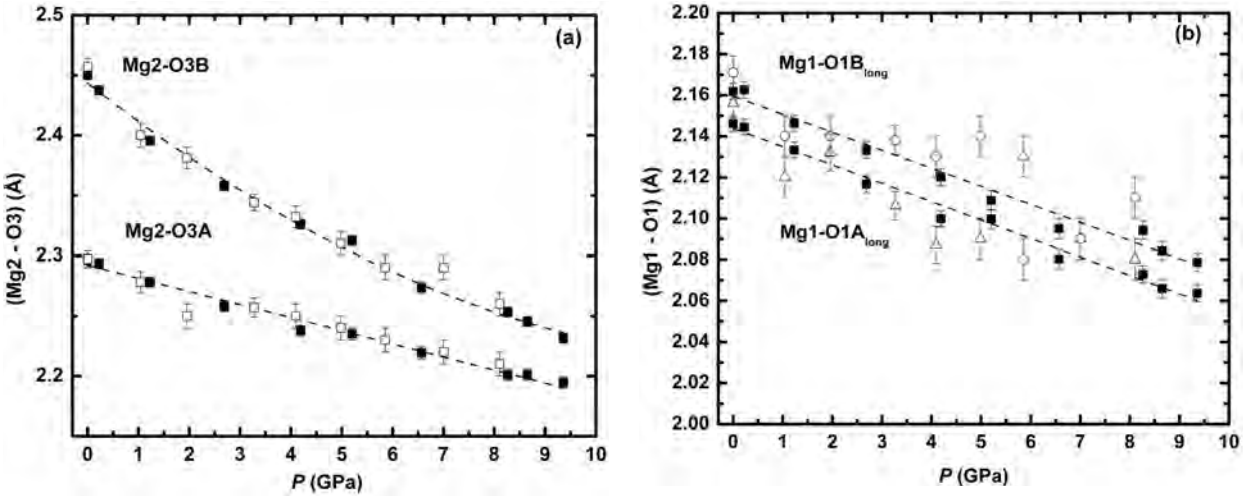

FIGURE 3. (**a**) Evolution of the Mg2-O3 bond distances as a function of pressure. (**b**) Evolution of the Mg1-O1 bond distances as a function of pressure. The filled symbols are used for the data of this work, the empty for the Hugh-Jones and Angel (1994) data.

were obviously influenced by significantly lower accuracy and were therefore misleading. As can be seen from Figure 5 they scatter around the trend determined in the present work and are in this respect not in contradiction with our conclusions, which are also in line with the behavior of a natural Fe- and Al-rich orthoenstatite (Nestola et al. 2008b).

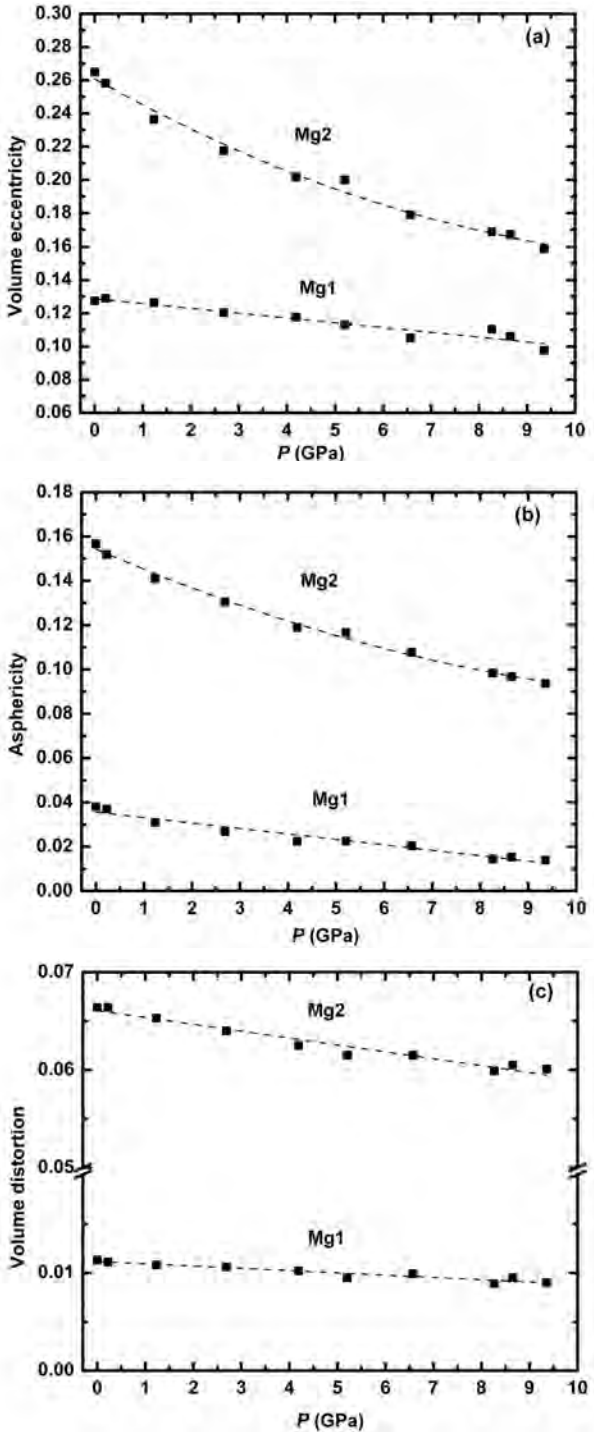

Figure 4. Evolution of (**a**) volume eccentricity, (**b**) asphericity, and (**c**) volume distortion for the Mg coordination polyhedra (this work).

In the orthopyroxene, the kinking of the tetrahedral chains plays a crucial role in the structural evolution as a function of pressure (Fig. 2). In Figure 6, the evolution of the kinking angle for the A and B chains for both data sets is shown. Our data show that the B chain undergoes the most pronounced kinking, with the O3B-O3B-O3B angle decreasing by about 3.3% with no discontinuities. The larger kinking angle of the A chain, O3A-O3A-O3A, decreases with pressure by only 0.3%. Again, there is a discrepancy in conclusions between the present and the previous work on the pure orthoenstatite. Whereas Hugh-Jones and Angel (1994) conclude that there is a well-defined change in both the degree of kinking of the tetrahedral chains (as measured by changes in the O3-O3-O3 chain extension angle) and the amount of tetrahedral tilt toward the (100) plane at about 4 GPa, our data show a practically uniform change of the kink angle throughout the whole pressure range up to 9.36 GPa. As seen from Figure 6, the data for O3B-O3B-O3B angle by Hugh-Jones and Angel (1994) indeed suggest a prominent change in slope between 4

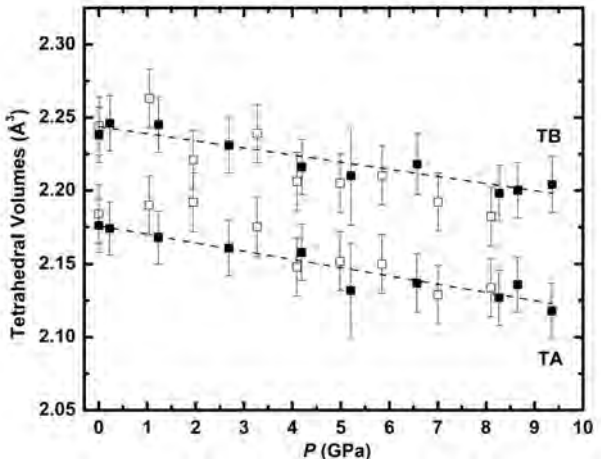

Figure 5. Evolution of tetrahedral volumes as a function of pressure. The filled symbols are used for the data of this work, the empty for the Hugh-Jones and Angel (1994) data.

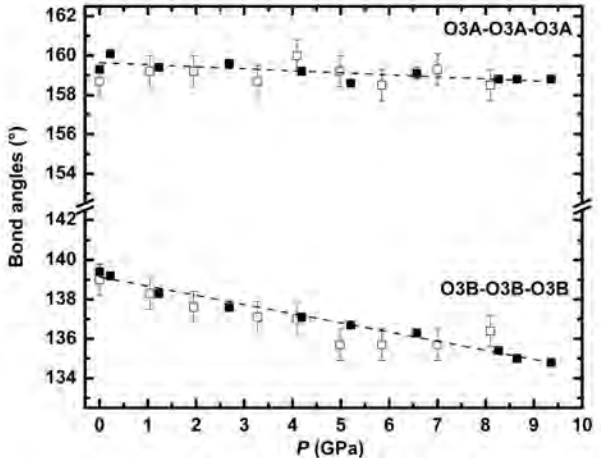

Figure 6. Evolution of the chain extension angle, O3-O3-O3, for the A and B tetrahedral chains. The filled symbols are used for the data of this work, the empty for the Hugh-Jones and Angel (1994) data.

and 5 GPa; in particular, this angle decreases to 4 GPa where it starts to increase up to 8 GPa. In light of the new data, it is clear that the accuracy of the previous data was slightly overestimated, and if slightly larger e.s.d.'s were assigned they are seen to follow the general trend of the new data.

The distortion parameters of the tetrahedral sites, showed in Figure 7, present an interesting behavior: the volume eccentricities (Fig. 7a) increase with pressure for both sites, whereas the volume distortion (Fig. 7b) slightly decreases for TB and it increases for TA. The larger TB tetrahedron evidently has a more regular arrangement of ligands (lower volume distortion) but at the same time a more eccentrically placed Si atom.

Concluding remarks

The re-investigation of the pure end-member $MgSiO_3$ is an example of the improvement on the data quality achieved during recent years with the single-crystal X-ray diffraction technique at high-pressure conditions. The determination of the crystal structure for the $MgSiO_3$ enstatite up to 9.36 GPa demonstrates how important it is to obtain accurate data, especially if they are to be used as a reference for the behavior of a mineral species under high pressure. The present data show that the previous results about the high-pressure behavior of the crystal structure of pure orthoenstatite (Hugh-Jones and Angel 1994) had higher uncertainties, which led to some erroneous conclusions. Thanks to the available higher precision of high-pressure diffraction data, our results on the pure orthoenstatite confirm that there is no evidence of any change in compression at about 4 GPa for the tetrahedral TA and TB coordinations, in contrast to the conclusions of Hugh-Jones and Angel (1994). Moreover, as found in Nestola et al. (2006, 2008b) for orthopyroxenes with different compositions, the compressibility of the octahedral sites smoothly decreases as a function of pressure without any significant changes in compression. The analysis of the pure end-member $MgSiO_3$ confirms that the longest bond Mg2-O3B undergoes the main compression in orthopyroxenes and this contraction is connected with changes in the kink of the B tetrahedral chain.

The crystal structure of the $MgSiO_3$ orthoenstatite can be considered a reference model for orthopyroxenes with different compositions. In particular, the accuracy of our structural results for the high-pressure pure orthoenstatite allows a better comparison of the mechanisms of compression among the orthopyroxenes having Ca, Al, and Fe substitutions to investigate the effect of these elements in the high-pressure behavior of orthoenstatite. Figure 8 presents the relative compression of the bond distance M2-O3B as a function of the V/V_0 ratio for the pure $MgSiO_3$ end-member of this study, the synthetic $Ca_{0.07}Mg_{1.93}Si_2O_6$ orthoenstatite (Nestola et al. 2006), the natural S95 orthoenstatite sample studied by Nestola et al. (2008b) with composition $^{M2}[Fe^{2+}_{0.818}Mg_{0.156}Ca_{0.010}Mn_{0.016}]^{M1}[Fe^{2+}_{0.081}Mg_{0.767}Al_{0.084}Fe^{3+}_{0.068}]^{TA}[Si]^{TB}[Si_{0.848}Al_{0.152}]O_6$ and a synthetic orthoenstatite of $(Mg_{0.99}\square_{0.01})^{M2}(Mg_{0.89}Al_{0.11})^{M1}(Al_{0.12}Si_{0.88})^{TB}Si^{TA}O_{5.97}(OH)_{0.03}$ composition (Balić-Žunić personal communication). The V/V_0 ratio is calculated from the equation of state of the orthopyroxenes (Angel and Jackson 2002; Nestola et al. 2006, 2008b; Balić-Žunić personal communication). Comparing the compressibility between these orthopyroxenes with different composition and our data of pure

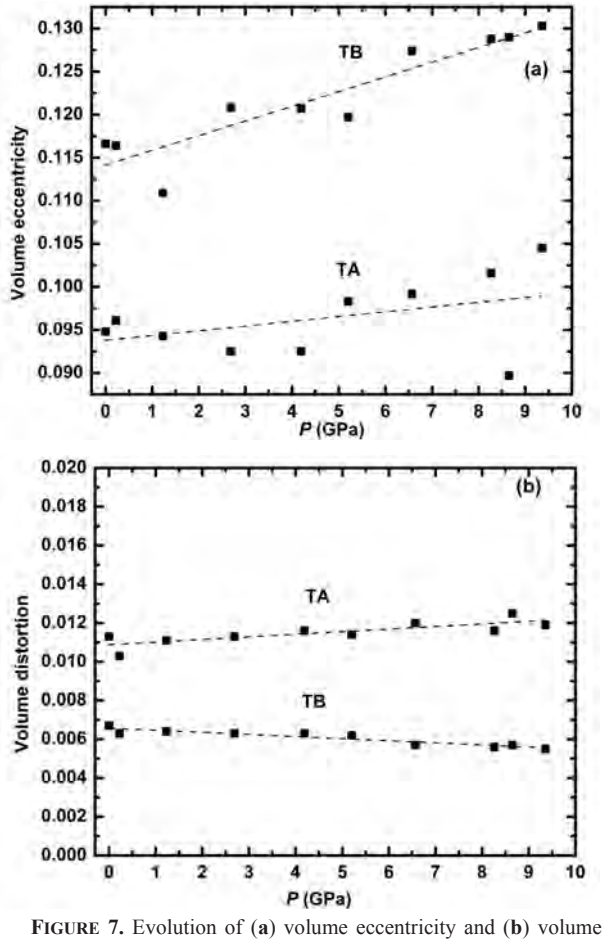

Figure 7. Evolution of (**a**) volume eccentricity and (**b**) volume distortion for the tetrahedral coordination (this work).

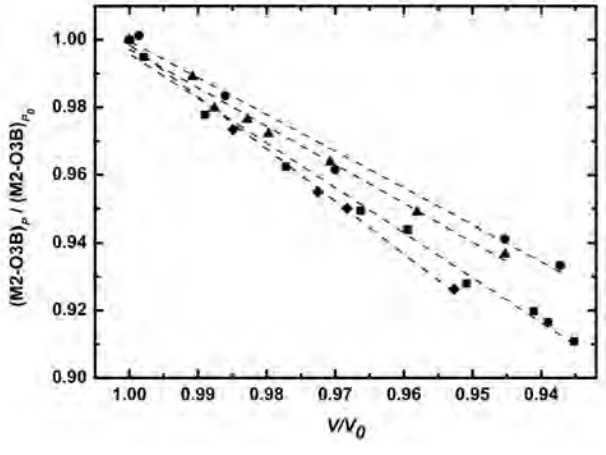

Figure 8. Relative compression of the bond distance M2-O3B as a function of the V/V_0 ratio in: pure $MgSiO_3$ orthoenstatite (squares; this work), Fe- and Al-rich S95 orthoenstatite (circles; Nestola et al. 2008b), Ca-bearing orthoenstatite (rhombs; Nestola et al. 2006) and Al- and H-rich orthopyroxene (triangles; Balić-Žunić personal communication). The lines are linear fits to the data.

orthoenstatite, it is evident that the M2-O3B compression is in all cases pronounced and one of the main deformation mechanisms. As noted earlier it is directly related to the kinking of the TB tetrahedral chain. In turn, the kinking of the B tetrahedral chain depends on the relative sizes of M2 and TB polyhedra, as the different linear trends in Figure 8 confirm. That it is the relative M2/TB size difference that influences the high-pressure behavior is confirmed by the fact that Ca substitution, which increases the difference, increases also the compression of the M2-O3B bond, whereas the substitution of Al in TB, which decreases the difference, diminishes the compression of the same bond as compared to the pure orthoenstatite.

Acknowledgments

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 'O'  'O'   0.0106   0.0060
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 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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 'x+1/2, -y+1/2, -z'
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 'x-1/2, y, -z-1/2'
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
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 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
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_refine_ls_weighting_details
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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
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_refine_ls_extinction_method      none
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Mg2 Mg 0.37691(11) 0.4868(2) 0.3589(3) 0.0096(5) Uani 1 1 d . . .
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SiB 0.0046(14) 0.0071(15) 0.0039(5) 0.0002(6) -0.0001(6) 0.0008(6)
Mg1 0.0051(16) 0.0105(17) 0.0050(7) 0.0010(8) 0.0002(7) 0.0007(7)
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 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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SiA Mg2 3.250(3) 2_564 ?
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SiB O1B 1.619(4) . ?
SiB 03B 1.671(4) . ?
SiB 03B 1.674(3) 8_566 ?
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SiB Mg2 3.238(3) 5_666 ?
SiB Mg1 3.245(2) 5_667 ?
Mg1 O2A 2.006(4) 1_556 ?
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Mg1 O2B 2.049(4) . ?
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 '-x, -y, -z'
 'x-1/2, y, -z-1/2'
 '-x-1/2, y-1/2, z'
 'x, -y-1/2, z-1/2'

_cell_length_a    18.2102
_cell_length_b     8.8196
_cell_length_c     5.1767
_cell_angle_alpha  90.000
_cell_angle_beta   90.000
_cell_angle_gamma  90.000

_shelx_F_squared_multiplier     1.000

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
   2   1   0      143.62      176.35     12.77 o
   4   1   0      143.40      131.10     14.87 o
   6   1   0    38331.80    35880.30    774.82 o
   8   1   0        0.58       18.62     48.27 o
   2   2   0        0.38        6.29      9.88 o
   4   2   0    16670.90    15489.01    145.61 o
   6   2   0      190.62      202.42     23.66 o
   8   2   0     1218.68     1280.05     91.57 o
  10   2   0      463.82      415.13     62.66 o
  12   2   0      275.71      256.75    108.84 o
   2   3   0     1058.03     1237.85     72.28 o
   4   3   0      811.02      874.60     32.43 o
   6   3   0     1450.65     1639.35     87.91 o
   8   3   0       19.82       31.56     27.88 o
  10   3   0      317.74      345.17     40.51 o
  12   3   0      354.59      395.32     75.11 o
  14   3   0     1784.83     1528.77    122.46 o
```

4	4	0	5485.44	5625.03	182.40	o
6	4	0	103.10	82.83	26.42	o
8	4	0	3962.85	4050.25	73.58	o
10	4	0	1757.64	1652.63	72.40	o
12	4	0	59.19	54.61	57.57	o
14	4	0	171.06	134.82	85.59	o
16	4	0	3738.90	3936.00	175.37	o
4	5	0	62.38	31.69	65.05	o
6	5	0	11138.94	10313.63	259.35	o
8	5	0	229.78	192.65	65.86	o
10	5	0	7035.05	6757.96	381.09	o
12	5	0	106.40	100.51	83.42	o
14	5	0	24346.71	21976.20	331.10	o
16	5	0	295.67	188.00	99.99	o
18	5	0	1370.97	1458.49	215.06	o
6	6	0	265.20	131.90	91.56	o
8	6	0	1081.36	1462.18	157.44	o
10	6	0	581.89	708.57	141.04	o
12	6	0	5704.18	5837.16	360.63	o
14	6	0	727.30	481.34	105.82	o
16	6	0	2072.34	1556.92	264.65	o
18	6	0	37.74	65.80	104.40	o
6	7	0	2199.49	2498.52	224.07	o
8	7	0	202.34	145.99	120.98	o
10	7	0	5526.80	5518.02	265.45	o
12	7	0	344.79	230.65	144.47	o
14	7	0	2298.54	2388.32	134.91	o
16	7	0	119.85	57.61	85.19	o
18	7	0	49.72	52.50	96.62	o
8	8	0	295.33	299.39	151.52	o
10	8	0	912.27	785.50	164.38	o
12	8	0	100.45	164.21	143.60	o
14	8	0	50.19	30.30	85.58	o
16	8	0	1608.53	1650.45	227.73	o
12	9	0	55.71	21.14	167.55	o
14	9	0	1259.15	1308.55	164.85	o
1	1	1	279.61	304.37	6.93	o
2	1	1	251.40	218.46	7.43	o
3	1	1	19.31	40.15	4.64	o
4	1	1	3118.36	3305.15	28.34	o
5	1	1	5080.21	5060.17	90.99	o
6	1	1	1066.63	961.43	28.63	o
7	1	1	2012.25	2008.59	78.93	o
8	1	1	1596.98	1468.56	106.70	o
9	1	1	296.41	305.85	54.82	o
0	2	1	12.69	14.10	14.36	o
1	2	1	5245.40	5192.33	106.46	o
3	2	1	9434.04	8844.43	120.34	o
4	2	1	7014.62	6726.44	103.96	o
5	2	1	8062.50	7698.81	94.57	o
6	2	1	174.73	147.70	10.59	o
7	2	1	2883.16	3087.37	47.66	o
8	2	1	3074.25	3051.79	51.41	o
9	2	1	0.14	12.92	20.17	o
10	2	1	596.11	716.00	41.73	o

11	2	1	280.44	271.34	53.21	o
12	2	1	1201.89	1137.40	97.73	o
1	3	1	12649.67	13615.70	237.37	o
2	3	1	2422.96	1977.51	49.96	o
3	3	1	1994.70	2569.93	42.91	o
4	3	1	1618.28	1933.32	33.88	o
5	3	1	8745.87	8898.58	149.90	o
6	3	1	12854.05	13310.29	143.79	o
7	3	1	6.73	8.92	15.31	o
8	3	1	5903.63	5786.92	55.53	o
9	3	1	9233.17	9132.09	85.82	o
10	3	1	22515.97	21087.89	344.17	o
11	3	1	27655.77	25285.32	298.55	o
12	3	1	16279.30	15100.64	207.12	o
13	3	1	1474.85	1372.22	80.21	o
14	3	1	40.66	72.75	70.60	o
15	3	1	423.70	525.41	143.28	o
3	4	1	781.38	806.26	46.68	o
4	4	1	1222.69	1192.16	35.85	o
5	4	1	4631.72	4768.15	92.94	o
6	4	1	681.23	739.27	28.11	o
7	4	1	1042.83	1009.40	32.96	o
8	4	1	237.86	249.64	35.57	o
9	4	1	179.27	175.67	34.03	o
10	4	1	109.33	131.83	31.34	o
11	4	1	79.09	43.16	34.96	o
12	4	1	61.57	90.16	37.37	o
13	4	1	148.66	118.80	46.94	o
14	4	1	520.66	590.13	70.91	o
15	4	1	8.35	9.77	77.87	o
16	4	1	1725.18	1660.12	115.67	o
17	4	1	611.33	297.86	165.57	o
4	5	1	1266.50	1177.47	86.15	o
5	5	1	1744.65	1780.79	74.91	o
6	5	1	294.43	280.43	35.64	o
7	5	1	1198.61	1194.63	52.87	o
8	5	1	564.04	622.69	45.60	o
9	5	1	526.53	495.82	43.59	o
11	5	1	102.86	113.46	51.63	o
12	5	1	26.28	29.22	50.74	o
13	5	1	38.97	52.71	60.23	o
14	5	1	2973.35	2589.52	105.82	o
15	5	1	452.66	423.11	74.78	o
16	5	1	313.33	151.07	79.72	o
17	5	1	1.66	14.16	81.66	o
18	5	1	11.68	51.13	80.60	o
19	5	1	22.02	44.34	148.21	o
5	6	1	7.75	14.91	61.94	o
6	6	1	225.56	210.73	73.70	o
7	6	1	48.50	53.77	42.76	o
8	6	1	254.59	264.99	52.27	o
9	6	1	140.75	154.32	73.62	o
10	6	1	54.76	44.97	66.24	o
11	6	1	127.90	211.48	89.83	o
12	6	1	445.37	400.43	62.72	o

13	6	1	117.81	138.24	54.21	o
14	6	1	127.33	153.67	54.85	o
15	6	1	137.23	52.86	80.99	o
16	6	1	6.99	54.61	84.04	o
17	6	1	69.98	51.11	88.40	o
18	6	1	48.30	73.93	90.76	o
19	6	1	28.23	63.26	92.69	o
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8	7	1	1172.92	1187.29	119.76	o
9	7	1	2232.57	2254.21	144.62	o
10	7	1	203.12	348.16	99.82	o
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12	7	1	1390.34	1461.84	118.72	o
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14	7	1	24.53	28.98	63.59	o
15	7	1	302.24	336.12	74.42	o
16	7	1	699.60	668.62	85.41	o
17	7	1	2.16	22.60	72.41	o
18	7	1	7.39	17.18	85.83	o
8	8	1	5566.84	5515.87	301.70	o
9	8	1	111.41	157.03	100.52	o
10	8	1	114.49	108.55	97.75	o
11	8	1	3.97	27.04	93.95	o
12	8	1	143.91	202.71	105.45	o
13	8	1	1389.24	1502.85	147.52	o
14	8	1	0.67	20.77	67.06	o
15	8	1	1003.80	1028.82	94.94	o
16	8	1	566.08	714.83	102.61	o
11	9	1	4540.66	5282.19	339.36	o
12	9	1	5328.89	5492.50	240.06	o
13	9	1	447.87	587.16	135.20	o
14	9	1	216.36	293.48	109.28	o
0	0	2	632.53	557.09	28.17	o
1	0	2	300.69	251.65	13.80	o
2	0	2	36855.70	33876.07	404.88	o
3	0	2	4548.48	3732.63	79.63	o
4	0	2	502.96	514.21	24.74	o
5	0	2	25154.24	25230.04	361.89	o
6	0	2	127.80	250.34	69.61	o
7	0	2	6114.05	5856.28	188.21	o
1	1	2	42.44	51.85	8.21	o
2	1	2	152.48	170.20	10.50	o
3	1	2	500.28	424.32	12.17	o
4	1	2	876.30	1071.34	24.09	o
5	1	2	5905.19	6353.15	86.82	o
6	1	2	453.04	485.07	26.10	o
7	1	2	40.89	37.50	25.14	o
8	1	2	5621.33	5692.38	196.26	o
9	1	2	1980.45	1912.45	96.44	o
10	1	2	98.58	130.58	82.37	o
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1	2	2	2.22	6.63	11.07	o
2	2	2	9.51	6.61	10.75	o
3	2	2	1260.48	1355.17	28.13	o
4	2	2	395.30	449.98	24.23	o

5	2	2	22.24	15.80	12.00	o
6	2	2	3448.72	3616.12	43.43	o
7	2	2	3578.95	3780.85	39.31	o
8	2	2	597.26	587.12	27.69	o
9	2	2	2729.67	2662.36	88.43	o
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3	3	2	1089.35	1220.74	33.78	o
4	3	2	718.99	755.45	25.11	o
5	3	2	508.13	555.93	20.55	o
6	3	2	74.04	62.31	14.10	o
7	3	2	233.51	252.96	20.40	o
8	3	2	272.15	336.62	24.13	o
9	3	2	337.72	336.65	32.60	o
10	3	2	57.43	30.60	31.75	o
11	3	2	127.52	126.96	40.95	o
12	3	2	0.55	15.09	46.40	o
13	3	2	0.97	48.79	46.73	o
14	3	2	0.18	11.19	55.89	o
15	3	2	137.13	12.00	119.98	o
1	4	2	1275.99	1465.58	137.38	o
2	4	2	4072.91	4264.19	507.74	o
3	4	2	2057.68	2072.70	63.71	o
4	4	2	5.49	23.25	26.88	o
5	4	2	154.22	127.09	20.54	o
6	4	2	1653.17	1642.46	38.61	o
7	4	2	1219.77	1251.56	39.21	o
8	4	2	72.64	94.69	26.74	o
9	4	2	148.85	154.66	45.33	o
10	4	2	1.00	24.90	37.88	o
11	4	2	6.27	45.96	46.06	o
12	4	2	93.32	91.39	44.14	o
13	4	2	281.81	339.16	58.87	o
14	4	2	612.20	494.30	70.40	o
15	4	2	48.91	105.22	71.45	o
16	4	2	51.86	64.51	93.23	o
17	4	2	218.12	227.50	157.27	o
3	5	2	9414.33	7224.72	238.76	o
4	5	2	49.43	19.33	50.01	o
5	5	2	1120.41	1255.67	48.57	o
6	5	2	5.74	7.92	34.71	o
7	5	2	246.85	265.97	43.02	o
8	5	2	7297.69	7053.38	101.91	o
9	5	2	8125.49	8014.80	152.23	o
11	5	2	3138.44	3309.69	71.97	o
12	5	2	9569.96	9161.62	397.37	o
13	5	2	153.39	91.33	58.08	o
14	5	2	137.92	144.82	68.95	o
15	5	2	366.29	371.47	74.63	o
16	5	2	848.34	767.79	126.29	o
17	5	2	2353.96	2407.32	183.79	o
18	5	2	326.04	309.27	122.77	o

5	6	2	5214.95	5633.91	253.71	o
6	6	2	0.61	29.79	48.67	o
7	6	2	2177.65	2089.51	81.77	o
8	6	2	295.23	254.66	54.84	o
9	6	2	8641.43	8749.41	149.73	o
10	6	2	950.62	1140.19	134.23	o
11	6	2	7028.58	7170.79	218.97	o
12	6	2	283.80	342.54	61.90	o
13	6	2	44.63	36.68	59.75	o
14	6	2	4.24	67.97	66.61	o
15	6	2	132.35	158.28	70.80	o
16	6	2	155.23	98.40	70.18	o
17	6	2	698.82	651.09	117.37	o
18	6	2	552.32	803.27	169.40	o
7	7	2	1216.26	1286.78	180.94	o
8	7	2	2237.66	2186.17	127.32	o
9	7	2	14.90	51.25	65.31	o
10	7	2	0.17	36.14	71.60	o
11	7	2	426.33	232.56	78.32	o
12	7	2	3125.99	3043.59	142.60	o
13	7	2	499.62	619.77	78.56	o
14	7	2	10.15	38.22	65.41	o
15	7	2	81.48	37.58	69.61	o
16	7	2	517.28	573.61	87.93	o
17	7	2	476.70	486.12	94.73	o
18	7	2	23.79	89.61	121.28	o
9	8	2	315.29	421.16	171.78	o
10	8	2	71.48	148.73	158.21	o
11	8	2	76.88	51.13	144.71	o
12	8	2	0.05	14.63	103.48	o
13	8	2	887.64	792.15	99.06	o
14	8	2	194.70	204.35	76.89	o
15	8	2	720.39	700.28	100.36	o
16	8	2	60.46	111.83	121.25	o
12	9	2	302.16	402.82	196.52	o
13	9	2	502.42	529.05	147.01	o
1	1	3	53.27	49.61	12.05	o
2	1	3	1411.60	1510.64	24.94	o
3	1	3	3185.96	3176.26	36.40	o
4	1	3	1.87	11.69	13.18	o
5	1	3	327.47	342.49	19.48	o
6	1	3	2090.08	2278.56	42.54	o
7	1	3	1033.13	1035.29	39.37	o
8	1	3	48.18	64.99	32.04	o
9	1	3	786.99	822.51	122.02	o
10	1	3	1536.74	1646.56	167.88	o
11	1	3	92.79	68.20	114.78	o
0	2	3	28587.58	27542.30	316.54	o
1	2	3	9781.77	9989.62	118.73	o
2	2	3	17.79	18.86	14.03	o
3	2	3	46.29	51.64	16.99	o
4	2	3	1190.60	1272.08	28.79	o
5	2	3	1103.76	1188.55	34.42	o
6	2	3	418.99	475.20	27.04	o
7	2	3	3969.90	3920.51	49.48	o

8	2	3	299.98	354.33	28.25	o
9	2	3	960.21	1021.91	45.22	o
10	2	3	672.42	720.93	51.45	o
11	2	3	282.57	268.49	73.11	o
12	2	3	1667.10	1623.15	128.02	o
13	2	3	3658.51	3855.07	250.37	o
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2	3	3	3711.33	3728.06	84.80	o
3	3	3	88.83	82.01	23.70	o
4	3	3	747.79	741.98	38.06	o
5	3	3	2389.89	2402.78	46.34	o
6	3	3	8304.40	8421.46	138.07	o
7	3	3	2523.73	2677.02	66.55	o
8	3	3	36.58	45.67	31.10	o
9	3	3	517.36	531.14	41.04	o
10	3	3	3934.82	3664.80	103.04	o
11	3	3	181.57	167.57	57.49	o
12	3	3	1006.53	960.00	148.65	o
13	3	3	8650.60	8606.43	314.16	o
14	3	3	9548.18	9318.71	245.98	o
15	3	3	2480.24	2657.26	231.77	o
0	4	3	13813.56	13756.46	341.49	o
1	4	3	3093.45	3143.68	109.39	o
2	4	3	92.92	55.22	43.53	o
3	4	3	2196.39	2253.15	96.70	o
4	4	3	1905.70	1869.34	48.86	o
5	4	3	792.30	793.68	37.33	o
6	4	3	113.44	155.91	36.28	o
7	4	3	1030.79	1177.69	56.08	o
8	4	3	3.00	29.76	42.80	o
9	4	3	1742.32	1561.24	77.96	o
10	4	3	656.81	666.41	62.56	o
11	4	3	195.61	136.43	63.37	o
12	4	3	835.04	958.91	97.40	o
13	4	3	971.09	1053.03	99.69	o
14	4	3	195.92	97.34	79.84	o
15	4	3	623.66	728.98	102.45	o
16	4	3	20.87	56.96	99.63	o
2	5	3	1905.16	1699.28	166.65	o
3	5	3	3796.90	3725.55	154.58	o
4	5	3	248.89	240.96	68.05	o
5	5	3	105.46	100.62	45.08	o
6	5	3	866.97	903.07	65.20	o
7	5	3	198.64	247.23	60.95	o
8	5	3	69.02	71.66	62.21	o
9	5	3	782.99	956.57	153.31	o
10	5	3	515.60	612.14	85.32	o
11	5	3	0.79	40.35	55.98	o
12	5	3	11.86	40.24	58.90	o
13	5	3	133.35	165.01	64.77	o
14	5	3	211.76	137.45	67.84	o
15	5	3	1287.72	1283.80	117.83	o
16	5	3	93.11	89.11	90.06	o
17	5	3	433.83	468.36	125.24	o
18	5	3	160.49	158.23	164.57	o

5	6	3	9.67	10.48	60.48	o
6	6	3	22.54	20.28	84.72	o
7	6	3	104.77	101.06	76.85	o
8	6	3	350.73	337.69	84.37	o
9	6	3	212.53	218.72	111.22	o
10	6	3	172.96	212.61	86.19	o
11	6	3	197.54	187.56	63.03	o
12	6	3	22.88	48.83	70.35	o
13	6	3	1.37	16.42	66.45	o
14	6	3	1.71	19.80	70.65	o
15	6	3	28.22	31.96	73.01	o
16	6	3	83.99	99.47	78.83	o
17	6	3	294.17	236.40	108.32	o
18	6	3	58.53	16.86	168.61	o
6	7	3	912.44	222.86	126.67	o
7	7	3	447.30	127.51	137.25	o
8	7	3	258.09	98.41	114.42	o
9	7	3	146.25	125.51	75.65	o
10	7	3	1370.82	1351.18	343.56	o
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16	7	3	3.95	35.29	166.03	o
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4	0	4	11581.29	11238.40	150.99	o
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6	0	4	349.09	340.56	40.07	o
7	0	4	1369.87	1236.63	61.05	o
8	0	4	5215.99	4870.10	244.41	o
9	0	4	3002.55	2446.33	205.76	o
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6	6	4	215.40	218.39	132.44	o
7	6	4	220.32	215.45	113.19	o
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3	5	5	29.13	62.07	67.79	o
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
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SiB Si 0.47323(8) 0.33712(19) 0.8004(2) 0.0049(4) Uani 1 1 d . . .
Mg1 Mg 0.37583(10) 0.6542(2) 0.8629(3) 0.0064(5) Uani 1 1 d . . .
Mg2 Mg 0.37713(11) 0.4853(2) 0.3555(3) 0.0095(5) Uani 1 1 d . . .
O1A O 0.1830(2) 0.3397(4) 0.0318(5) 0.0053(8) Uiso 1 1 d . . .
O2A O 0.3106(2) 0.5038(4) 0.0404(5) 0.0067(8) Uiso 1 1 d . . .
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O3A O 0.3030(2) 0.2233(4) 0.8272(5) 0.0062(8) Uiso 1 1 d . . .
O1B O 0.5626(2) 0.3391(4) 0.8018(5) 0.0059(8) Uiso 1 1 d . . .
O2B O 0.4324(2) 0.4831(4) 0.6875(5) 0.0066(8) Uiso 1 1 d . . .
03B O 0.4474(2) 0.1940(4) 0.6077(5) 0.0044(8) Uiso 1 1 d . . .

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SiB 0.0052(14) 0.0042(14) 0.0052(5) -0.0006(6) -0.0007(6) 0.0001(5)
Mg1 0.0071(16) 0.0062(16) 0.0060(7) 0.0004(8) -0.0013(7) 0.0006(7)
Mg2 0.0115(18) 0.0094(17) 0.0075(7) -0.0013(8) -0.0015(8) -0.0001(7)

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 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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   8   1   0        1.32        5.52     55.16 o
   2   2   0        0.02        4.77     12.50 o
   4   2   0    16335.88    14014.35    283.04 o
   6   2   0      205.67      216.21     24.23 o
   8   2   0     1242.72     1353.33     98.01 o
  10   2   0      481.31      471.69     64.78 o
  12   2   0      208.40      187.48    122.10 o
   2   3   0     1082.52     1268.39     74.45 o
   4   3   0      829.49      914.35     57.50 o
   6   3   0     1494.52     1622.06     92.52 o
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7	1	1	2144.42	2019.86	86.76	o
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2	3	1	2539.60	2220.44	75.46	o
4	3	1	1612.50	1877.15	35.16	o
5	3	1	8491.99	8781.12	157.82	o
7	3	1	9.66	19.44	16.23	o
8	3	1	5876.30	5443.05	106.06	o
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5	6	1	3.70	11.22	79.31	o
6	6	1	223.56	260.29	89.44	o
7	6	1	39.20	17.09	45.11	o
8	6	1	239.06	193.25	63.50	o
9	6	1	125.76	183.59	78.96	o
10	6	1	31.85	13.15	74.57	o
11	6	1	142.83	62.17	129.95	o
12	6	1	453.82	369.77	68.23	o

13	6	1	94.90	83.95	59.23	o
14	6	1	119.44	74.35	67.76	o
15	6	1	140.59	78.96	89.05	o
16	6	1	9.53	14.68	84.62	o
17	6	1	67.17	101.89	93.13	o
18	6	1	62.31	26.16	101.10	o
19	6	1	28.82	41.11	95.89	o
7	7	1	827.97	950.85	184.87	o
8	7	1	1313.56	1676.03	150.02	o
9	7	1	2603.06	2710.57	162.10	o
10	7	1	242.37	274.01	118.55	o
11	7	1	754.07	857.50	134.31	o
12	7	1	1530.97	1574.36	122.38	o
13	7	1	215.62	204.58	78.37	o
14	7	1	18.07	49.85	74.60	o
15	7	1	350.27	474.54	87.25	o
16	7	1	634.93	581.63	94.89	o
17	7	1	3.13	27.83	81.42	o
18	7	1	7.98	34.88	99.81	o
9	8	1	74.79	213.80	126.64	o
10	8	1	110.47	100.86	122.20	o
11	8	1	0.90	70.19	117.92	o
12	8	1	167.44	244.83	128.14	o
13	8	1	1344.00	1697.21	176.27	o
14	8	1	12.42	76.42	76.20	o
15	8	1	1154.04	1221.84	105.74	o
16	8	1	677.00	816.66	115.00	o
11	9	1	5371.65	6130.45	376.78	o
12	9	1	5617.32	6257.90	593.76	o
13	9	1	621.50	630.92	214.02	o
14	9	1	269.45	325.53	149.31	o
0	0	2	673.05	622.12	29.43	o
1	0	2	327.78	300.49	14.61	o
2	0	2	36946.93	33480.06	392.86	o
3	0	2	4383.14	3554.32	66.42	o
4	0	2	615.84	629.57	26.89	o
5	0	2	24831.51	25295.83	269.52	o
6	0	2	137.73	121.58	66.66	o
7	0	2	5904.99	5464.50	184.27	o
1	1	2	38.06	49.21	7.77	o
2	1	2	159.54	185.86	11.39	o
3	1	2	482.72	411.31	11.72	o
4	1	2	861.15	1078.96	22.56	o
5	1	2	5791.86	6284.17	157.53	o
6	1	2	476.35	497.65	26.83	o
7	1	2	46.16	56.41	26.81	o
8	1	2	5646.84	5782.17	172.15	o
9	1	2	1920.10	1874.67	99.71	o
10	1	2	115.29	94.87	84.14	o
0	2	2	94.89	115.20	20.90	o
1	2	2	1.51	10.81	11.51	o
2	2	2	6.75	9.33	11.29	o
3	2	2	1213.00	1308.78	27.93	o
4	2	2	428.07	528.39	26.63	o
5	2	2	26.06	27.23	12.62	o

6	2	2	3359.88	3656.54	47.86	o
7	2	2	3592.36	3666.44	84.01	o
8	2	2	677.76	744.18	30.93	o
9	2	2	2779.58	2748.80	79.26	o
10	2	2	1079.90	1199.83	80.64	o
11	2	2	164.37	131.02	55.12	o
12	2	2	247.79	212.11	64.25	o
1	3	2	52.27	70.17	28.43	o
2	3	2	0.05	13.86	23.37	o
3	3	2	1066.24	1150.12	28.97	o
4	3	2	696.79	729.27	22.12	o
5	3	2	497.69	552.24	19.47	o
6	3	2	90.05	87.57	15.21	o
7	3	2	229.13	273.75	23.24	o
8	3	2	298.86	344.34	25.73	o
9	3	2	315.53	353.87	34.07	o
10	3	2	47.51	68.25	33.61	o
11	3	2	162.46	165.58	44.62	o
12	3	2	2.19	33.74	45.75	o
13	3	2	0.08	48.94	49.45	o
14	3	2	0.37	32.71	66.59	o
1	4	2	1230.37	1046.62	115.88	o
2	4	2	4342.24	4348.23	190.81	o
3	4	2	2104.04	2098.20	105.74	o
4	4	2	5.32	16.51	27.10	o
5	4	2	178.14	170.58	21.75	o
6	4	2	1658.90	1721.36	40.01	o
7	4	2	1152.66	1170.70	39.45	o
8	4	2	87.67	106.40	29.82	o
9	4	2	157.59	170.17	45.13	o
10	4	2	0.11	22.43	39.83	o
11	4	2	2.98	26.15	49.94	o
12	4	2	89.55	122.48	48.04	o
13	4	2	303.29	336.91	70.71	o
14	4	2	651.58	607.94	78.70	o
15	4	2	47.49	57.84	71.02	o
16	4	2	51.99	49.92	88.65	o
3	5	2	9980.52	8348.46	270.48	o
4	5	2	111.35	103.32	54.29	o
5	5	2	1123.63	1236.00	48.13	o
6	5	2	10.75	20.27	36.61	o
7	5	2	238.09	283.54	44.46	o
8	5	2	7830.65	7091.19	235.84	o
9	5	2	8276.88	7564.41	149.32	o
10	5	2	23.55	84.06	62.80	o
11	5	2	3063.84	3147.47	79.35	o
12	5	2	9485.96	9366.44	143.13	o
13	5	2	151.60	163.84	62.77	o
14	5	2	132.92	146.13	70.86	o
15	5	2	436.73	403.13	79.46	o
16	5	2	839.05	861.13	134.22	o
17	5	2	2323.63	2139.19	239.23	o
18	5	2	336.34	277.43	113.88	o
5	6	2	5444.27	5047.78	248.29	o
6	6	2	2.66	48.79	55.94	o

7	6	2	2028.71	2089.74	99.61	o
8	6	2	313.77	286.07	57.56	o
9	6	2	8928.66	9040.39	156.45	o
10	6	2	977.20	1067.53	84.54	o
11	6	2	6888.84	6988.72	290.76	o
12	6	2	282.26	366.86	61.23	o
13	6	2	43.23	57.75	60.41	o
14	6	2	0.12	95.56	78.72	o
15	6	2	138.89	142.85	82.54	o
16	6	2	143.99	68.85	82.48	o
17	6	2	663.91	612.71	102.14	o
18	6	2	535.44	715.77	123.03	o
7	7	2	1340.01	1783.70	226.01	o
8	7	2	2472.92	2456.42	135.66	o
9	7	2	27.24	35.18	83.79	o
10	7	2	2.73	14.01	80.81	o
11	7	2	468.10	535.56	105.80	o
12	7	2	3226.38	3306.62	227.44	o
13	7	2	612.75	754.98	86.97	o
14	7	2	1.89	16.76	74.61	o
15	7	2	78.34	77.81	85.13	o
16	7	2	523.57	608.52	115.89	o
17	7	2	480.81	616.73	116.28	o
18	7	2	18.17	151.28	242.85	o
9	8	2	323.41	372.43	204.04	o
10	8	2	80.51	99.30	131.61	o
12	8	2	0.53	17.45	123.29	o
13	8	2	818.40	922.26	132.77	o
14	8	2	182.12	174.39	85.79	o
15	8	2	711.31	606.54	110.08	o
16	8	2	67.04	38.41	135.81	o
12	9	2	466.99	820.63	259.94	o
13	9	2	529.39	538.67	137.92	o
1	1	3	52.83	46.56	12.32	o
2	1	3	1305.05	1438.78	29.92	o
3	1	3	3271.84	3207.33	52.43	o
4	1	3	2.81	20.14	13.75	o
5	1	3	287.90	308.71	19.92	o
6	1	3	2116.47	2176.82	50.17	o
7	1	3	999.58	1117.87	44.85	o
8	1	3	50.16	36.81	28.06	o
9	1	3	854.35	951.99	127.94	o
10	1	3	1416.43	1301.89	160.41	o
11	1	3	105.70	134.43	119.40	o
1	2	3	9889.78	9788.80	144.58	o
2	2	3	19.36	25.34	14.32	o
4	2	3	1137.57	1226.00	30.77	o
5	2	3	1129.64	1216.42	35.03	o
6	2	3	384.05	423.36	28.26	o
7	2	3	4126.26	4126.27	62.40	o
8	2	3	276.23	641.25	108.11	o
9	2	3	942.08	1055.15	47.29	o
10	2	3	646.75	632.43	57.22	o
11	2	3	254.25	111.50	85.33	o
12	2	3	1567.32	1626.45	194.96	o

13	2	3	3420.55	3544.89	240.91	o
1	3	3	28022.19	27348.50	592.02	o
2	3	3	3484.61	3567.44	111.41	o
3	3	3	97.72	114.91	24.52	o
4	3	3	745.25	757.16	29.95	o
5	3	3	2440.84	2423.58	46.49	o
6	3	3	7867.75	8611.28	292.38	o
7	3	3	2478.51	2673.15	60.26	o
8	3	3	30.08	22.79	32.06	o
9	3	3	570.69	639.02	48.08	o
10	3	3	3858.31	3460.81	87.68	o
11	3	3	197.90	144.14	69.06	o
12	3	3	939.95	924.39	120.88	o
13	3	3	8798.32	8498.54	438.73	o
14	3	3	8927.27	9220.00	248.07	o
15	3	3	2466.75	2005.63	205.74	o
0	4	3	13735.28	12645.81	330.52	o
1	4	3	3110.47	3178.84	102.18	o
2	4	3	60.55	45.17	42.85	o
3	4	3	2312.52	2123.91	66.96	o
4	4	3	1937.74	1841.99	53.65	o
5	4	3	805.92	852.06	40.70	o
6	4	3	117.20	126.90	33.86	o
7	4	3	1062.56	1085.63	42.93	o
8	4	3	1.85	41.10	47.34	o
9	4	3	1748.18	1630.53	108.43	o
10	4	3	640.62	659.06	67.47	o
11	4	3	194.78	145.12	65.86	o
12	4	3	772.56	898.04	101.35	o
13	4	3	858.90	898.39	99.60	o
14	4	3	160.25	42.72	75.93	o
15	4	3	529.08	275.65	107.61	o
16	4	3	22.52	34.69	97.63	o
3	5	3	3744.83	3961.62	455.93	o
4	5	3	215.33	111.55	42.29	o
5	5	3	110.09	107.80	45.94	o
6	5	3	926.11	921.26	63.49	o
7	5	3	184.07	194.29	57.95	o
8	5	3	39.61	32.75	57.97	o
9	5	3	779.07	722.28	91.39	o
10	5	3	507.91	598.08	75.07	o
11	5	3	2.78	43.04	57.48	o
12	5	3	15.99	18.92	63.09	o
13	5	3	149.97	189.18	71.59	o
14	5	3	194.63	85.77	73.05	o
15	5	3	1343.61	1128.23	117.38	o
16	5	3	93.74	26.19	83.46	o
17	5	3	420.07	367.46	116.45	o
18	5	3	163.48	200.16	165.93	o
5	6	3	26.52	178.09	150.08	o
6	6	3	24.61	124.35	110.00	o
7	6	3	122.93	79.99	80.12	o
8	6	3	305.02	336.47	85.97	o
9	6	3	158.56	188.66	80.61	o
10	6	3	177.77	112.48	78.93	o

11	6	3	205.14	164.94	60.94	o
12	6	3	14.07	39.20	67.57	o
13	6	3	3.27	30.31	64.64	o
14	6	3	2.21	26.54	70.33	o
15	6	3	22.59	41.12	75.65	o
16	6	3	80.47	54.48	79.52	o
17	6	3	340.47	290.85	135.72	o
18	6	3	57.89	25.92	259.16	o
6	7	3	1170.62	1299.27	198.70	o
7	7	3	615.34	273.12	152.99	o
8	7	3	282.54	249.77	103.19	o
9	7	3	210.73	238.67	97.15	o
10	7	3	1437.97	1489.53	131.63	o
11	7	3	372.98	314.86	100.56	o
12	7	3	6.73	15.44	77.08	o
13	7	3	1414.12	1392.17	103.92	o
14	7	3	1623.68	1638.30	110.87	o
15	7	3	45.16	116.35	112.27	o
16	7	3	4.62	180.77	192.56	o
10	8	3	30.19	37.21	170.91	o
11	8	3	931.69	1095.86	182.91	o
12	8	3	532.18	371.19	136.32	o
13	8	3	2560.06	2387.42	163.91	o
14	8	3	9.10	18.03	180.32	o
0	0	4	2361.16	2443.33	79.28	o
1	0	4	15433.71	14790.37	196.09	o
2	0	4	479.06	478.61	31.50	o
3	0	4	3290.74	3475.27	66.37	o
4	0	4	11277.99	11155.00	188.62	o
5	0	4	213.39	269.16	37.17	o
6	0	4	322.95	268.45	41.77	o
7	0	4	1288.07	1209.60	63.02	o
9	0	4	2790.91	2757.60	216.75	o
1	1	4	4819.45	4711.05	61.58	o
2	1	4	142.24	168.03	21.63	o
3	1	4	1268.25	1443.64	40.22	o
4	1	4	0.33	19.70	23.50	o
5	1	4	3671.77	3861.84	60.22	o
6	1	4	1862.69	1854.54	89.00	o
7	1	4	2553.54	2414.22	69.73	o
8	1	4	32.38	30.77	37.62	o
9	1	4	519.28	248.85	103.03	o
10	1	4	4659.81	4757.53	264.94	o
11	1	4	3317.52	3400.45	245.89	o
12	1	4	4.37	6.63	66.31	o
0	2	4	175.26	170.71	32.12	o
1	2	4	867.12	854.50	29.38	o
2	2	4	4.08	26.46	21.62	o
3	2	4	24.36	34.23	25.47	o
4	2	4	321.17	326.37	37.46	o
5	2	4	3433.55	3436.22	67.73	o
6	2	4	6.93	39.12	30.24	o
7	2	4	781.36	813.76	46.18	o
8	2	4	1982.91	2177.16	112.22	o
9	2	4	57.24	79.83	57.12	o

10	2	4	0.59	13.27	58.74	o
11	2	4	2.22	11.56	115.58	o
12	2	4	31.04	98.42	122.93	o
13	2	4	10.81	24.71	133.23	o
1	3	4	81.08	73.27	35.67	o
2	3	4	103.98	102.90	38.21	o
3	3	4	137.42	94.08	37.47	o
4	3	4	3.42	9.24	33.17	o
5	3	4	91.34	74.21	31.57	o
6	3	4	248.03	261.34	36.32	o
7	3	4	217.86	203.84	50.13	o
8	3	4	0.26	67.97	53.31	o
9	3	4	190.25	318.04	99.88	o
10	3	4	14.22	75.24	60.23	o
11	3	4	169.56	141.00	94.44	o
12	3	4	13.80	31.99	93.73	o
13	3	4	224.06	199.05	148.26	o
14	3	4	63.03	102.30	140.61	o
15	3	4	424.68	148.19	162.11	o
0	4	4	1399.85	1344.67	247.76	o
1	4	4	166.77	107.93	54.35	o
2	4	4	0.01	61.26	46.26	o
3	4	4	50.47	64.48	49.66	o
4	4	4	217.25	172.52	46.90	o
5	4	4	2727.00	2771.90	114.65	o
6	4	4	13.47	29.28	50.98	o
7	4	4	16.94	45.02	46.38	o
8	4	4	1.35	19.66	45.09	o
9	4	4	1934.68	1846.11	135.14	o
10	4	4	11.07	22.20	79.71	o
11	4	4	17.09	36.81	82.83	o
12	4	4	64.41	98.62	101.31	o
13	4	4	510.84	412.73	166.21	o
14	4	4	8.10	14.00	98.96	o
15	4	4	1345.81	1405.86	161.97	o
16	4	4	15.18	15.93	159.32	o
1	5	4	2621.02	2352.26	227.70	o
2	5	4	2402.62	2068.00	232.06	o
3	5	4	3398.64	3712.87	206.22	o
4	5	4	0.33	12.58	63.80	o
5	5	4	1177.84	1231.64	92.65	o
6	5	4	943.59	1116.23	84.01	o
7	5	4	1610.16	1634.06	131.75	o
8	5	4	49.15	39.54	76.49	o
9	5	4	206.16	186.59	88.10	o
10	5	4	5838.85	5649.05	164.67	o
11	5	4	3432.03	3268.06	220.10	o
12	5	4	10.23	57.34	85.38	o
13	5	4	2224.90	2249.32	133.14	o
14	5	4	129.33	112.65	90.59	o
15	5	4	2260.26	2433.22	166.65	o
16	5	4	1.31	15.97	99.05	o
3	6	4	957.16	1052.67	197.08	o
4	6	4	5633.51	4886.41	297.97	o
5	6	4	412.93	485.08	267.71	o

6	6	4	195.71	115.44	115.46	o
7	6	4	166.06	98.42	110.11	o
8	6	4	3273.54	3230.01	192.75	o
9	6	4	3416.62	3159.32	158.83	o
10	6	4	85.91	60.51	88.41	o
11	6	4	4045.63	4120.49	149.48	o
12	6	4	1603.72	1726.96	167.68	o
13	6	4	1512.23	1359.89	115.82	o
14	6	4	45.04	36.48	88.02	o
15	6	4	25.30	41.48	104.75	o
6	7	4	3.63	15.98	159.80	o
7	7	4	10.56	17.56	175.61	o
8	7	4	7.24	15.19	107.34	o
9	7	4	571.19	563.49	169.83	o
10	7	4	544.59	522.20	122.13	o
11	7	4	2217.22	2164.13	196.62	o
12	7	4	22.50	69.83	92.85	o
13	7	4	85.65	16.92	97.53	o
9	8	4	215.89	171.91	188.34	o
1	1	5	127.46	146.43	32.80	o
2	1	5	2.42	31.65	37.49	o
3	1	5	366.69	339.54	38.71	o
4	1	5	233.57	253.21	36.88	o
5	1	5	408.53	367.13	44.12	o
6	1	5	1535.95	1535.11	70.30	o
7	1	5	302.83	310.78	109.11	o
8	1	5	524.83	554.24	69.39	o
9	1	5	103.44	83.79	70.89	o
10	1	5	3.11	13.44	134.36	o
11	1	5	20.98	12.92	129.17	o
0	2	5	180.14	165.98	53.36	o
1	2	5	146.05	155.27	37.69	o
2	2	5	2343.63	2289.03	64.02	o
3	2	5	18.84	24.29	35.01	o
4	2	5	4317.94	4334.64	70.94	o
5	2	5	122.14	111.62	40.40	o
6	2	5	349.06	384.65	50.30	o
7	2	5	204.62	211.19	52.41	o
8	2	5	511.96	567.67	80.80	o
9	2	5	2441.20	2591.61	204.28	o
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11	2	5	3522.81	3643.43	288.13	o
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6	3	5	3137.37	3333.57	92.45	o
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8	3	5	1533.35	1549.16	124.50	o
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
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 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
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   6   2   0      216.23      197.30     23.63 o
   8   2   0     1165.78     1325.05     99.38 o
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  12   2   0      242.39      272.71    118.49 o
   2   3   0      936.89     1121.59     71.42 o
   4   3   0      949.99     1044.22     61.56 o
   6   3   0     1516.79     1719.68     52.26 o
   8   3   0       19.47       28.83     27.63 o
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17	6	2	608.14	667.95	93.70	o
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_exptl_absorpt_process_details    ?

_exptl_special_details
;
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;


_diffrn_radiation_wavelength      0.71073
_diffrn_radiation_type            MoK\a
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_diffrn_reflns_limit_l_min        -6
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_computing_cell_refinement        ?
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_computing_publication_material   ?

_refine_special_details
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
;

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_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0593P)^2^+0.0000P] where P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     mixed
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_number_reflns          584
_refine_ls_number_parameters      61
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_refine_ls_wR_factor_ref          0.1080
_refine_ls_wR_factor_gt           0.0999
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SiB Si 0.47305(8) 0.3376(2) 0.8018(2) 0.0047(4) Uani 1 1 d . . .
Mg1 Mg 0.37601(10) 0.6550(2) 0.8608(3) 0.0060(5) Uani 1 1 d . . .
Mg2 Mg 0.37711(11) 0.4843(2) 0.3531(3) 0.0089(5) Uani 1 1 d . . .
O1A O 0.1827(2) 0.3397(4) 0.0288(5) 0.0054(8) Uiso 1 1 d . . .
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O1B O 0.5624(2) 0.3393(4) 0.8036(6) 0.0060(8) Uiso 1 1 d . . .
O2B O 0.4326(2) 0.4831(4) 0.6859(6) 0.0075(9) Uiso 1 1 d . . .
03B O 0.4471(2) 0.1929(4) 0.6103(5) 0.0041(8) Uiso 1 1 d . . .

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 _atom_site_aniso_U_12
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SiB 0.0048(14) 0.0045(15) 0.0049(6) -0.0003(6) -0.0005(6) 0.0002(6)
Mg1 0.0063(16) 0.0058(17) 0.0060(7) 0.0005(8) -0.0010(7) -0.0003(7)
Mg2 0.0122(18) 0.0069(18) 0.0077(7) 0.0007(8) -0.0014(9) -0.0004(8)

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;
 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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SiA Mg2 2.777(2) . ?
SiA Mg1 3.121(2) 2_564 ?
SiA Mg2 3.234(3) 2_564 ?
SiA Mg1 3.269(2) 7_654 ?
SiB O2B 1.583(4) . ?
SiB O1B 1.617(4) . ?
SiB 03B 1.669(4) . ?
SiB 03B 1.674(3) 8_566 ?
SiB Mg2 3.158(2) . ?
SiB Mg2 3.227(3) 5_666 ?
SiB Mg1 3.237(2) 5_667 ?
Mg1 O2A 1.987(4) 1_556 ?
Mg1 O1A 2.011(3) 2_565 ?
Mg1 O2B 2.027(4) . ?
Mg1 O1B 2.054(4) 5_667 ?
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Mg1 Mg2 2.936(2) 1_556 ?
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Mg1 Mg1 3.058(2) 8_575 ?
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Mg2 O3A 2.258(4) 8_565 ?
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Mg2 SiB 3.227(3) 5_666 ?
O1A Mg1 2.011(3) 2_564 ?
O1A Mg2 2.086(4) 2_564 ?
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O2A Mg1 1.987(4) 1_554 ?
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   4   1   0      177.35      159.44     16.35 o
   6   1   0    37281.87    35223.85    980.78 o
   8   1   0        0.41        4.74     47.44 o
   2   2   0        0.00       15.66     10.63 o
   4   2   0    15398.13    13841.06    138.55 o
   6   2   0      211.98      204.03     23.72 o
   8   2   0     1134.24     1402.45     98.95 o
  10   2   0      573.30      515.95     62.68 o
  12   2   0      229.30      219.84    110.50 o
   2   3   0      806.46     1056.55     69.53 o
   4   3   0     1055.33     1164.97     70.10 o
   6   3   0     1604.89     1764.13     68.77 o
   8   3   0       15.08       16.25     27.43 o
  10   3   0      659.28      715.96     49.11 o
  12   3   0      455.37      388.70     70.20 o
```

14	3	0	1608.39	1451.91	122.61	o
4	4	0	5885.69	6005.88	190.99	o
6	4	0	139.44	99.52	29.39	o
8	4	0	3844.97	3649.17	148.76	o
10	4	0	2145.17	2031.67	108.68	o
12	4	0	23.01	27.57	57.83	o
14	4	0	262.24	283.81	81.70	o
16	4	0	3980.72	3683.96	171.82	o
4	5	0	85.67	87.58	70.29	o
6	5	0	14183.01	14024.36	305.80	o
8	5	0	236.77	277.59	69.42	o
10	5	0	6377.96	6060.54	677.82	o
12	5	0	190.80	156.87	81.44	o
14	5	0	23885.68	22863.92	1357.12	o
16	5	0	356.21	321.20	100.18	o
18	5	0	1481.20	1583.05	225.54	o
6	6	0	440.37	450.51	114.75	o
8	6	0	1127.70	1356.14	157.84	o
10	6	0	857.26	922.67	150.92	o
12	6	0	6134.46	6410.64	200.63	o
14	6	0	828.98	772.42	95.61	o
16	6	0	1885.95	1799.55	151.42	o
18	6	0	54.06	131.88	113.62	o
8	7	0	194.34	215.16	129.25	o
10	7	0	5821.10	5544.41	285.14	o
12	7	0	422.75	542.74	186.11	o
14	7	0	2146.74	2057.28	132.71	o
16	7	0	211.81	173.85	93.05	o
18	7	0	45.12	69.76	120.08	o
10	8	0	1014.60	1080.60	187.71	o
12	8	0	68.34	3.61	148.65	o
14	8	0	44.73	62.96	91.78	o
16	8	0	1246.37	1276.94	163.43	o
12	9	0	117.99	234.25	214.04	o
14	9	0	1321.73	1210.14	169.06	o
1	1	1	332.22	359.47	8.79	o
2	1	1	274.76	247.94	7.99	o
3	1	1	21.38	38.97	4.81	o
4	1	1	2892.99	3059.16	38.75	o
5	1	1	5182.36	5050.92	98.99	o
6	1	1	1189.26	1084.84	30.63	o
7	1	1	2112.54	2001.29	87.54	o
8	1	1	1503.32	1408.79	75.52	o
9	1	1	357.72	405.24	58.60	o
0	2	1	31.97	13.24	16.00	o
3	2	1	9363.14	8916.74	122.37	o
5	2	1	8252.58	7899.48	147.71	o
6	2	1	210.36	180.82	12.16	o
7	2	1	2695.71	2874.83	72.34	o
8	2	1	3356.89	3250.14	77.61	o
9	2	1	12.11	15.62	14.87	o
10	2	1	635.90	754.94	42.08	o
11	2	1	304.08	306.35	69.31	o
12	2	1	1118.59	999.22	94.69	o
1	3	1	12809.06	12304.73	228.07	o

2	3	1	2529.33	2147.65	55.19	o
3	3	1	2266.39	2845.47	110.43	o
4	3	1	1426.41	1718.25	26.25	o
5	3	1	8226.51	8641.56	196.84	o
7	3	1	55.42	48.41	17.12	o
8	3	1	5311.38	4988.46	74.96	o
9	3	1	8622.01	8462.67	144.69	o
10	3	1	23954.35	23196.21	540.27	o
11	3	1	27143.55	25023.45	298.50	o
12	3	1	15224.52	13767.96	293.97	o
13	3	1	1605.59	1572.66	82.45	o
14	3	1	33.27	41.52	68.64	o
15	3	1	536.93	718.73	165.99	o
3	4	1	837.11	832.57	56.04	o
4	4	1	1176.34	1181.14	59.93	o
5	4	1	4442.56	4543.55	89.64	o
6	4	1	608.93	646.61	27.83	o
7	4	1	1011.19	942.39	32.78	o
8	4	1	247.38	265.62	36.10	o
9	4	1	185.28	224.21	36.31	o
10	4	1	114.55	119.15	31.90	o
11	4	1	55.63	91.77	37.21	o
12	4	1	27.17	26.30	37.22	o
13	4	1	182.23	132.32	49.02	o
14	4	1	576.66	603.95	69.28	o
15	4	1	1.52	79.37	81.31	o
17	4	1	518.78	505.57	185.36	o
4	5	1	1121.30	1265.71	172.07	o
5	5	1	1620.22	1700.89	106.31	o
6	5	1	251.30	266.16	41.09	o
7	5	1	1022.48	1084.13	52.28	o
8	5	1	510.88	542.96	42.86	o
9	5	1	420.33	334.97	43.97	o
10	5	1	135.71	114.43	44.44	o
11	5	1	106.70	125.23	52.27	o
12	5	1	11.99	19.75	53.36	o
13	5	1	13.18	81.32	59.94	o
14	5	1	2743.72	2404.52	106.58	o
15	5	1	307.21	316.87	67.26	o
16	5	1	303.29	359.73	85.71	o
17	5	1	1.34	18.12	82.96	o
18	5	1	10.11	112.27	87.44	o
19	5	1	4.81	160.32	178.48	o
5	6	1	4.04	34.80	67.32	o
6	6	1	217.14	293.68	94.89	o
7	6	1	42.67	43.91	40.15	o
8	6	1	149.72	186.88	56.00	o
9	6	1	89.42	122.46	67.44	o
10	6	1	40.66	13.70	96.66	o
11	6	1	182.78	198.08	95.04	o
12	6	1	591.67	584.29	69.58	o
13	6	1	82.30	101.59	56.05	o
14	6	1	151.52	133.03	66.43	o
15	6	1	72.17	61.90	79.76	o
16	6	1	22.62	13.69	79.01	o

17	6	1	66.96	67.31	80.90	o
18	6	1	64.56	74.56	93.47	o
19	6	1	40.40	38.75	111.32	o
7	7	1	803.11	919.51	171.12	o
8	7	1	1214.28	1343.94	127.20	o
9	7	1	2476.55	2441.37	154.79	o
10	7	1	251.31	220.34	104.58	o
11	7	1	926.96	1167.18	130.31	o
12	7	1	1414.71	1612.30	150.68	o
13	7	1	197.94	208.89	73.71	o
14	7	1	34.72	13.89	69.51	o
15	7	1	416.01	510.73	79.22	o
16	7	1	633.60	561.47	83.39	o
17	7	1	12.94	24.58	70.70	o
18	7	1	2.11	57.67	99.91	o
9	8	1	28.47	168.08	111.42	o
10	8	1	116.66	77.21	108.36	o
11	8	1	5.48	42.39	106.09	o
12	8	1	233.84	359.42	115.42	o
13	8	1	1423.60	1629.80	221.78	o
14	8	1	15.63	31.13	71.81	o
15	8	1	1130.73	1188.66	132.40	o
16	8	1	882.28	1033.57	115.45	o
11	9	1	5083.53	6469.02	396.59	o
12	9	1	5317.95	6161.21	513.86	o
13	9	1	476.74	510.93	161.16	o
14	9	1	212.42	145.53	139.75	o
0	0	2	861.28	820.04	32.09	o
1	0	2	565.22	518.27	17.76	o
2	0	2	37638.01	33635.46	448.80	o
3	0	2	3511.18	2715.47	35.36	o
4	0	2	1170.98	1208.52	38.36	o
5	0	2	24469.30	24179.10	306.05	o
6	0	2	128.86	150.71	65.98	o
7	0	2	5227.87	4673.92	172.26	o
1	1	2	12.67	21.51	7.56	o
2	1	2	201.11	231.71	11.97	o
3	1	2	660.74	552.01	12.92	o
4	1	2	835.15	1047.91	21.99	o
5	1	2	5709.93	6357.32	176.35	o
6	1	2	720.06	784.16	30.86	o
7	1	2	45.41	64.74	26.36	o
8	1	2	5917.92	5726.85	112.21	o
9	1	2	1750.14	1802.70	95.41	o
10	1	2	312.16	296.89	92.64	o
0	2	2	133.18	164.50	22.64	o
1	2	2	0.04	15.73	11.57	o
2	2	2	6.58	15.82	11.20	o
3	2	2	1115.13	1213.99	29.24	o
4	2	2	485.24	594.05	25.08	o
5	2	2	33.18	25.70	11.98	o
6	2	2	3377.12	3648.92	58.74	o
7	2	2	3391.72	3519.21	46.66	o
8	2	2	1033.83	1086.96	50.18	o
9	2	2	2244.66	2189.78	72.35	o

10	2	2	1040.86	1107.83	75.91	o
11	2	2	188.41	155.31	53.35	o
12	2	2	291.56	282.34	64.26	o
1	3	2	81.86	116.06	29.89	o
2	3	2	0.09	10.42	23.45	o
3	3	2	815.95	957.59	27.40	o
4	3	2	643.91	678.40	21.49	o
5	3	2	552.30	612.52	19.85	o
6	3	2	138.57	144.88	16.24	o
7	3	2	272.25	316.97	23.76	o
8	3	2	317.03	361.89	25.57	o
9	3	2	219.31	188.88	31.41	o
10	3	2	52.00	85.60	36.56	o
11	3	2	160.26	170.96	42.47	o
12	3	2	11.52	15.50	43.00	o
13	3	2	6.94	21.83	47.96	o
14	3	2	0.03	74.07	65.48	o
15	3	2	90.00	14.04	114.30	o
1	4	2	1104.08	977.47	121.04	o
2	4	2	4416.01	4220.08	128.01	o
3	4	2	1886.18	1831.92	57.40	o
4	4	2	0.19	8.38	25.29	o
5	4	2	183.08	161.56	20.97	o
6	4	2	1729.73	1805.76	65.95	o
7	4	2	1139.38	1132.89	37.30	o
8	4	2	103.79	130.73	32.10	o
9	4	2	175.95	222.19	44.97	o
10	4	2	0.03	40.09	39.80	o
11	4	2	0.02	48.75	50.13	o
12	4	2	120.94	110.41	45.83	o
13	4	2	279.20	280.82	64.57	o
14	4	2	651.66	630.51	75.51	o
15	4	2	73.11	125.47	72.06	o
16	4	2	67.07	32.76	93.04	o
3	5	2	10337.81	9818.72	283.07	o
4	5	2	170.58	207.01	52.97	o
5	5	2	1358.41	1499.14	59.40	o
6	5	2	0.05	30.36	34.58	o
7	5	2	314.46	366.77	43.86	o
8	5	2	7968.18	7352.57	223.81	o
9	5	2	7814.37	7341.13	158.40	o
10	5	2	141.03	177.36	60.28	o
11	5	2	2685.83	2872.80	120.47	o
12	5	2	9034.83	8286.33	366.72	o
13	5	2	243.64	266.36	61.92	o
14	5	2	155.74	107.97	64.64	o
15	5	2	555.08	552.49	77.59	o
16	5	2	903.01	921.41	110.15	o
17	5	2	2771.16	2498.07	184.23	o
18	5	2	574.63	734.18	138.59	o
5	6	2	5363.19	4698.48	229.71	o
6	6	2	0.37	29.01	51.79	o
7	6	2	1909.06	1836.97	78.77	o
8	6	2	405.80	380.39	63.21	o
9	6	2	8510.04	8284.62	254.91	o

10	6	2	926.56	1038.50	82.59	o
11	6	2	7767.50	8107.05	475.08	o
13	6	2	107.70	94.03	57.47	o
14	6	2	0.11	93.41	76.23	o
15	6	2	111.26	115.72	70.34	o
16	6	2	112.37	24.91	68.83	o
17	6	2	621.71	847.40	91.56	o
18	6	2	512.49	621.57	117.55	o
7	7	2	1202.57	936.27	185.79	o
8	7	2	2281.34	2131.38	126.59	o
9	7	2	0.13	14.61	66.26	o
10	7	2	5.01	19.13	69.17	o
11	7	2	339.89	289.62	84.97	o
12	7	2	3158.54	4082.61	413.20	o
13	7	2	549.86	699.18	83.03	o
14	7	2	0.72	21.57	70.16	o
15	7	2	131.33	113.19	78.42	o
16	7	2	464.78	540.93	89.84	o
17	7	2	548.60	493.98	112.93	o
10	8	2	63.16	134.74	185.94	o
12	8	2	0.64	43.11	92.85	o
13	8	2	738.92	751.08	101.64	o
14	8	2	158.64	197.32	81.39	o
15	8	2	715.99	751.33	143.00	o
16	8	2	62.72	465.19	206.43	o
12	9	2	584.63	966.79	253.19	o
1	1	3	38.16	35.45	12.59	o
2	1	3	1059.41	1149.11	23.78	o
3	1	3	3648.77	3683.75	82.96	o
4	1	3	0.38	14.02	14.02	o
5	1	3	260.45	247.57	20.43	o
6	1	3	1995.11	2085.12	46.82	o
7	1	3	1136.39	1182.85	48.79	o
8	1	3	40.13	48.29	27.63	o
9	1	3	1100.74	1102.73	130.89	o
10	1	3	1134.24	1080.39	134.96	o
11	1	3	92.10	158.18	122.51	o
1	2	3	11239.22	10964.12	208.38	o
2	2	3	34.43	28.08	14.24	o
4	2	3	1130.52	1217.40	29.62	o
5	2	3	1307.58	1301.26	35.18	o
6	2	3	450.09	520.54	28.79	o
7	2	3	5068.88	5027.37	73.10	o
8	2	3	262.83	297.69	30.01	o
9	2	3	840.51	910.14	48.08	o
10	2	3	771.02	733.28	58.51	o
11	2	3	261.47	152.89	82.64	o
12	2	3	1286.60	1466.52	170.30	o
13	2	3	3443.22	2901.29	228.80	o
1	3	3	31164.33	29222.47	544.06	o
2	3	3	2322.99	2306.50	69.30	o
3	3	3	108.58	106.65	24.60	o
4	3	3	703.49	743.77	29.38	o
5	3	3	2705.23	2747.14	66.40	o
6	3	3	6481.88	6393.13	200.95	o

7	3	3	2603.29	2724.43	65.58	o
8	3	3	31.23	23.16	32.39	o
9	3	3	845.12	907.80	53.05	o
10	3	3	3405.89	3270.40	97.40	o
11	3	3	170.78	124.05	66.83	o
12	3	3	883.65	802.23	88.65	o
13	3	3	10629.32	9961.52	357.45	o
14	3	3	7057.57	6802.01	219.78	o
15	3	3	2770.98	2024.90	209.60	o
0	4	3	11159.97	10645.85	305.66	o
1	4	3	3484.70	3513.24	108.90	o
2	4	3	95.64	82.57	43.46	o
3	4	3	2815.59	2643.58	70.95	o
4	4	3	1589.99	1520.41	51.30	o
5	4	3	874.75	893.58	40.05	o
6	4	3	143.07	174.20	33.61	o
7	4	3	1199.38	1215.38	45.49	o
8	4	3	1.89	11.12	46.88	o
9	4	3	1852.01	1768.54	99.28	o
10	4	3	702.06	649.62	67.99	o
11	4	3	237.57	198.69	79.91	o
12	4	3	638.34	717.63	92.55	o
13	4	3	782.32	1010.54	97.12	o
14	4	3	149.91	134.23	78.14	o
15	4	3	564.26	556.07	99.08	o
16	4	3	16.93	26.75	93.43	o
2	5	3	1271.33	1275.21	155.45	o
3	5	3	3911.65	3705.52	161.68	o
4	5	3	242.24	143.93	63.58	o
5	5	3	79.20	61.07	43.53	o
6	5	3	765.42	748.85	60.09	o
7	5	3	194.92	211.66	55.83	o
8	5	3	52.88	37.58	55.77	o
9	5	3	843.21	896.86	94.09	o
10	5	3	279.28	292.98	67.85	o
11	5	3	23.93	24.59	52.27	o
12	5	3	17.60	45.35	55.06	o
13	5	3	119.63	150.62	67.47	o
14	5	3	127.25	103.32	69.19	o
16	5	3	89.50	77.04	91.73	o
17	5	3	389.22	408.28	101.49	o
18	5	3	110.10	234.13	173.39	o
4	6	3	139.22	276.82	136.88	o
5	6	3	72.86	10.75	107.51	o
6	6	3	24.19	37.95	79.41	o
7	6	3	57.17	11.01	70.54	o
8	6	3	198.65	206.91	74.22	o
9	6	3	95.77	87.73	72.84	o
10	6	3	161.62	177.54	78.59	o
11	6	3	293.87	249.88	61.97	o
12	6	3	7.73	14.30	71.37	o
13	6	3	1.19	61.86	62.68	o
14	6	3	6.47	48.96	66.48	o
15	6	3	15.79	26.70	69.66	o
16	6	3	87.90	24.82	72.19	o

17	6	3	360.73	328.30	154.06	o
6	7	3	1187.34	818.07	148.04	o
7	7	3	783.24	561.04	152.01	o
8	7	3	234.72	217.36	135.16	o
9	7	3	258.55	319.71	90.79	o
10	7	3	1223.01	1330.51	182.06	o
11	7	3	392.60	383.65	91.83	o
12	7	3	4.06	88.69	67.50	o
13	7	3	1742.44	1738.04	107.89	o
14	7	3	1344.05	1313.16	99.52	o
15	7	3	52.62	116.65	99.51	o
16	7	3	0.03	77.28	165.97	o
10	8	3	55.18	160.22	142.03	o
11	8	3	847.12	909.63	144.67	o
12	8	3	508.72	441.89	111.51	o
13	8	3	2752.85	2864.70	484.33	o
14	8	3	17.65	16.02	160.22	o
0	0	4	1567.32	1662.44	72.78	o
1	0	4	15510.83	14941.82	219.03	o
2	0	4	1614.81	1708.54	61.87	o
3	0	4	2367.87	2356.95	59.96	o
4	0	4	10916.55	11036.48	220.29	o
5	0	4	54.35	66.19	34.47	o
6	0	4	373.77	390.14	45.18	o
7	0	4	639.11	579.25	55.23	o
9	0	4	3823.58	3604.12	236.43	o
1	1	4	4446.31	4398.13	56.86	o
2	1	4	115.96	126.79	21.15	o
3	1	4	1289.90	1411.93	44.29	o
4	1	4	17.22	15.16	24.61	o
5	1	4	4168.49	4336.78	109.21	o
6	1	4	1581.29	1714.88	58.56	o
7	1	4	2582.22	2479.43	76.04	o
8	1	4	199.61	160.94	42.97	o
9	1	4	351.19	391.27	83.62	o
10	1	4	4908.88	4841.11	266.09	o
11	1	4	2710.96	2762.65	233.32	o
0	2	4	152.29	177.49	33.16	o
1	2	4	712.04	718.41	28.77	o
2	2	4	8.82	23.45	22.24	o
3	2	4	58.77	52.57	24.25	o
4	2	4	210.27	213.81	35.37	o
5	2	4	3219.10	3158.46	115.20	o
6	2	4	29.65	38.95	31.22	o
7	2	4	876.78	921.47	47.40	o
8	2	4	1790.27	1975.58	108.71	o
9	2	4	34.10	31.68	53.38	o
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4	3	4	15.65	22.57	35.77	o

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6	3	4	241.72	230.59	36.11	o
7	3	4	206.69	198.59	50.06	o
8	3	4	0.06	29.37	50.77	o
9	3	4	198.25	203.00	172.61	o
10	3	4	13.01	31.67	56.51	o
11	3	4	258.83	255.12	104.64	o
12	3	4	41.23	11.02	86.07	o
13	3	4	211.11	119.66	144.98	o
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2	4	4	17.32	74.78	45.38	o
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4	4	4	243.15	240.17	48.54	o
5	4	4	2930.98	3122.96	130.83	o
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16	4	4	46.65	15.14	151.42	o
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12	5	4	24.42	41.54	78.67	o
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3	6	4	518.23	429.95	130.89	o
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6	6	4	179.77	139.87	97.22	o
7	6	4	46.87	13.38	94.58	o
8	6	4	2722.85	2808.30	171.42	o
9	6	4	4210.42	3921.20	165.10	o
10	6	4	102.57	40.48	86.72	o
11	6	4	4447.48	4527.59	402.02	o
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13	6	4	1415.12	1370.46	115.69	o

14	6	4	66.89	22.95	88.68	o
15	6	4	11.68	18.72	131.84	o
6	7	4	0.83	12.63	126.30	o
7	7	4	0.38	24.72	128.76	o
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11	7	4	1941.98	1887.86	124.16	o
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8	3	5	1365.64	1467.42	86.18	o
9	3	5	18.39	45.49	56.68	o
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4	4	5	1092.97	1191.95	94.80	o

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9	4	5	1244.12	1337.11	111.27	o
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6	2	6	385.05	414.89	56.82	o
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9	2	6	2.35	22.84	82.84	o
1	3	6	20.65	25.98	52.85	o
2	3	6	0.98	36.77	48.41	o

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7	4	6	890.93	1027.30	131.18	o
3	5	6	371.58	362.47	121.38	o
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 'O'  'O'   0.0106   0.0060
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 'Si'  'Si'   0.0817   0.0704
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 '-x, -y, -z'
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
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SiB Si 0.47285(9) 0.3375(2) 0.8025(2) 0.0053(4) Uani 1 1 d . . .
Mg1 Mg 0.37601(11) 0.6557(2) 0.8585(3) 0.0069(5) Uani 1 1 d . . .
Mg2 Mg 0.37721(11) 0.4837(2) 0.3510(3) 0.0088(6) Uani 1 1 d . . .
O1A O 0.1823(2) 0.3398(4) 0.0265(5) 0.0046(8) Uiso 1 1 d . . .
O2A O 0.3102(2) 0.5062(5) 0.0351(6) 0.0071(9) Uiso 1 1 d . . .
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O1B O 0.5621(2) 0.3391(4) 0.8053(6) 0.0059(8) Uiso 1 1 d . . .
O2B O 0.4326(2) 0.4835(4) 0.6850(6) 0.0078(9) Uiso 1 1 d . . .
03B O 0.4467(2) 0.1922(4) 0.6118(5) 0.0040(8) Uiso 1 1 d . . .

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SiB 0.0061(15) 0.0051(16) 0.0048(6) -0.0010(6) -0.0006(6) 0.0005(6)
Mg1 0.0071(17) 0.0079(18) 0.0058(7) -0.0002(8) -0.0011(7) 0.0003(7)
Mg2 0.0123(19) 0.0067(19) 0.0074(7) -0.0007(8) -0.0015(9) -0.0005(7)

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 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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SiA O3A 1.657(3) 8_565 ?
SiA Mg2 2.764(2) . ?
SiA Mg1 3.110(2) 2_564 ?
SiA Mg2 3.227(3) 2_564 ?
SiA Mg1 3.258(2) 7_654 ?
SiB O2B 1.581(4) . ?
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Mg1 O2A 1.979(4) 1_556 ?
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Mg1 O1B 2.052(4) 5_667 ?
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Mg2 O3A 2.238(4) 8_565 ?
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O1A Mg2 2.077(4) 2_564 ?
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O1B Mg1 2.052(4) 5_667 ?
O1B Mg2 2.053(4) 5_666 ?
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03B SiB 1.672(3) 8_565 ?
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   4   1   0      192.37      179.64     19.01 o
   8   1   0        0.11       49.39     51.12 o
   2   2   0        0.15       16.96     13.21 o
   4   2   0    14732.93    13080.69    402.50 o
   6   2   0      233.16      204.43     23.62 o
   8   2   0     1162.37     1380.88     97.92 o
  10   2   0      629.83      574.24     62.59 o
  12   2   0      186.95      114.82    109.37 o
   2   3   0      737.76      873.35     64.79 o
   4   3   0     1123.26     1215.22     77.43 o
   6   3   0     1691.12     1928.18     73.51 o
   8   3   0       22.11       38.30     27.22 o
  10   3   0      802.06      823.47     50.78 o
  12   3   0      471.07      472.38     69.53 o
  14   3   0     1509.59     1501.99    125.23 o
   4   4   0     6030.69     6337.87    192.60 o
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4	5	0	69.85	130.54	71.34	o
6	5	0	14703.42	14605.63	310.33	o
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10	5	0	6184.77	6039.28	515.46	o
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14	5	0	22521.18	19645.18	317.12	o
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18	5	0	1575.85	1667.12	224.09	o
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10	6	0	902.24	1047.84	149.95	o
12	6	0	6084.07	6922.46	212.21	o
14	6	0	818.84	682.47	99.04	o
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14	8	0	53.82	10.46	84.92	o
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3	1	1	21.43	37.35	4.67	o
4	1	1	2796.31	2936.63	41.85	o
5	1	1	5207.33	5080.04	102.39	o
6	1	1	1228.01	1080.98	30.16	o
7	1	1	2205.77	2104.53	53.45	o
8	1	1	1488.13	1358.71	73.97	o
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13	4	1	182.35	110.16	46.54	o
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12	8	1	229.40	250.30	112.11	o
13	8	1	1373.20	1735.75	159.04	o
14	8	1	17.94	42.70	68.23	o
15	8	1	1062.64	1021.18	95.54	o
16	8	1	808.78	909.33	166.17	o
11	9	1	5060.81	5799.10	368.78	o
12	9	1	5155.78	5833.46	258.57	o
13	9	1	505.26	547.68	144.78	o
0	0	2	951.97	894.91	36.31	o
1	0	2	690.93	618.13	18.53	o
3	0	2	3145.12	2248.26	78.62	o
4	0	2	1444.11	1475.19	49.67	o
5	0	2	24272.89	24467.24	481.35	o
6	0	2	137.22	130.14	66.01	o
7	0	2	4984.28	4828.91	174.02	o
1	1	2	5.76	12.29	7.71	o
2	1	2	200.51	218.19	11.96	o
3	1	2	720.75	585.34	13.62	o
4	1	2	823.81	1059.67	22.68	o
5	1	2	5654.47	6418.75	108.74	o
6	1	2	819.75	830.63	32.15	o
7	1	2	45.35	63.25	25.47	o
8	1	2	5998.86	5792.91	175.93	o
9	1	2	1702.40	1746.01	96.16	o
10	1	2	424.18	576.89	105.32	o
0	2	2	140.47	173.04	22.62	o
1	2	2	0.16	17.31	11.61	o
2	2	2	5.81	9.64	10.99	o
3	2	2	1065.50	1095.10	30.72	o
4	2	2	526.52	625.32	24.22	o
5	2	2	38.85	35.55	12.27	o
6	2	2	3315.22	3536.58	52.63	o
7	2	2	3291.36	3419.65	37.67	o
8	2	2	1147.37	1206.43	38.51	o
9	2	2	2030.82	1932.79	69.22	o
10	2	2	1025.87	1047.06	71.43	o
11	2	2	194.67	181.03	53.22	o
12	2	2	315.26	247.60	63.01	o
1	3	2	94.36	142.96	28.94	o
2	3	2	0.36	9.08	22.94	o

3	3	2	711.03	831.12	28.58	o
4	3	2	598.06	636.08	20.87	o
5	3	2	593.76	637.66	21.74	o
6	3	2	146.59	144.88	16.03	o
7	3	2	270.43	297.40	23.59	o
8	3	2	311.52	380.45	25.64	o
9	3	2	168.49	154.15	28.99	o
10	3	2	54.98	39.94	34.36	o
11	3	2	164.99	118.55	40.48	o
12	3	2	17.68	35.32	44.43	o
13	3	2	9.38	42.59	47.40	o
14	3	2	0.31	10.36	72.19	o
15	3	2	71.49	9.99	99.87	o
1	4	2	1091.59	1080.82	117.23	o
2	4	2	4438.75	4201.98	126.79	o
3	4	2	1740.30	1603.22	106.84	o
4	4	2	0.24	17.50	24.88	o
5	4	2	196.05	179.91	21.10	o
6	4	2	1726.97	1769.90	64.82	o
7	4	2	1083.43	1112.02	37.41	o
8	4	2	119.82	124.37	32.43	o
9	4	2	171.20	172.78	44.45	o
10	4	2	0.65	41.63	40.97	o
11	4	2	0.30	20.33	48.67	o
12	4	2	137.18	121.63	43.87	o
13	4	2	258.01	242.52	62.65	o
14	4	2	583.76	591.71	72.36	o
15	4	2	97.76	55.31	68.86	o
16	4	2	72.05	31.91	84.86	o
3	5	2	10268.52	9283.30	275.02	o
4	5	2	211.90	183.69	51.93	o
5	5	2	1340.76	1455.99	50.97	o
6	5	2	0.04	25.94	34.30	o
7	5	2	317.30	344.50	42.14	o
8	5	2	8031.66	7607.07	163.08	o
9	5	2	7523.44	7509.83	166.48	o
10	5	2	220.37	271.72	53.13	o
11	5	2	2432.46	2544.05	71.28	o
12	5	2	8629.79	8235.11	354.71	o
13	5	2	267.94	363.19	69.68	o
14	5	2	179.43	105.55	61.28	o
15	5	2	594.87	538.99	76.14	o
16	5	2	818.13	861.09	104.81	o
17	5	2	2612.44	2505.88	219.96	o
18	5	2	577.85	787.24	150.71	o
5	6	2	5250.40	4976.46	238.83	o
6	6	2	0.21	25.47	50.08	o
7	6	2	1778.11	1631.93	84.72	o
8	6	2	469.82	476.12	62.08	o
9	6	2	8144.78	7890.16	208.58	o
10	6	2	914.86	953.89	77.53	o
11	6	2	7734.55	7871.39	471.34	o
13	6	2	145.37	72.70	55.59	o
14	6	2	0.11	70.28	73.39	o
15	6	2	102.11	140.82	68.90	o

16	6	2	85.44	74.94	71.29	o
17	6	2	553.37	593.23	88.30	o
18	6	2	430.93	553.55	95.06	o
7	7	2	1173.42	1113.55	189.41	o
8	7	2	2245.27	2175.47	200.63	o
9	7	2	0.09	11.50	66.09	o
10	7	2	15.70	57.51	68.97	o
11	7	2	289.40	313.26	84.85	o
12	7	2	3135.75	3510.85	196.15	o
13	7	2	568.08	680.78	79.54	o
14	7	2	2.40	38.30	67.12	o
15	7	2	141.06	99.48	73.40	o
16	7	2	404.09	447.64	81.73	o
17	7	2	531.16	662.77	118.50	o
10	8	2	58.57	98.11	172.82	o
12	8	2	2.11	67.60	110.94	o
13	8	2	695.17	545.91	96.71	o
14	8	2	146.52	122.05	79.03	o
15	8	2	657.14	581.42	117.10	o
12	9	2	677.87	1057.87	238.13	o
1	1	3	36.29	25.15	13.01	o
2	1	3	955.61	1010.29	23.01	o
3	1	3	3773.02	3773.83	73.50	o
4	1	3	0.04	19.02	13.97	o
5	1	3	232.97	253.56	20.22	o
6	1	3	1948.85	1994.88	62.68	o
7	1	3	1175.92	1222.57	48.52	o
8	1	3	37.22	32.98	26.35	o
9	1	3	1238.48	1451.26	154.25	o
10	1	3	1025.20	1028.82	137.41	o
11	1	3	84.54	150.84	123.53	o
0	2	3	20564.76	19805.63	388.39	o
1	2	3	11684.11	11162.25	237.73	o
2	2	3	46.27	49.76	14.37	o
4	2	3	1119.52	1176.70	28.85	o
5	2	3	1369.41	1371.29	33.05	o
6	2	3	426.15	502.38	28.05	o
7	2	3	5199.11	5322.21	64.73	o
8	2	3	223.85	262.54	28.95	o
9	2	3	768.36	849.53	47.07	o
10	2	3	770.84	786.36	60.07	o
11	2	3	251.21	238.46	71.18	o
12	2	3	1168.51	1311.30	163.36	o
13	2	3	3260.96	2860.00	224.95	o
1	3	3	32102.36	30509.83	724.86	o
2	3	3	1800.62	1745.82	51.47	o
3	3	3	126.85	133.42	24.75	o
4	3	3	684.44	679.15	28.32	o
5	3	3	2805.80	2778.99	79.17	o
7	3	3	2590.77	2620.97	58.32	o
8	3	3	27.97	31.90	32.31	o
9	3	3	940.72	978.07	53.58	o
10	3	3	3229.70	3029.00	94.36	o
11	3	3	184.64	151.64	67.04	o
12	3	3	789.10	796.43	127.95	o

13	3	3	10993.04	10602.63	619.25	o
14	3	3	6004.12	6135.84	211.11	o
15	3	3	2798.80	1753.30	193.33	o
0	4	3	10214.56	9141.79	284.35	o
1	4	3	3719.02	3788.86	258.96	o
2	4	3	99.08	70.32	41.65	o
3	4	3	2932.67	2785.34	81.01	o
4	4	3	1555.87	1424.11	51.31	o
5	4	3	926.60	934.50	42.92	o
6	4	3	142.33	141.37	32.26	o
7	4	3	1177.62	1209.72	44.77	o
8	4	3	9.02	35.88	41.35	o
9	4	3	1882.39	1758.21	83.21	o
10	4	3	683.13	761.15	69.04	o
11	4	3	232.48	202.14	78.49	o
12	4	3	555.88	658.05	90.83	o
13	4	3	700.55	874.04	93.47	o
14	4	3	128.83	141.14	78.29	o
15	4	3	588.23	541.75	98.16	o
16	4	3	16.25	9.36	90.43	o
2	5	3	1074.10	1201.82	150.63	o
3	5	3	3943.52	3658.38	161.49	o
4	5	3	246.30	207.43	63.10	o
5	5	3	61.59	55.13	42.20	o
6	5	3	748.01	827.09	60.76	o
7	5	3	196.69	216.75	55.30	o
8	5	3	47.87	25.05	53.30	o
9	5	3	849.98	822.76	87.53	o
10	5	3	214.93	229.94	62.73	o
11	5	3	41.54	36.19	49.90	o
12	5	3	26.32	38.40	53.76	o
13	5	3	122.26	212.81	83.02	o
14	5	3	114.65	74.33	67.09	o
16	5	3	71.97	47.15	88.30	o
17	5	3	339.47	342.04	95.54	o
18	5	3	83.75	204.82	153.47	o
4	6	3	175.02	166.36	133.14	o
5	6	3	116.31	159.63	168.69	o
6	6	3	29.10	10.49	74.10	o
7	6	3	32.17	32.21	70.48	o
8	6	3	153.76	173.63	70.98	o
9	6	3	79.71	20.19	69.29	o
10	6	3	157.57	107.94	74.26	o
11	6	3	331.38	277.44	61.54	o
12	6	3	8.19	13.52	67.55	o
13	6	3	0.47	14.37	63.96	o
14	6	3	7.98	17.99	61.85	o
15	6	3	7.85	17.62	67.19	o
16	6	3	95.54	25.33	67.58	o
17	6	3	356.08	487.60	150.03	o
7	7	3	847.25	797.40	158.51	o
8	7	3	230.33	132.61	133.07	o
9	7	3	357.39	385.92	90.97	o
10	7	3	1182.04	1326.83	113.02	o
11	7	3	460.11	419.08	90.05	o

12	7	3	3.24	39.30	75.05	o
13	7	3	1743.72	1681.91	103.10	o
14	7	3	1208.54	1097.23	127.17	o
15	7	3	47.31	15.25	107.76	o
16	7	3	0.30	14.61	146.13	o
10	8	3	63.96	178.12	132.48	o
11	8	3	831.16	875.56	228.09	o
12	8	3	466.33	543.13	117.70	o
13	8	3	2621.74	2812.04	362.85	o
0	0	4	1243.86	1280.96	64.89	o
1	0	4	15435.37	14691.65	212.16	o
2	0	4	2094.14	2210.08	68.32	o
3	0	4	1877.85	1993.85	60.34	o
4	0	4	10666.51	10530.63	246.66	o
5	0	4	10.88	36.04	33.36	o
6	0	4	415.60	381.39	47.83	o
7	0	4	453.99	398.15	51.29	o
8	0	4	3952.04	3805.98	343.86	o
9	0	4	4052.09	3570.69	228.29	o
1	1	4	4228.38	4141.60	52.43	o
2	1	4	95.26	95.93	20.37	o
3	1	4	1354.22	1527.67	50.11	o
4	1	4	19.46	18.52	24.27	o
5	1	4	4302.23	4573.39	146.74	o
6	1	4	1451.68	1609.81	54.99	o
7	1	4	2601.12	2437.44	92.67	o
8	1	4	264.39	227.63	44.11	o
9	1	4	238.36	307.22	70.12	o
10	1	4	4921.58	4949.87	264.93	o
11	1	4	2383.37	2218.88	221.50	o
0	2	4	120.08	142.23	32.28	o
1	2	4	656.06	656.12	29.15	o
2	2	4	15.38	20.10	22.97	o
3	2	4	65.66	36.56	24.93	o
4	2	4	178.56	180.11	34.99	o
5	2	4	3066.00	3019.89	137.18	o
6	2	4	35.24	39.82	31.70	o
7	2	4	954.84	1085.71	49.29	o
8	2	4	1752.30	1961.97	77.24	o
9	2	4	24.27	14.50	53.10	o
10	2	4	0.28	36.88	59.01	o
11	2	4	1.60	10.84	108.41	o
12	2	4	2.72	11.10	111.04	o
13	2	4	48.51	148.92	137.15	o
1	3	4	35.78	48.94	36.07	o
2	3	4	25.46	55.74	39.55	o
3	3	4	156.74	125.84	35.90	o
4	3	4	20.20	53.21	35.94	o
5	3	4	130.19	72.96	36.30	o
6	3	4	259.51	231.30	36.09	o
7	3	4	196.18	204.39	51.47	o
8	3	4	0.04	50.71	53.84	o
9	3	4	200.90	330.14	172.24	o
10	3	4	12.57	15.08	56.98	o
11	3	4	273.45	321.54	94.77	o

12	3	4	57.10	94.36	90.69	o
13	3	4	202.54	213.51	105.35	o
14	3	4	9.81	12.64	126.45	o
15	3	4	440.04	397.23	165.69	o
0	4	4	1272.18	1341.07	94.04	o
1	4	4	143.97	226.56	65.60	o
2	4	4	31.10	27.61	44.15	o
3	4	4	33.05	38.59	47.69	o
4	4	4	266.55	287.25	49.27	o
5	4	4	2897.07	2997.95	117.56	o
6	4	4	78.07	92.12	52.88	o
7	4	4	1.56	13.82	45.65	o
8	4	4	29.41	34.73	43.68	o
9	4	4	1935.33	1848.23	93.87	o
10	4	4	39.75	61.27	81.71	o
11	4	4	26.95	11.39	82.45	o
12	4	4	8.08	11.44	95.14	o
13	4	4	461.70	412.82	117.48	o
14	4	4	8.50	91.97	100.53	o
15	4	4	1247.10	1349.95	155.30	o
16	4	4	51.06	14.92	149.22	o
1	5	4	2145.21	1466.39	179.02	o
2	5	4	2194.23	1780.82	195.66	o
3	5	4	3912.88	3784.43	244.88	o
4	5	4	1.90	11.38	56.86	o
5	5	4	1812.91	1753.19	97.36	o
6	5	4	833.66	930.00	88.53	o
7	5	4	1995.25	2094.12	152.77	o
8	5	4	271.99	158.35	79.71	o
9	5	4	11.25	21.82	77.17	o
10	5	4	5979.02	5795.96	223.74	o
11	5	4	2635.46	2504.68	128.60	o
12	5	4	53.55	66.30	77.14	o
13	5	4	2030.82	1929.71	166.34	o
14	5	4	53.60	46.90	78.54	o
15	5	4	2410.43	2590.96	146.57	o
16	5	4	9.61	97.78	102.27	o
4	6	4	5056.25	4105.32	259.52	o
5	6	4	178.60	153.63	91.69	o
6	6	4	185.28	173.65	99.67	o
7	6	4	14.77	13.03	92.13	o
8	6	4	2401.31	2224.68	258.19	o
9	6	4	4363.28	3930.06	164.02	o
10	6	4	120.64	94.13	82.74	o
11	6	4	4656.18	4735.58	308.55	o
12	6	4	1560.85	1649.77	117.56	o
13	6	4	1246.03	1212.72	109.50	o
14	6	4	91.07	20.40	87.22	o
15	6	4	4.19	9.26	124.63	o
6	7	4	2.58	32.57	123.07	o
7	7	4	2.30	12.95	129.50	o
8	7	4	76.60	176.51	183.28	o
9	7	4	387.42	444.30	117.44	o
10	7	4	641.31	539.33	105.65	o
11	7	4	1854.09	1663.06	117.07	o

12	7	4	5.07	28.46	83.25	o
13	7	4	30.53	16.29	114.28	o
1	1	5	110.68	136.16	35.02	o
2	1	5	2.40	23.03	33.48	o
3	1	5	351.08	328.68	39.88	o
4	1	5	225.91	243.32	37.37	o
5	1	5	687.94	688.65	46.95	o
6	1	5	1519.23	1609.62	73.27	o
7	1	5	105.10	177.42	58.67	o
8	1	5	423.14	385.06	64.20	o
9	1	5	133.46	126.00	67.16	o
10	1	5	18.79	32.11	135.09	o
11	1	5	60.96	113.79	130.29	o
0	2	5	131.56	101.67	52.24	o
1	2	5	301.44	339.08	39.46	o
2	2	5	1739.40	1643.27	58.19	o
3	2	5	62.08	41.88	35.65	o
4	2	5	5090.48	5222.77	109.01	o
5	2	5	0.13	25.83	36.53	o
6	2	5	340.83	427.65	51.84	o
7	2	5	315.30	327.19	55.55	o
8	2	5	496.10	461.32	92.06	o
9	2	5	2196.14	2189.57	133.71	o
10	2	5	98.65	152.37	79.54	o
11	2	5	2689.97	3067.53	271.97	o
12	2	5	1217.88	1472.95	214.37	o
13	2	5	2139.24	2412.72	254.07	o
1	3	5	1784.58	1824.50	67.87	o
2	3	5	1986.55	2018.18	74.40	o
3	3	5	4263.92	4127.07	91.62	o
4	3	5	0.11	32.61	44.70	o
5	3	5	74.16	104.25	46.47	o
6	3	5	3359.17	3854.13	194.69	o
7	3	5	40.74	76.26	54.68	o
8	3	5	1255.14	1239.01	75.67	o
9	3	5	1.28	36.77	57.08	o
10	3	5	13259.66	12913.09	444.29	o
11	3	5	623.50	661.48	173.37	o
12	3	5	1478.22	1481.97	220.85	o
13	3	5	449.17	376.77	178.28	o
0	4	5	497.25	421.90	84.99	o
1	4	5	111.48	106.43	45.05	o
2	4	5	1093.98	1146.61	89.58	o
3	4	5	7.73	41.30	62.83	o
4	4	5	1108.43	1197.92	93.30	o
5	4	5	6.67	13.96	56.89	o
6	4	5	103.66	79.70	60.82	o
7	4	5	176.09	106.85	65.34	o
8	4	5	34.54	46.73	53.36	o
9	4	5	1187.22	1293.34	143.90	o
10	4	5	6.99	69.31	89.75	o
11	4	5	1344.73	1430.42	171.15	o
12	4	5	179.85	56.16	93.69	o
13	4	5	1753.25	2285.85	279.28	o
2	5	5	255.16	280.86	144.06	o

3	5	5	69.51	146.64	66.64	o
4	5	5	38.04	38.84	65.46	o
5	5	5	138.43	131.30	66.51	o
6	5	5	612.45	632.53	82.35	o
7	5	5	445.96	398.20	92.99	o
8	5	5	29.18	17.49	87.69	o
9	5	5	253.65	188.67	95.50	o
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8	3	6	23.28	60.86	69.50	o
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 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
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 used when they are defined by crystal symmetry.  An approximate (isotropic)
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loop_
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   2   2   0        0.12        4.23     12.43 o
   4   2   0    14666.73    11584.77    452.82 o
   6   2   0      225.55      236.81     24.71 o
   8   2   0     1092.32     1093.09    183.35 o
  10   2   0      626.68      523.43     61.98 o
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   2   3   0      719.66      916.40     68.23 o
   4   3   0     1126.11     1201.88     37.83 o
   6   3   0     1641.15     1763.71     66.86 o
   8   3   0       12.93        8.67     27.85 o
  10   3   0      782.79      796.26     62.21 o
  12   3   0      500.11      503.97     74.36 o
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5	3	3	2934.57	2855.12	75.13	o
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
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 are estimated using the full covariance matrix.  The cell esds are taken
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 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
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   2   2   0        0.12        6.41     10.85 o
   6   2   0      232.32      251.40     21.48 o
   8   2   0     1207.74     1287.07     95.64 o
  12   2   0       86.23        6.80     67.98 o
   2   3   0      628.08      842.31     64.97 o
   4   3   0     1219.82     1316.28     92.68 o
   6   3   0     1652.38     1980.57     86.46 o
   8   3   0       17.08        6.26     25.44 o
  10   3   0      992.35      971.00     65.72 o
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4	1	1	2596.12	2768.64	36.68	o
0	2	1	51.53	37.16	16.93	o
3	2	1	9034.93	8683.93	157.96	o
4	2	1	8295.19	7750.73	108.07	o
5	2	1	7915.77	7444.63	163.25	o
6	2	1	236.37	229.51	11.56	o
7	2	1	2494.69	2682.33	43.43	o
8	2	1	3224.38	3287.57	63.76	o
9	2	1	17.69	29.71	15.09	o
11	2	1	341.32	74.87	73.95	o
1	3	1	12758.69	10206.62	204.93	o
2	3	1	2515.99	2048.22	150.89	o
3	3	1	2536.79	3266.76	65.36	o
4	3	1	1205.35	1477.46	31.79	o
5	3	1	8085.24	8526.24	152.85	o
7	3	1	150.01	143.90	18.26	o
8	3	1	4526.64	4389.91	66.60	o
9	3	1	7621.42	7659.47	79.78	o
10	3	1	24568.58	22698.97	494.04	o
11	3	1	24826.57	22622.42	574.37	o
14	3	1	9.10	30.76	57.42	o
15	3	1	316.40	7.75	77.47	o
3	4	1	839.69	812.11	53.86	o
4	4	1	1289.65	1271.67	49.23	o
5	4	1	4036.48	4154.40	86.80	o

6	4	1	542.93	539.33	26.66	o
7	4	1	1027.58	953.98	37.25	o
8	4	1	267.51	296.18	37.57	o
9	4	1	138.01	129.37	34.13	o
10	4	1	136.56	177.81	33.77	o
11	4	1	49.69	42.75	38.03	o
12	4	1	13.18	19.52	39.63	o
13	4	1	157.15	107.42	51.10	o
14	4	1	525.37	422.12	192.00	o
15	4	1	2.79	59.10	54.91	o
17	4	1	290.64	11.64	116.42	o
4	5	1	1025.10	880.97	208.64	o
5	5	1	1354.42	1323.51	105.77	o
6	5	1	236.38	253.04	39.82	o
7	5	1	882.07	937.66	48.77	o
8	5	1	529.28	542.33	43.71	o
9	5	1	318.51	246.97	44.76	o
10	5	1	61.09	59.53	56.26	o
11	5	1	78.10	128.32	50.21	o
12	5	1	5.59	11.54	62.74	o
13	5	1	4.20	19.84	68.53	o
14	5	1	2506.32	2188.42	101.72	o
15	5	1	160.94	103.66	61.02	o
16	5	1	221.53	79.86	83.30	o
17	5	1	0.34	23.41	64.48	o
18	5	1	17.92	59.66	66.77	o
19	5	1	10.14	10.87	108.67	o
5	6	1	0.70	11.97	82.98	o
6	6	1	171.80	164.13	75.59	o
7	6	1	45.98	54.94	44.60	o
8	6	1	92.91	94.89	54.08	o
9	6	1	55.66	48.28	62.61	o
10	6	1	65.17	35.06	113.34	o
11	6	1	250.31	294.07	143.17	o
12	6	1	652.03	742.74	81.00	o
13	6	1	63.10	52.69	63.16	o
14	6	1	171.88	159.68	77.02	o
15	6	1	9.01	42.98	75.86	o
16	6	1	68.03	23.91	84.19	o
17	6	1	68.91	9.46	66.80	o
18	6	1	41.29	13.06	74.71	o
19	6	1	29.96	58.71	96.92	o
7	7	1	901.46	909.81	167.31	o
8	7	1	1245.84	1442.24	216.56	o
9	7	1	2389.11	2500.02	159.47	o
10	7	1	186.52	253.08	101.96	o
11	7	1	1023.01	1078.43	127.48	o
12	7	1	1161.31	1656.23	154.06	o
13	7	1	154.13	193.88	90.54	o
14	7	1	25.97	60.31	83.04	o
15	7	1	371.44	369.41	91.63	o
16	7	1	547.74	483.31	95.95	o
17	7	1	0.07	59.25	79.75	o
18	7	1	1.93	18.84	131.37	o
9	8	1	1.98	62.82	103.11	o

10	8	1	131.66	94.40	105.23	o
11	8	1	12.92	55.93	108.11	o
12	8	1	221.07	292.90	120.07	o
13	8	1	1306.50	1707.27	183.28	o
14	8	1	20.34	27.63	83.57	o
15	8	1	923.76	1017.96	198.93	o
16	8	1	823.81	1176.31	249.99	o
11	9	1	4802.63	5791.75	380.17	o
12	9	1	5273.57	6094.13	265.48	o
13	9	1	404.31	442.83	143.41	o
0	0	2	994.22	939.78	33.19	o
1	0	2	830.52	744.49	21.61	o
3	0	2	2642.68	1928.16	47.51	o
4	0	2	1738.87	1826.42	61.87	o
5	0	2	23849.22	23453.71	585.71	o
6	0	2	147.78	179.73	64.99	o
7	0	2	4757.51	4643.49	171.82	o
1	1	2	2.62	8.27	7.75	o
2	1	2	206.24	238.07	12.12	o
3	1	2	789.07	682.64	14.23	o
4	1	2	787.12	1009.47	31.53	o
5	1	2	5715.24	6163.54	148.54	o
6	1	2	946.42	910.94	76.30	o
7	1	2	44.52	35.74	21.82	o
9	1	2	1511.29	1520.85	88.22	o
10	1	2	492.99	551.13	103.46	o
0	2	2	182.31	233.92	23.35	o
1	2	2	2.22	10.98	11.92	o
2	2	2	9.31	17.12	11.03	o
3	2	2	967.85	1058.71	32.04	o
4	2	2	535.22	623.33	23.22	o
5	2	2	57.25	42.91	12.80	o
6	2	2	3186.14	3408.39	61.32	o
7	2	2	3294.98	3134.38	104.97	o
8	2	2	1309.00	1240.25	86.02	o
11	2	2	169.48	116.73	52.13	o
12	2	2	269.76	168.46	91.95	o
1	3	2	97.36	108.62	33.21	o
2	3	2	0.28	7.94	23.21	o
3	3	2	622.55	689.51	26.91	o
4	3	2	576.07	580.42	20.16	o
5	3	2	651.67	645.83	21.76	o
6	3	2	177.57	169.39	16.42	o
7	3	2	268.68	336.50	26.59	o
8	3	2	306.41	357.11	28.50	o
9	3	2	112.75	89.40	30.78	o
10	3	2	40.94	41.88	33.09	o
11	3	2	163.59	111.86	42.08	o
12	3	2	22.00	32.09	38.11	o
13	3	2	10.58	22.82	43.39	o
14	3	2	0.95	8.81	62.08	o
15	3	2	57.27	50.45	116.37	o
1	4	2	1007.75	817.84	100.45	o
2	4	2	4552.30	4158.36	275.38	o
3	4	2	1696.86	1112.26	208.06	o

4	4	2	0.03	14.63	25.60	o
5	4	2	226.89	213.06	21.51	o
6	4	2	1735.98	1707.73	56.03	o
7	4	2	1097.47	1112.12	38.00	o
8	4	2	140.11	150.02	33.48	o
9	4	2	184.71	243.57	63.32	o
10	4	2	0.46	30.51	44.25	o
11	4	2	4.18	28.24	53.04	o
12	4	2	116.84	127.86	46.48	o
13	4	2	208.85	144.86	76.10	o
14	4	2	469.48	262.00	158.58	o
15	4	2	138.23	58.99	59.05	o
16	4	2	95.46	32.16	74.25	o
3	5	2	10331.78	9533.79	275.37	o
4	5	2	301.01	199.25	52.31	o
5	5	2	1466.70	1591.57	50.78	o
6	5	2	3.15	22.48	34.31	o
7	5	2	326.50	352.71	43.67	o
8	5	2	8039.30	6991.92	248.39	o
9	5	2	6981.73	7188.42	184.17	o
10	5	2	270.30	368.27	53.27	o
11	5	2	1999.08	2211.58	69.52	o
12	5	2	7773.11	7968.22	139.94	o
13	5	2	327.21	302.88	92.65	o
14	5	2	222.88	62.84	59.24	o
15	5	2	635.85	321.13	183.94	o
16	5	2	640.05	329.68	260.38	o
18	5	2	510.44	408.09	369.32	o
5	6	2	5062.99	4520.10	228.98	o
6	6	2	0.28	89.46	74.47	o
7	6	2	1704.85	1591.88	75.23	o
8	6	2	556.40	536.10	57.09	o
9	6	2	7955.44	8310.16	283.87	o
10	6	2	899.07	954.17	80.39	o
11	6	2	8045.85	8684.63	578.24	o
13	6	2	223.51	160.63	62.71	o
14	6	2	0.09	16.95	83.69	o
15	6	2	83.89	87.00	69.03	o
16	6	2	78.76	41.99	66.07	o
17	6	2	345.43	234.46	119.25	o
18	6	2	245.08	279.14	76.44	o
19	6	2	60.72	23.19	231.86	o
8	7	2	2261.72	1887.35	258.14	o
9	7	2	4.84	28.67	64.63	o
10	7	2	8.91	28.80	68.49	o
11	7	2	215.36	161.56	81.93	o
12	7	2	3012.19	3359.91	189.42	o
13	7	2	502.94	719.12	93.49	o
14	7	2	1.95	90.62	84.92	o
15	7	2	186.22	157.21	90.75	o
16	7	2	284.26	277.39	94.76	o
17	7	2	494.02	406.16	209.46	o
10	8	2	49.86	17.50	174.98	o
11	8	2	3.73	198.23	162.93	o
12	8	2	1.49	16.02	113.28	o

13	8	2	637.54	651.27	106.65	o
14	8	2	119.72	181.13	91.25	o
15	8	2	591.33	663.50	154.96	o
1	1	3	35.58	48.07	12.87	o
2	1	3	747.69	842.47	20.67	o
4	1	3	0.22	9.15	13.47	o
5	1	3	189.00	165.94	18.89	o
6	1	3	1802.48	1930.99	45.17	o
7	1	3	1228.98	1261.37	47.33	o
8	1	3	20.37	37.99	26.38	o
9	1	3	1310.94	1305.79	153.02	o
10	1	3	865.61	789.57	122.97	o
11	1	3	82.16	236.66	127.23	o
0	2	3	18366.90	17338.55	465.82	o
1	2	3	12184.72	11772.63	241.13	o
2	2	3	55.31	69.99	15.66	o
3	2	3	200.63	246.15	22.07	o
4	2	3	1054.78	1088.14	28.24	o
5	2	3	1425.42	1414.37	33.61	o
6	2	3	417.47	523.32	29.47	o
7	2	3	5393.52	5605.63	136.80	o
8	2	3	189.78	198.11	28.31	o
9	2	3	716.23	680.51	69.40	o
10	2	3	710.01	630.49	125.31	o
11	2	3	195.60	153.89	75.65	o
12	2	3	933.98	1117.76	154.48	o
13	2	3	2831.65	3088.99	226.31	o
1	3	3	33299.63	31008.04	754.06	o
2	3	3	1322.46	1243.59	84.94	o
3	3	3	113.19	118.28	25.46	o
4	3	3	697.66	714.05	28.90	o
5	3	3	3002.73	2896.99	66.44	o
7	3	3	2380.09	2612.88	88.92	o
8	3	3	27.75	47.31	33.62	o
9	3	3	1056.14	1041.57	62.58	o
10	3	3	2690.07	2635.41	102.59	o
11	3	3	172.06	79.96	56.38	o
12	3	3	671.45	520.94	235.75	o
14	3	3	4669.82	5327.35	445.72	o
15	3	3	2723.61	1606.69	184.07	o
0	4	3	9295.16	7893.82	265.32	o
1	4	3	3975.12	3920.05	97.89	o
2	4	3	124.78	147.52	44.57	o
3	4	3	3091.41	2984.24	72.30	o
4	4	3	1357.12	1256.12	48.42	o
5	4	3	996.69	946.80	47.81	o
6	4	3	156.93	191.87	32.46	o
7	4	3	1218.59	1207.85	45.18	o
8	4	3	12.95	23.50	43.07	o
9	4	3	1893.75	1728.81	81.93	o
10	4	3	595.20	612.64	80.94	o
11	4	3	194.99	146.44	86.20	o
12	4	3	415.64	441.39	128.43	o
13	4	3	549.42	536.57	241.70	o
14	4	3	91.91	86.10	65.02	o

15	4	3	529.71	386.26	164.39	o
16	4	3	3.14	12.94	91.45	o
2	5	3	813.14	614.94	126.17	o
3	5	3	3818.03	3539.50	160.84	o
4	5	3	221.18	170.82	62.00	o
5	5	3	41.41	25.26	40.80	o
6	5	3	635.99	637.70	59.77	o
7	5	3	212.11	241.83	58.01	o
8	5	3	53.18	59.67	54.90	o
9	5	3	786.55	784.65	86.45	o
10	5	3	148.66	176.22	60.35	o
11	5	3	51.10	35.16	53.62	o
12	5	3	25.63	29.74	55.68	o
13	5	3	154.63	111.46	66.81	o
14	5	3	97.45	51.45	61.00	o
16	5	3	39.87	39.36	80.52	o
17	5	3	290.97	246.92	126.25	o
18	5	3	71.39	79.92	162.84	o
4	6	3	195.98	163.79	127.51	o
5	6	3	142.05	108.63	93.71	o
6	6	3	21.26	36.41	78.24	o
7	6	3	28.49	46.20	71.85	o
8	6	3	122.29	119.90	70.12	o
9	6	3	52.98	25.07	69.23	o
10	6	3	126.34	132.19	77.40	o
11	6	3	397.12	392.54	67.08	o
12	6	3	3.17	89.58	86.12	o
13	6	3	0.06	14.59	64.62	o
14	6	3	15.02	12.56	65.20	o
15	6	3	0.03	39.03	69.09	o
16	6	3	90.34	28.36	72.62	o
17	6	3	296.77	98.96	120.71	o
7	7	3	1008.12	834.49	159.14	o
8	7	3	159.42	91.46	123.32	o
9	7	3	405.13	473.72	93.25	o
10	7	3	1087.52	1125.10	110.78	o
11	7	3	447.74	439.47	91.74	o
12	7	3	6.54	52.45	71.98	o
13	7	3	1723.61	1687.21	141.03	o
14	7	3	950.05	977.93	296.08	o
15	7	3	21.72	14.32	124.42	o
11	8	3	788.35	810.36	356.06	o
12	8	3	444.61	432.77	108.37	o
13	8	3	2548.98	3141.64	910.34	o
0	0	4	958.17	1076.02	58.62	o
1	0	4	14967.41	14348.58	225.77	o
2	0	4	2894.17	2877.88	51.55	o
3	0	4	1496.87	1622.15	59.94	o
4	0	4	10480.25	10123.49	218.54	o
5	0	4	1.57	23.52	32.99	o
6	0	4	503.76	470.60	49.96	o
7	0	4	245.43	206.50	47.18	o
8	0	4	3367.88	3402.91	164.92	o
9	0	4	3980.69	3273.50	219.32	o
1	1	4	3868.45	3921.43	68.62	o

2	1	4	93.63	117.86	20.72	o
3	1	4	1299.60	1475.93	34.17	o
4	1	4	35.78	28.38	24.91	o
5	1	4	4305.59	4545.73	71.29	o
6	1	4	1296.23	1430.60	54.44	o
7	1	4	2473.42	2289.97	115.77	o
8	1	4	360.29	420.51	51.53	o
9	1	4	152.33	95.08	70.61	o
10	1	4	4936.19	5280.53	267.05	o
11	1	4	1803.51	1927.57	207.85	o
0	2	4	114.51	83.82	35.23	o
1	2	4	598.67	586.54	30.30	o
2	2	4	21.57	35.11	24.32	o
3	2	4	83.23	63.30	27.69	o
4	2	4	109.43	114.23	35.33	o
5	2	4	2762.74	2822.89	112.36	o
6	2	4	52.65	44.11	33.42	o
7	2	4	1026.40	1060.85	48.24	o
8	2	4	1552.72	1879.71	167.40	o
9	2	4	15.81	68.51	54.91	o
10	2	4	0.13	43.38	58.51	o
11	2	4	0.21	11.09	110.88	o
12	2	4	0.57	10.90	109.03	o
13	2	4	43.34	50.22	124.24	o
1	3	4	18.05	30.52	35.77	o
2	3	4	15.48	32.79	38.02	o
3	3	4	155.81	118.54	38.18	o
4	3	4	18.96	28.29	35.32	o
5	3	4	147.69	131.41	38.00	o
6	3	4	238.02	232.89	40.41	o
7	3	4	175.60	208.98	51.18	o
8	3	4	0.30	16.77	61.88	o
9	3	4	197.40	362.35	162.75	o
10	3	4	12.02	37.13	56.88	o
11	3	4	298.11	310.12	94.95	o
12	3	4	69.85	89.24	90.55	o
13	3	4	165.18	107.13	98.46	o
14	3	4	2.62	109.77	126.11	o
15	3	4	418.51	274.05	149.88	o
0	4	4	1241.02	1256.23	94.53	o
1	4	4	145.99	194.67	66.78	o
2	4	4	51.90	29.00	45.36	o
3	4	4	25.63	79.13	50.26	o
4	4	4	332.82	326.58	56.62	o
5	4	4	2954.42	2773.63	150.21	o
6	4	4	124.79	132.14	59.19	o
7	4	4	1.02	25.19	47.48	o
8	4	4	31.87	64.61	48.29	o
9	4	4	1925.72	1891.49	105.49	o
10	4	4	49.70	37.04	77.22	o
11	4	4	42.92	9.07	78.38	o
12	4	4	1.35	26.47	92.50	o
13	4	4	364.48	179.66	112.09	o
14	4	4	2.72	13.65	96.53	o
15	4	4	1087.59	1227.79	190.59	o

16	4	4	38.64	63.29	148.44	o
2	5	4	2170.15	1671.11	189.96	o
3	5	4	4057.06	3892.77	449.07	o
4	5	4	4.84	63.07	60.12	o
5	5	4	2016.32	2060.77	112.10	o
6	5	4	722.63	796.14	97.61	o
7	5	4	1963.14	2112.26	151.51	o
8	5	4	378.73	287.96	87.72	o
9	5	4	0.48	12.32	73.41	o
10	5	4	5808.85	5631.66	151.27	o
11	5	4	2249.81	2256.60	120.89	o
12	5	4	89.25	26.41	71.82	o
13	5	4	1791.67	1919.23	151.97	o
14	5	4	33.60	21.58	76.91	o
15	5	4	2070.13	2693.31	190.00	o
16	5	4	10.16	91.71	104.08	o
4	6	4	5008.14	4395.09	265.82	o
5	6	4	138.69	101.81	98.77	o
6	6	4	212.69	264.68	143.06	o
7	6	4	1.60	12.93	91.34	o
8	6	4	2006.87	1775.01	154.48	o
9	6	4	4494.45	4479.79	302.99	o
10	6	4	148.81	147.38	88.66	o
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12	6	4	1422.88	1457.04	113.23	o
13	6	4	1186.85	1105.64	107.56	o
14	6	4	105.94	40.20	84.15	o
6	7	4	9.58	11.51	115.13	o
7	7	4	0.49	97.33	127.47	o
8	7	4	104.99	196.95	167.05	o
9	7	4	335.26	361.16	222.55	o
10	7	4	750.76	643.98	107.76	o
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1	1	5	104.04	122.12	34.54	o
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4	1	5	188.81	169.66	37.00	o
5	1	5	803.61	877.73	79.24	o
6	1	5	1428.55	1564.15	71.80	o
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9	1	5	129.69	123.17	70.14	o
10	1	5	15.03	11.66	116.63	o
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3	2	5	137.86	108.56	36.90	o
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5	2	5	15.41	54.71	35.14	o
6	2	5	317.54	400.18	52.17	o
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9	2	5	2024.71	2131.80	134.88	o

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6	3	5	3409.02	4050.88	176.42	o
7	3	5	31.35	23.95	55.04	o
8	3	5	1121.79	1148.70	76.25	o
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 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
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   2   2   0        0.03        9.59     10.34 o
   4   2   0    13308.84    11616.10    324.11 o
   6   2   0      274.59      272.34     22.33 o
  10   2   0      617.07      679.98     67.19 o
  12   2   0      131.13      170.11    107.75 o
   2   3   0      639.52      866.09     64.24 o
   4   3   0     1278.48     1423.21     88.07 o
   6   3   0     1770.67     1939.94     60.18 o
   8   3   0       11.63       31.35     27.19 o
  10   3   0     1193.35     1252.71     61.32 o
  12   3   0      590.50      547.66     64.31 o
  14   3   0     1434.95     1420.79    125.05 o
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   6   4   0      149.93      156.60     28.89 o
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12	3	1	13883.63	12614.31	454.56	o
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6	4	2	1675.84	1722.87	90.44	o
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_diffrn_ambient_temperature       293(2)
_cell_length_a                    17.916(3)
_cell_length_b                    8.5900(15)
_cell_length_c                    5.0726(4)
_cell_angle_alpha                 90.00
_cell_angle_beta                  90.00
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_cell_volume                      780.7(2)
_cell_formula_units_Z             8
_cell_measurement_temperature     293(2)
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_exptl_special_details
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_diffrn_reflns_limit_l_min        -6
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_reflns_number_total              560
_reflns_number_gt                 368
_reflns_threshold_expression      >2sigma(I)

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_computing_cell_refinement        ?
_computing_data_reduction         ?
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_computing_molecular_graphics     ?
_computing_publication_material   ?
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;
 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
;

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_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0662P)^2^+0.0000P] where P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     mixed
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_number_reflns          560
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Mg1 Mg 0.37631(11) 0.6571(2) 0.8548(3) 0.0063(6) Uani 1 1 d . . .
Mg2 Mg 0.37744(12) 0.4828(3) 0.3474(3) 0.0087(6) Uani 1 1 d . . .
O1A O 0.1818(2) 0.3400(5) 0.0214(6) 0.0063(9) Uiso 1 1 d . . .
O2A O 0.3098(2) 0.5093(5) 0.0312(6) 0.0072(10) Uiso 1 1 d . . .
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 _atom_site_aniso_U_33
 _atom_site_aniso_U_23
 _atom_site_aniso_U_13
 _atom_site_aniso_U_12
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SiB 0.0051(15) 0.0041(17) 0.0051(6) 0.0002(6) -0.0005(6) 0.0008(6)
Mg1 0.0086(18) 0.0045(19) 0.0058(8) -0.0006(8) -0.0014(8) 0.0001(8)
Mg2 0.017(2) 0.003(2) 0.0071(8) -0.0012(8) -0.0016(9) 0.0011(8)

_geom_special_details
;
 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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SiA O3A 1.653(4) 8_565 ?
SiA Mg2 2.740(3) . ?
SiA Mg1 3.090(2) 2_564 ?
SiA Mg2 3.199(3) 2_564 ?
SiA Mg1 3.228(3) 7_654 ?
SiB O2B 1.577(4) . ?
SiB O1B 1.600(5) . ?
SiB 03B 1.666(4) . ?
SiB 03B 1.669(3) 8_566 ?
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SiB Mg1 3.214(2) 5_667 ?
SiB Mg1 3.224(3) 4_646 ?
SiB Mg2 3.244(3) 8_566 ?
SiB Mg1 3.251(3) . ?
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Mg1 O1A 1.986(4) 2_565 ?
Mg1 O2B 2.000(4) . ?
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O1B Mg2 2.042(5) 5_666 ?
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SiB O1B Mg1 121.5(2) . 4_646 ?
Mg1 O1B Mg1 93.34(19) 5_667 4_646 ?
Mg2 O1B Mg1 97.10(19) 5_666 4_646 ?
SiB O2B Mg2 124.1(2) . . ?
SiB O2B Mg1 130.30(19) . . ?
Mg2 O2B Mg1 97.30(19) . . ?
SiB 03B SiB 124.4(2) . 8_565 ?
SiB 03B Mg2 111.22(17) . 8_566 ?
SiB 03B Mg2 124.2(2) 8_565 8_566 ?

_diffrn_measured_fraction_theta_max    0.577
_diffrn_reflns_theta_full              28.24
_diffrn_measured_fraction_theta_full   0.577
_refine_diff_density_max    0.899
_refine_diff_density_min   -0.595
_refine_diff_density_rms    0.152
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```
#
# h,k,l, Fc-squared, Fo-squared, sigma(Fo-squared) and status flag
#
data_enstatitep8.65
_shelx_title '  MgSiO3 (Pbca) at P=8.6 GPa in DBP DAC with 60 sec, 0.2∞-CPH'
_shelx_refln_list_code          4
_shelx_F_calc_maximum      159.49
_exptl_crystal_F_000       800.00
_reflns_d_resolution_high  0.7509

loop_
 _symmetry_equiv_pos_as_xyz
 'x, y, z'
 '-x+1/2, -y, z+1/2'
 'x+1/2, -y+1/2, -z'
 '-x, y+1/2, -z+1/2'
 '-x, -y, -z'
 'x-1/2, y, -z-1/2'
 '-x-1/2, y-1/2, z'
 'x, -y-1/2, z-1/2'

_cell_length_a    17.9164
_cell_length_b     8.5900
_cell_length_c     5.0726
_cell_angle_alpha  90.000
_cell_angle_beta   90.000
_cell_angle_gamma  90.000

_shelx_F_squared_multiplier     1.000

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
   2   1   0      137.92      181.94     10.51 o
   4   1   0      204.21      181.92     13.85 o
   8   1   0        0.06        5.05     50.46 o
   2   2   0        0.01        8.28     11.28 o
   4   2   0    13334.74    13208.12    134.03 o
   6   2   0      260.22      254.92     21.75 o
  10   2   0      628.47      696.63     68.54 o
  12   2   0      149.70      123.16    105.26 o
   2   3   0      605.52      723.40     61.78 o
   4   3   0     1369.53     1472.10     43.20 o
   6   3   0     1733.96     1970.01     67.20 o
   8   3   0       14.23        8.77     25.75 o
  10   3   0     1148.62     1115.42     59.76 o
  12   3   0      638.43      576.18     64.35 o
  14   3   0     1406.25     1218.82    121.22 o
   4   4   0     6406.25     7066.78    206.40 o
   6   4   0      150.49      148.88     29.65 o
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8	4	0	3385.11	3000.30	130.20	o
10	4	0	2486.18	2302.57	78.07	o
12	4	0	16.01	34.85	59.88	o
14	4	0	312.17	361.42	88.09	o
16	4	0	4026.68	4092.17	181.91	o
4	5	0	94.55	77.43	73.24	o
6	5	0	16797.96	17971.73	348.62	o
8	5	0	167.89	271.35	80.45	o
10	5	0	5560.93	5687.45	446.80	o
12	5	0	235.19	245.03	89.89	o
14	5	0	20907.32	18897.75	355.32	o
16	5	0	262.32	256.97	104.19	o
18	5	0	1474.62	1784.98	247.98	o
6	6	0	724.39	875.30	135.07	o
8	6	0	930.98	1231.63	157.50	o
10	6	0	1110.58	1357.28	183.47	o
12	6	0	6408.52	6798.29	207.94	o
14	6	0	906.63	676.24	120.91	o
16	6	0	1829.41	1723.05	148.55	o
18	6	0	126.16	182.81	119.43	o
8	7	0	254.67	94.42	132.48	o
10	7	0	5456.55	5186.30	278.96	o
12	7	0	533.38	594.61	179.50	o
14	7	0	1862.20	1839.55	275.78	o
16	7	0	189.56	260.51	101.67	o
18	7	0	7.77	20.95	160.11	o
10	8	0	1010.65	1032.80	193.00	o
12	8	0	19.25	14.84	148.40	o
14	8	0	62.17	21.44	95.44	o
16	8	0	754.00	907.94	217.17	o
12	9	0	252.87	408.90	214.79	o
14	9	0	1245.44	1158.69	234.45	o
1	1	1	355.79	374.61	10.53	o
2	1	1	329.16	286.33	8.27	o
3	1	1	22.26	37.24	4.76	o
4	1	1	2608.41	2658.25	34.72	o
5	1	1	5237.22	5211.99	85.78	o
6	1	1	1324.67	1128.88	33.89	o
7	1	1	2294.49	1956.99	162.26	o
8	1	1	1477.60	1444.94	74.66	o
9	1	1	460.12	475.32	61.19	o
0	2	1	67.91	50.02	18.39	o
1	2	1	5499.51	5447.60	194.58	o
4	2	1	8541.41	8178.66	134.58	o
6	2	1	266.89	237.76	12.10	o
7	2	1	2319.77	2600.78	76.33	o
8	2	1	3248.80	3353.92	78.16	o
9	2	1	57.03	48.65	15.88	o
10	2	1	699.78	777.78	50.69	o
11	2	1	363.59	339.75	58.59	o
12	2	1	929.09	818.06	88.82	o
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2	3	1	2554.19	1999.30	137.40	o
3	3	1	2599.41	3538.76	115.27	o
4	3	1	1162.79	1455.31	34.62	o

5	3	1	7832.59	8662.64	122.05	o
7	3	1	191.32	199.66	19.00	o
8	3	1	4459.69	4299.69	97.06	o
9	3	1	7546.66	7539.16	74.51	o
10	3	1	25416.83	23610.54	518.42	o
11	3	1	25438.21	23653.59	165.28	o
12	3	1	14167.85	13054.96	324.70	o
13	3	1	1619.76	1679.66	87.22	o
14	3	1	0.83	64.61	66.45	o
15	3	1	517.58	912.65	192.94	o
3	4	1	911.80	872.47	54.90	o
4	4	1	1343.61	1356.18	46.13	o
5	4	1	3968.59	3975.30	78.28	o
6	4	1	522.98	562.48	29.99	o
7	4	1	1069.45	997.02	38.81	o
8	4	1	230.33	277.42	34.04	o
9	4	1	145.01	165.57	34.74	o
10	4	1	194.07	225.14	33.61	o
11	4	1	54.89	49.78	36.89	o
12	4	1	10.81	51.98	38.86	o
13	4	1	201.40	163.89	48.25	o
14	4	1	592.24	687.70	73.56	o
15	4	1	0.03	31.92	74.08	o
17	4	1	340.23	164.21	204.54	o
4	5	1	1064.53	1098.27	92.11	o
5	5	1	1275.88	1239.24	165.70	o
6	5	1	230.62	204.61	40.41	o
7	5	1	794.92	837.84	47.31	o
8	5	1	534.25	578.70	45.33	o
9	5	1	293.38	247.94	44.62	o
10	5	1	39.97	61.18	50.46	o
11	5	1	107.59	71.31	47.43	o
12	5	1	2.24	24.79	55.34	o
13	5	1	0.61	36.94	61.80	o
14	5	1	2391.65	2078.85	102.55	o
15	5	1	148.85	105.63	62.06	o
16	5	1	213.91	135.32	86.41	o
17	5	1	0.09	12.59	84.61	o
18	5	1	9.11	42.37	87.91	o
19	5	1	1.02	103.12	208.65	o
5	6	1	1.74	41.22	107.35	o
6	6	1	208.34	256.74	82.12	o
7	6	1	23.34	13.94	44.77	o
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9	6	1	61.18	21.39	64.49	o
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11	6	1	282.01	399.91	118.21	o
12	6	1	625.94	520.22	75.27	o
13	6	1	43.90	54.53	57.35	o
14	6	1	136.32	122.46	66.57	o
15	6	1	14.68	21.17	65.89	o
16	6	1	78.90	51.69	79.37	o
17	6	1	78.21	91.83	92.91	o
18	6	1	84.18	42.34	100.67	o
19	6	1	35.52	15.97	112.95	o

7	7	1	993.80	984.04	176.19	o
8	7	1	1109.51	1364.96	133.05	o
9	7	1	2481.32	2621.73	162.36	o
10	7	1	169.33	293.24	108.03	o
11	7	1	1239.97	1426.48	138.50	o
12	7	1	1264.02	1402.45	170.75	o
13	7	1	176.22	161.88	80.23	o
14	7	1	31.96	16.95	71.62	o
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16	7	1	631.95	614.95	91.66	o
17	7	1	6.46	25.14	76.31	o
9	8	1	0.22	112.23	174.16	o
10	8	1	90.41	179.99	115.08	o
11	8	1	39.64	129.60	137.60	o
12	8	1	279.13	456.84	125.49	o
13	8	1	1326.39	1605.35	164.61	o
14	8	1	41.96	52.94	78.57	o
15	8	1	1051.76	1041.99	242.73	o
12	9	1	5424.43	6073.87	268.63	o
13	9	1	345.38	389.90	157.17	o
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3	0	2	2389.67	1788.62	60.24	o
4	0	2	2063.43	2105.84	45.47	o
5	0	2	23717.84	24954.05	342.58	o
6	0	2	96.80	130.04	66.19	o
7	0	2	4415.32	4080.07	163.54	o
1	1	2	0.04	7.04	7.99	o
2	1	2	235.54	275.38	12.54	o
3	1	2	869.37	751.08	14.91	o
4	1	2	787.49	991.68	22.24	o
5	1	2	5700.96	6312.14	126.29	o
6	1	2	1082.47	1124.93	35.43	o
7	1	2	48.93	60.32	26.53	o
8	1	2	6240.08	5936.71	298.85	o
9	1	2	1583.57	1750.87	142.59	o
10	1	2	653.45	639.91	109.90	o
0	2	2	202.32	272.34	25.00	o
1	2	2	4.58	14.84	12.38	o
2	2	2	6.82	10.67	11.72	o
3	2	2	928.68	1031.83	31.37	o
4	2	2	576.78	657.10	20.48	o
5	2	2	63.90	63.14	12.26	o
6	2	2	3212.48	3421.87	41.60	o
7	2	2	3188.49	3216.64	58.80	o
8	2	2	1477.66	1479.08	46.23	o
9	2	2	1615.49	1538.63	67.04	o
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12	2	2	377.19	345.67	65.98	o
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2	3	2	0.44	15.48	24.10	o
3	3	2	533.20	617.48	25.73	o
4	3	2	501.72	526.30	19.59	o
5	3	2	609.52	634.47	21.09	o

6	3	2	205.18	207.33	17.63	o
7	3	2	319.62	331.89	24.91	o
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15	3	2	46.59	11.72	117.22	o
1	4	2	1012.50	865.72	103.13	o
2	4	2	4543.64	4413.28	322.90	o
4	4	2	0.82	21.88	26.77	o
5	4	2	234.44	219.23	22.34	o
6	4	2	1731.57	1691.80	76.27	o
7	4	2	1028.64	1025.33	44.17	o
8	4	2	128.53	119.51	31.86	o
9	4	2	194.87	149.51	50.80	o
10	4	2	3.42	29.26	42.07	o
11	4	2	0.66	44.89	49.06	o
12	4	2	146.71	178.74	51.66	o
13	4	2	260.76	314.32	66.93	o
14	4	2	546.22	526.39	76.98	o
15	4	2	136.93	173.48	78.16	o
16	4	2	88.44	44.21	93.71	o
17	4	2	181.95	14.29	142.88	o
3	5	2	10482.85	9363.07	275.08	o
4	5	2	397.69	302.43	68.54	o
5	5	2	1518.36	1641.96	67.07	o
6	5	2	0.32	26.62	36.32	o
7	5	2	322.71	333.18	44.76	o
8	5	2	8205.47	7587.32	222.28	o
9	5	2	6698.45	6937.98	186.17	o
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11	5	2	1974.64	2040.52	78.41	o
12	5	2	7858.02	7805.10	270.51	o
13	5	2	323.87	255.19	70.05	o
14	5	2	236.38	204.23	68.50	o
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16	5	2	804.77	923.73	113.45	o
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18	5	2	712.15	892.12	161.89	o
5	6	2	5427.77	4762.53	238.00	o
6	6	2	1.05	89.68	70.61	o
7	6	2	1811.37	1746.31	112.58	o
8	6	2	537.55	623.73	60.33	o
9	6	2	7952.39	7873.40	427.00	o
10	6	2	858.85	938.30	84.31	o
11	6	2	8592.08	8733.47	378.20	o
13	6	2	293.81	179.54	70.37	o
14	6	2	5.51	106.40	74.68	o
15	6	2	74.86	154.07	75.74	o
16	6	2	64.54	35.69	73.40	o
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18	6	2	366.19	334.77	113.82	o

19	6	2	40.94	23.46	234.58	o
8	7	2	2212.29	1952.40	313.73	o
9	7	2	5.36	9.72	69.40	o
10	7	2	14.91	120.20	75.84	o
11	7	2	208.15	175.07	95.14	o
12	7	2	3086.37	3984.84	733.09	o
13	7	2	480.78	423.80	91.01	o
14	7	2	9.06	33.40	77.59	o
15	7	2	219.58	147.21	83.97	o
16	7	2	362.42	337.25	89.90	o
17	7	2	676.62	719.58	179.35	o
10	8	2	39.72	19.06	190.62	o
11	8	2	4.53	205.69	171.50	o
12	8	2	11.09	15.49	120.50	o
13	8	2	514.21	448.10	99.93	o
14	8	2	118.51	110.62	80.85	o
15	8	2	610.73	710.56	162.53	o
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2	1	3	737.94	787.59	20.16	o
3	1	3	4048.96	4030.51	72.19	o
4	1	3	0.14	17.77	14.49	o
5	1	3	176.31	183.76	19.99	o
6	1	3	1785.71	1811.29	45.20	o
7	1	3	1310.31	1274.30	60.28	o
8	1	3	23.63	38.57	26.62	o
9	1	3	1419.04	1391.01	156.92	o
10	1	3	803.50	766.14	128.84	o
11	1	3	87.23	211.84	126.76	o
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2	2	3	74.40	77.04	15.84	o
3	2	3	250.92	265.07	22.75	o
4	2	3	1052.39	1126.33	30.69	o
5	2	3	1441.74	1440.75	33.83	o
6	2	3	432.57	494.93	30.30	o
7	2	3	5920.54	6178.78	156.56	o
8	2	3	197.50	228.09	31.34	o
9	2	3	664.42	687.46	45.61	o
10	2	3	788.21	889.53	66.70	o
11	2	3	256.44	134.99	77.25	o
12	2	3	916.53	984.82	152.58	o
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2	3	3	1061.38	963.91	93.04	o
3	3	3	102.14	90.59	25.46	o
4	3	3	700.10	695.19	29.02	o
5	3	3	3200.48	3129.31	93.34	o
6	3	3	4740.96	4684.90	169.54	o
7	3	3	2520.72	2640.16	78.17	o
8	3	3	35.87	67.05	33.93	o
9	3	3	1226.35	1221.86	64.33	o
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12	3	3	664.21	713.84	86.61	o
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2	4	3	143.25	149.33	45.30	o
3	4	3	3216.77	3018.34	73.70	o
4	4	3	1287.12	1234.60	48.29	o
5	4	3	991.35	983.37	44.00	o
6	4	3	152.69	173.68	33.06	o
7	4	3	1305.13	1255.96	46.39	o
8	4	3	8.75	34.88	41.21	o
9	4	3	1949.24	1840.18	85.52	o
10	4	3	652.73	630.74	78.12	o
11	4	3	196.94	167.72	80.42	o
12	4	3	445.42	563.30	87.75	o
13	4	3	588.35	678.93	92.83	o
14	4	3	111.33	146.89	83.75	o
15	4	3	653.45	579.44	123.50	o
16	4	3	13.68	83.90	92.36	o
2	5	3	702.07	520.12	128.92	o
3	5	3	3822.38	3408.55	164.56	o
4	5	3	269.88	281.59	66.54	o
5	5	3	37.98	19.20	39.76	o
6	5	3	631.85	664.74	61.34	o
7	5	3	211.53	185.27	59.20	o
8	5	3	63.55	33.23	67.88	o
9	5	3	819.03	882.43	92.80	o
10	5	3	129.02	120.71	61.94	o
11	5	3	91.42	65.02	55.34	o
12	5	3	20.43	18.07	55.50	o
13	5	3	116.30	134.26	63.08	o
14	5	3	59.66	37.13	68.11	o
16	5	3	52.10	9.67	91.04	o
17	5	3	284.21	378.34	98.93	o
4	6	3	200.32	12.15	121.47	o
5	6	3	193.11	219.83	129.90	o
6	6	3	21.21	9.06	83.50	o
7	6	3	23.21	53.41	77.26	o
8	6	3	71.25	77.72	71.95	o
9	6	3	23.18	14.08	72.84	o
10	6	3	157.49	161.50	91.03	o
11	6	3	390.37	438.49	67.78	o
12	6	3	2.16	14.37	64.03	o
13	6	3	0.08	41.87	65.97	o
14	6	3	8.80	64.52	69.87	o
15	6	3	2.48	13.75	72.41	o
16	6	3	71.31	58.78	89.57	o
17	6	3	406.49	195.00	147.32	o
7	7	3	1074.65	934.26	167.52	o
8	7	3	192.25	76.38	132.23	o
9	7	3	488.56	612.12	99.75	o
10	7	3	959.43	1011.10	127.83	o
11	7	3	541.33	627.46	100.86	o
12	7	3	1.17	26.25	69.31	o
13	7	3	2107.99	1961.46	119.26	o
14	7	3	882.31	776.40	138.80	o

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6	0	4	454.18	451.60	50.31	o
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5	4	6	24.06	17.19	76.71	o
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
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SiB Si 0.47243(9) 0.3381(2) 0.8048(2) 0.0050(5) Uani 1 1 d . . .
Mg1 Mg 0.37650(11) 0.6575(2) 0.8544(3) 0.0065(5) Uani 1 1 d . . .
Mg2 Mg 0.37753(12) 0.4824(3) 0.3466(3) 0.0089(6) Uani 1 1 d . . .
O1A O 0.1821(2) 0.3400(5) 0.0207(6) 0.0047(8) Uiso 1 1 d . . .
O2A O 0.3093(2) 0.5091(5) 0.0306(6) 0.0080(10) Uiso 1 1 d . . .
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O1B O 0.5619(2) 0.3386(5) 0.8100(6) 0.0060(8) Uiso 1 1 d . . .
O2B O 0.4331(2) 0.4855(4) 0.6809(6) 0.0070(9) Uiso 1 1 d . . .
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SiB 0.0070(15) 0.0031(16) 0.0049(6) -0.0005(6) -0.0006(6) 0.0000(6)
Mg1 0.0084(18) 0.0057(19) 0.0055(7) -0.0007(8) -0.0014(8) -0.0006(8)
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 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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SiA Mg1 3.090(2) 2_564 ?
SiA Mg2 3.197(3) 2_564 ?
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   2   2   0        0.16        9.41     10.89 o
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  10   2   0      634.51      683.96     65.30 o
  12   2   0      102.06       12.95     99.70 o
   2   3   0      552.34      656.18     62.17 o
   4   3   0     1337.47     1324.44     40.47 o
   6   3   0     1735.47     1966.65     59.37 o
   8   3   0        6.81        8.17     26.59 o
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  12   3   0      654.31      559.65     63.37 o
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12	5	1	0.12	16.92	55.97	o
13	5	1	1.36	12.42	61.65	o
14	5	1	2334.64	2081.92	103.96	o
15	5	1	114.56	95.93	71.91	o
16	5	1	228.14	100.97	80.54	o
17	5	1	0.31	35.13	78.36	o
18	5	1	6.80	70.81	87.81	o
19	5	1	2.62	9.58	197.48	o
5	6	1	1.94	13.27	132.66	o
6	6	1	212.65	359.67	98.33	o
7	6	1	20.44	14.01	63.48	o
8	6	1	66.23	40.01	63.76	o
9	6	1	47.45	40.19	70.50	o
10	6	1	41.45	43.15	113.84	o
11	6	1	301.01	355.84	109.90	o
12	6	1	697.75	733.39	75.23	o
13	6	1	30.99	74.53	56.58	o
14	6	1	136.01	137.28	68.98	o
15	6	1	14.47	14.36	63.86	o
16	6	1	91.25	66.19	79.30	o
17	6	1	75.60	14.72	84.86	o

18	6	1	104.39	46.49	95.27	o
19	6	1	33.53	65.66	118.70	o
7	7	1	953.59	1028.95	220.76	o
8	7	1	1139.02	1411.32	153.59	o
9	7	1	2475.51	2755.61	169.82	o
10	7	1	199.59	305.52	125.35	o
11	7	1	1301.57	1610.52	166.63	o
12	7	1	1282.73	1498.05	223.18	o
13	7	1	166.63	91.81	78.13	o
14	7	1	32.52	43.32	73.57	o
15	7	1	432.63	436.94	99.64	o
16	7	1	585.53	562.79	86.53	o
17	7	1	3.11	58.03	84.85	o
9	8	1	0.03	74.28	206.49	o
10	8	1	97.50	156.87	135.95	o
11	8	1	29.40	17.79	125.67	o
12	8	1	250.06	673.42	152.17	o
13	8	1	1322.38	1785.28	193.03	o
14	8	1	44.51	44.15	85.42	o
15	8	1	942.81	957.59	261.04	o
12	9	1	5407.17	6281.49	281.74	o
13	9	1	334.28	525.75	191.98	o
0	0	2	1100.54	1087.10	38.82	o
1	0	2	1019.55	955.49	36.50	o
3	0	2	2286.36	1664.74	47.79	o
4	0	2	2265.73	2260.30	72.99	o
6	0	2	90.69	167.04	73.33	o
7	0	2	4417.41	4067.48	163.02	o
1	1	2	0.22	9.65	8.42	o
2	1	2	237.20	285.32	12.98	o
3	1	2	882.57	785.92	15.22	o
4	1	2	779.08	995.89	26.11	o
5	1	2	5723.83	6456.70	121.77	o
6	1	2	1107.77	1174.04	36.27	o
7	1	2	51.97	75.15	26.57	o
8	1	2	6253.12	6157.42	297.87	o
9	1	2	1598.09	1571.14	95.78	o
0	2	2	188.04	242.43	24.76	o
1	2	2	8.03	30.35	12.90	o
2	2	2	5.16	11.22	12.00	o
3	2	2	926.14	1054.89	31.05	o
4	2	2	595.17	680.62	21.23	o
5	2	2	63.75	55.58	12.59	o
6	2	2	3109.06	3272.09	64.79	o
7	2	2	3138.97	3227.55	55.90	o
8	2	2	1487.46	1564.23	39.15	o
9	2	2	1571.39	1575.56	53.89	o
10	2	2	1034.15	1052.18	74.87	o
11	2	2	215.59	179.74	55.68	o
12	2	2	368.75	354.26	65.36	o
1	3	2	124.59	132.97	34.70	o
2	3	2	0.66	7.42	24.38	o
3	3	2	519.17	607.74	26.11	o
4	3	2	507.85	511.67	19.87	o
5	3	2	637.89	665.24	22.05	o

6	3	2	211.36	179.22	17.81	o
7	3	2	334.47	357.68	27.29	o
8	3	2	355.38	354.61	26.13	o
9	3	2	96.12	83.68	29.49	o
10	3	2	45.69	53.94	35.24	o
11	3	2	196.74	158.69	40.89	o
12	3	2	40.25	29.72	47.40	o
13	3	2	9.01	29.45	48.67	o
14	3	2	3.65	55.41	82.14	o
15	3	2	34.30	11.94	119.37	o
1	4	2	963.81	833.83	105.42	o
2	4	2	4646.65	4317.57	222.78	o
3	4	2	1480.04	1457.67	117.20	o
4	4	2	0.05	18.66	28.82	o
5	4	2	249.20	259.20	23.71	o
6	4	2	1685.03	1714.83	81.02	o
7	4	2	984.09	1020.24	38.02	o
8	4	2	128.21	120.74	31.86	o
9	4	2	207.75	175.08	53.06	o
10	4	2	1.95	34.86	42.02	o
11	4	2	0.77	23.36	48.65	o
12	4	2	157.87	195.22	51.83	o
13	4	2	268.81	277.82	65.09	o
14	4	2	522.04	462.18	72.60	o
15	4	2	143.49	147.58	76.64	o
16	4	2	102.92	76.10	91.28	o
17	4	2	152.26	13.89	138.95	o
3	5	2	10384.97	8811.31	270.25	o
4	5	2	398.76	361.92	71.78	o
5	5	2	1557.45	1645.38	58.60	o
6	5	2	5.41	21.62	39.13	o
7	5	2	327.15	387.85	48.53	o
8	5	2	8227.80	7901.38	211.52	o
9	5	2	6621.70	6761.61	166.71	o
10	5	2	426.88	535.23	54.37	o
11	5	2	1891.82	2077.26	90.31	o
12	5	2	7859.00	7791.37	179.05	o
13	5	2	340.52	315.52	70.88	o
14	5	2	205.54	187.19	67.13	o
15	5	2	773.09	724.56	98.64	o
16	5	2	783.28	969.02	109.31	o
17	5	2	2727.03	3062.75	198.04	o
18	5	2	719.26	977.47	340.52	o
5	6	2	5155.10	4758.19	240.50	o
6	6	2	0.17	63.67	69.63	o
7	6	2	1750.82	1643.71	83.36	o
8	6	2	571.80	707.88	66.95	o
9	6	2	7838.55	8316.34	481.62	o
10	6	2	881.14	1025.46	120.22	o
11	6	2	8552.09	8957.50	498.27	o
14	6	2	4.64	54.54	70.04	o
15	6	2	83.73	115.44	70.76	o
16	6	2	55.35	55.52	71.04	o
17	6	2	356.95	451.07	85.80	o
18	6	2	309.32	400.25	104.52	o

19	6	2	42.70	21.31	213.14	o
8	7	2	2080.38	1959.21	159.43	o
9	7	2	7.28	30.67	79.04	o
10	7	2	13.12	52.55	78.69	o
11	7	2	192.83	176.84	95.37	o
12	7	2	2971.47	2897.09	190.51	o
13	7	2	439.04	587.59	90.76	o
14	7	2	10.68	42.50	80.34	o
15	7	2	211.07	122.45	85.06	o
16	7	2	343.32	285.78	86.07	o
17	7	2	631.02	874.25	185.43	o
10	8	2	44.08	22.86	228.62	o
12	8	2	11.39	134.93	148.77	o
13	8	2	434.90	434.10	107.45	o
14	8	2	79.07	138.27	90.20	o
15	8	2	622.06	937.12	282.81	o
1	1	3	25.24	24.09	13.21	o
2	1	3	691.17	747.99	20.01	o
3	1	3	4076.14	4073.58	75.03	o
4	1	3	0.48	22.57	14.70	o
5	1	3	174.27	169.27	20.17	o
6	1	3	1797.56	1813.87	45.85	o
7	1	3	1297.12	1275.52	59.76	o
8	1	3	24.58	36.46	26.55	o
9	1	3	1563.66	1672.02	166.46	o
10	1	3	795.51	833.56	136.77	o
11	1	3	116.01	118.12	134.31	o
0	2	3	15757.75	15898.85	336.52	o
1	2	3	12652.75	12836.04	214.98	o
2	2	3	77.97	93.12	16.39	o
3	2	3	271.96	295.02	24.13	o
4	2	3	1029.54	1093.14	28.73	o
5	2	3	1463.85	1420.29	33.17	o
6	2	3	416.33	524.48	30.66	o
7	2	3	6005.84	6376.33	118.69	o
8	2	3	187.97	215.49	31.42	o
9	2	3	676.58	752.87	46.88	o
10	2	3	741.86	793.95	62.87	o
11	2	3	218.76	182.38	68.03	o
12	2	3	900.53	889.99	159.02	o
13	2	3	2969.25	2882.86	230.53	o
2	3	3	940.98	840.26	74.31	o
3	3	3	94.74	88.41	26.16	o
4	3	3	704.57	752.06	30.03	o
5	3	3	3221.21	3062.02	72.00	o
6	3	3	4551.68	4687.65	182.26	o
7	3	3	2397.79	2609.53	80.77	o
8	3	3	40.50	30.35	36.63	o
9	3	3	1222.62	1285.34	65.44	o
10	3	3	2548.07	2372.76	87.62	o
11	3	3	172.12	177.06	68.53	o
12	3	3	690.15	628.82	82.60	o
13	3	3	12184.75	11566.39	998.72	o
14	3	3	4280.78	4636.35	191.48	o
15	3	3	3059.49	2231.55	216.79	o

0	4	3	8034.62	7598.66	264.30	o
1	4	3	4239.10	3988.91	230.26	o
2	4	3	146.80	136.76	45.77	o
3	4	3	3182.58	3057.28	74.38	o
4	4	3	1205.37	1167.13	48.17	o
5	4	3	975.57	921.16	51.61	o
6	4	3	150.27	172.57	34.74	o
7	4	3	1275.18	1325.88	53.57	o
8	4	3	10.01	43.13	38.75	o
9	4	3	2000.84	1753.20	82.99	o
10	4	3	612.91	542.66	76.96	o
11	4	3	186.11	149.88	78.77	o
12	4	3	416.82	466.49	84.87	o
13	4	3	547.63	734.58	176.24	o
14	4	3	91.37	104.15	80.71	o
15	4	3	649.39	629.68	108.68	o
16	4	3	9.06	92.05	97.90	o
2	5	3	618.32	543.76	133.63	o
3	5	3	3617.04	3346.74	164.01	o
4	5	3	263.30	192.48	67.10	o
5	5	3	33.26	10.29	39.37	o
6	5	3	600.98	583.49	63.07	o
7	5	3	235.26	251.78	64.68	o
8	5	3	49.05	55.46	74.19	o
9	5	3	797.23	844.84	110.11	o
10	5	3	98.78	95.63	56.63	o
11	5	3	95.63	98.18	55.68	o
12	5	3	24.15	14.06	53.96	o
13	5	3	133.94	149.37	61.94	o
14	5	3	58.90	21.77	65.56	o
15	5	3	1093.18	1174.24	129.18	o
16	5	3	47.77	100.13	93.26	o
17	5	3	247.75	408.92	102.63	o
4	6	3	211.82	13.22	132.23	o
5	6	3	213.54	293.08	137.24	o
6	6	3	21.43	89.52	87.87	o
7	6	3	29.67	15.94	79.10	o
8	6	3	65.11	66.56	74.45	o
9	6	3	9.98	23.49	75.80	o
10	6	3	147.27	79.32	82.54	o
11	6	3	418.73	387.44	68.36	o
12	6	3	0.35	22.26	68.94	o
13	6	3	0.02	64.30	66.42	o
14	6	3	13.22	70.37	68.81	o
15	6	3	0.68	137.82	75.24	o
16	6	3	87.33	20.87	83.01	o
17	6	3	426.28	335.13	259.85	o
7	7	3	1072.95	779.10	168.47	o
8	7	3	151.57	202.01	142.47	o
9	7	3	511.44	579.55	102.13	o
10	7	3	949.83	973.55	129.33	o
11	7	3	539.44	467.30	101.29	o
12	7	3	1.89	16.11	71.47	o
13	7	3	2244.83	2129.61	114.53	o
14	7	3	855.83	887.47	161.88	o

15	7	3	34.10	31.06	123.02	o
11	8	3	815.80	730.78	181.02	o
12	8	3	449.76	457.91	116.24	o
13	8	3	2626.06	3268.85	354.84	o
0	0	4	733.32	766.37	57.12	o
1	0	4	14701.57	13905.32	325.56	o
2	0	4	3888.74	3817.32	59.40	o
3	0	4	1143.11	1198.40	49.00	o
4	0	4	10336.27	10285.81	186.33	o
5	0	4	21.42	35.02	36.03	o
6	0	4	473.12	440.93	50.63	o
7	0	4	138.53	123.72	46.71	o
8	0	4	2891.92	2760.58	214.46	o
9	0	4	4522.24	3527.92	228.89	o
1	1	4	3744.47	3799.48	44.98	o
2	1	4	84.08	106.86	21.40	o
3	1	4	1285.10	1485.43	41.56	o
4	1	4	41.72	30.40	26.26	o
5	1	4	4604.01	4847.45	149.89	o
6	1	4	1099.51	1215.76	51.98	o
7	1	4	2445.11	2324.00	72.58	o
8	1	4	537.76	559.70	50.60	o
9	1	4	91.36	100.37	55.80	o
10	1	4	5069.90	5042.40	272.01	o
11	1	4	1699.05	1655.92	201.05	o
0	2	4	113.51	98.69	37.41	o
1	2	4	519.39	568.27	31.04	o
2	2	4	44.02	21.67	26.71	o
3	2	4	96.67	84.12	29.75	o
4	2	4	87.74	90.25	37.87	o
5	2	4	2634.72	2559.02	149.46	o
6	2	4	61.67	62.46	33.91	o
7	2	4	1096.72	1194.10	50.27	o
8	2	4	1468.39	1661.09	89.29	o
9	2	4	5.58	29.65	55.73	o
10	2	4	0.32	47.59	60.70	o
11	2	4	1.27	195.22	133.29	o
12	2	4	2.23	31.19	125.39	o
13	2	4	82.11	156.59	141.79	o
1	3	4	6.07	33.95	37.26	o
2	3	4	1.99	27.52	37.36	o
3	3	4	177.95	148.54	38.79	o
4	3	4	24.96	25.11	37.48	o
5	3	4	168.17	152.84	39.61	o
6	3	4	234.02	233.64	39.12	o
7	3	4	190.65	219.42	49.60	o
8	3	4	5.35	37.97	63.87	o
9	3	4	188.53	350.23	169.35	o
10	3	4	14.23	44.98	59.67	o
11	3	4	397.64	462.96	100.56	o
12	3	4	90.32	113.84	93.25	o
13	3	4	199.62	119.40	100.86	o
14	3	4	0.92	14.21	142.05	o
15	3	4	425.05	163.74	171.76	o
0	4	4	1211.52	1118.30	90.32	o

1	4	4	101.45	171.25	67.53	o
2	4	4	131.29	134.79	50.41	o
3	4	4	11.09	52.49	52.70	o
4	4	4	320.37	313.34	58.98	o
5	4	4	3021.16	3154.60	116.17	o
6	4	4	147.72	135.34	62.60	o
7	4	4	4.91	30.82	48.00	o
8	4	4	63.01	72.57	51.58	o
9	4	4	1913.52	1835.92	106.62	o
10	4	4	58.81	13.72	83.16	o
11	4	4	30.78	30.80	84.49	o
12	4	4	1.93	25.88	80.21	o
13	4	4	414.62	216.38	110.88	o
14	4	4	2.10	27.85	101.37	o
15	4	4	1135.86	1106.90	147.06	o
16	4	4	72.77	17.16	171.62	o
2	5	4	2055.07	1683.94	194.39	o
3	5	4	4271.32	3289.28	494.92	o
4	5	4	14.34	32.39	57.63	o
5	5	4	2227.94	2278.99	128.54	o
6	5	4	669.86	691.13	88.63	o
7	5	4	2021.52	2214.95	161.68	o
8	5	4	558.97	465.82	93.89	o
9	5	4	16.83	13.99	80.73	o
10	5	4	5905.25	5524.70	244.54	o
11	5	4	2087.66	1994.64	117.52	o
12	5	4	194.15	176.22	83.09	o
13	5	4	1756.80	1841.63	117.50	o
14	5	4	10.83	32.13	80.31	o
15	5	4	2458.62	2589.45	147.13	o
16	5	4	33.28	19.24	135.89	o
4	6	4	4784.97	3788.89	261.85	o
5	6	4	71.13	60.54	96.88	o
6	6	4	203.98	198.89	107.77	o
7	6	4	5.03	41.07	98.99	o
8	6	4	1632.01	1595.10	149.29	o
9	6	4	4911.30	4936.90	308.37	o
10	6	4	160.01	50.64	92.26	o
11	6	4	5194.73	4985.57	288.65	o
12	6	4	1425.62	1455.43	117.22	o
13	6	4	1114.66	965.35	109.10	o
14	6	4	108.42	45.79	105.52	o
7	7	4	0.62	12.49	137.34	o
8	7	4	121.66	110.35	155.48	o
9	7	4	231.41	383.90	121.29	o
10	7	4	799.46	761.71	116.55	o
11	7	4	1478.88	1424.00	119.29	o
12	7	4	22.47	87.21	109.07	o
1	1	5	95.20	113.96	35.25	o
2	1	5	1.17	38.32	32.79	o
3	1	5	335.89	330.44	38.34	o
4	1	5	182.60	164.59	37.25	o
5	1	5	903.94	858.03	54.96	o
6	1	5	1480.34	1546.22	71.23	o
7	1	5	18.07	32.93	55.87	o

8	1	5	359.12	361.31	66.58	o
9	1	5	177.70	178.08	66.71	o
10	1	5	33.81	56.36	138.03	o
11	1	5	117.19	81.15	117.42	o
0	2	5	90.13	37.53	50.45	o
1	2	5	474.03	515.61	42.34	o
2	2	5	1262.01	1273.15	53.44	o
3	2	5	262.12	287.97	40.96	o
4	2	5	5295.58	5292.38	132.47	o
5	2	5	80.21	93.58	36.81	o
6	2	5	308.09	289.24	52.92	o
7	2	5	347.13	366.31	70.66	o
8	2	5	458.84	510.28	93.70	o
9	2	5	2065.33	2145.70	137.13	o
10	2	5	132.15	133.86	84.13	o
11	2	5	2070.34	2169.89	260.84	o
12	2	5	1154.63	1101.13	206.69	o
13	2	5	2207.93	2254.19	247.22	o
1	3	5	2154.97	2160.72	72.37	o
2	3	5	1941.02	1947.06	75.67	o
3	3	5	3602.41	3528.63	111.01	o
4	3	5	44.90	73.76	48.60	o
5	3	5	9.22	20.76	53.07	o
6	3	5	3515.24	4018.02	214.88	o
7	3	5	18.10	14.99	56.60	o
8	3	5	987.40	1056.33	74.81	o
9	3	5	167.72	79.69	62.95	o
10	3	5	13320.64	13375.45	578.88	o
11	3	5	1557.86	1826.64	246.37	o
12	3	5	597.96	752.25	194.14	o
13	3	5	470.45	536.94	191.89	o
0	4	5	378.54	377.00	85.12	o
1	4	5	232.63	191.77	80.44	o
2	4	5	847.81	803.35	87.57	o
3	4	5	66.43	73.89	69.87	o
4	4	5	1134.78	1269.78	96.65	o
5	4	5	47.49	49.89	60.18	o
6	4	5	59.02	44.25	61.72	o
7	4	5	176.17	179.49	63.14	o
8	4	5	38.83	54.27	68.06	o
9	4	5	1232.59	1311.35	109.70	o
10	4	5	5.84	44.64	94.11	o
11	4	5	1174.31	1256.56	132.21	o
12	4	5	169.33	89.45	97.50	o
2	5	5	212.41	117.27	145.82	o
3	5	5	115.46	180.01	69.93	o
4	5	5	29.61	13.82	69.07	o
5	5	5	182.68	176.33	74.53	o
6	5	5	400.37	476.59	78.53	o
7	5	5	296.11	369.62	97.05	o
8	5	5	14.62	28.13	94.07	o
9	5	5	189.19	561.57	314.40	o
10	5	5	96.95	113.14	100.18	o
11	5	5	0.06	17.58	175.78	o
4	6	5	65.73	111.03	152.30	o

5	6	5	228.34	210.24	167.54	o
6	6	5	5.96	85.29	106.90	o
7	6	5	299.07	213.65	121.84	o
8	6	5	0.89	52.74	164.47	o
0	0	6	12387.34	12253.66	361.78	o
1	0	6	5126.14	5419.58	114.82	o
2	0	6	10.31	57.74	54.17	o
3	0	6	767.95	783.24	74.14	o
4	0	6	609.31	685.89	72.60	o
5	0	6	534.52	547.38	76.68	o
6	0	6	21.97	65.71	67.81	o
7	0	6	3887.63	3622.75	362.53	o
1	1	6	3554.96	3314.07	83.40	o
2	1	6	171.56	173.86	43.21	o
3	1	6	484.68	500.32	48.05	o
4	1	6	41.16	41.16	39.99	o
5	1	6	7.54	80.56	42.96	o
6	1	6	738.12	797.59	65.93	o
7	1	6	448.21	442.32	65.90	o
8	1	6	10.28	19.31	60.86	o
9	1	6	1463.92	1287.85	219.83	o
0	2	6	16.99	50.50	58.83	o
1	2	6	64.39	60.58	45.29	o
2	2	6	96.71	143.41	43.56	o
3	2	6	712.16	782.73	54.34	o
4	2	6	582.90	980.66	157.74	o
5	2	6	34.64	26.59	48.31	o
6	2	6	282.05	236.27	56.03	o
7	2	6	1034.76	1079.68	98.60	o
8	2	6	116.40	135.40	68.44	o
9	2	6	10.48	19.95	140.57	o
1	3	6	23.37	72.89	55.12	o
2	3	6	0.48	48.60	50.29	o
3	3	6	24.78	55.06	49.80	o
4	3	6	255.46	178.79	55.28	o
5	3	6	9.46	29.43	62.06	o
6	3	6	92.70	68.03	64.73	o
7	3	6	159.95	118.11	72.15	o
8	3	6	13.51	38.85	108.09	o
9	3	6	8.00	17.05	170.52	o
0	4	6	40.12	119.20	89.58	o
1	4	6	540.08	599.89	103.02	o
2	4	6	74.06	113.64	100.07	o
3	4	6	874.52	886.75	87.96	o
4	4	6	247.52	253.45	81.57	o
5	4	6	13.16	47.46	87.91	o
6	4	6	28.39	16.82	118.88	o
7	4	6	902.06	1016.78	209.55	o