Title

PREPARATION AND CRYSTAL STRUCTURE OF THE MIXED-VALENCE Yb(III,II) TETRANUCLEAR COMPLEX, (Me5C5)6Yb4(u-F)4

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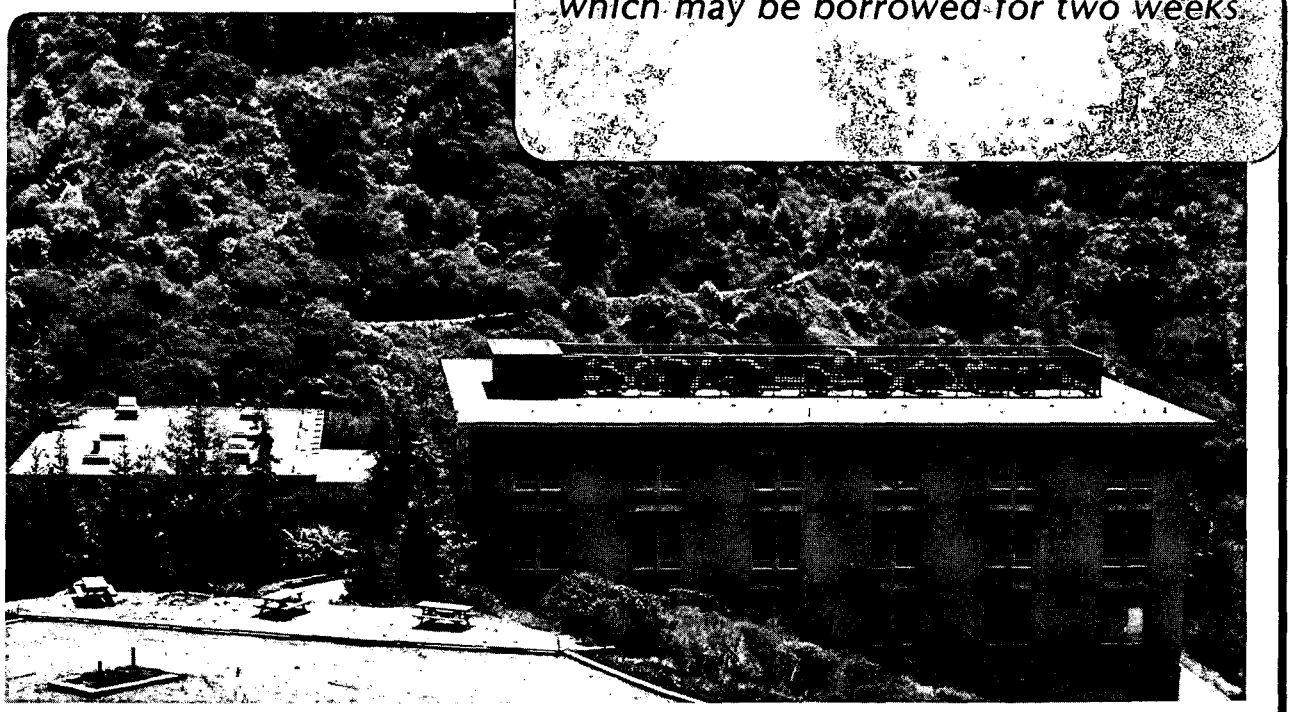

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DISCLAIMER

LBL-22007

Preparation and Crystal Structure of the Mixed-Valence [Yb(III,II)] Tetranuclear Complex, $(Me_5C_5)_6Yb_4(\mu\text{-}F)_4$.

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Silver fluoride and $(Me_5C_5)_2Yb$ in toluene give the novel, tetranuclear, mixed-valence complex $(Me_5C_5)_6Yb_4(\mu\text{-}F)_4$ as shown by single crystal X-ray crystallography.

Binary transition-metal fluorides form a wide range of interesting solid state structures.[1] It is generally observed that those compounds in oxidation state less than six form M-F-M bridge bonds. These bridge bonds have been likened to the bridge bonding in metal alkyls with the important difference that a bridging methyl group has one σ-orbital and an electron for bonding and fluorine has two σ-orbitals, two π-orbitals and seven electrons for bonding.[2] With this analogy in mind we decided to try to prepare $(Me_5C_5)_2YbF$ since $(Me_5C_5)_2LuMe$ is a molecule which has a terminal methyl group and a methyl group that bridges the two lanthanide centers in a near-linear fashion, the Lu-C(Me)-Lu angle being 170(4)°, and the ytterbium methyl is thought to have a similar structure, $(Me_5C_5)_4Yb_2(Me)(\mu\text{-}Me)$.[3]. The pentamethylcyclopentadienyl ligand is crutial for giving the unusual bridging methyl since $(C_5H_5)_4Yb_2(\mu\text{-}Me)_2$ has two normal bridge bonds in which the Yb-C(Me)-Yb angle is 86.5(5)°.[4]

We have used silver (I) salts to oxidize $(Me_5C_5)_2Yb(L)$ to $(Me_5C_5)_2Yb(L)(X)$, where L is a Lewis base[5] and others have used silver (II) salts to oxidize $Cp_2Yb(L)_2$.[6] Hence reaction of base-free $(Me_5C_5)_2Yb$[7] with AgF in hydrocarbons was a rational synthetic route to the target molecule.

Stirring $(Me_5C_5)_2Yb$(0.30g) with one or up to four molar equivalents of AgF in toluene for 8h yielded a brown solution and silver metal. Crystallization of the brown solution yielded brown blocks and red needles. The brown blocks, the identity of which is currently under study, may be converted to the red needles (total yield, 0.08g) by heating in toluene. The red needles do not melt to 350°C, do not give an understandable mass spectrum, and are not soluble enough in aromatic solvents to give a satisfactory ^{1}HNMR spectrum and were shown by single crystal X-ray crystallography to be the tetranuclear complex $(Me_5C_5)_6Yb_4(\mu\text{-}F)_4(PhMe)_2$. Crystal data: $C_{74}H_{106}F_4Yb_4$,

M=1763.96, monoclinic, space group $C_{2/c}$, a=26.805(3), b=10.285(1), c=24.621(2)Å, β=104.53(1)°, U=6570(2)Å^3, D_c=1.78g cm^{-3}, Mo-K_α radiation, R=0.71073Å, μ(Mo-K_α)=59.7cm^{-1}. The structure was solved by a combination of Patterson and Fourier methods and refined using 3305 unique reflections [$Fo^2 > 3\sigma(Fo^2)$] measured on a CAD4 diffractometer (2θ max 45°). An analytical absorption correction was applied to the data, all non-hydrogen atoms were refined anisotropically and the hydrogen atoms on the Me_5C_5-rings on Yb(1) were located, included in the structure factor calculations with isotropic thermal parameters but were not refined. The hydrogen atoms on the Me_5C_5-ring on Yb(2) were not located. The current R value is 0.027 for 329 variables.‡ An ORTEP diagram is shown in the Figure.

The structure consists of two trivalent ytterbium fragments, $(Me_5C_5)_2YbF$, and two divalent ytterbium fragments, $(Me_5C_5)YbF$, connected by way of near-linear bridging fluorides, Yb(2)F(2)Yb(1)=160.0(2)° and Yb(2)F(1)Yb(1)=157.3(2)°. The molecule has idealized C_{2h} symmetry, the inversion centre being located in the centre of the Yb_4F_4 ring. The eight-membered Yb_4F_4 ring is non-planar, the dihedral angle formed by intersection of the plane defined by F(1)F(1')F(2)F(2') and Yb(2)F(1)F(2) is 104°. In addition Yb(1) and Yb(1') are out of the plane defined by F(1)F(1')F(2)F(2') by -0.63Å and +0.63Å, respectively, and Yb(2) and Yb(2') are out of this plane by +1.34Å and -1.34Å, respectively.

The coordination of Yb(2) is distorted tetrahedral, defining the Me_5C_5 ring centroid as occupying one coordination site. The averaged Me_5C_5 ring centroid-Yb(2)-Me_5C_5 ring centroid angle is 138.4°, the averaged Me_5C_5 ring centroid-Yb(2)-F angle is 104.3° and the F(2)-Yb(2)-F(1) angle is 91.9°. The coordination of Yb(1) is near-trigonal planar, the averaged Me_5C_5 ring centroid-Yb-F angle is 127.1° and the F(2)-Yb(1)-F91)- angle is 105.9(1).°

Alternatively, the two $(Me_5C_5)_2Yb(2)F_2$ tetrahedra and the two $(Me_5C_5)Yb(1)F_2$ trigonal planar units are fused so that they share common vertices. The four fluoride atoms are at the corners of a rectangle with F(1)F(1') and F(2)F(2') being 3.061(5) and 3.544(5)Å, respectively, and F(1)F(2)F(1') and F(2)F(1)F(2') being 90.20(5) and 89.88(5)°, respectively.

The average oxidation state of the ytterbium atoms in the tetranuclear complex is 2.5. The Yb(2) atoms are most reasonably described as being trivalent with a coordination number of eight, defining a Me_5C_5-group as occupying three coordination sites, and the Yb(1) atoms being divalent with coordination number five since the radius of Yb(III) in eight coordination is nearly the same as that of Yb(II) in five coordination.[8] Thus the averaged Yb(2)-C and Yb(1)-C distances are 2.62∓0.02Å and 2.65∓0.02Å, respectively, and the averaged Yb(2)-F and Yb(1)-F distances are 2.129∓0.002Å and 2.22⁰∓0.001Å, respectively. Not surprisingly, Yb(1), in an attempt to increase its coordination number, has two close Yb...C(17,18) contact distances of 3,124(7)Å and 3.232(7)Å, respectively. All other intra- and inter- molecular contacts are >3.6Å.

Variable temperature magnetic susceptibility studies are consistent with the Yb(II,III) mixed-valence formulation with non-interacting spins, i.e., a class I or trapped-valence complex.[9] Powdered samples follow Curie-Weiss behavior and the shape of the plot of χ_m^{-1} vs. T(K) is as expected for isolated Yb(III) paramagnets, μ_B=3.67 [per Yb(III)] and θ=-3K from 7-35K and μ_B=4.95 and θ=-37K from 80-280K at a field strength of 5Kgauss. The magnetic susceptibility is highly anisotropic since measurement of χ_m on randomly orientated crystals gives μ_B=3.87 [per Yb(III)] and θ=-2K from 7-30K and μ_B=6.06 and θ=-64K from 80-200K. The anisotropy in the magnetic moment is not unusual in lanthanide magnetism.[10]

We thank the Fannie and John Hertz Foundation (C.J.B.) and NSERC (Canada) (D.J.B.) for fellowships and Dr. F.J. Hollander, staff crystallographer of the University of California X-ray facility, for his help. This work was supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Chemical Sciences Division of the U.S. Department of Energy under contract DE-AC03-76SF 00098.

‡ The atomic coordinates for this work are available on request from the Director of the Cambridge Crystallographic Data Centre, University Chemical Laboratory, Lensfield Road, Cambridge CB2 1EW. Any request should be accompanied by the full literature citation for this communication.

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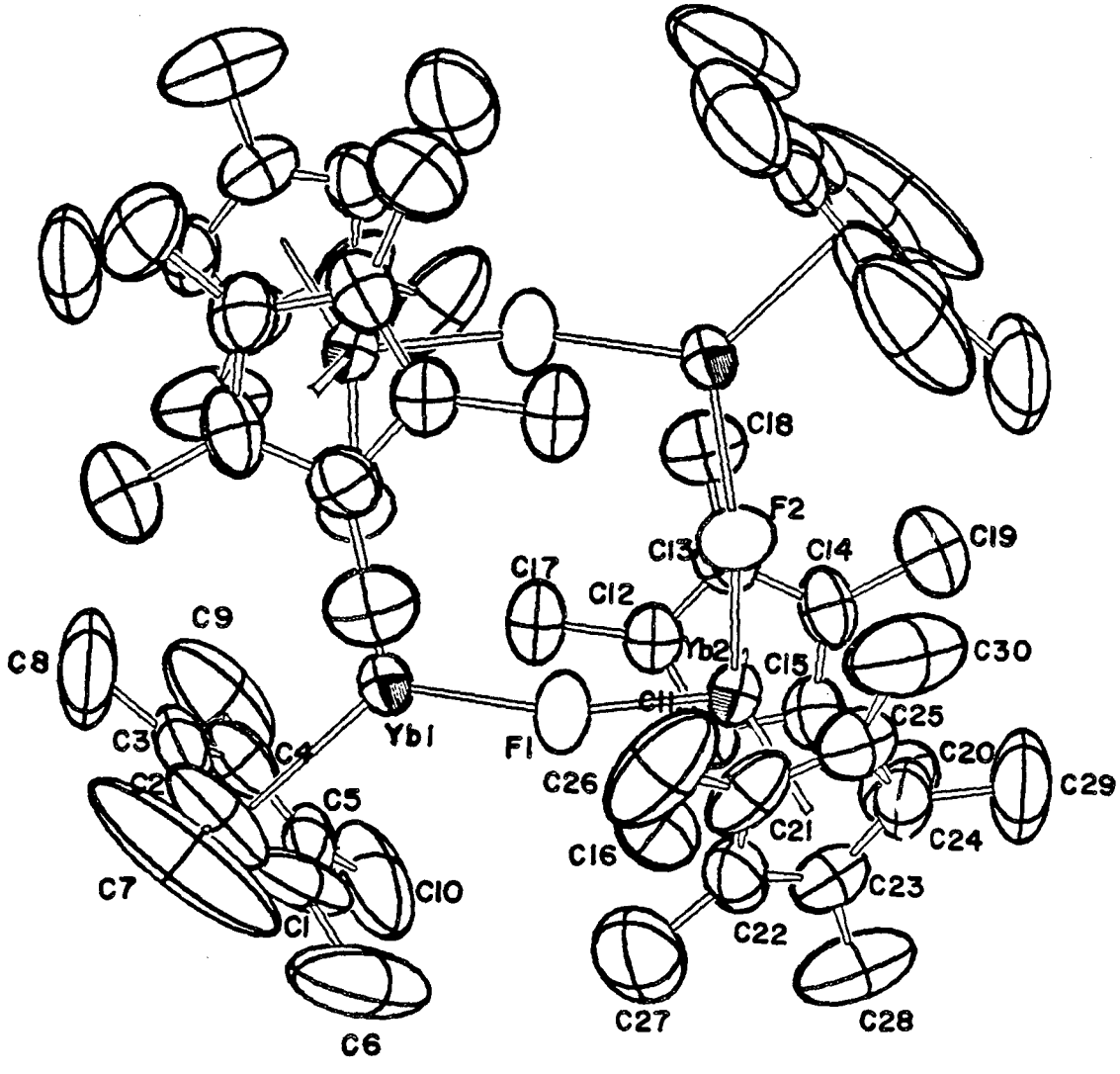
Figure Caption. The averaged Yb(2)-Me_5C_5 ring centroid and the Yb(1)-Me_5C_5 ring centroid distances are 2.33Å and 2.39Å, respectively.


C18
F2
C13
C14
C19
C17
C12
C9
C8
Yb2
C15
C30
C11
C25
C3
Yb1
F1
C20
C29
C4
C26
C2
C5
C21
C24
C16
C7
C10
C23
C1
C22
C6
C27
C28

XBL 868-2844

Supplementary Material for

Preparation and Crystal Structure of the Mixed-Valence [Yb(III,II)] Tetranuclear Complex, $(Me_5C_5)_6Yb_4(\mu\text{-}F)_4$.

C.J. Burns , D.J. Berg and R.A. Andersen

Atomic Coordinates
Bond Lengths and Angles
Thermal Parameters
Structure Factor Tables
Full Experimental Details

Table I. Crystal Data (25°C) for $[(Me_5C_5)_3Yb_2F_2]_2(PhMe)_2$

Space Group	C2/c
a, Å	26.805(3)
b, Å	10.285(1)
c, Å	24.621(2)
α, deg	90
β, deg	104.530(9)
γ, deg	90
V, Å^3	6570(2)
Z	4
fw	1763.96
d (calc.), g/cm^3	1.78
μ (calc.), 1/cm	59.7
size, mm	0.12 x 0.24 x 0.30
radiation	MoKα (λ = 0.71073Å)
monochromator	highly oriented graphite
scan range, type	$3^0 \leq 2\theta \leq 45^0$, θ-2θ
scan speed, deg/min	0.69-6.7, variable
scan width, deg	$\Delta\theta = 0.55 + 0.35 \tan\theta$
reflections collected	4690; ±h, +k, +l
unique reflections	4287
reflections, $F_o^2 > 3\sigma(F_o^2)$	3305
R, %	0.0272
R_w, %	0.0356
GOF	1.58
g	3.07×10^{-8}

largest Δ/σ in final least squares cycle	9.71

Intensity Standards: 3, 7, -3; 0, 0, 12; 12, 0, 2: measured every two hours of x-ray exposure time. Over the period of data collection 2.4 % decay in intensity was observed. A linear decay correction was applied to the raw data.

Orientation Standards: 3 reflections were checked after every 250 measurements. Crystal orientation was redetermined if any of the reflections were offset from their predicted positions by more than 0.1^{0}. No reorientation was required during data collection.

X-Ray Crystallography of $[(Me_5C_5)_3Yb_2F_2]_2(PhMe)_2$

Red needles of the compound were grown by slow cooling of a hot toluene solution to room temperature. A large needle was cleaved, yielding a fragment of approximate dimensions 0.12 mm x 0.24 mm x 0.30 mm suitable for diffraction. This fragment was lodged in a 0.3 mm thin walled quartz capillary in a nitrogen-filled drybox, and the capillary was flame sealed.

Precession photographs indicated monoclinic Laue symmetry, and yielded preliminary cell dimensions.

The crystal was transferred to an Enraf-Nonius automated diffractometer[1] and centered in the beam. Automatic peak indexing procedures yielded the same unit cell as the precession photographs and confirmed the Laue symmetry. Examination of the h0l and hil zones showed the following systematic absences: h0l; l = 2n+1, hkl; h + k = 2n + 1, consistent with both space groups Cc and C2/c. Selection of the space group C2/c for data refinement was proven correct by successful convergence of the solution. Accurate cell parameters and the orientation matrix were determined by a least-squares fit to the setting angles of the unresolved MoKα components of 24 symmetry related reflections with 2θ between 28 and 29°C. The results are given in Table (I) along with the parameters used for data collection.

The 4690 raw data were converted to structure factor amplitudes and their esd's by correcting for scan speed, background, and Lorentz-polarization effects.[2,4] Analysis of the azimuthal scan data[5] showed a variation of I_{min}/I_{max} of 0.559 in the average relative intensity curve. An analytical absorption correction was applied to the data using the dimensions of the indexed faces of the crystal and a 12 x 12 x 6 Gaussian grid of internal points.[3] The maximum and minimum transmission factors were 0.549 and 0.268, respectively.

The unique set of 4287 data was used to solve and refine the structure. The ytterbium atoms were located through the use of a three-dimensional Patterson map. The remaining non-hydrogen

atoms were located through the use of standard Fourier techniques.

During the course of the refinement, the difference Fourier map indicated the presence of one disordered molecule of toluene per asymmetric unit. The toluene was placed and refined isotropically as two half-occupancy molecules related by the two-fold axis. The C-C-C angles were constrained to be 120°, the C_{ring}-C_{ring} bond lengths to be 1.40Å, and the C_{ring}-C_{Me} length to be 1.50Å during least-squares refinement. The ring carbons were furthermore constrained to have the same isotropic thermal parameter. The three largest peaks in the final difference Fourier map were all around the disordered ring, indicating that there may have been another disordered position, but no other ring model could be fitted successfully.

The hydrogen atoms on the pentamethylcyclopentadienyl rings on Yb(1) were located. These atoms were placed and included in the structure factor calculations with isotropic thermal parameters, but were not refined.

The final residuals for 329 variables refined against the 3305 data for which $F_o^2 > 3\sigma(F_o^2)$ were R = 0.0272, wR = 0.0356, and GOF = 1.58. The R value for all 4287 data was 0.0508.

The quantity minimized by the least-squares program was $\Sigma w(|F_o| - |F_c|)^2$, where w is the weight of a given observation. The p-factor[6], used to reduce the weight of intense reflections, was set to 0.03 throughout the refinement. The analytical forms for the scattering factor tables for the neutral atoms[7] were used and all non-hydrogen scattering factors were corrected for both the real and imaginary components of anomalous dispersion.[8]

Inspection of the residuals ordered in ranges of $\sin\theta/\lambda$, $|F_o|$, and parity and value of the individual indexes showed no unusual features or trends. There was evidence of secondary extinction in the low-angle, high-intensity data, and a secondary extinction correction was applied to the data[9]. The secondary extinction coefficient was refined in the least-squares calculations to a value of 3.07×10^{-8}.

The largest peak in the final difference Fourier map had an electron density of 0.837 $e^{-1}/Å^3$. and was associated with the disordered toluene molecule.

1.) Instrumentation at the University of California Chemistry Department X-ray Crystallographic Facility (CHEXRAY) consists of two Enraf-Nonius CAD-4 diffractometers, one controlled by a DEC PDP 8/a with an RK05 disk and the other by a DEC PDP 8/e with a RL01 disk. Both use Enraf-Nonius software as described in the CAD-4 Operation Manual, Enraf-Nonius, Delft, Nov. 1977, updated Jan. 1980.

2.) All calculation were performed on a PDP 11/60 equipped with 128 kilowords of memory, twin RK07 28 MByte disk drives, Versatec printer/plotter and TU10 tape drive using locally-modified Nonius-SDP[3] software operating under RSX-11M.

3.) Structure Determination Package User's Guide, 1982, B. A. Frenz and Associates, College Station, TX 77840.

4.) The data reduction formulae are:

$$F_0^2 = \frac{\omega}{Lp}(C - 2B) \qquad \sigma_0(F_0^2) = \frac{\omega}{Lp}(C + 4B)^{1/2}$$

$$F_0 = \sqrt{F_0^2} \qquad \sigma_0(F) = \frac{\sigma_0(F_0^2)}{2F_0}$$

where C is the total count in the scan, B the sum of the two background counts, ω the scan speed used in deg/min, and

$$\frac{1}{Lp} = \frac{\sin 2\theta\,(1 + \cos^2 2\theta_m)}{1 + \cos^2 2\theta_m - \sin^2 2\theta}$$

is the correction for Lorentz and polarization effects for a reflection with scattering angle 2r and radiation monochromatized with a 50% perfect single crystal monochrometer with scattering angle $2r_m$.

5.) Reflections used for azimuthal scans were located near x = 90° and the intensities were measured at 10° increments of rotation of the crystal about the diffraction vector.

6.)

$$R = \frac{\Sigma||F_o| - |F_c||}{\Sigma|F_o|} \qquad wR = \frac{\Sigma w(|F_o| - |F_c|)^2}{\Sigma w F_o^2}^{1/2}$$

$$GOF = \frac{\Sigma w(|F_o| - |F_c|)^2}{(n_o - n_v)}^{1/2}$$

where n_o is the number of observations, n_v the number of variable parameters, and the weights w were given by:

$$w = \frac{4F_o^2}{\sigma^2(F_o^2)}, \quad \sigma^2(F_o^2) = \sigma_o^2(F_o^2) + (pF^2)^2$$

where p is the factor used to lower the weight of intense reflections.

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Intramolecular Distances

ATOM 1	ATOM 2	DISTANCE
YB1	F1	2.221(3)
YB1	F2	2.219(3)
YB1	C1	2.684(10)
YB1	C2	2.637(9)
YB1	C3	2.653(7)
YB1	C4	2.631(7)
YB1	C5	2.667(8)
YB1	CP1	2.386
YB2	F1	2.132(3)
YB2	F2	2.126(3)
YB2	C11	2.630(6)
YB2	C12	2.629(6)
YB2	C13	2.631(6)
YB2	C14	2.639(6)
YB2	C15	2.669(6)
YB2	C21	2.580(7)
YB2	C22	2.570(7)
YB2	C23	2.601(7)
YB2	C24	2.611(7)
YB2	C25	2.612(6)
YB2	CP2	2.357
YB2	CP3	2.311
C1	C2	1.406(20)
C2	C3	1.318(14)
C3	C4	1.364(11)
C4	C5	1.365(12)
C5	C1	1.371(18)
C1	C6	1.473(17)
C2	C7	1.501(16)
C3	C8	1.534(13)
C4	C9	1.563(13)
C5	C10	1.612(16)
C11	C12	1.400(9)
C12	C13	1.390(9)
C13	C14	1.407(9)
C14	C15	1.402(10)
C15	C11	1.388(9)
C11	C16	1.509(10)
C12	C17	1.514(8)
C13	C18	1.493(9)
C14	C19	1.502(9)
C15	C20	1.511(10)
C21	C22	1.380(10)
C22	C23	1.372(10)
C23	C24	1.400(10)
C24	C25	1.393(10)
C25	C21	1.405(11)
C21	C26	1.502(11)
C22	C27	1.520(12)
C23	C28	1.529(11)
C24	C29	1.497(10)
C25	C30	1.449(11)

Intramolecular Angles

ATOM 1	ATOM 2	ATOM 3	ANGLE
F1	YB1	F2	105.95(14)
F1	YB2	F2	91.94(14)
YB1	F1	YB2	157.29(18)
YB1	F2	YB2	159.95(18)
F1	YB1	CP1	129.15
F2	YB1	CP1	124.88
F1	YB2	CP2	103.72
F1	YB2	CP3	104.00
F2	YB2	CP2	103.98
F2	YB2	CP3	105.44
CP2	YB2	CP3	138.40
C5	C1	C2	104.7(9)
C1	C2	C3	109.5(12)
C2	C3	C4	109.1(10)
C3	C4	C5	107.1(9)
C4	C5	C1	109.5(11)
C2	C1	C6	137.7(24)
C5	C1	C6	117.0(23)
C3	C2	C7	138.1(19)
C1	C2	C7	111.7(19)
C4	C3	C8	125.3(12)
C2	C3	C8	125.5(13)
C5	C4	C9	128.9(12)
C3	C4	C9	123.6(11)
C1	C6	C10	133.5(15)
C4	C5	C10	116.7(14)
C15	C11	C12	108.9(6)
C11	C12	C13	107.5(6)
C12	C13	C14	108.3(6)
C13	C14	C15	107.6(6)
C14	C15	C11	107.6(6)
C12	C11	C16	124.9(7)
C15	C11	C16	126.0(7)
C13	C12	C17	126.3(7)
C11	C12	C17	126.0(6)
C14	C13	C18	125.9(7)
C12	C13	C18	125.8(6)
C15	C14	C19	125.9(7)
C13	C14	C19	126.3(7)
C11	C15	C20	126.4(7)
C14	C15	C20	124.9(7)
C25	C21	C22	107.6(6)
C21	C22	C23	109.6(7)
C22	C23	C24	107.2(7)
C23	C24	C25	108.5(6)
C24	C25	C21	107.0(6)
C22	C21	C26	124.2(10)
C25	C21	C26	127.9(9)
C23	C22	C27	125.2(9)
C21	C22	C27	124.8(9)
C24	C23	C28	126.5(8)
C22	C23	C28	125.3(9)
C25	C24	C29	125.7(9)
C23	C24	C29	124.9(8)
C21	C25	C30	124.3(9)
C24	C25	C30	128.6(9)

Table of Positional Parameters and Their Estimated Standard Deviations

Atom	x	y	z	B(Å^2)
YB1	Ø.19Ø86(1)	Ø.16551(3)	Ø.Ø7565(1)	4.411(8)
YB2	Ø.34782(1)	Ø.1Ø367(3)	Ø.Ø7363(1)	3.932(7)
F1	Ø.2759(1)	Ø.1567(4)	Ø.Ø896(2)	5.4(1)
F2	Ø.1613(2)	Ø.2582(4)	-Ø.ØØ76(2)	5.4(1)
C1	Ø.1741(4)	Ø.11Ø(2)	Ø.1761(4)	14.3(4)
C2	Ø.1376(4)	Ø.2Ø4(1)	Ø.15Ø9(4)	1Ø.5(3)
C3	Ø.1Ø38(3)	Ø.1521(9)	Ø.1Ø81(4)	7.Ø(2)
C4	Ø.1177(3)	Ø.Ø265(9)	Ø.1Ø16(4)	6.6(2)
C5	Ø.16Ø1(3)	Ø.ØØØ(1)	Ø.1442(4)	9.5(3)
C6	Ø.2158(5)	Ø.Ø96(2)	Ø.2277(6)	28.Ø(9)
C7	Ø.1439(7)	Ø.328(1)	Ø.1844(5)	24.9(5)
C8	Ø.Ø548(4)	Ø.219(2)	Ø.Ø737(6)	15.9(4)
C9	Ø.Ø851(5)	-Ø.Ø69(1)	Ø.Ø57Ø(6)	14.5(4)
C1Ø	Ø.1796(5)	-Ø.148(1)	Ø.15Ø7(6)	17.6(4)
C11	Ø.32ØØ(3)	-Ø.1422(7)	Ø.Ø667(3)	5.1(2)
C12	Ø.2855(3)	-Ø.Ø8Ø1(7)	Ø.Ø221(3)	4.4(2)
C13	Ø.3131(3)	-Ø.Ø414(8)	-Ø.Ø159(3)	4.8(2)
C14	Ø.3648(3)	-Ø.Ø791(7)	Ø.ØØ52(4)	5.4(2)
C15	Ø.3684(3)	-Ø.1444(7)	Ø.Ø56Ø(4)	5.3(2)
C16	Ø.3Ø52(4)	-Ø.2Ø59(9)	Ø.1157(4)	7.6(3)
C17	Ø.2278(3)	-Ø.Ø677(8)	Ø.Ø144(4)	5.9(2)
C18	Ø.2912(4)	Ø.Ø244(8)	-Ø.Ø7Ø8(4)	6.6(2)
C19	Ø.4Ø76(4)	-Ø.Ø621(9)	-Ø.Ø235(4)	7.5(3)
C2Ø	Ø.414Ø(4)	-Ø.2247(9)	Ø.Ø865(4)	7.7(3)
C21	Ø.3826(3)	Ø.2866(8)	Ø.1448(4)	6.3(2)
C22	Ø.3798(3)	Ø.1771(9)	Ø.1763(4)	6.2(2)
C23	Ø.416Ø(3)	Ø.Ø883(8)	Ø.1695(4)	5.8(2)
C24	Ø.4421(3)	Ø.1431(8)	Ø.1325(4)	5.8(2)
C25	Ø.4219(3)	Ø.2663(8)	Ø.1172(4)	6.Ø(2)
C26	Ø.3513(5)	Ø.4Ø8(1)	Ø.1453(6)	11.2(4)
C27	Ø.3461(5)	Ø.164(2)	Ø.2172(5)	12.2(4)
C28	Ø.4311(5)	-Ø.Ø35(1)	Ø.2Ø46(5)	1Ø.8(4)
C29	Ø.4897(4)	Ø.Ø88(1)	Ø.12ØØ(5)	11.7(4)
C3Ø	Ø.4388(5)	Ø.363(1)	Ø.Ø828(5)	11.2(4)
C31	Ø.5ØØ	Ø.368Ø(2)	Ø.25Ø	11.6(3)*
C32	Ø.4635(1)	Ø.4Ø34(2)	Ø.28Ø1(1)	11.6*
C33	Ø.45148(8)	Ø.5366(4)	Ø.2853(1)	11.6*
C34	Ø.4793(2)	Ø.6316(2)	Ø.2656(2)	11.6*

Table of Positional Parameters and Their Estimated Standard Deviations (cont.)

Atom	x	y	z	$B(A^2)$
C35	Ø.518ØØ(9)	Ø.595Ø(2)	Ø.2389(1)	11.6*
C36	Ø.52798(6)	Ø.4618(2)	Ø.2315Ø(9)	11.6*
C37	Ø.5684(3)	Ø.4234(3)	Ø.2Ø26(4)	19(1)*

* -- Atoms refined with isotropic thermal parameters.

Anisotropically refined atoms are given in the form of the isotropic equivalent thermal parameter defined as:

$$(4/3) * [a^2*B(1,1) + b^2*B(2,2) + c^2*B(3,3) + ab(\cos \text{gamma})*B(1,2) + ac(\cos \text{beta})*B(1,3) + bc(\cos \text{alpha})*B(2,3)]$$

Table of Positional Parameters and Their Estimated Standard Deviations (cont.)

Atom	x	y	z	$B(A^2)$
H161	0.2959	-0.2945	0.1087	10.0**
H162	0.3335	-0.2027	0.1495	10.0**
H163	0.2766	-0.1617	0.1253	10.0**
H171	0.2098	-0.1388	-0.0046	10.0**
H172	0.2200	-0.0599	0.0508	10.0**
H173	0.2149	0.0114	-0.0059	10.0**
H181	0.2805	-0.0397	-0.1002	10.0**
H182	0.2626	0.0764	-0.0696	10.0**
H183	0.3169	0.0777	-0.0811	10.0**
H191	0.4100	-0.1339	-0.0472	10.0**
H192	0.4031	0.0157	-0.0462	10.0**
H193	0.4406	-0.0535	0.0036	10.0**
H201	0.4125	-0.3095	0.0710	10.0**
H202	0.4463	-0.1851	0.0822	10.0**
H203	0.4162	-0.2294	0.1252	10.0**
H261	0.3684	0.4656	0.1747	15.0**
H262	0.3440	0.4514	0.1108	15.0**
H263	0.3182	0.3856	0.1535	15.0**
H271	0.3625	0.1944	0.2534	15.0**
H272	0.3144	0.2140	0.2038	15.0**
H273	0.3354	0.0751	0.2201	15.0**
H281	0.4572	-0.0136	0.2384	15.0**
H282	0.4021	-0.0693	0.2157	15.0**
H283	0.4445	-0.0985	0.1846	15.0**
H291	0.5206	0.1128	0.1478	15.0**
H292	0.4895	-0.0079	0.1205	15.0**
H293	0.4938	0.1128	0.0841	15.0**
H301	0.4659	0.4149	0.1040	15.0**
H302	0.4508	0.3210	0.0532	15.0**
H303	0.4107	0.4188	0.0648	15.0**
CP1	0.1387	0.0987	0.1362	
CP2	0.3304	-0.0974	0.0268	
CP3	0.4085	0.1923	0.1481	

** -- Atoms included but not refined.

Table of General Temperature Factor Expressions - B's (Continued)

Name	B(1,1)	B(2,2)	B(3,3)	B(1,2)	B(1,3)	B(2,3)	Beqv
C15	5.2(4)	4.Ø(3)	6.7(4)	Ø.8(3)	1.8(3)	-Ø.1(3)	5.3(2)
C16	9.2(5)	5.7(4)	8.5(5)	-1.4(4)	3.2(4)	Ø.4(4)	7.6(3)
C17	4.2(3)	5.5(4)	8.1(5)	-Ø.1(3)	1.7(3)	-1.5(4)	5.9(2)
C18	8.1(5)	5.Ø(4)	6.Ø(5)	-Ø.5(4)	Ø.8(4)	-Ø.9(4)	6.6(2)
C19	7.5(4)	6.8(5)	9.3(5)	-Ø.5(4)	4.3(4)	-1.1(4)	7.5(3)
C2Ø	8.Ø(5)	5.4(4)	9.1(6)	2.8(4)	1.Ø(5)	-Ø.4(4)	7.7(3)
C21	5.6(4)	4.2(3)	7.1(5)	Ø.2(3)	-2.Ø(4)	-1.3(4)	6.3(2)
C22	4.3(3)	9.Ø(5)	5.2(4)	-1.1(4)	1.4(3)	-1.6(4)	6.2(2)
C23	5.6(4)	5.5(4)	5.3(4)	-Ø.Ø(3)	-Ø.3(4)	Ø.6(3)	5.8(2)
C24	3.5(3)	7.3(5)	6.6(4)	-Ø.Ø(3)	1.2(3)	-Ø.7(4)	5.8(2)
C25	5.6(4)	5.8(4)	6.Ø(4)	-2.2(3)	Ø.1(4)	1.Ø(4)	6.Ø(2)
C26	9.8(7)	7.8(6)	12.6(8)	2.Ø(5)	-3.9(6)	-3.7(5)	11.2(4)
C27	8.9(7)	2Ø(1)	7.9(6)	-2.2(8)	2.3(5)	-4.3(7)	12.2(4)
C28	13.4(9)	8.6(6)	7.7(6)	-Ø.9(7)	-2.8(6)	2.3(5)	1Ø.8(4)
C29	4.4(4)	19(1)	12.2(8)	Ø.8(6)	2.6(5)	-4.1(7)	11.7(4)
C3Ø	11.Ø(7)	12.2(7)	8.4(6)	-6.1(5)	-1.7(6)	3.4(5)	11.2(4)

The form of the anisotropic thermal parameter is:

$$\exp[-Ø.25(h^2 a^{*2} B(1,1) + k^2 b^{*2} B(2,2) + l^2 c^{*2} B(3,3) + 2hka^*b^*B(1,2) + 2hla^*c^*B(1,3) + 2klb^*c^*B(2,3))]$$, where a*,b*, and c* are reciprocal lattice constants.

Table of General Temperature Factor Expressions - B's

Name	B(1,1)	B(2,2)	B(3,3)	B(1,2)	B(1,3)	B(2,3)	Beqv
YB1	3.48(1)	5.62(2)	4.38(1)	-Ø.Ø7(1)	1.46(1)	Ø.13(1)	4.411(8)
YB2	3.18(1)	3.81(1)	4.73(1)	Ø.29(1)	Ø.85(1)	-Ø.Ø5(1)	3.932(7)
F1	3.7(2)	5.8(2)	6.9(2)	Ø.3(2)	1.4(2)	-1.6(2)	5.4(1)
F2	6.2(2)	4.7(2)	5.1(2)	-Ø.2(2)	Ø.8(2)	Ø.7(2)	5.4(1)
C1	7.5(4)	32(1)	3.6(4)	-1Ø.(6)	1.7(4)	-Ø.9(7)	14.3(4)
C2	13.4(5)	11.1(6)	1Ø.2(5)	-6.1(5)	8.9(4)	-5.1(5)	1Ø.5(3)
C3	6.2(4)	8.1(5)	8.4(4)	1.2(4)	5.Ø(3)	1.4(4)	7.Ø(2)
C4	7.3(4)	6.5(4)	7.4(4)	-2.2(4)	4.6(3)	-Ø.9(4)	6.6(2)
C5	5.6(3)	14.2(6)	1Ø.4(4)	4.4(4)	5.4(3)	8.4(4)	9.5(3)
C6	11.6(7)	65(3)	6.6(7)	-1(1)	Ø.1(6)	6(1)	28.Ø(9)
C7	5Ø(1)	12.1(7)	23.5(7)	-15.(8)	3Ø.Ø(6)	-11.(6)	24.9(5)
C8	8.2(5)	2Ø(1)	23(1)	7.7(6)	9.1(5)	11.1(8)	15.9(4)
C9	15.8(7)	16.2(8)	14.7(7)	-1Ø.(6)	1Ø.Ø(5)	-6.4(7)	14.5(4)
C1Ø	18.1(7)	16.6(8)	24.2(8)	1Ø.5(6)	16.5(5)	13.8(6)	17.6(4)
C11	5.9(3)	3.2(3)	7.2(4)	Ø.2(3)	3.4(3)	Ø.2(3)	5.1(2)
C12	4.1(3)	3.8(3)	5.4(4)	-Ø.4(3)	1.2(3)	-1.2(3)	4.4(2)
C13	5.5(4)	4.7(3)	4.4(3)	Ø.2(3)	1.5(3)	-Ø.9(3)	4.8(2)
C14	5.Ø(3)	4.2(4)	7.7(4)	Ø.Ø(3)	3.1(3)	-1.Ø(3)	5.4(2)

Values of Fobs and Fcalc (x20.)

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
-28	0	2	1674	1635	68	-26	2	1	2005	1921	63	-25	3	2	2798	2828	42	-24	2	13	497*	253	569
-28	0	4	432*	156	506	-26	2	2	663*	144	427	-25	3	3	630*	62	111	-24	2	14	1208	1226	96
-28	0	6	1323	1252	67	-26	2	3	4704	4868	48	-25	3	4	3729	3748	37	-24	2	15	3405	3363	56
-28	0	8	1374	1438	65	-26	2	4	388*	607	700	-25	3	5	2328	2524	42	-24	2	16	1057	1032	123
-28	0	10	0*	501	4240	-26	2	5	4106	4142	38	-25	3	6	1400	1422	59	-24	2	17	3588	3615	55
-28	0	12	980	1022	95	-26	2	6	460*	558	159	-25	3	7	2499	2688	43	-24	2	18	775*	289	421
-28	2	3	1132	1163	101	-26	2	7	0*	228	4102	-25	3	8	2263	2252	48	-24	4	1	1475	1522	61
-28	2	4	1572	1544	76	-26	2	8	0*	166	4095	-25	3	9	490*	500	167	-24	4	2	736	867	100
-28	2	5	1231	1270	84	-26	2	9	4534	4484	47	-25	3	10	3688	3671	42	-24	4	3	1017	938	71
-28	2	6	915	1020	97	-26	2	10	0*	636	4672	-25	3	11	1639	1759	67	-24	4	4	2143	2119	45
-28	2	7	0*	504	4696	-26	2	11	4517	4401	47	-25	3	12	2191	2021	58	-24	4	5	2314	2240	44
-28	2	8	404*	373	662	-26	2	12	560*	827	667	-25	3	13	2396	2307	56	-24	4	6	3243	3254	38
-28	2	9	841	760	129	-26	2	13	997	967	131	-25	3	14	1011	935	112	-24	4	7	1603	1594	54
-28	2	10	1795	1763	77	-26	2	14	0*	287	4293	-25	3	15	1322	1285	93	-24	4	8	1477	1431	57
-27	1	1	2872	2804	59	-26	2	15	2827	2818	62	-25	3	16	2900	2862	57	-24	4	9	0*	360	3731
-27	1	2	1728	1611	77	-26	2	16	0*	270	4164	-25	5	1	2192	2245	51	-24	4	10	1332	1281	68
-27	1	3	1074	616	100	-26	4	1	329*	655	717	-25	5	2	1377	1344	65	-24	4	11	2088	2083	54
-27	1	4	2579	2625	57	-26	4	2	2097	2124	51	-25	5	3	182*	827	1304	-24	4	12	2895	2785	47
-27	1	5	1973	1781	56	-26	4	3	840	692	95	-25	5	4	720	778	109	-24	4	13	2193	2119	54
-27	1	6	1747	1620	57	-26	4	4	256*	336	906	-25	5	5	1442	1450	64	-24	4	14	2281	2215	57
-27	1	7	2736	2836	43	-26	4	5	441*	86	510	-25	5	6	0*	400	4675	-24	4	15	0*	263	4157
-27	1	8	0*	606	4067	-26	4	6	2872	2897	43	-25	5	7	2401	2381	47	-24	4	16	0*	116	4338
-27	1	9	1392	1444	77	-26	4	7	968	730	87	-25	5	8	1331	1283	68	-24	6	3	1232	1193	71
-27	1	10	2452	2372	54	-26	4	8	3163	3140	43	-25	5	9	1304	1249	70	-24	6	4	2080	2078	50
-27	1	11	532*	1310	712	-26	4	9	1149	1148	81	-25	5	10	1361	1247	67	-24	6	5	0*	116	4481
-27	1	12	2097	2068	66	-26	4	10	609*	555	400	-25	5	11	0*	723	5032	-24	6	6	0*	172	1521
-27	1	13	2641	2726	61	-26	4	11	279*	435	908	-24	0	2	2356	2370	44	-24	6	7	1469	1421	64
-27	1	14	510*	110	232	-26	4	12	2153	2233	60	-24	0	4	2300	2407	43	-24	6	8	2031	2033	52
-27	3	1	2115	2102	56	-25	1	1	3863	3717	48	-24	0	6	5848	6032	60	-23	1	1	1560	1641	75
-27	3	2	1987	2029	57	-25	1	2	3353	3180	49	-24	0	8	3633	3666	38	-23	1	2	1784	1738	66
-27	3	3	1932	1973	57	-25	1	3	761*	621	132	-24	0	10	503*	1286	417	-23	1	3	0*	305	3655
-27	3	4	2178	2060	50	-25	1	4	3939	3819	44	-24	0	12	4414	4451	43	-23	1	4	1145	998	81
-27	3	5	407*	192	544	-25	1	5	3513	3626	42	-24	0	14	4231	4223	41	-23	1	5	2272	2291	44
-27	3	6	494*	565	163	-25	1	6	507*	784	428	-24	0	16	894	806	117	-23	1	6	1135	1213	64
-27	3	7	1712	1672	56	-25	1	7	4839	5014	47	-24	0	18	2705	2820	57	-23	1	7	2952	3060	44
-27	3	8	1846	1787	59	-25	1	8	3152	3259	43	-24	2	1	3164	3235	44	-23	1	8	2381	2376	51
-27	3	9	2212	2149	55	-25	1	9	1911	1914	60	-24	2	2	1444	1427	68	-23	1	9	1343	1363	83
-27	3	10	2682	2682	51	-25	1	10	4003	3974	44	-24	2	3	5228	5193	51	-23	1	10	1594	1615	74
-27	3	11	766*	928	139	-25	1	11	2259	2265	59	-24	2	4	609*	938	403	-23	1	11	837	835	130
-26	0	2	3368	3222	44	-25	1	12	1896	1734	66	-24	2	5	2963	3083	37	-23	1	12	0*	149	3332
-26	0	4	1624	1549	57	-25	1	13	4101	4080	49	-24	2	6	270*	574	243	-23	1	13	2308	2347	59
-26	0	6	5283	5377	57	-25	1	14	1384	1265	92	-24	2	7	2284	2362	45	-23	1	14	1351	1305	81
-26	0	8	4618	4783	45	-25	1	15	2678	2685	60	-24	2	8	1963	1990	53	-23	1	15	1641	1507	73
-26	0	10	317*	155	613	-25	1	16	3180	3092	56	-24	2	9	4815	4733	50	-23	1	16	1589	1621	76
-26	0	12	3820	3893	43	-25	1	17	662*	761	188	-24	2	10	1636	1712	70	-23	1	17	0*	497	3328
-26	0	14	4526	4524	49	-25	1	18	2191	2182	72	-24	2	11	3378	3264	49	-23	1	18	680*	700	164
-26	0	16	1690	1586	72	-25	3	1	1920	1904	55	-24	2	12	376*	39	712	-23	1	19	1505	1610	80

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
-23	1	20	751*	629	148	-22	2	3	413*	802	546	-22	6	12	534*	691	168	-21	5	3	2789	2779	38
-23	3	1	1303	1431	62	-22	2	4	1584	1595	51	-22	6	13	1445	1592	69	-21	5	4	3611	3642	35
-23	3	2	1380	1382	55	-22	2	5	539*	734	352	-22	6	14	2455	2400	53	-21	5	5	2104	2185	44
-23	3	3	3367	3476	35	-22	2	6	1301	1333	61	-21	1	1	1556	1452	79	-21	5	6	3344	3343	36
-23	3	4	2963	2994	37	-22	2	7	0*	186	4001	-21	1	2	3202	3130	49	-21	5	7	0*	210	3835
-23	3	5	2623	2530	38	-22	2	8	3160	3245	42	-21	1	3	2254	2289	57	-21	5	8	0*	381	3585
-23	3	6	1820	1869	48	-22	2	9	189*	487	1430	-21	1	4	2602	2594	49	-21	5	9	1550	1511	54
-23	3	7	536*	341	320	-22	2	10	3051	3007	47	-21	1	5	3469	3408	36	-21	5	10	2880	2904	41
-23	3	8	491*	256	400	-22	2	11	0*	151	1198	-21	1	6	0*	503	3727	-21	5	11	1445	1388	61
-23	3	9	2611	2634	42	-22	2	12	791	615	123	-21	1	7	1806	1830	60	-21	5	12	3682	3759	41
-23	3	10	2355	2327	47	-22	2	13	0*	117	3700	-21	1	8	2964	2971	50	-21	5	13	0*	130	4339
-23	3	11	2362	2304	49	-22	2	14	1744	1758	67	-21	1	9	1775	1762	70	-21	5	14	1596	1574	62
-23	3	12	2521	2563	49	-22	2	15	0*	139	3100	-21	1	10	2340	2312	59	-21	5	15	1198	1256	86
-23	3	13	402*	382	225	-22	2	16	2016	1757	60	-21	1	11	3002	3052	52	-21	5	16	1316	1253	78
-23	3	14	0*	252	4136	-22	2	17	226*	57	1415	-21	1	12	753*	813	145	-21	5	17	1524	1546	79
-23	3	15	1415	1410	77	-22	2	18	452*	585	714	-21	1	13	2244	2413	62	-21	5	18	2468	2340	56
-23	3	16	1961	1856	64	-22	2	19	0*	261	1339	-21	1	14	1195	1137	91	-21	7	1	3145	3103	42
-23	3	17	2143	2016	63	-22	2	20	720*	543	158	-21	1	15	0*	59	3465	-21	7	2	0*	183	4642
-23	3	18	1847	1752	76	-22	4	1	2752	2681	39	-21	1	16	2181	2244	57	-21	7	3	2722	2798	44
-23	3	19	1205	1237	101	-22	4	2	1128	1123	60	-21	1	17	1898	1904	64	-21	7	4	1086	1003	75
-23	5	1	2429	2410	44	-22	4	3	1487	1549	51	-21	1	18	907	952	114	-21	7	5	0*	192	4194
-23	5	2	1470	1448	58	-22	4	4	0*	489	3903	-21	1	19	1709	1721	67	-21	7	6	1160	1185	77
-23	5	3	1704	1759	51	-22	4	5	4120	4258	41	-21	1	20	663*	746	437	-21	7	7	2451	2442	47
-23	5	4	1957	1967	47	-22	4	6	711	695	97	-21	1	21	0*	264	4135	-21	7	8	604*	334	133
-23	5	5	0*	398	4003	-22	4	7	3209	3217	38	-21	1	22	1318	1358	92	-21	7	9	3282	3184	42
-23	5	6	3920	3892	37	-22	4	8	1184	1150	64	-21	3	1	4233	4325	41	-21	7	10	326*	573	685
-23	5	7	1722	1698	53	-22	4	9	533*	171	123	-21	3	2	2841	2943	37	-21	7	11	1397	1490	71
-23	5	8	2596	2642	44	-22	4	10	591*	661	388	-21	3	3	2200	2242	41	-20	0	2	860	816	87
-23	5	9	1390	1379	65	-22	4	11	3513	3484	39	-21	3	4	579*	53	314	-20	0	4	6930	7076	70
-23	5	10	184*	616	1260	-22	4	12	0*	188	4025	-21	3	5	1697	1602	48	-20	0	6	7974	8133	77
-23	5	11	0*	65	1511	-22	4	13	3593	3563	41	-21	3	6	2703	2717	39	-20	0	8	2258	2260	42
-23	5	12	3158	3095	45	-22	4	14	395*	449	691	-21	3	7	2905	3104	38	-20	0	10	4057	4138	39
-23	5	13	1638	1642	68	-22	4	15	755*	758	130	-21	3	8	3266	3362	38	-20	0	12	5949	6083	62
-23	5	14	2656	2649	50	-22	4	16	588*	652	527	-21	3	9	1993	1849	48	-20	0	14	3165	3163	44
-23	5	15	2130	2014	58	-22	4	17	1648	1759	76	-21	3	10	806	580	100	-20	0	16	2622	2726	52
-22	0	2	624*	478	118	-22	4	18	0*	266	4343	-21	3	11	0*	214	3479	-20	0	18	5159	5265	52
-22	0	4	1432	1339	54	-22	6	1	888	901	93	-21	3	12	1973	2118	56	-20	0	20	3352	3267	49
-22	0	6	1347	1086	53	-22	6	2	4063	4057	40	-21	3	13	2723	2781	47	-20	0	22	392*	251	258
-22	0	8	0*	31	3665	-22	6	3	0*	611	4778	-21	3	14	2457	2479	52	-20	2	1	6725	6806	72
-22	0	10	734	763	111	-22	6	4	2817	2813	44	-21	3	15	3003	2942	46	-20	2	2	1438	1404	60
-22	0	12	0*	276	3717	-22	6	5	1724	1712	54	-21	3	16	1181	949	82	-20	2	3	6475	6786	66
-22	0	14	0*	620	1169	-22	6	6	1017	1011	81	-21	3	17	855	866	117	-20	2	4	0*	676	3731
-22	0	16	582*	583	449	-22	6	7	1631	1615	58	-21	3	18	864	623	127	-20	2	5	1145	1010	60
-22	0	18	377*	474	730	-22	6	8	3932	3917	39	-21	3	19	939	861	123	-20	2	6	0*	52	3767
-22	0	20	111*	26	924	-22	6	9	0*	289	4495	-21	3	20	1666	1568	80	-20	2	7	5146	4998	52
-22	2	1	316*	300	736	-22	6	10	3727	3726	41	-21	5	1	531*	810	342	-20	2	8	1381	1200	67
-22	2	2	2833	2966	42	-22	6	11	1405	1349	70	-21	5	2	997	949	69	-20	2	9	6220	6184	62

Reflections flagged with an asterisk were considered unobserved.

Values of Fobs and Fcalc (x20.)

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
-20	2	10	2009	2079	59	-20	6	15	1256	1158	80	-19	5	1	891	1006	81	-18	2	3	4888	4993	49
-20	2	11	2692	2495	49	-20	6	16	1518	1567	72	-19	5	2	2124	2054	41	-18	2	4	1001	858	56
-20	2	12	1217	1115	92	-19	1	1	1133	1105	95	-19	5	3	2019	2056	41	-18	2	5	1186	1222	55
-20	2	13	2663	2450	52	-19	1	2	5561	5423	54	-19	5	4	703	714	93	-18	2	6	2447	2347	37
-20	2	14	413*	927	836	-19	1	3	4264	4198	43	-19	5	5	3747	3798	40	-18	2	7	7140	7178	73
-20	2	15	5816	5946	58	-19	1	4	2595	2489	47	-19	5	6	1041	987	67	-18	2	8	1624	1610	56
-20	2	16	1393	1485	86	-19	1	5	6973	7132	69	-19	5	7	2087	2093	42	-18	2	9	6825	6710	66
-20	2	17	3344	3388	50	-19	1	6	3312	3257	44	-19	5	8	2102	2123	44	-18	2	10	0*	453	1160
-20	2	18	0*	365	3496	-19	1	7	4307	4201	46	-19	5	9	939	945	80	-18	2	11	1300	1375	77
-20	2	19	625*	692	160	-19	1	8	6266	6363	58	-19	5	10	1660	1708	50	-18	2	12	1232	1363	85
-20	2	20	0*	354	3790	-19	1	9	1976	1841	62	-19	5	11	2999	2902	40	-18	2	13	5058	5127	51
-20	2	21	2897	2795	56	-19	1	10	4620	4525	47	-19	5	12	253*	41	779	-18	2	14	1683	1503	73
-20	2	22	561*	665	200	-19	1	11	5961	6023	62	-19	5	13	2714	2660	42	-18	2	15	6983	6953	71
-20	4	1	1695	1787	49	-19	1	12	395*	234	752	-19	5	14	1050	1096	80	-18	2	16	0*	232	3748
-20	4	2	0*	180	3940	-19	1	13	5366	5274	49	-19	5	15	0*	106	1237	-18	2	17	3061	3148	51
-20	4	3	425*	561	153	-19	1	14	3934	4005	45	-19	5	16	911	957	96	-18	2	18	0*	714	3655
-20	4	4	3928	3901	35	-19	1	15	402*	140	271	-19	5	17	2035	1999	59	-18	2	19	1755	1900	69
-20	4	5	2528	2481	38	-19	1	16	3762	3777	46	-19	5	18	0*	136	4340	-18	2	20	817	898	128
-20	4	6	4187	4095	43	-19	1	17	4171	4435	44	-19	5	19	2162	2022	59	-18	2	21	3791	3759	49
-20	4	7	2449	2529	40	-19	1	18	517*	301	182	-19	7	1	269*	78	240	-18	2	22	766*	565	435
-20	4	8	1094	1125	69	-19	1	19	3903	3861	45	-19	7	2	0*	350	3746	-18	2	23	2503	2678	61
-20	4	9	617*	563	116	-19	1	20	2429	2531	53	-19	7	3	681	752	99	-18	4	1	0*	457	3447
-20	4	10	2208	2224	45	-19	1	21	1281	1127	85	-19	7	4	0*	514	1354	-18	4	2	1972	1986	41
-20	4	11	1285	1265	68	-19	1	22	2869	2903	57	-19	7	5	1020	1021	71	-18	4	3	2778	2812	34
-20	4	12	3638	3629	40	-19	1	23	1494	1461	85	-19	7	6	0*	140	1317	-18	4	4	3962	3980	39
-20	4	13	1808	1876	58	-19	3	1	1105	1081	67	-19	7	7	750	556	90	-18	4	5	2632	2642	35
-20	4	14	2409	2360	49	-19	3	2	5331	5412	55	-19	7	8	0*	462	4092	-18	4	6	3160	3182	33
-20	4	15	928	753	93	-19	3	3	2709	2714	35	-19	7	9	569*	50	346	-18	4	7	464*	201	435
-20	4	16	450*	743	570	-19	3	4	2677	2779	35	-19	7	10	532*	357	139	-18	4	8	0*	128	3335
-20	4	17	792	952	122	-19	3	5	3955	4032	38	-19	7	11	0*	550	4220	-18	4	9	2059	2095	45
-20	4	18	2303	2263	57	-19	3	6	2048	2019	42	-19	7	12	0*	177	3971	-18	4	10	3913	3801	36
-20	4	19	1527	1539	81	-19	3	7	1938	1891	44	-19	7	13	544*	313	411	-18	4	11	3495	3365	37
-20	4	20	1802	1763	70	-19	3	8	5112	5014	53	-19	7	14	240*	621	385	-18	4	12	4453	4468	43
-20	6	1	1376	1257	54	-19	3	9	1610	1483	55	-18	0	2	2307	2376	34	-18	4	13	1183	1279	75
-20	6	2	1883	1937	47	-19	3	10	3507	3493	38	-18	0	4	7941	8099	73	-18	4	14	1387	1428	67
-20	6	3	2244	2234	42	-19	3	11	3732	3905	42	-18	0	6	7561	7776	64	-18	4	15	1521	1548	62
-20	6	4	967	995	73	-19	3	12	0*	616	3858	-18	0	8	695	778	94	-18	4	16	2274	2209	50
-20	6	5	612*	1072	351	-19	3	13	3357	3260	43	-18	0	10	5808	6015	56	-18	4	17	1518	1527	67
-20	6	6	807	904	87	-19	3	14	4779	4670	47	-18	0	12	6986	7058	69	-18	4	18	2943	2938	48
-20	6	7	824	875	84	-19	3	15	0*	739	3500	-18	0	14	1790	1896	62	-18	4	19	499*	584	198
-20	6	8	2330	2399	44	-19	3	16	3618	3630	44	-18	0	16	3411	3588	45	-18	4	20	1196	1227	93
-20	6	9	2108	2148	46	-19	3	17	2052	2147	59	-18	0	18	5347	5401	55	-18	4	21	704*	595	150
-20	6	10	2016	2027	48	-19	3	18	389*	75	245	-18	0	20	3353	3304	48	-18	6	1	2285	2284	40
-20	6	11	1799	1824	53	-19	3	19	2055	2143	63	-18	0	22	432*	676	601	-18	6	2	2943	2977	36
-20	6	12	0*	174	4082	-19	3	20	2132	2063	67	-18	0	24	3100	3162	56	-18	6	3	1135	1094	60
-20	6	13	568*	297	390	-19	3	21	686*	615	160	-18	2	1	7109	7131	74	-18	6	4	1041	1102	66
-20	6	14	1354	1352	72	-19	3	22	2490	2519	64	-18	2	2	1429	1416	50	-18	6	5	1140	1071	60

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
-18	6	6	1712	1597	46	-17	1	24	496*	348	581	-17	7	3	3211	3269	36	-16	2	22	1448	1397	76
-18	6	7	2873	2905	37	-17	3	1	4155	4140	41	-17	7	4	1965	1894	44	-16	2	23	898	585	111
-18	6	8	2387	2445	41	-17	3	2	3910	3945	38	-17	7	5	544*	491	121	-16	2	24	0*	43	3860
-18	6	9	1969	2069	47	-17	3	3	3853	3984	41	-17	7	6	938	1004	76	-16	4	1	369*	482	152
-18	6	10	1350	1334	57	-17	3	4	3404	3356	35	-17	7	7	3217	3231	38	-16	4	2	1425	1375	45
-18	6	11	534*	206	124	-17	3	5	641	681	89	-17	7	8	765	648	91	-16	4	3	5616	5811	61
-18	6	12	955	1013	85	-17	3	6	251*	253	667	-17	7	9	3579	3599	37	-16	4	4	0*	260	3384
-18	6	13	1663	1678	54	-17	3	7	2600	2628	36	-17	7	10	1662	1605	53	-16	4	5	6027	5912	55
-18	6	14	2076	2221	51	-17	3	8	3073	3146	34	-17	7	11	626*	728	344	-16	4	6	827	1015	75
-18	6	15	1368	1386	73	-17	3	9	4575	4717	48	-17	7	12	1279	1338	66	-16	4	7	1619	1577	45
-18	6	16	1261	1287	81	-17	3	10	3987	3874	39	-17	7	13	2475	2478	47	-16	4	8	1095	1112	62
-18	6	17	202*	280	1268	-17	3	11	3066	2923	39	-17	7	14	0*	36	4372	-16	4	9	4031	3883	40
-18	6	18	0*	362	4577	-17	3	12	1387	1400	69	-17	7	15	3161	3077	46	-16	4	10	952	783	76
-18	8	1	661*	765	112	-17	3	13	1083	1092	84	-17	7	16	1243	1186	80	-16	4	11	5622	5641	57
-18	8	2	991	901	77	-17	3	14	2658	2631	47	-16	0	2	1876	1718	33	-16	4	12	652*	66	330
-18	8	3	1255	1249	64	-17	3	15	2661	2667	48	-16	0	4	1768	1768	29	-16	4	13	2517	2501	44
-18	8	4	0*	438	4325	-17	3	16	3801	3689	43	-16	0	6	270*	146	157	-16	4	14	704*	542	119
-18	8	5	2135	2093	47	-17	3	17	2055	2043	56	-16	0	8	0*	427	2560	-16	4	15	2070	1989	51
-18	8	6	0*	86	4377	-17	3	18	1465	1476	73	-16	0	10	476*	375	397	-16	4	16	0*	465	3889
-18	8	7	905	965	91	-17	3	19	0*	500	3439	-16	0	12	565*	137	397	-16	4	17	3860	3931	41
-18	8	8	450*	539	535	-17	3	20	945	959	113	-16	0	14	0*	532	3307	-16	4	18	693*	438	368
-18	8	9	503*	593	152	-17	3	21	1334	1313	88	-16	0	16	371*	662	268	-16	4	19	2451	2387	51
-18	8	10	566*	592	144	-17	3	22	1975	2063	72	-16	0	18	739*	926	133	-16	4	20	0*	180	3330
-18	8	11	1589	1575	63	-17	3	23	1656	1563	75	-16	0	20	1206	1291	80	-16	4	21	0*	570	3682
-17	1	1	481*	703	172	-17	5	1	2525	2565	37	-16	0	22	0*	50	3467	-16	4	22	629*	614	494
-17	1	2	2779	2893	43	-17	5	2	1069	1077	65	-16	0	24	0*	664	4184	-16	6	1	0*	245	4045
-17	1	3	3034	3048	38	-17	5	3	350*	414	186	-16	2	1	0*	333	2592	-16	6	2	5730	5723	56
-17	1	4	0*	370	2936	-17	5	4	4375	4455	45	-16	2	2	3389	3396	34	-16	6	3	2366	2352	39
-17	1	5	5187	5059	48	-17	5	5	2397	2378	38	-16	2	3	1101	1090	44	-16	6	4	690	747	100
-17	1	6	3337	3257	40	-17	5	6	3907	3860	39	-16	2	4	945	957	49	-16	6	5	2676	2617	37
-17	1	7	2649	2644	45	-17	5	7	2972	2961	36	-16	2	5	1837	1830	34	-16	6	6	4292	4364	42
-17	1	8	3680	3563	40	-17	5	8	357*	439	191	-16	2	6	3351	3345	32	-16	6	7	506*	613	409
-17	1	9	322*	1307	848	-17	5	9	618*	603	117	-16	2	7	1067	939	58	-16	6	8	5562	5554	56
-17	1	10	677*	889	142	-17	5	10	3289	3312	37	-16	2	8	3642	3677	35	-16	6	9	1716	1641	50
-17	1	11	3669	3516	42	-17	5	11	2047	2136	48	-16	2	9	429*	273	451	-16	6	10	2172	2146	43
-17	1	12	2194	2318	54	-17	5	12	4164	4091	42	-16	2	10	2353	2231	41	-16	6	11	2417	2399	43
-17	1	13	3359	3366	44	-17	5	13	3112	3251	40	-16	2	11	607*	866	136	-16	6	12	2806	2926	41
-17	1	14	2480	2311	51	-17	5	14	1360	1312	64	-16	2	12	1923	1811	53	-16	6	13	567*	958	426
-17	1	15	458*	273	219	-17	5	15	1549	1535	59	-16	2	13	319*	262	819	-16	6	14	4621	4729	49
-17	1	16	1019	1035	106	-17	5	16	1550	1566	62	-16	2	14	3972	4024	43	-16	6	15	498*	340	454
-17	1	17	2705	2702	51	-17	5	17	656*	915	371	-16	2	15	436*	586	649	-16	6	16	2792	2783	46
-17	1	18	287*	615	1059	-17	5	18	2647	2681	50	-16	2	16	2111	1955	60	-16	6	17	1337	1236	73
-17	1	19	3460	3478	45	-17	5	19	2163	2126	57	-16	2	17	1194	1092	94	-16	6	18	712*	678	129
-17	1	20	2102	2035	57	-17	5	20	1845	1754	65	-16	2	18	945	1061	115	-16	6	19	1048	1214	103
-17	1	21	1345	1276	75	-17	5	21	1459	1478	80	-16	2	19	360*	271	666	-16	8	1	0*	630	3801
-17	1	22	1731	1778	65	-17	7	1	4153	4219	43	-16	2	20	2194	2309	56	-16	8	2	1751	1839	49
-17	1	23	1167	1100	91	-17	7	2	867	833	79	-16	2	21	740*	1129	400	-16	8	3	3628	3616	39

Reflections flagged with an asterisk were considered unobserved.

Values of Fobs and Fclc (x20.)

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
-16	8	4	135*	250	521	-15	3	12	4305	4389	42	-15	7	13	3666	3685	40	-14	2	20	1506	1562	72
-16	8	5	3554	3541	37	-15	3	13	4333	4452	46	-15	7	14	496*	112	461	-14	2	21	3448	3479	46
-16	8	6	1419	1467	57	-15	3	14	3255	3277	41	-15	7	15	3191	3106	45	-14	2	22	1057	1158	97
-16	8	7	954	940	76	-15	3	15	2032	2010	55	-15	7	16	1117	1067	82	-14	2	23	846	1016	120
-16	8	8	2028	1944	48	-15	3	16	1030	1362	98	-15	7	17	0*	517	4241	-14	2	24	0*	146	3713
-16	8	9	2161	2137	47	-15	3	17	944	854	106	-15	7	18	1162	1240	90	-14	2	25	1395	1401	84
-16	8	10	886	799	94	-15	3	18	3236	3309	46	-15	9	1	211*	377	348	-14	4	1	0*	73	2680
-16	8	11	3392	3430	43	-15	3	19	2286	2428	55	-15	9	2	2336	2355	45	-14	4	2	2771	2955	32
-16	8	12	988	904	87	-15	3	20	1673	1694	66	-15	9	3	553*	531	143	-14	4	3	3053	3071	31
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-16	8	14	1539	1625	68	-15	3	22	442*	140	685	-15	9	5	917	864	92	-14	4	5	4429	4536	44
-15	1	1	2070	2103	40	-15	3	23	0*	94	3714	-15	9	6	1932	1935	51	-14	4	6	3228	3136	31
-15	1	2	3660	3693	34	-15	3	24	1459	1344	82	-15	9	7	486*	760	474	-14	4	7	1221	1280	47
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-15	1	4	1521	1419	34	-15	5	2	4470	4478	46	-15	9	9	0*	366	4227	-14	4	9	2907	2901	33
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-15	1	6	2518	2299	37	-15	5	4	5581	5679	57	-14	0	2	7738	7583	66	-14	4	11	3710	3788	38
-15	1	7	616*	590	319	-15	5	5	527*	233	315	-14	0	4	10816	11342	60	-14	4	12	4272	4276	43
-15	1	8	4041	3860	41	-15	5	6	2104	2183	39	-14	0	6	4797	4674	50	-14	4	13	2491	2493	42
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-15	1	10	1482	1397	57	-15	5	8	3208	3257	34	-14	0	10	10063	10108	81	-14	4	15	407*	375	207
-15	1	11	2726	2635	41	-15	5	9	2990	3031	37	-14	0	12	5276	5296	51	-14	4	16	2929	2878	44
-15	1	12	544*	717	471	-15	5	10	5293	5448	54	-14	0	14	1680	1784	58	-14	4	17	3079	2972	45
-15	1	13	0*	96	3285	-15	5	11	1137	1184	70	-14	0	16	6146	6195	60	-14	4	18	2842	2798	47
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-15	1	15	2868	3018	46	-15	5	13	1293	1188	65	-14	0	20	486*	548	543	-14	4	20	0*	737	3508
-15	1	16	1395	1632	75	-15	5	14	590*	649	135	-14	0	22	3066	3092	48	-14	4	21	0*	241	3746
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-15	1	18	0*	151	3401	-15	5	16	3359	3249	42	-14	2	1	10257	10407	66	-14	4	23	1436	1463	86
-15	1	19	139*	35	685	-15	5	17	1022	1098	90	-14	2	2	2765	2892	27	-14	6	1	2760	2849	35
-15	1	20	1130	1053	86	-15	5	18	3268	3220	45	-14	2	3	3807	3835	37	-14	6	2	2762	2822	34
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-15	1	22	955	1048	104	-15	5	20	468*	492	548	-14	2	5	6086	5944	60	-14	6	4	0*	142	3576
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-15	1	24	0*	124	4247	-15	5	22	1840	1821	71	-14	2	7	10553	10371	73	-14	6	6	2679	2720	36
-15	1	25	383*	433	636	-15	7	1	5094	5139	50	-14	2	8	2975	2943	31	-14	6	7	2766	2818	36
-15	3	1	4131	4100	41	-15	7	2	555*	952	363	-14	2	9	5081	5013	47	-14	6	8	3548	3493	39
-15	3	2	319*	543	407	-15	7	3	1502	1593	51	-14	2	10	1142	1185	59	-14	6	9	3147	3203	36
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-15	3	4	2462	2571	28	-15	7	5	2925	3034	37	-14	2	12	452*	707	428	-14	6	11	621*	739	116
-15	3	5	5396	5406	57	-15	7	6	1508	1471	53	-14	2	13	6380	6166	65	-14	6	12	2201	2194	45
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-15	3	7	5744	5685	54	-15	7	8	0*	183	4258	-14	2	15	5659	5716	54	-14	6	14	3375	3279	39
-15	3	8	2427	2441	33	-15	7	9	3204	3163	37	-14	2	16	2560	2588	52	-14	6	15	2004	1938	49
-15	3	9	2109	1941	37	-15	7	10	1988	1925	44	-14	2	17	598*	175	449	-14	6	16	1805	1830	54
-15	3	10	1935	2001	44	-15	7	11	1111	1077	66	-14	2	18	726*	139	369	-14	6	17	1138	1275	78
-15	3	11	2409	2216	41	-15	7	12	1665	1712	53	-14	2	19	3503	3440	45	-14	6	18	815	792	110

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
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-14	6	20	2120	2112	59	-13	3	7	648	606	71	-13	7	8	563*	656	335	-12	2	11	5385	5354	54
-14	8	1	1462	1439	51	-13	3	8	5818	5793	58	-13	7	9	496*	44	354	-12	2	12	1735	1740	45
-14	8	2	580*	655	355	-13	3	9	4625	4715	48	-13	7	10	320*	370	214	-12	2	13	8569	8594	79
-14	8	3	2603	2562	39	-13	3	10	471*	388	119	-13	7	11	1015	970	70	-12	2	14	611*	555	358
-14	8	4	798	734	84	-13	3	11	5130	4984	50	-13	7	12	393*	493	526	-12	2	15	5314	5208	54
-14	8	5	2061	2104	44	-13	3	12	5165	5196	50	-13	7	13	596*	878	424	-12	2	16	1206	1148	84
-14	8	6	1799	1757	47	-13	3	13	1796	1665	50	-13	7	14	0*	282	3704	-12	2	17	1460	1538	76
-14	8	7	0*	62	3636	-13	3	14	6282	6108	62	-13	7	15	466*	331	159	-12	2	18	1420	1425	78
-14	8	8	1237	1347	62	-13	3	15	1731	1663	59	-13	7	16	387*	194	551	-12	2	19	6070	6168	60
-14	8	9	2423	2411	42	-13	3	16	0*	1181	3933	-13	7	17	0*	722	4164	-12	2	20	0*	525	3503
-14	8	10	309*	213	625	-13	3	17	3124	3191	45	-13	7	18	0*	533	1474	-12	2	21	4514	4471	47
-14	8	11	2288	2286	45	-13	3	18	3322	3328	44	-13	7	19	1114	966	87	-12	2	22	532*	549	176
-14	8	12	523*	668	483	-13	3	19	1784	1751	64	-13	9	1	429*	612	464	-12	2	23	465*	413	190
-14	8	13	0*	497	4099	-13	3	20	4046	3948	45	-13	9	2	1053	842	69	-12	2	24	253*	614	398
-14	8	14	1052	1026	88	-13	3	21	0*	453	3258	-13	9	3	658*	761	356	-12	2	25	2247	2212	59
-14	8	15	1351	1300	71	-13	3	22	1610	1604	70	-13	9	4	466*	622	433	-12	4	1	3712	3751	39
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-13	1	5	9610	9390	75	-13	5	3	4741	4695	47	-13	9	9	409*	482	557	-12	4	6	0*	118	2393
-13	1	6	8587	8392	80	-13	5	4	416*	268	365	-13	9	10	609*	774	133	-12	4	7	2251	2164	30
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-13	1	8	6852	6827	67	-13	5	6	1615	1588	41	-13	9	12	271*	151	766	-12	4	9	1893	1844	37
-13	1	9	7670	7515	78	-13	5	7	1673	1753	42	-12	0	2	13277	13570	58	-12	4	10	7252	7171	69
-13	1	10	1821	1587	47	-13	5	8	2535	2481	35	-12	0	4	13473	13613	56	-12	4	11	783	849	85
-13	1	11	6420	6399	67	-13	5	9	4580	4449	45	-12	0	6	4063	4313	42	-12	4	12	3128	3109	35
-13	1	12	6139	6194	64	-13	5	10	1135	1139	61	-12	0	8	8859	9161	73	-12	4	13	2123	1954	43
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-13	1	18	2409	2366	53	-13	5	16	1903	1964	54	-12	0	20	0*	319	3346	-12	4	19	0*	435	3392
-13	1	19	2920	2988	49	-13	5	17	2688	2654	45	-12	0	22	4265	4444	42	-12	4	20	832	668	102
-13	1	20	3715	3831	43	-13	5	18	438*	404	182	-12	0	24	3597	3577	47	-12	4	21	1289	1255	77
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-13	1	22	1911	1919	60	-13	5	20	1171	1264	86	-12	2	1	10698	10920	59	-12	4	23	725*	697	149
-13	1	23	3448	3441	46	-13	5	21	669*	1139	423	-12	2	2	1057	1002	35	-12	4	24	2247	2189	63
-13	1	24	0*	771	3764	-13	5	22	1053	1119	103	-12	2	3	196*	483	462	-12	6	1	1756	1727	39
-13	1	25	1786	1852	71	-13	7	1	257*	216	243	-12	2	4	3346	3451	35	-12	6	2	619	799	95
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-13	3	3	6063	6077	57	-13	7	4	440*	652	149	-12	2	7	13156	12827	69	-12	6	5	3157	3164	32
-13	3	4	2752	2784	25	-13	7	5	1709	1683	45	-12	2	8	484*	502	324	-12	6	6	2487	2539	36
-13	3	5	4841	4871	50	-13	7	6	1530	1498	51	-12	2	9	3744	3607	36	-12	6	7	3232	3157	33

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
-12	6	8	915	792	71	-11	1	13	341*	541	550	-11	5	9	3208	3300	32	-10	0	2	2830	2815	30
-12	6	9	378*	334	171	-11	1	14	3947	3953	38	-11	5	10	5102	5262	56	-10	0	4	4623	4415	50
-12	6	10	1389	1269	54	-11	1	15	4415	4515	44	-11	5	11	4131	4093	42	-10	0	6	1776	1836	29
-12	6	11	1700	1560	49	-11	1	16	510*	508	496	-11	5	12	2750	2706	37	-10	0	8	1404	1345	36
-12	6	12	2110	2145	45	-11	1	17	4978	4936	52	-11	5	13	1751	1843	49	-10	0	10	4771	4926	46
-12	6	13	2549	2500	43	-11	1	18	2919	3062	45	-11	5	14	0*	333	3540	-10	0	12	958	795	61
-12	6	14	815	831	93	-11	1	19	1855	1996	61	-11	5	15	1655	1640	59	-10	0	14	3442	3344	37
-12	6	15	1407	1393	60	-11	1	20	2839	2802	48	-11	5	16	2591	2622	46	-10	0	16	3308	3394	37
-12	6	16	0*	161	3535	-11	1	21	1886	1973	61	-11	5	17	2638	2757	47	-10	0	18	1750	1751	57
-12	6	17	192*	457	1178	-11	1	22	287*	398	792	-11	5	18	2547	2557	47	-10	0	20	385*	183	228
-12	6	18	0*	676	3917	-11	1	23	2718	2780	48	-11	5	19	2056	1985	53	-10	0	22	1284	1287	75
-12	6	19	1403	1446	72	-11	1	24	698*	1306	439	-11	5	20	0*	221	3961	-10	0	24	360*	1017	825
-12	6	20	705*	789	141	-11	1	25	1535	1596	76	-11	5	21	0*	8	3648	-10	0	26	530*	307	471
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-12	8	4	0*	80	1194	-11	3	4	0*	220	1944	-11	7	3	151*	418	1213	-10	2	5	4127	4309	41
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-12	8	6	550*	506	335	-11	3	6	5623	5571	57	-11	7	5	3698	3724	37	-10	2	7	4015	3970	43
-12	8	7	174*	164	360	-11	3	7	6105	5863	59	-11	7	6	691	679	97	-10	2	8	996	865	45
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-12	8	10	0*	72	3347	-11	3	10	1050	1145	55	-11	7	9	1400	1435	55	-10	2	11	4887	4815	48
-12	8	11	789	951	94	-11	3	11	1230	1271	49	-11	7	10	1793	1790	48	-10	2	12	3932	3998	43
-12	8	12	403*	467	173	-11	3	12	3958	3936	44	-11	7	11	2353	2404	42	-10	2	13	3722	3704	37
-12	8	13	0*	111	1273	-11	3	13	3120	3136	38	-11	7	12	488*	174	412	-10	2	14	2541	2412	39
-12	8	14	425*	483	539	-11	3	14	4665	4702	47	-11	7	13	3504	3511	38	-10	2	15	754	777	100
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-12	8	16	0*	215	4366	-11	3	16	2155	2188	50	-11	7	15	2191	2173	48	-10	2	17	1205	1280	83
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-12	10	2	1287	1230	68	-11	3	18	1552	1452	68	-11	7	17	620*	482	377	-10	2	19	2354	2422	55
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-11	1	3	9817	9664	56	-11	3	24	0*	31	3490	-11	9	4	2742	2705	38	-10	2	25	612*	1012	489
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-11	1	8	4642	4864	46	-11	5	4	5442	5636	57	-11	9	9	821	692	93	-10	4	5	3126	2897	32
-11	1	9	7380	7285	72	-11	5	5	4152	4264	42	-11	9	10	2731	2751	44	-10	4	6	2861	2845	26
-11	1	10	2764	2825	35	-11	5	6	2251	2278	31	-11	9	11	490*	220	366	-10	4	7	5006	4985	50
-11	1	11	5859	5589	59	-11	5	7	644	598	77	-11	9	12	1186	1165	72	-10	4	8	3851	3816	40
-11	1	12	6930	6820	69	-11	5	8	3089	3123	29	-11	9	13	296*	610	287	-10	4	9	8378	8400	73

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
-10	4	10	1352	1400	45	-10	8	12	1804	1803	50	-9	3	8	3979	3732	39	-9	7	7	5713	5701	56
-10	4	11	3725	3788	37	-10	8	13	1061	1130	72	-9	3	9	1427	1478	38	-9	7	8	2028	1905	41
-10	4	12	1434	1385	47	-10	8	14	1495	1498	60	-9	3	10	3081	3107	31	-9	7	9	355*	54	513
-10	4	13	1621	1568	47	-10	8	15	3055	3069	45	-9	3	11	4566	4599	47	-9	7	10	1690	1686	51
-10	4	14	2286	2224	43	-10	8	16	440*	62	526	-9	3	12	730	734	75	-9	7	11	4523	4549	42
-10	4	15	4310	4317	46	-10	8	17	253*	2579	53	-9	3	13	3912	3795	38	-9	7	12	510*	83	402
-10	4	16	1432	1442	66	-10	10	1	1300	1278	65	-9	3	14	913	909	76	-9	7	13	4961	4906	50
-10	4	17	3870	3893	40	-10	10	2	1112	1085	75	-9	3	15	171*	253	1240	-9	7	14	1355	1420	62
-10	4	18	0*	84	3438	-10	10	3	1733	1667	54	-9	3	16	2765	2699	42	-9	7	15	1148	1301	74
-10	4	19	553*	138	417	-10	10	4	1761	1592	53	-9	3	17	2567	2426	47	-9	7	16	1615	1574	57
-10	4	20	1350	1118	68	-10	10	5	446*	603	546	-9	3	18	2068	2166	57	-9	7	17	2470	2434	47
-10	4	21	2685	2624	50	-10	10	6	2873	2913	44	-9	3	19	2592	2794	52	-9	7	18	839	767	109
-10	4	22	880	989	118	-10	10	7	1043	814	80	-9	3	20	455*	374	567	-9	7	19	3539	3400	47
-10	4	23	2325	2327	62	-10	10	8	1894	1787	53	-9	3	21	1210	1152	80	-9	7	20	558*	94	470
-10	4	24	0*	317	3772	-9	1	1	2098	2176	21	-9	3	22	1353	1356	75	-9	9	1	473*	585	386
-10	6	1	1626	1578	39	-9	1	2	2374	2249	22	-9	3	23	676*	547	386	-9	9	2	4463	4543	48
-10	6	2	1687	1665	39	-9	1	3	2343	2534	22	-9	3	24	1335	1244	86	-9	9	3	336*	667	580
-10	6	3	2970	3136	30	-9	1	4	2968	2717	29	-9	3	25	1376	1527	87	-9	9	4	3006	3072	37
-10	6	4	4674	4615	48	-9	1	5	1306	1192	37	-9	5	1	3902	3787	41	-9	9	5	1700	1673	48
-10	6	5	2553	2604	34	-9	1	6	2990	2872	28	-9	5	2	7469	7799	66	-9	9	6	568*	816	328
-10	6	6	7071	7169	67	-9	1	7	4185	4241	43	-9	5	3	0*	47	2571	-9	9	7	870	898	83
-10	6	7	0*	222	3245	-9	1	8	1976	2005	34	-9	5	4	5485	5539	59	-9	9	8	3793	3860	37
-10	6	8	3348	3306	32	-9	1	9	466*	572	316	-9	5	5	3866	3938	39	-9	9	9	532*	239	393
-10	6	9	2206	2250	39	-9	1	10	1307	1275	48	-9	5	6	2485	2516	28	-9	9	10	3535	3489	40
-10	6	10	3012	3032	35	-9	1	11	1574	1474	44	-9	5	7	3484	3421	34	-9	9	11	735	755	107
-10	6	11	2266	2243	42	-9	1	12	1422	1125	47	-9	5	8	8168	8128	73	-9	9	12	619*	547	357
-10	6	12	5892	5865	57	-9	1	13	1186	1253	56	-9	5	9	474*	239	320	-9	9	13	466*	661	538
-10	6	13	0*	414	3465	-9	1	14	2393	2554	39	-9	5	10	5875	6026	63	-9	9	14	2158	2150	55
-10	6	14	4092	3973	42	-9	1	15	1934	1978	46	-9	5	11	1916	1985	42	-8	0	2	11818	12048	44
-10	6	15	1378	1363	64	-9	1	16	1629	1596	52	-9	5	12	261*	132	235	-8	0	4	9922	9770	52
-10	6	16	0*	108	3438	-9	1	17	0*	425	3060	-9	5	13	2062	2159	43	-8	0	6	1905	1958	27
-10	6	17	2008	2016	52	-9	1	18	553*	168	422	-9	5	14	4213	4236	39	-8	0	8	10927	10980	67
-10	6	18	3257	3077	44	-9	1	19	498*	868	546	-9	5	15	1257	1275	70	-8	0	10	5878	5988	54
-10	6	19	348*	598	731	-9	1	20	0*	531	3631	-9	5	16	5063	4996	48	-8	0	12	788	598	71
-10	6	20	2803	2785	50	-9	1	21	680*	878	411	-9	5	17	1454	1483	63	-8	0	14	6149	6146	61
-10	6	21	613*	699	160	-9	1	22	0*	430	3191	-9	5	18	1637	1649	58	-8	0	16	6311	6309	58
-10	8	1	4319	4300	42	-9	1	23	0*	31	3263	-9	5	19	2048	2054	51	-8	0	18	1713	1761	55
-10	8	2	815	924	86	-9	1	24	0*	80	3656	-9	5	20	2033	1923	54	-8	0	20	2525	2429	48
-10	8	3	5660	5615	59	-9	1	25	0*	668	3494	-9	5	21	1201	1171	82	-8	0	22	3150	3253	47
-10	8	4	1679	1559	49	-9	1	26	573*	393	503	-9	5	22	2656	2703	56	-8	0	24	1374	1337	68
-10	8	5	2788	2821	37	-9	3	1	1720	1665	24	-9	5	23	0*	117	1411	-8	0	26	589*	668	159
-10	8	6	2430	2409	38	-9	3	2	4723	4903	50	-9	7	1	3361	3361	35	-8	2	1	5461	5724	51
-10	8	7	2341	2309	40	-9	3	3	3800	3637	39	-9	7	2	2021	2156	38	-8	2	2	390*	579	71
-10	8	8	1400	1260	55	-9	3	4	5160	5048	51	-9	7	3	2357	2261	35	-8	2	3	2524	2619	25
-10	8	9	4722	4744	46	-9	3	5	6637	6695	60	-9	7	4	1662	1589	43	-8	2	4	5735	5604	54
-10	8	10	570*	583	358	-9	3	6	887	819	42	-9	7	5	6912	6897	71	-8	2	5	9529	9428	55
-10	8	11	2505	2508	41	-9	3	7	4234	4036	44	-9	7	6	202*	53	314	-8	2	6	5803	5603	51

Reflections flagged with an asterisk were considered unobserved.

Values of Fobs and Fclc (x20.)

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
-8	2	7	8444	8274	62	-8	6	4	4283	4320	45	-7	1	1	12838	12747	43	-7	3	22	209*	630	1385
-8	2	8	283*	472	409	-8	6	5	1548	1667	39	-7	1	2	226*	37	377	-7	3	23	2103	2238	58
-8	2	9	1222	1277	41	-8	6	6	5645	5754	55	-7	1	3	12585	11885	48	-7	3	24	2365	2249	58
-8	2	10	3139	3039	30	-8	6	7	3319	3308	30	-7	1	4	5261	5499	48	-7	3	25	657*	1187	509
-8	2	11	5574	5422	56	-8	6	8	2308	2414	36	-7	1	5	2786	2617	30	-7	5	1	3808	3999	36
-8	2	12	3093	3177	33	-8	6	9	2439	2444	35	-7	1	6	10981	10704	61	-7	5	2	3401	3416	33
-8	2	13	5497	5422	57	-8	6	10	2126	2074	40	-7	1	7	11338	10848	65	-7	5	3	2541	2541	27
-8	2	14	2569	2631	37	-8	6	11	0*	327	3527	-7	1	8	4333	3998	43	-7	5	4	2176	2093	27
-8	2	15	1368	1412	55	-8	6	12	4600	4540	47	-7	1	9	9601	9392	73	-7	5	5	1521	1321	31
-8	2	16	0*	383	2840	-8	6	13	2658	2698	40	-7	1	10	5296	5198	52	-7	5	6	5331	5243	55
-8	2	17	3520	3507	41	-8	6	14	3362	3395	39	-7	1	11	2240	2303	35	-7	5	7	4370	4458	42
-8	2	18	1624	1691	65	-8	6	15	2459	2447	46	-7	1	12	8782	8815	84	-7	5	8	2942	3012	34
-8	2	19	4217	4229	42	-8	6	16	895	927	87	-7	1	13	5317	5295	54	-7	5	9	3777	3718	41
-8	2	20	1704	1658	66	-8	6	17	595*	487	347	-7	1	14	4868	4780	46	-7	5	10	0*	156	2890
-8	2	21	1725	1768	61	-8	6	18	3141	3199	45	-7	1	15	7824	7907	78	-7	5	11	1030	1014	56
-8	2	22	398*	330	202	-8	6	19	1014	1000	87	-7	1	16	1273	1125	61	-7	5	12	2450	2363	36
-8	2	23	531*	655	170	-8	6	20	2424	2387	53	-7	1	17	3778	3842	40	-7	5	13	2656	2574	37
-8	2	24	965	1059	103	-8	6	21	1408	1338	78	-7	1	18	3941	4004	39	-7	5	14	3258	3316	37
-8	2	25	1811	1698	66	-8	6	22	751*	644	383	-7	1	19	1203	1327	78	-7	5	15	2926	2970	41
-8	2	26	1319	1329	86	-8	8	1	4185	4238	42	-7	1	20	2979	2976	46	-7	5	16	1319	1329	68
-8	4	1	4514	4722	47	-8	8	2	439*	409	405	-7	1	21	3791	3801	43	-7	5	17	1030	923	81
-8	4	2	6358	6525	59	-8	8	3	3810	3750	39	-7	1	22	199*	424	1463	-7	5	18	823	994	107
-8	4	3	6837	6936	60	-8	8	4	1964	1879	43	-7	1	23	2452	2506	51	-7	5	19	1169	1183	75
-8	4	4	4374	4410	45	-8	8	5	0*	79	3819	-7	1	24	2247	2194	53	-7	5	20	1702	1673	61
-8	4	5	2539	2583	27	-8	8	6	2381	2399	39	-7	1	25	0*	10	4048	-7	5	21	1931	1895	59
-8	4	6	324*	163	341	-8	8	7	3232	3317	35	-7	1	26	2047	2160	63	-7	5	22	1093	1157	102
-8	4	7	4386	4396	43	-8	8	8	782	744	83	-7	3	1	5839	5923	53	-7	5	23	1350	1200	81
-8	4	8	5068	5110	51	-8	8	9	3375	3351	36	-7	3	2	2796	2620	28	-7	7	1	927	820	61
-8	4	9	6600	6442	63	-8	8	10	1429	1371	53	-7	3	3	5461	5674	54	-7	7	2	710	753	81
-8	4	10	5138	5329	55	-8	8	11	1132	1058	63	-7	3	4	8333	8633	54	-7	7	3	2835	2916	32
-8	4	11	3723	3779	38	-8	8	12	1830	1782	48	-7	3	5	1884	1681	24	-7	7	4	1424	1405	45
-8	4	12	2281	2212	34	-8	8	13	1711	1642	49	-7	3	6	8283	8119	58	-7	7	5	2880	2811	33
-8	4	13	158*	548	1163	-8	8	14	0*	795	4208	-7	3	7	3907	3582	39	-7	7	6	970	988	65
-8	4	14	2036	1917	44	-8	8	15	2758	2749	46	-7	3	8	2047	2029	27	-7	7	7	1143	1215	58
-8	4	15	3535	3390	37	-8	8	16	677*	624	359	-7	3	9	6302	6449	59	-7	7	8	0*	226	3355
-8	4	16	3153	3215	41	-8	8	17	1858	1677	59	-7	3	10	5787	5995	57	-7	7	9	1080	962	60
-8	4	17	2819	2792	44	-8	8	18	1449	1380	72	-7	3	11	4717	4772	46	-7	7	10	1072	1020	66
-8	4	18	1391	1397	68	-8	10	1	1227	1169	65	-7	3	12	7400	7348	69	-7	7	11	2191	2130	44
-8	4	19	616*	361	133	-8	10	2	615*	742	314	-7	3	13	612	597	92	-7	7	12	1152	1133	66
-8	4	20	250*	642	352	-8	10	3	1622	1605	53	-7	3	14	2732	2606	35	-7	7	13	1138	1056	68
-8	4	21	2158	2174	54	-8	10	4	2314	2318	45	-7	3	15	3507	3493	36	-7	7	14	178*	271	1046
-8	4	22	1642	1627	67	-8	10	5	911	829	85	-7	3	16	2997	2881	40	-7	7	15	577*	740	344
-8	4	23	2378	2279	60	-8	10	6	1761	1681	53	-7	3	17	3221	3321	42	-7	7	16	1195	1127	69
-8	4	24	1486	1446	82	-8	10	7	677	578	111	-7	3	18	4699	4723	50	-7	7	17	1616	1714	62
-8	6	1	2777	2845	29	-8	10	8	0*	304	4332	-7	3	19	0*	277	3607	-7	7	18	811	891	113
-8	6	2	687	654	65	-8	10	9	1450	1382	64	-7	3	20	2897	2812	48	-7	7	19	1245	1215	82
-8	6	3	1334	1384	40	-8	10	10	1797	1815	56	-7	3	21	2022	1893	56	-7	7	20	0*	369	4040

Reflections flagged with an asterisk were considered unobserved.

Values of Fobs and Fcalc (x20.)

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
-7	9	1	1193	1070	57	-6	2	20	550*	418	456	-6	6	17	1755	1722	55	-5	1	14	1187	1218	54
-7	9	2	1606	1518	49	-6	2	21	1899	1979	57	-6	6	18	307*	425	256	-5	1	15	5855	5903	60
-7	9	3	1498	1543	52	-6	2	22	286*	673	914	-6	6	19	1686	1598	58	-5	1	16	3135	3340	37
-7	9	4	0*	428	1176	-6	2	23	2583	2504	50	-6	6	20	0*	300	3675	-5	1	17	3261	3372	39
-7	9	5	357*	249	167	-6	2	24	0*	191	4287	-6	6	21	211*	206	1130	-5	1	18	4155	4181	41
-7	9	6	1083	1062	63	-6	2	25	3482	3362	48	-6	6	22	574*	694	542	-5	1	19	0*	749	3198
-7	9	7	675	922	102	-6	2	26	0*	153	4082	-6	8	1	739	813	84	-5	1	20	1971	2117	57
-7	9	8	1623	1583	53	-6	4	1	2846	2961	26	-6	8	2	717	769	87	-5	1	21	3918	3923	42
-7	9	9	900	803	79	-6	4	2	7659	7890	56	-6	8	3	1709	1693	45	-5	1	22	1417	1419	70
-7	9	10	861	831	84	-6	4	3	862	776	38	-6	8	4	614	522	97	-5	1	23	2714	2726	48
-7	9	11	602*	356	341	-6	4	4	2362	2334	24	-6	8	5	1472	1483	49	-5	1	24	2449	2551	52
-7	9	12	0*	345	3707	-6	4	5	1383	1268	30	-6	8	6	469*	59	128	-5	1	25	447*	284	199
-7	9	13	95*	112	797	-6	4	6	5997	5928	54	-6	8	7	0*	359	3475	-5	1	26	1632	1624	70
-7	9	14	1318	1207	73	-6	4	7	2389	2440	25	-6	8	8	584*	440	322	-5	3	1	5877	5954	49
-7	9	15	0*	439	4610	-6	4	8	9355	9238	66	-6	8	9	983	1122	72	-5	3	2	0*	357	1681
-6	0	2	14705	14698	39	-6	4	9	818	629	54	-6	8	10	505*	308	347	-5	3	3	365*	196	210
-6	0	4	6980	7180	50	-6	4	10	5610	5572	57	-6	8	11	0*	758	3679	-5	3	4	6477	6160	53
-6	0	6	1373	1721	34	-6	4	11	2377	2136	31	-6	8	12	466*	354	409	-5	3	5	4142	4176	44
-6	0	8	13627	13407	65	-6	4	12	825	873	67	-6	8	13	442*	91	469	-5	3	6	9885	9835	56
-6	0	10	11496	11617	72	-6	4	13	1616	1562	42	-6	8	14	0*	435	1239	-5	3	7	6331	6306	60
-6	0	12	1170	1202	48	-6	4	14	5028	5058	51	-6	8	15	502*	529	364	-5	3	8	3698	3533	37
-6	0	14	11575	11788	84	-6	4	15	608*	479	358	-6	8	16	585*	232	409	-5	3	9	4062	3977	40
-6	0	16	9207	9532	90	-6	4	16	4358	4304	45	-6	8	17	0*	462	4127	-5	3	10	3884	3746	41
-6	0	18	2147	2312	48	-6	4	17	0*	106	3234	-6	8	18	0*	48	3838	-5	3	11	739	810	65
-6	0	20	4409	4493	43	-6	4	18	837	654	103	-6	10	1	303*	597	600	-5	3	12	8001	7782	78
-6	0	22	5310	5389	52	-6	4	19	1188	1064	77	-6	10	2	1322	1320	60	-5	3	13	4259	4223	44
-6	0	24	1858	1868	58	-6	4	20	2814	2760	46	-6	10	3	351*	409	555	-5	3	14	3509	3476	34
-6	0	26	1684	1618	70	-6	4	21	0*	349	1228	-6	10	4	0*	219	1384	-5	3	15	3069	3141	35
-6	2	1	3071	2890	27	-6	4	22	3083	3041	49	-6	10	5	992	932	76	-5	3	16	1243	1184	70
-6	2	2	1709	1678	21	-6	4	23	0*	569	3920	-6	10	6	1395	1405	62	-5	3	17	675*	136	346
-6	2	3	9351	9003	47	-6	4	24	1228	1110	90	-6	10	7	627*	585	320	-5	3	18	4433	4398	41
-6	2	4	4990	4783	44	-6	6	1	1043	955	41	-6	10	8	1421	1354	61	-5	3	19	2508	2563	51
-6	2	5	15027	14798	51	-6	6	2	0*	174	2083	-6	10	9	0*	63	4236	-5	3	20	3692	3707	44
-6	2	6	1479	1432	28	-6	6	3	2516	2466	27	-6	10	10	541*	540	150	-5	3	21	2807	2831	49
-6	2	7	9859	9552	59	-6	6	4	1197	1237	42	-5	1	1	11325	11514	37	-5	3	22	545*	91	155
-6	2	8	1653	1609	30	-6	6	5	4054	4027	41	-5	1	2	8393	7984	39	-5	3	23	0*	835	3562
-6	2	9	4399	4341	43	-6	6	6	1136	1214	47	-5	1	3	7055	7075	44	-5	3	24	1991	1914	60
-6	2	10	1132	1155	43	-6	6	7	1571	1640	37	-5	1	4	8514	8143	48	-5	3	25	756*	797	401
-6	2	11	11187	11340	75	-6	6	8	761	745	68	-5	1	5	4119	3577	41	-5	5	1	2197	2289	24
-6	2	12	369*	24	405	-6	6	9	1110	1176	58	-5	1	6	2330	2547	26	-5	5	2	5790	6033	54
-6	2	13	8499	8439	83	-6	6	10	1760	1727	42	-5	1	7	6018	5800	55	-5	5	3	4138	4124	38
-6	2	14	1349	1290	52	-6	6	11	2819	2775	36	-5	1	8	733	888	64	-5	5	4	5342	5385	57
-6	2	15	806	657	83	-6	6	12	842	973	86	-5	1	9	8044	8049	70	-5	5	5	2443	2331	27
-6	2	16	1185	1105	66	-6	6	13	2589	2571	40	-5	1	10	7320	7373	73	-5	5	6	358*	649	321
-6	2	17	6142	6137	59	-6	6	14	482*	149	393	-5	1	11	2151	2130	34	-5	5	7	2664	2655	28
-6	2	18	532*	399	498	-6	6	15	466*	139	432	-5	1	12	6912	7124	72	-5	5	8	6001	5944	56
-6	2	19	6709	6830	70	-6	6	16	372*	503	207	-5	1	13	4485	4506	43	-5	5	9	5121	5086	50

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
-5	5	10	4732	4771	49	-5	9	14	1640	1693	61	-4	4	8	4403	4431	45	-4	8	9	4081	4132	39
-5	5	11	2650	2599	33	-5	9	15	637*	561	138	-4	4	9	6052	5949	60	-4	8	10	2213	2159	42
-5	5	12	963	865	67	-4	0	2	10361	10407	36	-4	4	10	872	839	52	-4	8	11	445*	515	151
-5	5	13	599*	514	113	-4	0	4	5566	4538	48	-4	4	11	0*	292	2254	-4	8	12	1818	1925	49
-5	5	14	2364	2331	42	-4	0	6	2905	2765	29	-4	4	12	3133	3041	33	-4	8	13	2907	2929	42
-5	5	15	3061	3063	39	-4	0	8	6885	7243	66	-4	4	13	5119	5186	54	-4	8	14	321*	506	239
-5	5	16	2981	3019	42	-4	0	10	5307	5294	52	-4	4	14	3218	3187	36	-4	8	15	3405	3397	42
-5	5	17	3025	3067	42	-4	0	12	2505	2450	31	-4	4	15	5304	5301	56	-4	8	16	1021	1015	93
-5	5	18	1025	1159	87	-4	0	14	5362	5524	53	-4	4	16	1104	1295	77	-4	8	17	1335	1277	71
-5	5	19	0*	101	3127	-4	0	16	3868	4120	40	-4	4	17	1140	1152	76	-4	8	18	1358	1345	73
-5	5	20	878	876	103	-4	0	18	751	932	105	-4	4	18	529*	596	495	-4	10	1	1890	1868	47
-5	5	21	1878	1892	62	-4	0	20	2660	2668	47	-4	4	19	2542	2538	49	-4	10	2	867	925	84
-5	5	22	1580	1553	72	-4	0	22	2801	2895	46	-4	4	20	2210	2252	54	-4	10	3	829	773	82
-5	5	23	1316	1429	87	-4	0	24	294*	727	295	-4	4	21	3027	2886	47	-4	10	4	2939	2966	40
-5	7	1	2246	2263	33	-4	0	26	774*	989	394	-4	4	22	1200	1341	88	-4	10	5	432*	704	522
-5	7	2	626	704	85	-4	2	1	0*	357	1573	-4	4	23	1139	1177	93	-4	10	6	2385	2356	45
-5	7	3	1891	2000	37	-4	2	2	2217	2397	23	-4	4	24	0*	287	3457	-4	10	7	1861	1743	51
-5	7	4	927	893	62	-4	2	3	5193	5301	45	-4	6	1	2872	2810	28	-4	10	8	512*	232	140
-5	7	5	4546	4569	42	-4	2	4	6826	6619	47	-4	6	2	3134	3247	30	-4	10	9	1169	1137	71
-5	7	6	1819	1849	40	-4	2	5	5236	5190	52	-4	6	3	3224	3182	32	-4	10	10	1788	1708	55
-5	7	7	2545	2729	35	-4	2	6	4549	4188	48	-4	6	4	7842	7897	69	-4	10	11	191*	262	1218
-5	7	8	1318	1379	51	-4	2	7	1034	1087	37	-4	6	5	230*	255	567	-3	1	1	2519	2153	24
-5	7	9	1112	1080	59	-4	2	8	941	1031	43	-4	6	6	5478	5720	52	-3	1	2	6028	5837	34
-5	7	10	596*	315	310	-4	2	9	2542	2466	25	-4	6	7	2074	2044	32	-3	1	3	268*	440	68
-5	7	11	3432	3464	36	-4	2	10	4343	4437	45	-4	6	8	944	1005	53	-3	1	4	3619	3116	34
-5	7	12	1179	1063	64	-4	2	11	4092	4137	44	-4	6	9	2818	2935	33	-3	1	5	2022	1981	23
-5	7	13	3050	3134	38	-4	2	12	3737	3708	41	-4	6	10	5652	5741	55	-3	1	6	4278	4326	46
-5	7	14	1424	1456	56	-4	2	13	1867	1852	38	-4	6	11	1130	1236	67	-3	1	7	3567	3497	36
-5	7	15	576*	544	351	-4	2	14	513*	63	312	-4	6	12	5791	5808	55	-3	1	8	4818	4485	52
-5	7	16	325*	401	670	-4	2	15	1299	1271	56	-4	6	13	330*	494	612	-3	1	9	1460	1280	36
-5	7	17	1820	1803	54	-4	2	16	2323	2368	41	-4	6	14	1068	1032	74	-3	1	10	332*	442	134
-5	7	18	652*	649	141	-4	2	17	2720	2779	45	-4	6	15	1466	1368	59	-3	1	11	2847	2745	30
-5	7	19	1966	1885	58	-4	2	18	2292	2363	51	-4	6	16	3543	3634	40	-3	1	12	1125	1114	50
-5	7	20	697*	898	387	-4	2	19	3106	3145	44	-4	6	17	1587	1519	59	-3	1	13	2008	1998	38
-5	9	1	1603	1532	46	-4	2	20	0*	149	1141	-4	6	18	3692	3801	41	-3	1	14	1189	1107	55
-5	9	2	3074	3175	36	-4	2	21	0*	428	3692	-4	6	19	0*	17	3446	-3	1	15	0*	364	2143
-5	9	3	0*	161	3519	-4	2	22	1145	1212	78	-4	6	20	1206	1175	84	-3	1	16	597*	658	114
-5	9	4	1438	1456	52	-4	2	23	1780	1770	59	-4	6	21	1176	1075	85	-3	1	17	1561	1619	57
-5	9	5	1488	1560	51	-4	2	24	1622	1564	65	-4	6	22	1309	1172	81	-3	1	18	511*	159	416
-5	9	6	1122	1093	63	-4	2	25	1490	1629	79	-4	8	1	5585	5646	60	-3	1	19	814	881	109
-5	9	7	1175	1328	63	-4	4	1	8347	8388	54	-4	8	2	666	535	93	-3	1	20	464*	560	600
-5	9	8	2617	2576	40	-4	4	2	1624	1806	25	-4	8	3	4030	3968	44	-3	1	21	336*	602	732
-5	9	9	302*	359	659	-4	4	3	5591	5904	56	-4	8	4	2479	2632	37	-3	1	22	819	746	100
-5	9	10	1750	1721	48	-4	4	4	2228	2345	22	-4	8	5	911	945	73	-3	1	23	1013	1057	86
-5	9	11	524*	661	132	-4	4	5	2650	2820	24	-4	8	6	2346	2484	39	-3	1	24	507*	210	463
-5	9	12	0*	322	3444	-4	4	6	4719	4580	48	-4	8	7	4402	4295	41	-3	1	25	0*	786	4423
-5	9	13	1194	1165	73	-4	4	7	8206	7947	63	-4	8	8	490*	74	133	-3	1	26	482*	137	576

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
-3	3	1	1699	1667	19	-3	5	23	1166	971	87	-2	0	22	1868	1833	55	-2	4	20	1505	1530	67
-3	3	2	6476	6261	48	-3	7	1	729	879	72	-2	0	24	0*	177	3369	-2	4	21	3064	3100	49
-3	3	3	6377	6174	49	-3	7	2	2536	2498	31	-2	0	26	1489	1344	74	-2	4	22	1384	1395	81
-3	3	4	1524	1539	23	-3	7	3	7014	7168	65	-2	2	1	4059	4426	39	-2	4	23	1270	1411	91
-3	3	5	6187	6028	53	-3	7	4	374*	569	398	-2	2	2	2148	2131	21	-2	4	24	0*	431	3902
-3	3	6	2186	1998	22	-3	7	5	7051	7107	67	-2	2	3	8969	8484	42	-2	6	1	3328	3383	32
-3	3	7	299*	309	348	-3	7	6	1425	1322	47	-2	2	4	3416	3328	33	-2	6	2	5616	5752	61
-3	3	8	4691	4960	45	-3	7	7	1832	1785	40	-2	2	5	8095	7956	49	-2	6	3	1854	1771	30
-3	3	9	4055	3949	40	-3	7	8	2168	2234	38	-2	2	6	3935	3867	40	-2	6	4	8333	8384	68
-3	3	10	2528	2520	27	-3	7	9	4386	4419	47	-2	2	7	904	1060	40	-2	6	5	3668	3751	36
-3	3	11	6095	6235	65	-3	7	10	1077	1231	74	-2	2	8	1402	1294	31	-2	6	6	4550	4564	43
-3	3	12	1802	1815	36	-3	7	11	6227	6347	65	-2	2	9	6333	6440	58	-2	6	7	2158	2115	30
-3	3	13	3106	2970	31	-3	7	12	1031	974	75	-2	2	10	5391	5465	55	-2	6	8	1322	1153	42
-3	3	14	3514	3573	34	-3	7	13	2882	2860	39	-2	2	11	6572	6521	64	-2	6	9	329*	240	168
-3	3	15	2093	2012	42	-3	7	14	1981	2052	48	-2	2	12	3735	3716	38	-2	6	10	5514	5561	54
-3	3	16	1906	1910	51	-3	7	15	1855	1785	51	-2	2	13	1792	1939	39	-2	6	11	1959	1932	43
-3	3	17	3336	3428	41	-3	7	16	775	960	108	-2	2	14	459*	752	418	-2	6	12	4303	4322	42
-3	3	18	591*	1021	467	-3	7	17	4064	3978	40	-2	2	15	2235	2297	40	-2	6	13	2485	2465	40
-3	3	19	2067	2100	54	-3	7	18	0*	414	1425	-2	2	16	2102	2107	45	-2	6	14	642*	316	112
-3	3	20	2055	2064	56	-3	7	19	2790	2710	50	-2	2	17	3267	3141	41	-2	6	15	906	921	90
-3	3	21	411*	68	572	-3	7	20	1201	1094	81	-2	2	18	1805	2009	58	-2	6	16	3614	3562	39
-3	3	22	1264	1412	79	-3	9	1	322*	288	563	-2	2	19	2011	1900	54	-2	6	17	707*	1058	357
-3	3	23	1587	1661	72	-3	9	2	4424	4414	44	-2	2	20	0*	382	3499	-2	6	18	3498	3475	43
-3	3	24	0*	104	3820	-3	9	3	1657	1657	46	-2	2	21	343*	469	679	-2	6	19	1480	1528	68
-3	3	25	1192	1368	97	-3	9	4	0*	638	3484	-2	2	22	1112	1135	82	-2	6	20	954	1155	104
-3	5	1	314*	92	103	-3	9	5	1253	1239	58	-2	2	23	1900	1767	58	-2	6	21	920	936	105
-3	5	2	7539	7896	61	-3	9	6	3731	3682	37	-2	2	24	1729	1733	65	-2	8	1	5054	5159	52
-3	5	3	3954	3889	39	-3	9	7	292*	184	603	-2	2	25	1096	1139	101	-2	8	2	2145	2128	38
-3	5	4	238*	58	391	-3	9	8	4405	4441	45	-2	4	1	8409	8641	52	-2	8	3	2130	2089	39
-3	5	5	5199	5242	51	-3	9	9	905	842	81	-2	4	2	6861	7077	54	-2	8	4	3084	3133	34
-3	5	6	7439	7665	66	-3	9	10	1586	1642	53	-2	4	3	4945	4927	49	-2	8	5	2656	2611	35
-3	5	7	1676	1532	32	-3	9	11	1547	1530	53	-2	4	4	2591	2541	27	-2	8	6	1627	1527	47
-3	5	8	7347	7461	71	-3	9	12	2033	1959	51	-2	4	5	4998	5056	52	-2	8	7	5273	5198	49
-3	5	9	2347	2316	31	-3	9	13	0*	835	4677	-2	4	6	3087	3048	33	-2	8	8	1321	1376	57
-3	5	10	3114	3159	29	-3	9	14	3494	3533	44	-2	4	7	8107	8426	62	-2	8	9	2854	2792	38
-3	5	11	3614	3565	37	-3	9	15	0*	196	1494	-2	4	8	5934	5735	59	-2	8	10	2351	2372	41
-3	5	12	3329	3327	36	-3	11	1	0*	269	4003	-2	4	9	6660	6647	61	-2	8	11	1602	1490	51
-3	5	13	1666	1752	48	-2	0	2	12799	14710	117	-2	4	10	3392	3206	34	-2	8	12	1499	1406	58
-3	5	14	5684	5599	57	-2	0	4	930	636	28	-2	4	11	388*	475	117	-2	8	13	3703	3723	38
-3	5	15	1496	1313	55	-2	0	6	6336	6150	57	-2	4	12	180*	129	279	-2	8	14	0*	339	3590
-3	5	16	2813	2749	43	-2	0	8	8544	8638	63	-2	4	13	5584	5664	61	-2	8	15	2797	2809	45
-3	5	17	2794	2833	45	-2	0	10	1094	1040	43	-2	4	14	2746	2738	38	-2	8	16	1321	1539	78
-3	5	18	1034	1052	85	-2	0	12	5570	5416	56	-2	4	15	5242	5225	51	-2	8	17	534*	342	409
-3	5	19	1462	1610	68	-2	0	14	5590	5855	57	-2	4	16	2210	2129	47	-2	8	18	1487	1443	72
-3	5	20	2997	2990	47	-2	0	16	2557	2635	37	-2	4	17	1370	1359	67	-2	10	1	1675	1643	48
-3	5	21	548*	26	472	-2	0	18	1189	1117	69	-2	4	18	0*	138	3317	-2	10	2	2352	2349	43
-3	5	22	2390	2407	58	-2	0	20	2994	2849	44	-2	4	19	2295	2264	49	-2	10	3	1388	1513	56

Reflections flagged with an asterisk were considered unobserved.

Values of Fobs and Fcalc (x20.)

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
-2	10	4	2527	2489	42	-1	3	15	3576	3695	38	-1	7	15	2296	2226	47	0	2	12	1638	1771	40
-2	10	5	528*	197	341	-1	3	16	4764	4760	49	-1	7	16	914	784	89	0	2	13	721	729	74
-2	10	6	749	720	98	-1	3	17	1903	1938	54	-1	7	17	2365	2280	50	0	2	14	1197	1141	53
-2	10	7	1321	1464	68	-1	3	18	3140	3137	44	-1	7	18	285*	28	912	0	2	15	5768	5813	54
-2	10	8	1377	1369	65	-1	3	19	1114	1202	87	-1	7	19	1053	956	89	0	2	16	0*	397	2597
-2	10	9	1411	1348	62	-1	3	20	435*	349	199	-1	7	20	602*	598	499	0	2	17	6597	6682	73
-2	10	10	2595	2444	47	-1	3	21	2511	2516	52	-1	9	1	1088	1033	58	0	2	18	592*	594	150
-2	10	11	0*	285	4826	-1	3	22	2709	2731	51	-1	9	2	1646	1610	46	0	2	19	3156	3150	46
-1	1	1	14303	14146	114	-1	3	23	1461	1422	75	-1	9	3	0*	685	3848	0	2	20	479*	550	562
-1	1	2	9530	9041	31	-1	3	24	1900	1824	66	-1	9	4	897	911	72	0	2	21	2522	2405	48
-1	1	3	1807	1718	18	-1	5	1	5058	5136	52	-1	9	5	466*	110	366	0	2	22	0*	66	3231
-1	1	4	9818	9355	42	-1	5	2	1731	1765	25	-1	9	6	2628	2700	38	0	2	23	3694	3685	45
-1	1	5	9258	9167	48	-1	5	3	875	881	42	-1	9	7	1078	1104	64	0	2	24	366*	552	784
-1	1	6	4405	4355	46	-1	5	4	5146	5147	50	-1	9	8	1916	2005	47	0	2	25	2148	2112	62
-1	1	7	11067	10754	58	-1	5	5	4929	4826	46	-1	9	9	1657	1686	50	0	4	0	11722	11976	51
-1	1	8	3633	3628	38	-1	5	6	5760	5886	58	-1	9	10	0*	91	3834	0	4	1	1312	1539	26
-1	1	9	3095	3048	32	-1	5	7	5240	5358	54	-1	9	11	809	800	92	0	4	2	5429	5567	54
-1	1	10	8373	8282	72	-1	5	8	2560	2524	28	-1	9	12	1708	1640	58	0	4	3	2125	2073	22
-1	1	11	5444	5315	51	-1	5	9	1069	926	45	-1	9	13	571*	361	385	0	4	4	3437	3417	35
-1	1	12	5472	5375	60	-1	5	10	1591	1557	39	-1	9	14	1782	1736	60	0	4	5	2246	2247	23
-1	1	13	8282	8307	73	-1	5	11	3392	3364	34	-1	9	15	538*	702	163	0	4	6	9943	9972	60
-1	1	14	0*	430	2111	-1	5	12	3792	3778	37	-1	11	1	876	911	90	0	4	7	0*	298	1783
-1	1	15	4482	4488	43	-1	5	13	3307	3324	36	-1	11	2	960	987	83	0	4	8	8907	8771	67
-1	1	16	3382	3461	35	-1	5	14	2925	2824	38	0	0	2	13862	14444	120	0	4	9	2283	2335	29
-1	1	17	0*	449	3010	-1	5	15	1324	1290	63	0	0	4	8150	8394	46	0	4	10	1290	1309	40
-1	1	18	3943	3960	45	-1	5	16	0*	201	3037	0	0	6	17506	17168	55	0	4	11	1317	1217	43
-1	1	19	3601	3587	41	-1	5	17	1543	1514	61	0	0	8	11738	11804	63	0	4	12	5822	5819	59
-1	1	20	1214	1277	80	-1	5	18	2464	2495	46	0	0	10	1389	1323	37	0	4	13	387*	269	433
-1	1	21	3039	3017	45	-1	5	19	2786	2861	47	0	0	12	12098	12119	77	0	4	14	5297	5311	51
-1	1	22	1547	1513	61	-1	5	20	2232	2205	54	0	0	14	11958	11830	84	0	4	15	1697	1638	51
-1	1	23	539*	151	402	-1	5	21	1542	1552	68	0	0	16	3283	3391	35	0	4	16	1847	1814	49
-1	1	24	1987	2001	60	-1	5	22	605*	632	438	0	0	18	3904	3893	41	0	4	17	1123	1184	81
-1	1	25	1692	1647	67	-1	5	23	0*	280	3542	0	0	20	6565	6699	66	0	4	18	2169	2203	51
-1	3	1	6890	7024	45	-1	7	1	3148	3176	33	0	0	22	3007	3072	46	0	4	19	0*	30	3273
-1	3	2	12303	12284	46	-1	7	2	2667	2617	31	0	0	24	1239	955	76	0	4	20	3643	3714	43
-1	3	3	3612	3637	34	-1	7	3	4674	4772	45	0	2	0	1754	1499	18	0	4	21	554*	756	163
-1	3	4	12294	11962	50	-1	7	4	1511	1586	40	0	2	1	8797	8835	37	0	4	22	1614	1716	71
-1	3	5	4653	4737	47	-1	7	5	2706	2691	32	0	2	2	961	1032	24	0	4	23	693*	662	413
-1	3	6	2118	2214	23	-1	7	6	828	787	67	0	2	3	15037	15124	41	0	6	0	468	377	73
-1	3	7	8532	8396	59	-1	7	7	563*	473	101	0	2	4	4591	4515	41	0	6	1	2508	2537	26
-1	3	8	6195	6107	55	-1	7	8	1773	1669	43	0	2	5	10676	10132	49	0	6	2	581	544	68
-1	3	9	6901	7010	67	-1	7	9	3237	3259	35	0	2	6	2774	2677	26	0	6	3	4289	4405	41
-1	3	10	8841	8660	70	-1	7	10	760	717	88	0	2	7	3739	3470	38	0	6	4	1929	1926	30
-1	3	11	1910	1967	34	-1	7	11	2951	2876	38	0	2	8	651	808	58	0	6	5	2449	2547	28
-1	3	12	3123	3177	30	-1	7	12	535*	139	396	0	2	9	12511	12309	65	0	6	6	2467	2455	28
-1	3	13	3014	2980	31	-1	7	13	0*	134	3326	0	2	10	0*	542	1762	0	6	7	1353	1268	39
-1	3	14	3066	3044	33	-1	7	14	284*	623	258	0	2	11	10567	10374	74	0	6	8	1507	1640	40

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
0	6	9	3055	3049	33	1	1	5	6578	6648	51	1	5	1	6144	6176	60	1	9	5	1370	1250	53
0	6	10	457*	112	381	1	1	6	5034	4324	50	1	5	2	5184	5430	54	1	9	6	2177	2126	41
0	6	11	2411	2401	39	1	1	7	11563	11260	59	1	5	3	2840	2771	28	1	9	7	1065	1100	68
0	6	12	515*	474	129	1	1	8	8500	8101	64	1	5	4	916	961	41	1	9	8	1688	1774	49
0	6	13	1075	1092	72	1	1	9	5304	5394	55	1	5	5	2251	2286	26	1	9	9	202*	136	317
0	6	14	347*	360	643	1	1	10	7236	7436	64	1	5	6	1330	1366	35	1	9	10	422*	98	152
0	6	15	1281	1143	63	1	1	11	4739	4774	47	1	5	7	4704	4679	51	1	9	11	0*	743	3969
0	6	16	240*	338	323	1	1	12	3203	3198	31	1	5	8	3668	3668	37	1	9	12	1151	1228	77
0	6	17	2047	2084	51	1	1	13	8744	8734	85	1	5	9	1656	1652	36	1	9	13	862	828	97
0	6	18	752	727	113	1	1	14	3506	3625	33	1	5	10	2613	2646	31	1	9	14	1297	1265	70
0	6	19	1032	895	82	1	1	15	4128	4260	44	1	5	11	1591	1736	42	1	11	0	400*	504	187
0	6	20	0*	381	3665	1	1	16	5268	5298	58	1	5	12	1149	1093	60	1	11	1	411*	204	502
0	6	21	213*	512	1111	1	1	17	1225	1164	73	1	5	13	3208	3251	36	1	11	2	1534	1407	60
0	8	0	0*	538	3543	1	1	18	2991	3180	44	1	5	14	2935	2848	39	2	0	0	11992	11777	113
0	8	1	333*	48	474	1	1	19	4203	4338	40	1	5	15	2106	2055	47	2	0	2	6950	6235	40
0	8	2	324*	380	182	1	1	20	640*	701	376	1	5	16	2151	2116	49	2	0	4	5174	4655	46
0	8	3	543*	224	320	1	1	21	3177	3000	44	1	5	17	0*	157	3528	2	0	6	7310	7639	61
0	8	4	264*	333	641	1	1	22	2786	2758	47	1	5	18	600*	493	419	2	0	8	6159	6000	60
0	8	5	866	942	74	1	1	23	0*	185	3282	1	5	19	1707	1671	58	2	0	10	3037	2908	32
0	8	6	1041	955	64	1	1	24	1778	1818	63	1	5	20	1105	1049	85	2	0	12	8300	8484	80
0	8	7	0*	588	3788	1	1	25	1568	1568	72	1	5	21	1560	1607	69	2	0	14	6482	6532	68
0	8	8	657	574	98	1	3	0	891	836	30	1	5	22	1257	1226	84	2	0	16	575*	81	344
0	8	9	468*	735	426	1	3	1	124*	503	616	1	7	0	1142	1280	45	2	0	18	3723	3624	40
0	8	10	0*	376	3206	1	3	2	11099	10760	47	1	7	1	1333	1325	39	2	0	20	4147	4174	42
0	8	11	1194	1292	61	1	3	3	8962	8466	49	1	7	2	691	726	74	2	0	22	1277	1300	71
0	8	12	0*	184	3539	1	3	4	11669	11445	51	1	7	3	3343	3404	30	2	0	24	946	774	99
0	8	13	578*	831	417	1	3	5	11107	10641	53	1	7	4	1460	1418	44	2	2	0	2482	2763	25
0	8	14	0*	465	3974	1	3	6	4527	4505	46	1	7	5	2360	2387	34	2	2	1	4097	3751	35
0	8	15	431*	230	494	1	3	7	7052	7170	61	1	7	6	876	911	67	2	2	2	787	609	33
0	8	16	657*	347	372	1	3	8	5716	5580	56	1	7	7	612	499	90	2	2	3	6281	6552	45
0	8	17	644*	370	376	1	3	9	897	642	47	1	7	8	343*	468	569	2	2	4	2348	2423	24
0	10	0	1179	1161	59	1	3	10	8577	8543	71	1	7	9	2722	2813	37	2	2	5	6408	6214	53
0	10	1	486*	640	423	1	3	11	4871	4857	49	1	7	10	1786	1782	49	2	2	6	569	636	53
0	10	2	601*	503	106	1	3	12	4805	4855	48	1	7	11	2307	2337	43	2	2	7	5250	5203	54
0	10	3	971	999	71	1	3	13	4292	4309	40	1	7	12	1920	1987	47	2	2	8	3970	3953	41
0	10	4	531*	610	127	1	3	14	1558	1503	48	1	7	13	853	960	88	2	2	9	9829	9862	68
0	10	5	598*	455	115	1	3	15	0*	432	3059	1	7	14	0*	378	3459	2	2	10	4063	3992	39
0	10	6	1313	1190	61	1	3	16	4881	4854	47	1	7	15	619*	636	344	2	2	11	5487	5314	56
0	10	7	143*	328	497	1	3	17	1844	1950	57	1	7	16	509*	622	419	2	2	12	1342	1385	44
0	10	8	1234	1165	67	1	3	18	4239	4253	44	1	7	17	1344	1227	70	2	2	13	921	984	63
0	10	9	941	950	85	1	3	19	2833	2805	46	1	7	18	407*	550	644	2	2	14	1577	1594	49
0	10	10	313*	405	242	1	3	20	286*	453	846	1	7	19	916	800	104	2	2	15	4605	4815	48
1	1	0	2639	3163	24	1	3	21	1103	1173	88	1	9	0	2474	2385	37	2	2	16	2109	2166	50
1	1	1	11863	11535	103	1	3	22	2038	2019	58	1	9	1	0*	101	1185	2	2	17	3653	3875	42
1	1	2	16762	16126	138	1	3	23	487*	625	198	1	9	2	1454	1576	49	2	2	18	0*	760	3483
1	1	3	1833	1718	21	1	3	24	2373	2159	57	1	9	3	1062	1101	63	2	2	19	0*	408	1135
1	1	4	9198	9172	44	1	5	0	5369	5382	52	1	9	4	468*	448	128	2	2	20	654*	701	370

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H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
2	2	21	2136	2191	54	2	6	19	914	760	97	3	1	15	850	798	84	3	5	13	1013	1095	78
2	2	22	1297	1336	77	2	6	20	534*	515	167	3	1	16	1412	1447	61	3	5	14	4811	4746	45
2	2	23	2047	2108	58	2	6	21	1330	1167	77	3	1	17	484*	161	465	3	5	15	2117	2121	48
2	2	24	369*	716	775	2	8	0	0*	613	3752	3	1	18	591*	207	401	3	5	16	0*	234	3510
2	4	0	4874	4979	47	2	8	1	4058	4081	40	3	1	19	896	751	103	3	5	17	1810	1849	54
2	4	1	4857	5247	47	2	8	2	2615	2581	34	3	1	20	1316	1343	70	3	5	18	2997	2971	44
2	4	2	314*	647	281	2	8	3	303*	450	614	3	1	21	565*	939	460	3	5	19	286*	192	299
2	4	3	3536	3618	34	2	8	4	2581	2730	37	3	1	22	947	961	91	3	5	20	2753	2670	51
2	4	4	6299	6391	59	2	8	5	3715	3707	37	3	1	23	368*	561	247	3	5	21	1049	941	89
2	4	5	9762	9840	60	2	8	6	547*	783	353	3	1	24	0*	236	3895	3	5	22	0*	842	4219
2	4	6	6512	6501	64	2	8	7	4717	4832	45	3	3	0	2383	2412	24	3	7	0	2618	2625	31
2	4	7	6746	6796	66	2	8	8	1171	1183	63	3	3	1	4815	4814	43	3	7	1	6105	6324	59
2	4	8	2911	2827	29	2	8	9	1653	1535	47	3	3	2	416	647	61	3	7	2	1045	879	55
2	4	9	1465	1506	36	2	8	10	1781	1732	46	3	3	3	6777	7121	52	3	7	3	7610	7798	76
2	4	10	3166	3260	31	2	8	11	1840	1930	50	3	3	4	5027	4939	48	3	7	4	1361	1402	48
2	4	11	3512	3564	36	2	8	12	904	818	82	3	3	5	3182	2895	31	3	7	5	3080	3133	32
2	4	12	4992	4899	45	2	8	13	2688	2682	44	3	3	6	3042	3112	31	3	7	6	2074	2063	38
2	4	13	4299	4194	40	2	8	14	755	604	106	3	3	7	2291	2387	25	3	7	7	3389	3395	33
2	4	14	2468	2386	40	2	8	15	1329	1437	73	3	3	8	736	668	53	3	7	8	382*	185	517
2	4	15	953	1110	83	2	8	16	1300	1280	76	3	3	9	5836	5743	62	3	7	9	6325	6396	64
2	4	16	1164	1087	72	2	8	17	462*	374	552	3	3	10	2317	2327	30	3	7	10	2105	2116	44
2	4	17	1868	1814	55	2	10	0	0*	20	1236	3	3	11	3519	3577	32	3	7	11	4305	4252	39
2	4	18	2474	2456	49	2	10	1	870	885	78	3	3	12	3438	3387	37	3	7	12	1841	1933	52
2	4	19	2784	2734	46	2	10	2	2527	2501	40	3	3	13	405*	66	135	3	7	13	770	822	96
2	4	20	1603	1806	67	2	10	3	523*	273	345	3	3	14	1056	1214	71	3	7	14	994	944	81
2	4	21	1355	1375	75	2	10	4	2704	2721	42	3	3	15	2582	2472	42	3	7	15	3773	3721	42
2	4	22	373*	298	690	2	10	5	1234	1296	68	3	3	16	1431	1526	66	3	7	16	617*	39	376
2	4	23	530*	433	180	2	10	6	862	912	92	3	3	17	2601	2663	48	3	7	17	3019	2977	47
2	6	0	2677	2744	28	2	10	7	0*	815	4419	3	3	18	1944	1961	54	3	7	18	582*	778	421
2	6	1	4274	4339	43	2	10	8	1173	1154	73	3	3	19	0*	463	3183	3	9	0	4830	4754	47
2	6	2	7433	7483	67	2	10	9	363*	470	218	3	3	20	1215	1265	75	3	9	1	1304	1261	54
2	6	3	1600	1591	33	2	10	10	2042	2060	54	3	3	21	1329	1236	71	3	9	2	1398	1428	52
2	6	4	4681	4655	44	3	1	0	4795	4591	32	3	3	22	0*	116	3581	3	9	3	1683	1628	46
2	6	5	1093	1222	44	3	1	1	1318	1378	15	3	3	23	1716	1631	67	3	9	4	3224	3197	36
2	6	6	1557	1365	36	3	1	2	1788	1779	18	3	5	0	9147	9093	60	3	9	5	999	909	70
2	6	7	2888	2852	30	3	1	3	6635	6628	44	3	5	1	4138	4113	42	3	9	6	4805	4951	45
2	6	8	5001	4975	50	3	1	4	5666	5588	51	3	5	2	3027	3021	27	3	9	7	0*	643	3875
2	6	9	2304	2289	37	3	1	5	0*	208	1398	3	5	3	5116	5119	50	3	9	8	2312	2275	43
2	6	10	4907	5037	49	3	1	6	5526	5098	52	3	5	4	4507	4524	44	3	9	9	1546	1563	53
2	6	11	0*	45	3018	3	1	7	5927	5659	56	3	5	5	1262	1213	35	3	9	10	1444	1477	61
2	6	12	1117	1125	67	3	1	8	2248	2262	28	3	5	6	7888	8134	69	3	9	11	1295	1318	71
2	6	13	2042	1997	47	3	1	9	2439	2545	28	3	5	7	1399	1493	38	3	9	12	3274	3158	43
2	6	14	2650	2670	43	3	1	10	0*	396	1617	3	5	8	4355	4310	43	3	9	13	646*	296	400
2	6	15	1796	1820	53	3	1	11	482*	130	311	3	5	9	2808	2873	30	3	11	0	777	616	96
2	6	16	3485	3475	42	3	1	12	2364	2218	36	3	5	10	1582	1708	41	4	0	0	12580	12102	38
2	6	17	334*	329	240	3	1	13	1736	1701	44	3	5	11	1204	1287	57	4	0	2	265*	360	340
2	6	18	1758	1757	59	3	1	14	2849	2812	36	3	5	12	5969	5956	58	4	0	4	5247	4917	53

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
4	0	6	1029	954	45	4	4	12	1201	1293	56	4	8	15	985	1061	94	5	3	11	1860	1869	38
4	0	8	3957	3777	40	4	4	13	4614	4652	46	4	8	16	1484	1533	73	5	3	12	2024	2070	38
4	0	10	2886	2737	30	4	4	14	2143	2104	45	4	10	0	2029	2002	44	5	3	13	3184	3194	36
4	0	12	3969	4072	41	4	4	15	1654	1652	56	4	10	1	1575	1488	53	5	3	14	3927	3968	37
4	0	14	2688	2627	38	4	4	16	1329	1413	71	4	10	2	2993	2955	39	5	3	15	2422	2458	45
4	0	16	308*	118	683	4	4	17	2170	2094	50	4	10	3	693	325	102	5	3	16	3024	3023	43
4	0	18	1618	1563	60	4	4	18	511*	392	430	4	10	4	1527	1453	57	5	3	17	0*	199	1163
4	0	20	589*	940	420	4	4	19	3146	3113	45	4	10	5	1625	1550	54	5	3	18	0*	118	3040
4	0	22	246*	250	315	4	4	20	0*	1211	4032	4	10	6	966	991	82	5	3	19	2227	2186	50
4	0	24	0*	620	4196	4	4	21	1865	1727	63	4	10	7	1284	1227	66	5	3	20	1907	1909	58
4	2	0	0*	562	1539	4	4	22	835	740	119	4	10	8	2494	2428	47	5	3	21	2017	1906	59
4	2	1	4279	4368	40	4	6	0	3762	3977	36	4	10	9	329*	32	670	5	3	22	1916	1863	64
4	2	2	5927	5809	46	4	6	1	446*	365	245	5	1	0	4248	3963	41	5	3	23	763*	725	132
4	2	3	3613	3644	34	4	6	2	8616	8649	69	5	1	1	2644	2821	28	5	5	0	1967	1951	25
4	2	4	4283	4242	43	4	6	3	1864	1988	32	5	1	2	5093	5742	48	5	5	1	1663	1699	28
4	2	5	3378	3497	33	4	6	4	5728	5759	57	5	1	3	5842	5806	52	5	5	2	1885	1945	27
4	2	6	1779	1797	27	4	6	5	3041	3150	29	5	1	4	11233	10747	54	5	5	3	4396	4553	44
4	2	7	242*	406	472	4	6	6	574	651	84	5	1	5	5183	5286	52	5	5	4	6415	6529	58
4	2	8	4871	4870	50	4	6	7	1040	1073	59	5	1	6	569	864	67	5	5	5	4467	4694	45
4	2	9	5171	5098	52	4	6	8	5232	5157	54	5	1	7	4722	4812	50	5	5	6	5402	5315	56
4	2	10	3818	3940	40	4	6	9	1285	1192	55	5	1	8	5655	6139	63	5	5	7	1222	1281	43
4	2	11	2874	2785	31	4	6	10	4874	4911	45	5	1	9	1607	1554	37	5	5	8	647	610	76
4	2	12	1555	1485	41	4	6	11	2539	2552	41	5	1	10	8095	7820	78	5	5	9	2484	2531	33
4	2	13	1068	1032	60	4	6	12	822	755	88	5	1	11	7004	6908	73	5	5	10	4673	4595	48
4	2	14	1482	1433	51	4	6	13	2018	1983	47	5	1	12	1200	1413	55	5	5	11	3173	3240	35
4	2	15	2026	2039	48	4	6	14	3623	3641	38	5	1	13	5340	5316	52	5	5	12	3901	3899	35
4	2	16	2253	2197	47	4	6	15	0*	414	3332	5	1	14	2382	2485	42	5	5	13	1145	1208	72
4	2	17	2232	2236	52	4	6	16	4393	4454	44	5	1	15	355*	726	612	5	5	14	1029	1046	80
4	2	18	1051	944	87	4	6	17	1405	1445	68	5	1	16	3690	3549	40	5	5	15	1390	1456	64
4	2	19	0*	532	3178	4	6	18	1798	1770	59	5	1	17	3103	3020	43	5	5	16	2088	2151	52
4	2	20	877	923	98	4	6	19	1354	1114	72	5	1	18	1995	2061	57	5	5	17	2183	2208	50
4	2	21	1038	1024	90	4	6	20	212*	1012	1378	5	1	19	3087	3083	45	5	5	18	2732	2792	48
4	2	22	1548	1600	68	4	8	0	1798	1800	43	5	1	20	809	824	103	5	5	19	1339	1448	75
4	2	23	1170	999	88	4	8	1	3235	3231	33	5	1	21	721	610	112	5	5	20	1265	1231	83
4	2	24	953	1025	107	4	8	2	3161	3237	33	5	1	22	1772	1659	62	5	5	21	215*	44	1027
4	4	0	4074	3751	40	4	8	3	1689	1687	47	5	1	23	1184	1194	89	5	7	0	2067	2148	35
4	4	1	4968	5124	49	4	8	4	1872	1907	44	5	3	0	7434	7470	50	5	7	1	5072	5070	52
4	4	2	3711	3716	39	4	8	5	5347	5354	55	5	3	1	6574	6554	51	5	7	2	1262	1116	50
4	4	3	3221	3148	32	4	8	6	650	501	102	5	3	2	8169	8205	52	5	7	3	4347	4475	43
4	4	4	521	314	59	4	8	7	3938	4013	45	5	3	3	541	776	54	5	7	4	687	570	80
4	4	5	8960	9021	63	4	8	8	2143	2186	43	5	3	4	2949	3015	29	5	7	5	394*	133	415
4	4	6	3053	3198	29	4	8	9	83*	273	772	5	3	5	6205	6104	52	5	7	6	589*	1019	339
4	4	7	7378	7191	68	4	8	10	2031	1970	45	5	3	6	2549	2609	25	5	7	7	3390	3375	33
4	4	8	5267	5179	52	4	8	11	3404	3303	38	5	3	7	8442	8373	66	5	7	8	827	766	85
4	4	9	670	540	64	4	8	12	367*	74	602	5	3	8	7342	7393	70	5	7	9	3850	3841	37
4	4	10	983	1011	54	4	8	13	3425	3358	42	5	3	9	3336	3200	33	5	7	10	565*	415	125
4	4	11	4486	4428	48	4	8	14	1601	1513	64	5	3	10	4021	4041	40	5	7	11	1403	1368	59

Reflections flagged with an asterisk were considered unobserved.

Values of Fobs and Fcalc (x20.)

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
5	7	12	178*	564	1136	6	2	14	0*	36	3132	6	6	15	1781	1737	55	7	1	17	3830	3838	41
5	7	13	2152	2041	47	6	2	15	6846	6918	71	6	6	16	1242	1125	69	7	1	18	0*	769	3842
5	7	14	1184	1209	73	6	2	16	962	898	96	6	6	17	1215	1203	75	7	1	19	3641	3761	44
5	7	15	3101	2986	44	6	2	17	4212	4261	41	6	6	18	0*	609	3879	7	1	20	2329	2417	50
5	7	16	0*	436	4157	6	2	18	152*	208	577	6	6	19	0*	15	3647	7	1	21	0*	1034	4267
5	7	17	1476	1497	72	6	2	19	1048	1062	82	6	8	0	986	1058	67	7	1	22	2360	2327	55
5	7	18	418*	560	522	6	2	20	0*	221	3750	6	8	1	789	744	76	7	1	23	1265	1455	92
5	9	0	2535	2410	38	6	2	21	3543	3674	46	6	8	2	956	878	68	7	3	0	7216	7370	53
5	9	1	1319	1224	54	6	2	22	297*	399	952	6	8	3	2015	2001	41	7	3	1	149*	199	564
5	9	2	645	547	91	6	2	23	2635	2651	55	6	8	4	594*	186	300	7	3	2	10381	10367	56
5	9	3	410*	187	144	6	4	0	7657	7785	57	6	8	5	838	867	84	7	3	3	5712	5896	51
5	9	4	2910	2871	37	6	4	1	2766	2639	27	6	8	6	461*	576	142	7	3	4	5875	5867	54
5	9	5	767	825	89	6	4	2	767	812	42	6	8	7	480*	507	129	7	3	5	6111	6117	56
5	9	6	2500	2443	41	6	4	3	750	355	46	6	8	8	720	661	88	7	3	6	3570	3582	35
5	9	7	1399	1324	54	6	4	4	6854	6994	64	6	8	9	846	862	84	7	3	7	803	931	54
5	9	8	107*	375	620	6	4	5	2350	2213	26	6	8	10	0*	148	3405	7	3	8	8050	8192	74
5	9	9	1156	1055	69	6	4	6	9184	9145	68	6	8	11	1000	1041	76	7	3	9	2259	2451	32
5	9	10	1619	1482	58	6	4	7	2800	2821	30	6	8	12	0*	600	3839	7	3	10	4707	4702	46
5	9	11	0*	321	4280	6	4	8	3153	3032	29	6	8	13	694*	730	122	7	3	11	3960	3868	40
5	9	12	2025	1971	55	6	4	9	290*	807	500	6	8	14	684*	680	383	7	3	12	378*	101	175
5	9	13	0*	372	3807	6	4	10	3190	3176	30	6	8	15	0*	152	3820	7	3	13	2973	3076	38
6	0	0	14647	14274	47	6	4	11	1001	1115	66	6	10	0	1510	1508	56	7	3	14	4454	4588	44
6	0	2	2937	2561	31	6	4	12	5580	5525	53	6	10	1	715	698	100	7	3	15	0*	576	3431
6	0	4	11431	11222	63	6	4	13	1818	1866	51	6	10	2	443*	242	160	7	3	16	4389	4341	46
6	0	6	16084	15265	70	6	4	14	3296	3145	38	6	10	3	252*	210	762	7	3	17	2754	2667	46
6	0	8	2635	2802	30	6	4	15	1249	1150	69	6	10	4	510*	1037	495	7	3	18	398*	1119	696
6	0	10	6998	7381	72	6	4	16	848	821	96	6	10	5	0*	274	1446	7	3	19	2056	2055	55
6	0	12	12253	12223	87	6	4	17	331*	137	582	6	10	6	1460	1439	62	7	3	20	1945	1838	60
6	0	14	5083	5116	50	6	4	18	3069	3052	44	6	10	7	495*	710	483	7	3	21	0*	219	3819
6	0	16	2109	2104	50	6	4	19	936	1020	105	6	10	8	850	741	95	7	3	22	2428	2388	58
6	0	18	6077	6010	59	6	4	20	2340	2419	56	7	1	0	7826	7526	47	7	5	0	5227	5087	51
6	0	20	3937	3853	43	6	4	21	1140	973	90	7	1	1	3883	3848	41	7	5	1	2191	2350	27
6	0	22	337*	145	243	6	6	0	434*	307	293	7	1	2	11731	11426	51	7	5	2	2995	2988	28
6	2	0	1361	1303	24	6	6	1	2965	2927	28	7	1	3	4037	4169	39	7	5	3	2068	2044	29
6	2	1	13099	13138	47	6	6	2	1311	1422	39	7	1	4	3828	3661	37	7	5	4	1231	1275	41
6	2	2	663	412	42	6	6	3	3033	3111	31	7	1	5	10507	10207	63	7	5	5	4668	4814	49
6	2	3	12158	11836	52	6	6	4	1726	1711	35	7	1	6	5225	5246	54	7	5	6	3509	3565	36
6	2	4	1431	1259	29	6	6	5	425*	786	354	7	1	7	6168	6187	63	7	5	7	3300	3309	31
6	2	5	3200	3223	31	6	6	6	503*	396	308	7	1	8	8855	8579	75	7	5	8	3298	3304	34
6	2	6	0*	548	1747	6	6	7	2342	2357	35	7	1	9	2773	2926	31	7	5	9	255*	161	232
6	2	7	10142	10366	66	6	6	8	722	602	86	7	1	10	4177	4209	40	7	5	10	158*	648	1167
6	2	8	485*	88	259	6	6	9	3374	3325	34	7	1	11	7418	7498	76	7	5	11	2553	2541	39
6	2	9	11598	11594	74	6	6	10	967	1003	75	7	1	12	511*	723	377	7	5	12	1781	1891	50
6	2	10	2251	2210	34	6	6	11	1669	1629	49	7	1	13	5879	5946	58	7	5	13	2517	2430	43
6	2	11	3300	3435	36	6	6	12	0*	218	3510	7	1	14	4884	4886	52	7	5	14	2522	2534	44
6	2	12	736	938	86	6	6	13	953	976	83	7	1	15	364*	11	587	7	5	15	557*	584	139
6	2	13	3913	4039	38	6	6	14	605*	821	132	7	1	16	4090	4213	44	7	5	16	1006	860	79

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
7	5	17	1522	143Ø	63	8	2	1	891Ø	887Ø	53	8	6	4	1393	1382	45	9	1	1Ø	Ø*	76	2425
7	5	18	646*	4ØØ	127	8	2	2	6534	6467	56	8	6	5	2638	2668	33	9	1	11	1485	1628	52
7	5	19	2ØØ7	1952	59	8	2	3	5945	5941	59	8	6	6	3157	322Ø	34	9	1	12	1918	1773	52
7	5	2Ø	Ø*	951	46Ø7	8	2	4	779	761	44	8	6	7	3245	3183	34	9	1	13	1929	2Ø38	55
7	7	Ø	Ø*	413	3Ø75	8	2	5	2282	2297	25	8	6	8	3843	3924	4Ø	9	1	14	1671	1997	61
7	7	1	1127	1137	51	8	2	6	4635	4795	47	8	6	9	1357	14Ø1	57	9	1	15	Ø*	45	1114
7	7	2	1Ø2Ø	991	56	8	2	7	7194	7164	61	8	6	1Ø	2Ø91	2124	45	9	1	16	737	427	112
7	7	3	2383	2464	36	8	2	8	2682	27Ø7	29	8	6	11	12Ø6	123Ø	67	9	1	17	1168	1168	77
7	7	4	774	796	81	8	2	9	4231	4341	44	8	6	12	14Ø2	1188	56	9	1	18	1175	989	77
7	7	5	14Ø5	13Ø7	49	8	2	1Ø	836	797	68	8	6	13	1866	1959	52	9	1	19	14Ø6	16Ø5	72
7	7	6	674	33Ø	88	8	2	11	1544	1492	45	8	6	14	3162	3273	42	9	1	2Ø	937	1176	1Ø1
7	7	7	696	857	1Ø1	8	2	12	1267	1236	57	8	6	15	386*	894	621	9	1	21	235*	669	4Ø6
7	7	8	1ØØ3	952	71	8	2	13	3896	3841	39	8	6	16	2Ø41	2Ø61	56	9	1	22	737*	782	129
7	7	9	1958	188Ø	45	8	2	14	1582	1741	62	8	6	17	Ø*	348	1402	9	3	Ø	271*	162	1Ø3
7	7	1Ø	136Ø	1335	57	8	2	15	4928	5Ø77	5Ø	8	6	18	Ø*	292	3751	9	3	1	6634	6558	59
7	7	11	1526	1484	54	8	2	16	1Ø42	1126	98	8	8	Ø	1427	1447	53	9	3	2	4288	4192	45
7	7	12	Ø*	428	3418	8	2	17	1789	1762	59	8	8	1	1642	1649	47	9	3	3	59Ø5	5699	56
7	7	13	Ø*	116	3334	8	2	18	Ø*	268	33Ø9	8	8	2	2Ø92	2158	42	9	3	4	4655	4694	48
7	7	14	Ø*	414	37Ø8	8	2	19	173Ø	1674	59	8	8	3	2Ø3Ø	2ØØ1	42	9	3	5	Ø*	74	636
7	7	15	965	991	93	8	2	2Ø	1ØØ6	1184	99	8	8	4	951	924	69	9	3	6	516	493	81
7	7	16	67Ø*	531	364	8	2	21	2885	2832	52	8	8	5	3666	3845	4Ø	9	3	7	4651	4696	45
7	7	17	572*	796	159	8	2	22	582*	732	176	8	8	6	973	961	69	9	3	8	1818	189Ø	37
7	9	Ø	1574	1427	46	8	4	Ø	1354	1327	29	8	8	7	2Ø74	2Ø83	43	9	3	9	4325	4284	44
7	9	1	Ø*	39	3473	8	4	1	Ø*	28Ø	196Ø	8	8	8	1697	1647	5Ø	9	3	1Ø	3929	3869	38
7	9	2	Ø*	559	37Ø1	8	4	2	4931	4833	5Ø	8	8	9	565*	779	344	9	3	11	2521	2609	4Ø
7	9	3	1Ø33	1Ø76	67	8	4	3	4377	446Ø	45	8	8	1Ø	1233	1121	66	9	3	12	1741	1728	5Ø
7	9	4	923	94Ø	73	8	4	4	7248	7Ø83	68	8	8	11	2432	2397	46	9	3	13	1Ø49	1161	8Ø
7	9	5	919	989	77	8	4	5	5757	5827	62	8	8	12	Ø*	1Ø4	3738	9	3	14	191Ø	193Ø	53
7	9	6	1464	1481	55	8	4	6	255Ø	266Ø	29	8	8	13	1997	1892	55	9	3	15	3326	327Ø	43
7	9	7	Ø*	271	1234	8	4	7	16Ø1	1621	37	8	8	14	2Ø2*	893	1356	9	3	16	2521	253Ø	47
7	9	8	363*	495	585	8	4	8	1233	1394	46	8	1Ø	Ø	1389	1431	62	9	3	17	1415	15Ø6	69
7	9	9	393*	422	191	8	4	9	2922	2847	32	8	1Ø	1	31Ø*	3ØØ	572	9	3	18	1219	1241	8Ø
7	9	1Ø	552*	599	144	8	4	1Ø	385Ø	3774	4Ø	8	1Ø	2	2376	2344	46	9	3	19	8Ø3	595	1Ø6
7	9	11	6Ø4*	729	142	8	4	11	4ØØ2	398Ø	43	8	1Ø	3	1413	1482	64	9	3	2Ø	Ø*	338	3412
8	Ø	Ø	9625	9Ø45	55	8	4	12	4149	419Ø	41	8	1Ø	4	1621	151Ø	55	9	3	21	1767	1632	69
8	Ø	2	2155	2279	27	8	4	13	22Ø4	22Ø9	46	8	1Ø	5	1145	1181	74	9	5	Ø	4196	4338	41
8	Ø	4	12746	12569	68	8	4	14	8Ø4	731	99	8	1Ø	6	Ø*	352	1445	9	5	1	4Ø22	4171	4Ø
8	Ø	6	99Ø5	9886	76	8	4	15	1264	12ØØ	69	9	1	Ø	2899	2862	27	9	5	2	2155	2177	29
8	Ø	8	972	88Ø	57	8	4	16	2486	2459	47	9	1	1	811	836	42	9	5	3	2Ø93	2Ø93	31
8	Ø	1Ø	7Ø33	6894	75	8	4	17	221Ø	2377	53	9	1	2	1192	1191	34	9	5	4	74Ø7	7462	74
8	Ø	12	6814	7347	66	8	4	18	2524	246Ø	5Ø	9	1	3	753	774	48	9	5	5	1597	1559	4Ø
8	Ø	14	255Ø	2447	44	8	4	19	12Ø1	1245	86	9	1	4	1617	1627	31	9	5	6	6Ø35	6ØØ6	56
8	Ø	16	3368	3351	43	8	4	2Ø	9Ø5	859	1Ø5	9	1	5	3861	3916	4Ø	9	5	7	319Ø	3186	32
8	Ø	18	4581	4785	42	8	6	Ø	4884	4977	49	9	1	6	4413	415Ø	44	9	5	8	Ø*	52	2696
8	Ø	2Ø	28Ø2	28ØØ	48	8	6	1	2776	2736	28	9	1	7	2Ø7Ø	2133	33	9	5	9	1773	1749	45
8	Ø	22	56Ø*	432	44Ø	8	6	2	5542	5615	53	9	1	8	1179	1313	48	9	5	1Ø	3783	3826	42
8	2	Ø	4612	451Ø	46	8	6	3	457*	315	1Ø8	9	1	9	527*	374	98	9	5	11	1ØØ8	941	77

Reflections flagged with an asterisk were considered unobserved.

Values of Fobs and Fclc (x20.)

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
9	5	12	4584	4565	49	10	2	0	4097	4227	42	10	6	5	1927	2059	42	11	1	15	1888	1902	59
9	5	13	2533	2565	44	10	2	1	3394	3404	33	10	6	6	4915	4943	47	11	1	16	2373	2314	52
9	5	14	1300	1421	66	10	2	2	3244	3424	33	10	6	7	227*	153	892	11	1	17	2000	2099	55
9	5	15	1527	1547	62	10	2	3	1649	1689	29	10	6	8	5489	5440	54	11	1	18	0*	38	3202
9	5	16	1862	1796	54	10	2	4	970	980	44	10	6	9	1689	1777	52	11	1	19	730*	648	125
9	5	17	668*	220	128	10	2	5	419*	650	315	10	6	10	2014	1920	47	11	1	20	993	1054	100
9	5	18	2735	2622	51	10	2	6	3468	3515	37	10	6	11	1788	1796	50	11	1	21	304*	609	899
9	5	19	637*	956	420	10	2	7	2537	2516	30	10	6	12	2617	2601	44	11	3	0	8033	8145	62
9	7	0	1264	1218	51	10	2	8	4521	4506	44	10	6	13	563*	461	395	11	3	1	3513	3437	37
9	7	1	6850	6859	71	10	2	9	1373	1531	49	10	6	14	4154	4088	44	11	3	2	2081	2010	28
9	7	2	834	879	78	10	2	10	2403	2422	38	10	6	15	858	805	109	11	3	3	2249	2225	28
9	7	3	4258	4316	41	10	2	11	237*	320	909	10	6	16	2247	2219	56	11	3	4	3503	3549	35
9	7	4	2236	2219	39	10	2	12	737	780	102	10	6	17	1388	1247	75	11	3	5	4465	4731	44
9	7	5	1583	1628	49	10	2	13	0*	213	2947	10	8	0	2825	2847	37	11	3	6	5697	5850	60
9	7	6	1266	1181	60	10	2	14	2746	2646	45	10	8	1	572*	427	110	11	3	7	3720	3544	37
9	7	7	4785	4971	53	10	2	15	614*	818	154	10	8	2	2484	2575	39	11	3	8	2478	2530	34
9	7	8	478*	334	453	10	2	16	1247	1284	76	10	8	3	4561	4604	48	11	3	9	1138	1031	60
9	7	9	4418	4323	42	10	2	17	0*	524	1188	10	8	4	0*	151	3541	11	3	10	1485	1609	55
9	7	10	1410	1338	58	10	2	18	804	732	104	10	8	5	4040	4013	41	11	3	11	2523	2687	43
9	7	11	595*	488	118	10	2	19	550*	175	473	10	8	6	1752	1721	49	11	3	12	3128	3156	41
9	7	12	1342	1320	64	10	2	20	1411	1362	81	10	8	7	305*	706	687	11	3	13	3791	3750	40
9	7	13	3124	3099	45	10	2	21	745*	386	402	10	8	8	1827	1794	49	11	3	14	2335	2287	50
9	7	14	0*	238	4266	10	4	0	2772	2751	28	10	8	9	2633	2486	42	11	3	15	853	995	98
9	7	15	3356	3359	47	10	4	1	641	610	58	10	8	10	0*	425	4734	11	3	16	396*	67	602
9	7	16	862	883	114	10	4	2	0*	281	2247	10	8	11	3500	3392	43	11	3	17	1459	1444	67
9	9	0	2395	2393	40	10	4	3	6418	6481	61	10	8	12	996	1074	94	11	3	18	1670	1585	68
9	9	1	1183	1073	59	10	4	4	2440	2609	29	10	8	13	1615	1686	68	11	3	19	1945	1944	67
9	9	2	1761	1749	49	10	4	5	7786	7922	74	10	10	0	2785	2796	44	11	3	20	1613	1580	74
9	9	3	638*	663	108	10	4	6	2851	2810	30	10	10	1	569*	406	133	11	5	0	930	985	51
9	9	4	4170	4074	42	10	4	7	2224	2249	34	10	10	2	2461	2235	45	11	5	1	4419	4316	44
9	9	5	468*	166	435	10	4	8	1368	1307	49	10	10	3	1454	1509	63	11	5	2	5053	5139	51
9	9	6	2777	2754	42	10	4	9	4086	4073	42	10	10	4	0*	49	3984	11	5	3	5095	5128	53
9	9	7	954	892	82	10	4	10	0*	72	3250	11	1	0	5344	5568	53	11	5	4	5310	5343	53
9	9	8	0*	413	4006	10	4	11	5921	5926	59	11	1	1	2510	2464	25	11	5	5	1887	1749	40
9	9	9	1039	1103	84	10	4	12	804	766	102	11	1	2	5930	5823	57	11	5	6	1106	1077	62
9	9	10	2588	2620	49	10	4	13	2318	2348	49	11	1	3	6525	6585	60	11	5	7	1831	1775	42
10	0	0	963	853	42	10	4	14	1589	1444	55	11	1	4	383*	278	334	11	5	8	3036	3218	36
10	0	2	2388	2414	29	10	4	15	1487	1580	59	11	1	5	3847	4004	39	11	5	9	2715	2758	40
10	0	4	2474	2385	30	10	4	16	0*	340	3008	11	1	6	3620	3669	37	11	5	10	4431	4484	46
10	0	6	582	607	96	10	4	17	2874	2796	46	11	1	7	1856	1828	38	11	5	11	248*	866	1034
10	0	8	1204	918	53	10	4	18	358*	674	847	11	1	8	4574	4710	45	11	5	12	1741	1758	54
10	0	10	2075	2028	43	10	4	19	1960	2010	66	11	1	9	5504	5484	54	11	5	13	617*	1062	399
10	0	12	764	843	102	10	6	0	6899	6977	65	11	1	10	2668	2441	38	11	5	14	1128	1069	70
10	0	14	666*	993	407	10	6	1	1120	959	54	11	1	11	4096	4205	42	11	5	15	1939	1876	55
10	0	16	618*	405	140	10	6	2	7075	7034	68	11	1	12	851	1035	105	11	5	16	2240	2235	59
10	0	18	530*	468	406	10	6	3	2461	2580	35	11	1	13	857	657	104	11	5	17	1530	1508	74
10	0	20	510*	267	441	10	6	4	693	727	86	11	1	14	2336	2412	51	11	5	18	1918	1860	63

Reflections flagged with an asterisk were considered unobserved.

Values of Fobs and Fclc (x20.)

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
11	7	0	1873	1957	43	12	2	12	0*	165	3306	12	8	3	1729	1738	48	13	3	18	1509	1644	82
11	7	1	5442	5493	54	12	2	13	5701	5672	56	12	8	4	0*	392	3762	13	5	0	2824	2781	31
11	7	2	629*	682	106	12	2	14	743*	1007	134	12	8	5	1043	1047	67	13	5	1	2109	2200	36
11	7	3	1237	1226	58	12	2	15	4234	4030	41	12	8	6	283*	549	247	13	5	2	952	1035	65
11	7	4	2314	2215	40	12	2	16	456*	543	560	12	8	7	0*	449	3391	13	5	3	4104	4149	44
11	7	5	3054	3107	37	12	2	17	0*	149	3254	12	8	8	0*	247	3894	13	5	4	1709	1752	46
11	7	6	1384	1469	57	12	2	18	0*	138	3754	12	8	9	1438	1462	65	13	5	5	3435	3426	37
11	7	7	4273	4278	44	12	2	19	2455	2399	57	12	8	10	603*	354	131	13	5	6	2420	2394	40
11	7	8	0*	140	3646	12	2	20	0*	554	3589	12	8	11	1213	1106	76	13	5	7	490*	298	375
11	7	9	2141	2070	45	12	4	0	1025	1096	44	13	1	0	9302	9324	65	13	5	8	1813	1827	49
11	7	10	1383	1303	60	12	4	1	0*	111	2111	13	1	1	5313	5387	55	13	5	9	2748	2751	41
11	7	11	1319	1439	68	12	4	2	6572	6668	63	13	1	2	4762	4663	48	13	5	10	0*	41	3225
11	7	12	1241	1237	76	12	4	3	3328	3224	31	13	1	3	9705	9555	73	13	5	11	2381	2366	44
11	7	13	3045	3002	48	12	4	4	7249	7429	67	13	1	4	3586	3516	38	13	5	12	1380	1458	62
11	7	14	0*	275	3938	12	4	5	3378	3336	33	13	1	5	5655	5705	55	13	5	13	333*	335	585
11	9	0	299*	550	640	12	4	6	3030	3040	33	13	1	6	8243	8144	72	13	5	14	1074	1036	82
11	9	1	1021	949	68	12	4	7	1402	1475	50	13	1	7	2198	2343	40	13	5	15	1748	1663	61
11	9	2	2331	2511	44	12	4	8	1695	1752	49	13	1	8	5711	5757	57	13	5	16	360*	276	712
11	9	3	0*	44	3850	12	4	9	1707	1654	51	13	1	9	6364	6373	64	13	7	0	899	981	76
11	9	4	3365	3261	39	12	4	10	4236	4355	38	13	1	10	437*	296	572	13	7	1	1047	1053	66
11	9	5	1021	948	78	12	4	11	1988	2076	52	13	1	11	5147	5089	54	13	7	2	719	698	91
11	9	6	1519	1342	58	12	4	12	3715	3658	39	13	1	12	3653	3617	44	13	7	3	750	913	88
11	9	7	593*	1079	434	12	4	13	883	745	93	13	1	13	0*	506	3786	13	7	4	236*	201	711
11	9	8	1247	1146	71	12	4	14	199*	334	370	13	1	14	3883	3769	43	13	7	5	449*	54	401
12	0	0	1578	1789	33	12	4	15	0*	355	3334	13	1	15	2839	2924	48	13	7	6	701	797	101
12	0	2	11203	11146	74	12	4	16	2607	2512	49	13	1	16	0*	773	3618	13	7	7	511*	407	123
12	0	4	12901	12675	80	12	4	17	1549	1507	72	13	1	17	3256	3155	45	13	7	8	510*	317	385
12	0	6	4331	4451	46	12	4	18	2186	2108	60	13	1	18	1499	1483	73	13	7	9	827	809	93
12	0	8	5600	5371	55	12	6	0	3347	3436	37	13	1	19	1318	1365	83	13	7	10	0*	324	3713
12	0	10	8297	8540	84	12	6	1	3027	3072	33	13	3	0	8942	9006	68	13	7	11	721	700	114
12	0	12	4925	4932	48	12	6	2	2643	2712	35	13	3	1	3554	3468	33	13	7	12	198*	451	1169
12	0	14	1615	1436	63	12	6	3	1546	1544	46	13	3	2	4939	5036	52	13	7	13	0*	62	4410
12	0	16	4515	4630	45	12	6	4	0*	12	3386	13	3	3	6489	6464	65	13	9	0	561*	612	129
12	0	18	3476	3474	46	12	6	5	986	1049	75	13	3	4	2221	2258	33	13	9	1	437*	58	497
12	0	20	0*	575	4058	12	6	6	2283	2307	41	13	3	5	3072	2936	31	13	9	2	255*	45	754
12	2	0	1387	1353	33	12	6	7	2921	2899	38	13	3	6	6363	6299	59	13	9	3	258*	604	938
12	2	1	12153	11966	64	12	6	8	2624	2701	41	13	3	7	914	1022	76	13	9	4	518*	334	147
12	2	2	1138	1024	40	12	6	9	2132	2192	45	13	3	8	4826	4683	51	13	9	5	324*	595	706
12	2	3	3409	3397	33	12	6	10	401*	431	499	13	3	9	3630	3677	39	13	9	6	630*	286	328
12	2	4	0*	153	2032	12	6	11	0*	27	1189	13	3	10	280*	20	272	14	0	0	3086	3097	31
12	2	5	6679	6511	65	12	6	12	1275	1398	69	13	3	11	3922	3934	43	14	0	2	10148	9874	81
12	2	6	896	1004	65	12	6	13	1283	1388	71	13	3	12	3936	3977	39	14	0	4	9612	9324	86
12	2	7	8648	8536	81	12	6	14	1588	1527	67	13	3	13	532*	299	463	14	0	6	1336	1088	62
12	2	8	2719	2675	35	12	6	15	1298	1284	81	13	3	14	4146	4096	44	14	0	8	6110	6066	63
12	2	9	4098	3972	46	12	8	0	1132	1173	58	13	3	15	2009	2127	55	14	0	10	7020	7006	74
12	2	10	1772	1772	50	12	8	1	621*	953	323	13	3	16	1070	887	80	14	0	12	2667	2643	48
12	2	11	2373	2219	44	12	8	2	0*	225	3297	13	3	17	1941	1976	64	14	0	14	2700	2804	48

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
14	0	16	4302	4215	43	14	6	8	1398	1250	57	15	3	11	0*	417	3689	16	0	16	618*	244	151
14	0	18	2414	2525	56	14	6	9	0*	325	3500	15	3	12	1572	1571	61	16	2	0	4057	4144	42
14	2	0	2832	2785	29	14	6	10	0*	347	3860	15	3	13	2611	2666	48	16	2	1	865	839	61
14	2	1	8457	8366	70	14	6	11	1615	1618	59	15	3	14	2014	2076	53	16	2	2	415*	595	398
14	2	2	722	574	65	14	6	12	1556	1550	65	15	3	15	1936	1939	61	16	2	3	585*	542	304
14	2	3	601	472	81	14	6	13	1427	1263	69	15	3	16	635*	823	156	16	2	4	2226	2205	39
14	2	4	1984	2052	36	14	6	14	768*	1204	394	15	3	17	0*	262	3765	16	2	5	640*	626	108
14	2	5	6863	6797	71	14	8	0	1504	1450	50	15	5	0	514*	401	306	16	2	6	3328	3386	37
14	2	6	2044	2099	42	14	8	1	1043	1051	69	15	5	1	682	621	91	16	2	7	774	735	104
14	2	7	6795	6891	70	14	8	2	925	930	76	15	5	2	4758	4923	48	16	2	8	2052	2108	49
14	2	8	797	734	96	14	8	3	2294	2344	44	15	5	3	1864	1935	47	16	2	9	1463	1531	65
14	2	9	1512	1578	60	14	8	4	0*	407	4201	15	5	4	5253	5332	52	16	2	10	0*	142	3576
14	2	10	502*	324	482	14	8	5	1381	1418	64	15	5	5	2311	2388	43	16	2	11	573*	792	423
14	2	11	3915	3934	41	14	8	6	1047	1198	81	15	5	6	1797	1820	49	16	2	12	1793	1935	58
14	2	12	1282	1220	77	14	8	7	0*	253	3747	15	5	7	635*	713	113	16	2	13	0*	171	3384
14	2	13	5394	5420	52	14	8	8	826	890	100	15	5	8	2306	2403	45	16	2	14	1134	1199	85
14	2	14	752*	871	125	14	8	9	1379	1312	69	15	5	9	1044	1023	79	16	2	15	0*	311	3447
14	2	15	2290	2420	53	15	1	0	1935	1919	31	15	5	10	3715	3595	39	16	2	16	0*	257	3368
14	2	16	596*	336	468	15	1	1	1818	1756	34	15	5	11	1886	1915	55	16	2	17	699*	400	379
14	2	17	803	954	127	15	1	2	411*	439	363	15	5	12	1599	1585	60	16	4	0	1444	1547	49
14	2	18	795*	743	133	15	1	3	4245	4201	42	15	5	13	967	1091	98	16	4	1	4305	4244	43
14	4	0	2102	2238	33	15	1	4	3305	3285	35	15	5	14	0*	728	4559	16	4	2	0*	85	3625
14	4	1	2433	2581	31	15	1	5	3141	3226	34	15	5	15	210*	50	1337	16	4	3	4540	4543	46
14	4	2	5386	5408	57	15	1	6	3913	3945	40	15	7	0	814	705	81	16	4	4	1215	1275	61
14	4	3	3182	3210	32	15	1	7	673	530	106	15	7	1	3808	3938	38	16	4	5	1677	1641	48
14	4	4	3916	3991	40	15	1	8	1218	1143	73	15	7	2	1921	1924	43	16	4	6	1936	1923	47
14	4	5	576*	731	320	15	1	9	2221	2271	51	15	7	3	0*	300	1213	16	4	7	2346	2347	43
14	4	6	0*	187	3303	15	1	10	1365	1285	70	15	7	4	1435	1309	53	16	4	8	1197	1245	71
14	4	7	2057	2141	44	15	1	11	2116	2146	55	15	7	5	3363	3359	38	16	4	9	4445	4409	42
14	4	8	3389	3342	37	15	1	12	2319	2374	53	15	7	6	401*	43	527	16	4	10	0*	536	3626
14	4	9	2732	2807	42	15	1	13	0*	199	1099	15	7	7	3340	3379	41	16	4	11	2502	2484	47
14	4	10	4088	3987	40	15	1	14	795	698	111	15	7	8	418*	680	560	16	4	12	1047	1039	81
14	4	11	1779	1794	53	15	1	15	1593	1625	65	15	7	9	1067	1000	83	16	4	13	200*	423	1182
14	4	12	1125	1184	72	15	1	16	210*	791	1502	15	7	10	0*	728	4586	16	4	14	0*	541	1404
14	4	13	267*	520	294	15	1	17	1835	1829	64	15	7	11	1784	1636	58	16	4	15	1900	1902	63
14	4	14	1679	1753	59	15	1	18	1440	1468	79	15	9	0	646*	528	121	16	6	0	5909	5902	59
14	4	15	1286	1100	73	15	3	0	3827	3898	39	15	9	1	520*	725	154	16	6	1	2131	2087	41
14	4	16	2200	2183	58	15	3	1	4599	4684	44	15	9	2	2795	2806	44	16	6	2	1492	1517	53
14	4	17	0*	590	4056	15	3	2	3645	3521	37	15	9	3	376*	165	560	16	6	3	2668	2583	38
14	6	0	3953	3992	36	15	3	3	1269	1166	51	16	0	0	304*	540	525	16	6	4	2796	2868	40
14	6	1	463*	635	411	15	3	4	536*	479	100	16	0	2	603*	474	103	16	6	5	1310	1222	59
14	6	2	1956	1977	42	15	3	5	2220	2245	39	16	0	4	556*	588	134	16	6	6	4401	4383	41
14	6	3	1642	1680	48	15	3	6	2807	2715	37	16	0	6	182*	209	1246	16	6	7	1004	990	78
14	6	4	1843	1802	47	15	3	7	4025	4090	45	16	0	8	0*	106	3095	16	6	8	2492	2385	44
14	6	5	2929	3031	38	15	3	8	2493	2472	45	16	0	10	0*	40	3391	16	6	9	1799	1764	54
14	6	6	2703	2671	39	15	3	9	3017	2992	41	16	0	12	529*	158	473	16	6	10	1181	1279	78
14	6	7	2107	2014	44	15	3	10	403*	662	540	16	0	14	0*	527	3591	16	6	11	1015	896	91

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
16	6	12	3025	2973	48	17	5	6	1260	1150	62	18	4	6	0*	112	3305	19	3	9	3015	2964	44
16	8	0	1873	1844	48	17	5	7	1975	1866	48	18	4	7	1303	1448	65	19	3	10	2137	2229	55
16	8	1	2706	2678	43	17	5	8	3815	3780	40	18	4	8	2831	2803	43	19	3	11	1389	1330	76
16	8	2	0*	351	1502	17	5	9	1149	1031	70	18	4	9	2252	2173	47	19	3	12	2901	2827	50
16	8	3	3404	3381	41	17	5	10	2375	2404	49	18	4	10	2748	2875	46	19	3	13	0*	666	4925
16	8	4	1181	1200	73	17	5	11	468*	544	192	18	4	11	1245	1246	79	19	5	0	1800	1825	45
16	8	5	1331	1353	68	17	5	12	0*	354	4405	18	4	12	0*	688	4187	19	5	1	3222	3240	36
16	8	6	1631	1574	58	17	5	13	1314	1473	83	18	4	13	208*	49	1174	19	5	2	0*	169	3315
17	1	0	4138	4106	44	17	7	0	540*	713	406	18	6	0	2085	2084	42	19	5	3	2588	2614	41
17	1	1	2590	2625	34	17	7	1	1764	1655	48	18	6	1	1688	1803	49	19	5	4	1502	1537	54
17	1	2	2363	2375	38	17	7	2	1495	1499	55	18	6	2	0*	266	1133	19	5	5	595*	77	317
17	1	3	2483	2468	39	17	7	3	1595	1674	55	18	6	3	491*	165	331	19	5	6	2037	1891	48
17	1	4	825	707	89	17	7	4	1482	1482	58	18	6	4	1467	1514	56	19	5	7	1769	1830	56
17	1	5	171*	339	1326	17	7	5	3313	3343	42	18	6	5	1737	1680	51	19	5	8	0*	553	4147
17	1	6	2633	2676	44	17	7	6	0*	614	4605	18	6	6	2450	2372	46	19	5	9	1859	1825	56
17	1	7	1857	1882	55	17	7	7	2382	2373	49	18	6	7	1899	1823	51	19	5	10	0*	818	4480
17	1	8	2348	2310	50	17	7	8	476*	713	476	18	6	8	922	993	97	19	5	11	0*	595	4311
17	1	9	2803	2733	47	18	0	0	3993	3984	41	18	6	9	0*	565	3842	19	7	0	0*	153	4178
17	1	10	0*	293	3514	18	0	2	7179	7308	74	18	6	10	1107	1025	86	19	7	1	0*	787	4326
17	1	11	1037	1055	93	18	0	4	4820	4824	48	18	8	0	758	595	103	19	7	2	0*	264	1364
17	1	12	1989	1903	57	18	0	6	1514	1521	71	18	8	1	1609	1685	59	19	7	3	713	821	115
17	1	13	595*	562	440	18	0	8	5525	5546	51	18	8	2	322*	240	702	19	7	4	0*	766	4263
17	1	14	1751	1724	65	18	0	10	4413	4400	43	18	8	3	1397	1314	65	19	7	5	0*	385	4469
17	1	15	1206	1084	91	18	0	12	465*	250	494	19	1	0	4259	4417	44	19	7	6	405*	528	201
17	1	16	434*	595	711	18	0	14	2908	2858	53	19	1	1	5737	5641	58	20	0	0	5540	5484	54
17	3	0	1472	1310	46	18	2	0	1804	1792	44	19	1	2	551*	95	401	20	0	2	7173	7339	80
17	3	1	0*	249	1099	18	2	1	4129	4202	44	19	1	3	5694	5702	56	20	0	4	2723	2638	48
17	3	2	1873	1784	43	18	2	2	463*	460	142	19	1	4	4411	4421	45	20	0	6	3408	3360	45
17	3	3	3469	3539	34	18	2	3	2011	1972	42	19	1	5	806	727	109	20	0	8	5271	5202	45
17	3	4	3214	3187	36	18	2	4	1298	1157	64	19	1	6	4589	4623	46	20	0	10	3003	3020	48
17	3	5	3841	3747	37	18	2	5	6138	6194	59	19	1	7	4157	4050	41	20	0	12	809	951	129
17	3	6	2249	2152	43	18	2	6	2190	1998	49	19	1	8	1154	1015	81	20	2	0	389*	290	515
17	3	7	2079	2008	49	18	2	7	5051	5082	50	19	1	9	4433	4413	46	20	2	1	1848	1799	48
17	3	8	0*	186	3677	18	2	8	1227	1218	74	19	1	10	2566	2564	50	20	2	2	1069	1033	74
17	3	9	1549	1454	58	18	2	9	0*	150	3142	19	1	11	1735	1719	66	20	2	3	4461	4389	47
17	3	10	1913	1983	55	18	2	10	337*	309	734	19	1	12	3270	3283	48	20	2	4	1477	1324	61
17	3	11	2849	2914	45	18	2	11	3512	3510	43	19	1	13	1509	1486	79	20	2	5	6367	6302	63
17	3	12	1840	1814	57	18	2	12	708*	754	389	19	1	14	1596	1569	76	20	2	6	0*	396	4149
17	3	13	1541	1650	71	18	2	13	3365	3318	49	19	3	0	3694	3759	40	20	2	7	2630	2618	46
17	3	14	489*	294	185	18	2	14	0*	621	4183	19	3	1	3901	3899	39	20	2	8	514*	201	433
17	3	15	407*	225	236	18	2	15	984	867	113	19	3	2	865	893	85	20	2	9	1644	1758	63
17	5	0	3322	3282	34	18	4	0	1985	2019	42	19	3	3	3426	3454	36	20	2	10	407*	692	643
17	5	1	2147	2178	42	18	4	1	1835	1872	45	19	3	4	4270	4365	43	20	2	11	3806	3773	46
17	5	2	4658	4731	45	18	4	2	4426	4548	48	19	3	5	460*	475	464	20	2	12	301*	639	965
17	5	3	1200	1153	66	18	4	3	2240	2227	43	19	3	6	3655	3646	39	20	2	13	2880	2781	55
17	5	4	2730	2769	40	18	4	4	3167	3188	39	19	3	7	2321	2301	47	20	4	0	3819	3764	37
17	5	5	0*	632	3391	18	4	5	1054	997	74	19	3	8	0*	330	3733	20	4	1	1973	2015	47

Reflections flagged with an asterisk were considered unobserved.

Values of Fobs and Fcalc (x20.)

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
20	4	2	4028	4095	42	21	5	4	2045	2090	49	23	3	0	1222	1181	65	26	0	4	1818	1827	74
20	4	3	715	752	101	21	5	5	951	895	86	23	3	1	1457	1428	59	26	2	0	536*	563	494
20	4	4	0*	994	4030	21	5	6	991	975	90	23	3	2	2559	2564	43	26	2	1	2200	2166	53
20	4	5	180*	483	1150	21	5	7	733*	529	370	23	3	3	2448	2486	46	26	2	2	681*	618	141
20	4	6	2475	2471	45	21	5	8	2721	2729	51	23	3	4	1534	1497	60	26	2	3	4234	4331	46
20	4	7	1475	1411	63	21	7	0	1064	915	78	23	3	5	1874	1790	56	26	2	4	0*	150	4744
20	4	8	3176	3163	44	21	7	1	874	880	97	23	3	6	464*	685	193	26	4	0	2800	2727	46
20	4	9	1139	1012	86	22	0	0	733*	777	125	23	3	7	0*	29	1402	27	1	0	737*	834	132
20	4	10	1781	1651	62	22	0	2	631*	567	145	23	3	8	1490	1408	70	27	1	1	2466	2346	54
20	4	11	543*	273	166	22	0	4	349*	66	720	23	5	0	3308	3329	42	27	1	2	2389	2393	55
20	6	0	956	1008	74	22	0	6	0*	606	3534	23	5	1	1157	1147	77						
20	6	1	249*	568	737	22	0	8	736*	679	137	23	5	2	2429	2370	49						
20	6	2	358*	484	586	22	0	10	0*	338	3907	23	5	3	734	773	119						
20	6	3	1942	1936	51	22	2	0	1017	938	74	23	5	4	194*	334	1281						
20	6	4	1206	1281	74	22	2	1	435*	674	168	24	0	0	4887	4736	49						
20	6	5	1609	1644	62	22	2	2	1525	1604	58	24	0	2	3449	3493	45						
20	6	6	1204	1109	77	22	2	3	1022	1045	81	24	0	4	806	532	116						
20	6	7	520*	224	408	22	2	4	2654	2684	45	24	0	6	3120	3118	55						
21	1	0	948	785	81	22	2	5	816	918	103	24	0	8	2848	2750	57						
21	1	1	4121	4066	43	22	2	6	1818	1803	57	24	2	0	0*	707	3927						
21	1	2	1996	1908	50	22	2	7	539*	60	152	24	2	1	507*	599	152						
21	1	3	3266	3201	42	22	2	8	0*	111	3614	24	2	2	620*	516	377						
21	1	4	2898	2911	45	22	2	9	625*	758	446	24	2	3	3386	3344	41						
21	1	5	467*	137	530	22	2	10	1521	1361	73	24	2	4	1697	1671	64						
21	1	6	1382	1313	66	22	4	0	244*	552	837	24	2	5	2836	2843	50						
21	1	7	2264	2286	51	22	4	1	3947	3961	36	24	2	6	1256	1319	85						
21	1	8	709*	710	132	22	4	2	565*	412	383	24	2	7	105*	464	917						
21	1	9	2376	2245	52	22	4	3	2427	2353	44	24	4	0	2895	2844	42						
21	1	10	1753	1836	69	22	4	4	719	866	113	24	4	1	2662	2700	46						
21	1	11	827	722	123	22	4	5	940	994	91	24	4	2	2366	2319	49						
21	1	12	1386	1536	85	22	4	6	1044	1063	87	24	4	3	1477	1467	65						
21	3	0	3228	3162	37	22	4	7	2997	2990	47	24	4	4	478*	81	507						
21	3	1	2456	2387	42	22	4	8	435*	459	221	24	4	5	830	795	111						
21	3	2	822	798	89	22	6	0	1800	1787	56	25	1	0	658*	385	125						
21	3	3	429*	477	455	22	6	1	1777	1815	56	25	1	1	4106	4026	40						
21	3	4	1757	1792	52	22	6	2	1402	1395	68	25	1	2	2706	2601	48						
21	3	5	2760	2670	42	22	6	3	269*	1159	964	25	1	3	964	857	104						
21	3	6	2451	2402	45	23	1	0	1135	1172	71	25	1	4	3269	3239	49						
21	3	7	2474	2496	47	23	1	1	1578	1495	57	25	1	5	2388	2404	58						
21	3	8	1069	959	87	23	1	2	355*	337	216	25	1	6	1224	1429	100						
21	3	9	0*	698	4371	23	1	3	0*	187	3626	25	3	0	327*	110	242						
21	3	10	888	865	109	23	1	4	1307	1338	73	25	3	1	2514	2545	47						
21	3	11	958	1011	111	23	1	5	1447	1321	67	25	3	2	2665	2690	48						
21	5	0	2068	2239	45	23	1	6	1220	1320	82	25	3	3	1333	1244	73						
21	5	1	1169	1155	63	23	1	7	1377	1295	79	25	3	4	2804	2733	50						
21	5	2	3328	3313	39	23	1	8	780	473	125	26	0	0	5499	5411	53						
21	5	3	1606	1636	57	23	1	9	690*	366	393	26	0	2	2923	2772	52						

Reflections flagged with an asterisk were considered unobserved.

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