

# Chapter 8

## Crystal Structure of 1-Benzyl-4-Phenyl-1,2,3- Triazole

### 8.1 Introduction

Continuing our studies on triazoles, we present crystal structure of 1-benzyl-4-phenyl-1,2,3-triazole in this chapter. Upon controlled crystallization we get single crystals using the solvent ether.

### 8.2 Experimental

#### 8.2.1 Data Collection

A colourless rectangular crystal of  $C_{15}H_{13}N_3$  having approximate dimensions of 0.35 x 0.25 x 0.20 mm was mounted on a glass fiber. All measurements were made on a Rigaku AFC7S diffractometer with graphite monochromated *Mo-K $\alpha$*  radiation.

Cell constants and an orientation matrix for data collection, obtained from a least-squares refinement using the setting angles of 22 carefully centered reflections in the range  $13.93 < 2\theta < 17.62^\circ$  corresponded to a

primitive monoclinic cell with dimensions:  $a = 6.038(2) \text{ \AA}$ ,  $b = 8.094(3) \text{ \AA}$ ,  $c = 25.62(1) \text{ \AA}$ ,  $\beta = 93.80(4)^\circ$ ,  $V = 1249.1(9) \text{ \AA}^3$ ,  $Z = 4$  and  $F.W. = 235.29$ , the calculated density is  $1.25 \text{ g/cm}^3$ . The systematic absences

$$\begin{aligned} hol & l \neq 2n \\ 0k0 & k \neq 2n \end{aligned}$$

uniquely determine the space group to be

$$P2_1/c \text{ (#14)}.$$

The data were collected at a temperature of  $20 \pm 1^\circ\text{C}$  using the  $\omega$  scan technique to a maximum  $2\theta$  value of  $50.0^\circ$ . Omega scans of several intense reflections, made prior to data collection, had an average width at half-height of  $0.38^\circ$  with a take-off angle of  $6.0^\circ$ . Scans of  $(1.15 + 0.14 \tan \theta)^\circ$  were made at a speed of  $16.0^\circ/\text{min}$  (in omega). The weak reflections ( $I < 15.0\sigma(I)$ ) were rescanned (maximum of 4 scans) and the counts were accumulated to ensure good counting statistics. Stationary background counts were recorded on each side of the reflection. The ratio of peak counting time to background counting time was 2:1. The diameter of the incident beam collimator was 1.0 mm and the crystal to detector distance was 400 mm, The computer-controlled slits were set to 9.0 mm (horizontal) and 13.0 mm (vertical).

### 8.2.2 Data Reduction

Of the 2608 reflections which were collected, 2372 were unique ( $R_{int} = 0.017$ ). The intensities of three representative reflections were measured after every 150 reflections. Certain class of reflections  $h + k + l = 2n$  were affected by pseudotranslational effects. Pseudotranslational symmetry will be neglected in subsequent steps. Over the course of data collection, the standards increased by 2.3%. A linear correction factor was applied to the data to account for this phenomenon.

Data were reduced by teXsan data reduction program[125]. Wilson plot[103] gave the temperature factor, B and scale factor. K as  $3.89 \text{ \AA}^2$  and 1.853 respectively. The linear absorption coefficient,  $\mu$ , for Mo— $K\alpha$  radiation is  $0.7 \text{ cm}^{-1}$ . An empirical absorption correction[125] based on azimuthal scans of several reflections was applied which resulted in transmission factors

ranging from 0.93 to 1.00. The data were corrected for Lorentz and polarization effects. A correction for secondary extinction was applied (coefficient =  $1.24531 \times 10^{-6}$ ).

### 8.2.3 Structure Solution and Refinement

The structure was solved by direct methods, SIR92[124] and expanded using Fourier techniques. Of the 10 phase sets that were refined, one set had a maximum combined figure of merit of 0.862. This was used to compute the E-map further. All the non-hydrogen atoms were revealed in the first map itself. Full-matrix least-squares refinement based on 1644 observed reflections ( $I > 3\sigma(I)$ ) with isotropic temperature factors for all the atoms converged to the residuals to  $R = 0.127$ , and  $R_w = 0.15$ . At this stage the hydrogen atoms were generated and placed at a distance of 0.98Å from the parent atom. The isotropic temperature factors of the hydrogen atoms were set to 1.2 times of the equivalent isotropic temperature factor of the parent atom. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included but not refined. The final cycle of full-matrix least-squares refinement[129] was based on 1644 observed reflections ( $I > 3\sigma(I)$ ) and 164 variable parameters and converged (largest parameter shift was 0.83 times its esd) with unweighted and weighted agreement factors of:

$$R = \frac{\sum ||F_o| - |F_c||}{\sum |F_o|} = 0.074$$

$$R_w = \sqrt{\frac{\sum w(|F_o| - |F_c|)^2}{\sum w F_o^2}} = 0.085$$

After the final cycle least-squares refinement the GooF = 3.39. The standard deviation of an observation of unit weight[128] was 5.00. The weighting scheme was based on counting statistics and included a factor ( $p = 0.009$ ) to downweight the intense reflections. Plots of  $\sum w(|F_o| - |F_c|)^2$  versus  $|F_o|$ , reflection order in data collection,  $\sin\theta/\lambda$  and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.42 and  $-0.36 \text{ e}^-/\text{\AA}^3$ , respectively.

Neutral atom scattering factors were taken from Cromer and Waber[130]. The values for the mass attenuation coefficients are those of Creagh and Hubbel[131]. All calculations were performed using the teXsan[125] crystallographic software package of Molecular Structure Corporation.

### 8.3 Results and Discussion

Table 8.1 contains the details of crystal data, data collection and refinement. The final coordinates with equivalent isotropic temperature factors for all atoms are given in Table 8.2. Anisotropic thermal parameters( $U_{ij}$ ) for the non-hydrogen atoms are listed in Table 8.3. Table 8.4 and 8.5 give the bond distances and angles of non-hydrogen atoms. Table 8.6 shows selected torsion angles. Non-bonded contacts and the least square planes are listed in Table 8.7 and 8.8 respectively. The final observed( $F_o$ ) and calculated structure factors ( $F_c$ ) are given in Table 8.9. Figure 8.1 represents the ORTEP diagram of the molecules with thermal ellipsoid at 50% probability. Figure 8.2 represents the packing of the molecule in the unit cell. Figures 8.3, 8.4 and 8.5 show the packing of the molecules, which are projected along a, b and c-axes respectively.

The bond distances and angles are in good agreement when compared with those of other triazoles. Table 8.7 shows the shortest intermolecular interactions responsible for bending the molecules to form crystalline state.

The dihedral angle between plane 1 (C1 C2 C3 C4 C5 C6) and 2 (C7 C8 N9 N10 N11) is  $2.96^\circ$ . The dihedral angle between the planes 1 and 3 (C13 C14 C15 C16 C17 C18) is  $90^\circ$ . and plane 1 is perpendicular to plane 3. The two phenyl and five membered rings are independently planar.

Table 8.1: Experimental Details

**Crystal Data**

Empirical Formula	$C_{15}H_{13}N_3$
Formula Weight	235.29
Crystal Color, Habit	Colourless, rectangular
Crystal Dimensions	0.35 x 0.25 x 0.20 mm
Crystal System	Monoclinic
Lattice Type	Primitive
No. of Reflections Used for Unit	
Cell Determination ( $2\theta$ range)	22(13.9 - 17.6°)
Omega Scan Peak Width at Half-height	0.38°
Lattice Parameters	$a = 6.038(2) \text{ \AA}$ $b = 8.094(3) \text{ \AA}$ $c = 25.62(1) \text{ \AA}$ $\beta = 93.80(4)^\circ$ $V = 1249.1(9) \text{ \AA}^3$
Space Group	$P2_1/c(\#14)$
Z value	4
$D_{\text{calc}}$	1.251 g/cm <sup>3</sup>
$F_{000}$	496.00
$\mu(MoK\alpha)$	0.71 cm <sup>-1</sup>
<b>Intensity Measurements</b>	
Diffractometer	Rigaku AFC7S
Radiation	$MoK\alpha$ ( $\lambda = 0.71069 \text{ \AA}$ ) Graphite monochromated
Attenuator	Zr foil (factor = 8.21)
Take-off Angle	6.0°
Detector Aperture	9.0 mm horizontal 13.0 mm vertical

Crystal to Detector Distance	400 mm
Voltage. Current	50 kV, 40 mA
Temperature	20.0° C
Scan Type	$w$
Scan Rate	16.0°/min(inw)(upto4scans)
Scan Width	(1.15 + 0.14 tan $\theta$ )°
$2\theta_{max}$	50.0°
No. of Reflections Measured	Total: 2608 Unique: 2372 ( $R_{int} = 0.017$ )
Corrections	Lorentz-polarization Absorption (trans, factors: 0.9321 - 1.0000) Decay (2.35% increase) Secondary Extinction (coefficient: 1.24531 x 10 <sup>-6</sup> )

### Structure Solution and Refinement

Structure Solution	Direct Methods ( <i>SIR92</i> )
Refinement	Full-matrix least-squares
Function Minimized	$\sum w( F_o  -  F_c )^2$
Least Squares Weights	$w = \frac{1}{\sigma^2(F_o)} = \left[ \sigma_c^2(F_o) + \frac{P^2}{4} F_o^2 \right]^{-1}$
p-factor	0.0090
Anomalous Dispersion	All non-hydrogen atoms
No. Observations ( $I > 3.00\sigma(I)$ )	1644
No. Variables	164
Reflection/Parameter Ratio	10.02
Residuals: $R$ : $R_w$	0.074 ; 0.085
Goodness of Fit Indicator	5.00
Max Shift/Error in Final Cycle	0.83
Maximum peak in Final Diff. Map	0.42 e <sup>-</sup> Å <sup>-3</sup>
Minimum peak in Final Diff. Map	-0.36 e <sup>-</sup> Å <sup>-3</sup>

Table 8.2: Atomic coordinates and  $B_{eq}$ 

Atom	$x$	$y$	$z$	$B_{eq}$
N(9)	0.0472(5)	0.2886(4)	0.0755(1)	4.62(8)
N(10)	0.2091(5)	0.1881(4)	0.0951(1)	3.59(7)
N(11)	0.1785(6)	0.1495(5)	0.1462(1)	5.9(1)
C(1)	-0.0478(7)	0.1574(5)	0.2490(2)	4.7(1)
C(2)	-0.1588(8)	0.1623(6)	0.2946(2)	5.8(1)
C(3)	-0.3564(8)	0.2464(6)	0.2960(2)	5.5(1)
C(4)	-0.4422(7)	0.3265(6)	0.2523(2)	5.4(1)
C(5)	-0.3339(6)	0.3234(5)	0.2062(2)	4.55(10)
C(6)	-0.1330(6)	0.2374(4)	0.2044(1)	3.67(9)
C(7)	-0.0170(5)	0.2335(4)	0.1554(1)	3.45(8)
C(8)	-0.0861(5)	0.3143(4)	0.1120(1)	3.02(7)
C(12)	0.3943(6)	0.1397(5)	0.0643(2)	4.22(9)
C(13)	0.4330(6)	-0.0444(4)	0.0650(1)	3.47(8)
C(14)	0.2694(6)	-0.1527(5)	0.0466(1)	4.29(10)
C(15)	0.3062(7)	-0.3208(5)	0.0459(2)	4.9(1)
C(16)	0.5113(8)	-0.3817(5)	0.0635(2)	4.9(1)
C(17)	0.6770(7)	-0.2760(5)	0.0817(2)	4.9(1)
C(18)	0.6371(6)	-0.1074(5)	0.0823(1)	4.16(9)

Table 8.2: Atomic coordinates and  $B_{eq}$  (continued)

Atom	$x$	$y$	$z$	$B_{eq}$
H(1)	0.0902	0.0972	0.2481	5.7354
H(2)	-0.0943	0.1060	0.3255	7.0516
H(3)	-0.4354	0.2480	0.3283	6.6634
H(4)	-0.5808	0.3859	0.2535	6.8834
H(5)	-0.3952	0.3806	0.1748	5.9028
H(6)	-0.2196	0.3809	0.1080	3.8118
H(7)	0.3617	0.1746	0.0278	5.3357
H(8)	0.5269	0.1956	0.0763	5.3357
H(9)	0.1267	-0.1086	0.0343	5.1390
H(10)	0.1902	-0.3964	0.0326	5.8207
H(11)	0.5387	-0.4991	0.0622	5.8094
H(12)	0.8218	-0.3213	0.0944	6.0366
H(13)	0.7554	-0.0322	0.0958	5.2408

Table 8.3: Anisotropic Displacement Parameters

Atom	$U_{11}$	$U_{22}$	$U_{33}$	$U_{12}$	$U_{13}$	$U_{23}$
N(9)	0.061(2)	0.053(2)	0.060(2)	0.012(2)	-0.005(2)	0.012(2)
N(10)	0.052(2)	0.042(2)	0.043(2)	0.002(2)	0.008(1)	0.002(1)
N(11)	0.078(3)	0.069(3)	0.077(3)	-0.001(2)	0.015(2)	-0.006(2)
C(1)	0.064(3)	0.061(3)	0.055(2)	0.007(2)	0.009(2)	0.003(2)
C(2)	0.096(4)	0.068(3)	0.055(3)	0.000(3)	0.009(2)	0.002(2)
C(3)	0.083(3)	0.063(3)	0.067(3)	-0.011(3)	0.030(3)	-0.012(2)
C(4)	0.060(3)	0.067(3)	0.082(3)	0.002(2)	0.023(2)	-0.012(3)
C(5)	0.053(2)	0.058(3)	0.062(3)	0.005(2)	0.007(2)	-0.006(2)
C(6)	0.045(2)	0.042(2)	0.052(2)	-0.003(2)	0.005(2)	-0.008(2)
C(7)	0.034(2)	0.038(2)	0.060(2)	0.002(2)	0.005(2)	-0.011(2)
C(8)	0.032(2)	0.044(2)	0.039(2)	0.019(2)	0.006(1)	0.008(2)
C(12)	0.056(2)	0.044(2)	0.063(3)	-0.000(2)	0.022(2)	0.001(2)
C(13)	0.046(2)	0.041(2)	0.046(2)	0.000(2)	0.014(2)	-0.001(2)
C(14)	0.048(2)	0.053(3)	0.063(3)	0.001(2)	0.007(2)	-0.001(2)
C(15)	0.071(3)	0.046(2)	0.071(3)	-0.010(2)	0.012(2)	-0.006(2)
C(16)	0.083(3)	0.040(2)	0.065(3)	0.010(2)	0.018(2)	0.003(2)
C(17)	0.061(3)	0.062(3)	0.063(3)	0.015(2)	0.005(2)	0.006(2)
C(18)	0.050(2)	0.052(2)	0.056(2)	-0.001(2)	0.006(2)	-0.003(2)

Table 8.4: Bond Lengths(Å)

Atom	Atom	Distance
N(9)	N(10)	1.343(4)
N(9)	C(8)	1.291(4)
N(10)	N(11)	1.372(4)
N(10)	C(12)	1.463(4)
N(11)	C(7)	1.396(4)
C(1)	C(2)	1.386(5)
C(1)	C(6)	1.382(5)
C(2)	C(3)	1.376(6)
C(3)	C(4)	1.365(6)
C(4)	C(5)	1.388(5)
C(5)	C(6)	1.401(5)
C(6)	C(7)	1.477(5)
C(7)	C(8)	1.334(4)
C(12)	C(13)	1.508(5)
C(13)	C(14)	1.380(5)
C(13)	C(18)	1.380(5)
C(14)	C(15)	1.379(5)
C(15)	C(16)	1.380(6)
C(16)	C(17)	1.373(6)
C(17)	C(18)	1.386(5)

Table 8.5: Bond Angles in degrees.

Atom	Atom	Atom	Angle
N(10)	N(9)	C(8)	107.4(3)
N(9)	N(10)	N(11)	110.8(3)
N(9)	N(10)	C(12)	121.6(3)
N(11)	N(10)	C(12)	127.5(3)
N(10)	N(11)	C(7)	102.7(3)
C(2)	C(1)	C(6)	120.6(4)
C(1)	C(2)	C(3)	120.4(4)
C(2)	C(3)	C(4)	119.7(4)
C(3)	C(4)	C(5)	121.0(4)
C(4)	C(5)	C(6)	119.6(4)
C(1)	C(6)	C(5)	118.8(4)
C(1)	C(6)	C(7)	121.3(3)
C(5)	C(6)	C(7)	119.9(3)
N(11)	C(7)	C(6)	127.5(3)
N(11)	C(7)	C(8)	108.6(3)
C(6)	C(7)	C(8)	123.9(3)
N(9)	C(8)	C(7)	110.5(3)
N(10)	C(12)	C(13)	112.4(3)
C(12)	C(13)	C(14)	121.1(3)
C(12)	C(13)	C(18)	120.2(3)
C(14)	C(13)	C(18)	118.6(3)
C(13)	C(14)	C(15)	121.2(4)
C(14)	C(15)	C(16)	119.3(4)
C(15)	C(16)	C(17)	120.4(4)
C(16)	C(17)	C(18)	119.6(4)
C(13)	C(18)	C(17)	120.8(4)

Table 8.6: Torsion Angles in degrees.

Atom	Atom	Atom	Atom	Angle
N(9)	N(10)	N(11)	C(7)	0.7(4)
N(9)	N(10)	C(12)	C(13)	-130.4(4)
N(9)	C(8)	C(7)	N(11)	0.5(4)
N(9)	C(8)	C(7)	C(6)	180.0(3)
N(10)	N(9)	C(8)	C(7)	-0.0(4)
N(10)	N(11)	C(7)	C(6)	179.8(3)
N(10)	N(11)	C(7)	C(8)	-0.7(4)
N(10)	C(12)	C(13)	C(14)	59.8(5)
N(10)	C(12)	C(13)	C(18)	-122.7(4)
N(11)	N(10)	N(9)	C(8)	-0.5(4)
N(11)	N(10)	C(12)	C(13)	53.3(5)
N(11)	C(7)	C(6)	C(1)	2.5(6)
N(11)	C(7)	C(6)	C(5)	-177.4(4)
C(1)	C(2)	C(3)	C(4)	-0.6(7)
C(1)	C(6)	C(5)	C(4)	0.0(6)
C(1)	C(6)	C(7)	C(8)	-176.9(4)
C(2)	C(1)	C(6)	C(5)	-0.1(6)
C(2)	C(1)	C(6)	C(7)	-180.0
C(2)	C(3)	C(4)	C(5)	0.5(7)
C(3)	C(2)	C(1)	C(6)	0.4(7)
C(3)	C(4)	C(5)	C(6)	-0.2(6)
C(4)	C(5)	C(6)	C(7)	179.9(4)
C(5)	C(6)	C(7)	C(8)	3.2(6)
C(7)	N(11)	N(10)	C(12)	177.4(3)
C(8)	N(9)	N(10)	C(12)	-177.3(3)
C(12)	C(13)	C(14)	C(15)	178.4(4)
C(12)	C(13)	C(18)	C(17)	-178.0(4)
C(13)	C(14)	C(15)	C(16)	-0.8(6)
C(13)	C(18)	C(17)	C(16)	0.0(6)
C(14)	C(13)	C(18)	C(17)	-0.5(6)
C(14)	C(15)	C(16)	C(17)	0.3(6)
C(15)	C(14)	C(13)	C(18)	0.9(6)
C(15)	C(16)	C(17)	C(18)	0.1(6)

Table 8.7: Non-bonded Contacts out to 3.60Å

Atom	Atom	Distance	ADC	Atom	Atom	Distance	ADC
N(11)	C(5)	3.523(6)	65501	C(8)	C(12)	3.581(5)	45501
C(13)	C(13)	3.553(7)	65503				

The ADC (atom designator code) specifies the position of an atom in a crystal. The 5-digit number shown in the table is a composite of three one-digit numbers and one two-digit number: TA (first digit) + TB (second digit) + TC (third digit) + SN (last two digits). TA, TB and TC are the crystal lattice translation digits along cell edges a, b and c. A translation digit of 5 indicates the origin unit cell. If TA = 4, this indicates a translation of one unit cell length along the a-axis in the negative direction. Each translation digit can range in value from 1 to 9 and thus  $\pm 4$  lattice translations from the origin (TA=5, TB=5, TC=5) can be represented.

The SN, or symmetry operator number, refers to the number of the symmetry operators used to generate the coordinates of the target atom. A list of symmetry operators relevant to this structure are given below.

For a given intermolecular contact, the first atom (origin atom) is located in the origin unit cell and its position can be generated using the identity operator (SN=1). Thus, the ADC for an origin atom is always 55501. The position of the second atom (target atom) can be generated by using the ADC and the coordinates of the atom in the parameter table. For example, an ADC of 47502 refers to the target atom moved through symmetry operator two, then translated -1 cell translations along the a axis, +2 cell translations along the b axis, and 0 cell translations along the c axis.

An ADC of 1 indicates an intermolecular contact between two fragments (eg. cation and anion) that reside in the same asymmetric unit.

#### Symmetry Operators:

- |                |                      |
|----------------|----------------------|
| (1) X, Y, Z    | (2) -X, 1/2+Y, 1/2-Z |
| (3) -X, -Y, -Z | (4) X, 1/2-Y, 1/2+Z  |

Table 8.8: Least Squares Planes  
Plane number 1

**Plane number 1**

$$2.9212x + 6.6975y + 6.4597z = 2.5229$$

Atoms defining plane	Distance
C(1)	-0.001(4)
C(2)	0.002(5)
C(3)	-0.003(4)
C(4)	0.002(4)
C(5)	0.000(4)
C(6)	-0.001(4)

**Plane number 2**

$$3.2407x + 6.4533y - 6.9399z = 2.5344$$

N(9)	0.002(3)
N(10)	-0.003(3)
N(11)	0.005(4)
C(7)	-0.003(3)
C(8)	0.001(4)

**Plane number 3**

$$2.2738x - 0.63248y - 24.234z = -0.61546$$

C(13)	-0.003(3)
C(14)	0.005(4)
C(15)	-0.003(4)
C(16)	-0.001(4)
C(17)	0.002(4)
C(18)	0.001(4)

## Summary

plane	mean deviation	$x^2$
1	0.0013	0.7
2	0.0028	3.9
3	0.0022	2.8

## Dihedral angles between planes (°)

Plane	1	2
2	2.96	
3	90.91	91.36

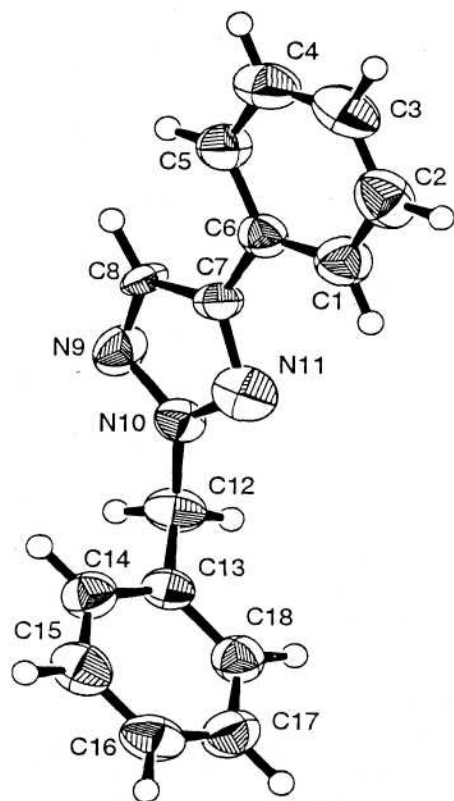


Figure 8.1: ORTEP diagram of the molecule.

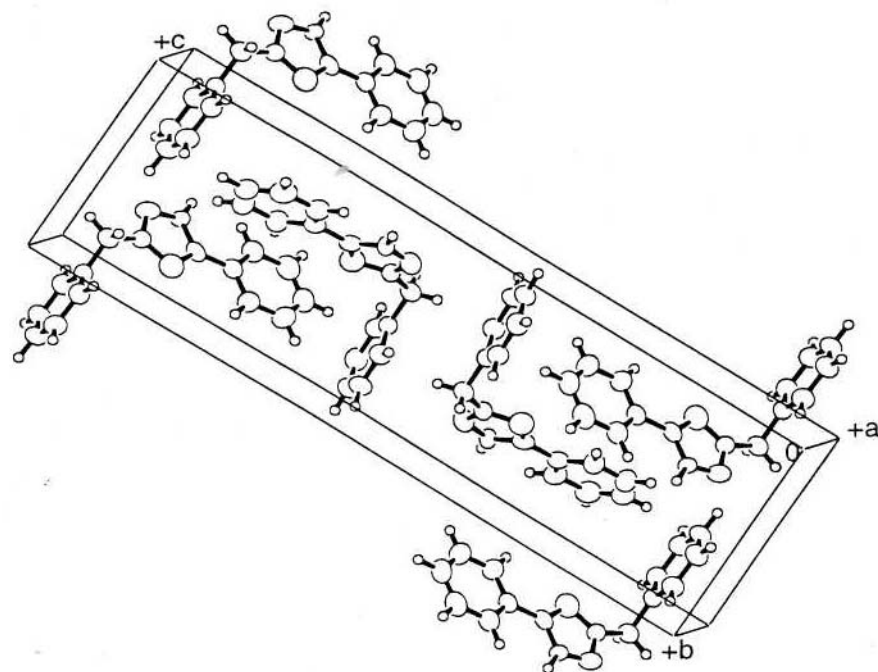


Figure 8.2: Packing of the molecules in the unit cell.

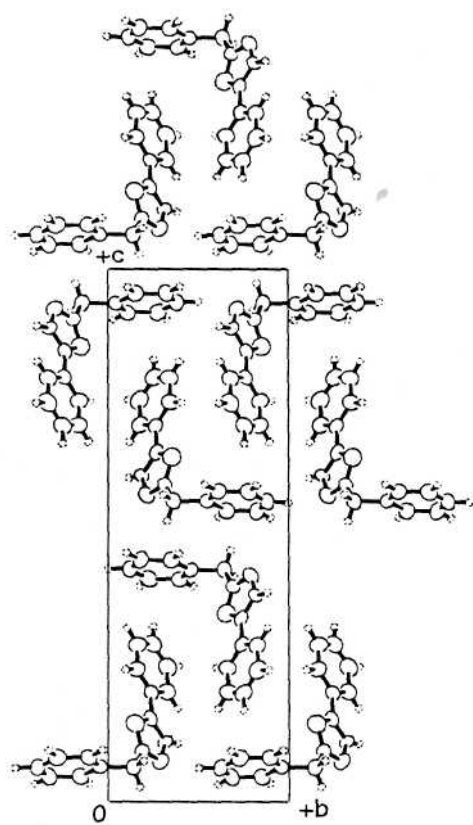


Figure 8.3: Packing of the molecules down a.

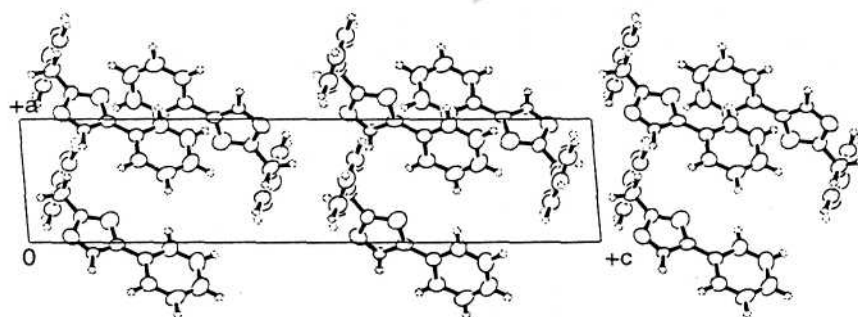


Figure 8.4: Packing of the molecules down b.

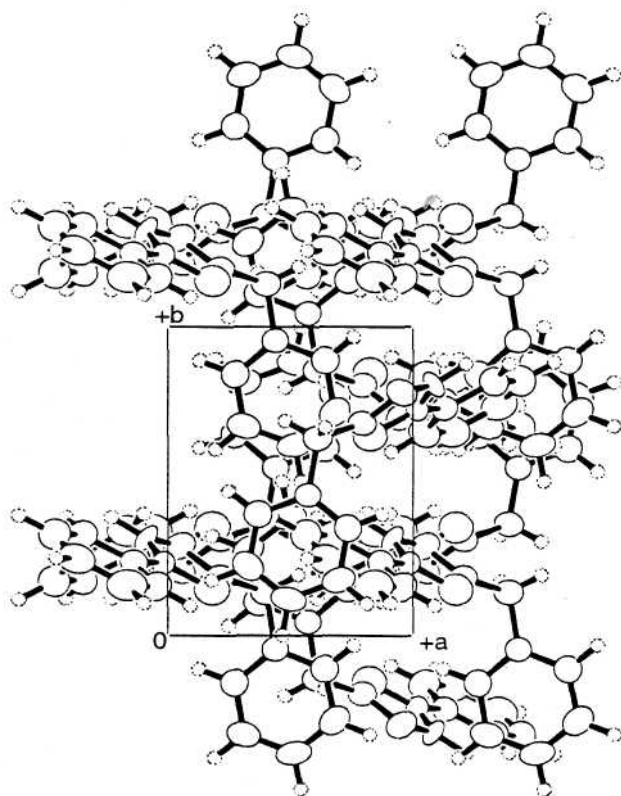


Figure 8.5: Packing of the molecules down c.

Table 8.9: Observed and Calculated structure factors

$h$	$k$	$l$	$F_o$	$F_c$	$\sigma F$	$h$	$k$	$l$	$F_o$	$F_c$	$\sigma F$
0	1	-2	47.77	46.74	0.24	0	0	4	9.94	10.44	0.10
1	0	0	10.96	12.48	0.11	0	1	3	12.18	12.96	0.11
1	0	-2	12.44	14.12	0.11	1	0	2	82.47	86.49	0.40
0	1	-4	40.15	39.55	0.21	1	1	0	36.05	35.35	0.19
1	1	-1	3.43	2.05	0.11	1	1	1	36.85	36.83	0.20
1	1	-2	28.41	28.11	0.17	1	0	-4	8.67	7.68	0.12
1	1	2	140.58	138.77	0.66	0	1	-5	32.71	32.66	0.19
1	1	-3	17.47	17.94	0.13	0	0	-6	134.50	134.54	0.63
1	0	4	65.98	66.63	0.33	1	1	3	26.79	30.12	0.17
0	2	0	157.05	158.27	0.73	0	2	1	23.38	24.69	0.15
1	1	-4	96.01	95.51	0.46	0	2	-2	37.94	38.68	0.21
0	1	6	69.04	68.32	0.34	1	1	4	44.52	46.94	0.24
0	2	-3	6.97	8.21	0.13	1	1	-5	19.30	18.92	0.15
1	0	-6	85.57	84.46	0.42	1	1	5	18.53	17.92	0.15
0	2	-4	8.35	7.80	0.13	1	0	6	2.96	4.51	0.09
1	2	0	47.24	45.46	0.25	1	2	1	78.14	81.80	0.38
1	1	-6	28.42	28.73	0.18	1	2	-2	20.59	23.38	0.15
1	2	2	3.61	0.95	0.11	0	0	8	86.16	85.85	0.42
0	2	-5	1.32	1.93	0.12	1	2	-3	27.47	25.96	0.18
1	1	6	37.76	36.53	0.22	1	2	3	98.26	98.05	0.47
1	2	-4	18.68	19.34	0.15	2	0	0	9.48	7.45	0.14
1	1	-7	22.74	21.96	0.17	2	0	-2	10.74	8.40	0.14
0	1	8	11.80	10.84	0.14	0	2	6	25.06	23.41	0.17
1	2	4	42.88	41.31	0.24	1	0	-8	103.86	101.86	0.50
2	0	2	25.05	29.17	0.19	1	2	-5	2.24	2.56	0.09
1	1	7	16.08	18.26	0.16	2	1	-1	29.14	26.64	0.18
2	1	0	7.24	4.15	0.14	2	0	-4	7.17	8.69	0.14
2	1	-2	30.86	29.83	0.19	1	2	5	3.85	6.38	0.11
1	0	8	10.30	9.17	0.15	1	1	-8	30.57	31.41	0.20
2	1	-3	14.66	13.79	0.15	2	1	2	17.83	15.14	0.16
0	2	7	17.07	16.78	0.16	1	2	-6	3.96	4.30	0.10
0	3	-1	8.40	6.20	0.14	0	1	9	18.68	18.65	0.16
2	0	4	7.68	10.92	0.17	2	1	-4	12.60	14.09	0.15
0	3	2	41.90	39.84	0.23	2	1	3	11.32	12.01	0.15
1	1	8	3.04	3.90	0.09	1	2	6	16.03	15.33	0.16
0	3	3	5.81	3.59	0.15	0	0	10	14.40	15.44	0.15
2	0	-6	42.66	42.44	0.24	2	1	-5	8.86	10.31	0.15
2	1	4	28.07	25.36	0.20	1	2	-7	5.81	7.28	0.16
1	1	-9	6.52	6.87	0.16	0	2	8	15.95	16.84	0.16
0	3	-4	27.92	26.88	0.19	1	3	0	14.98	13.50	0.16
1	3	-1	16.53	19.18	0.16	1	3	1	25.55	25.34	0.19
0	1	-10	3.12	2.40	0.10	1	3	-2	3.17	3.12	0.10
1	2	7	25.40	25.73	0.19	2	1	-6	2.45	4.27	0.14
2	2	-1	3.14	2.50	0.10	2	2	0	6.77	7.46	0.14
1	0	-10	23.54	23.81	0.19	2	1	5	37.25	37.84	0.23
1	3	2	45.36	45.04	0.25	2	2	-2	19.44	17.23	0.17
2	2	1	12.81	11.72	0.16	1	1	9	6.93	7.56	0.16
2	0	6	5.54	3.21	0.18	0	3	-5	10.94	11.26	0.16
1	3	-3	24.62	23.92	0.18	1	2	-8	1.41	1.52	0.11
2	2	-3	7.69	9.79	0.15	2	2	2	17.21	17.25	0.16
1	3	3	30.60	32.32	0.20	0	2	-9	6.79	8.64	0.16
1	3	-4	19.84	18.11	0.17	1	1	-10	11.86	12.70	0.17
2	1	-7	18.41	17.45	0.17	2	2	-4	19.66	20.51	0.17
1	0	10	10.49	8.15	0.16	2	2	3	25.97	26.06	0.19
2	1	6	24.40	26.37	0.20	0	3	6	9.14	10.08	0.15
1	3	4	29.48	29.86	0.20	1	2	8	16.87	16.30	0.17
2	0	-8	3.62	4.34	0.11	1	3	-5	8.32	6.20	0.16
2	2	-5	19.43	18.91	0.17	2	2	4	24.79	25.65	0.19

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$h$	$k$	$l$	$F_o$	$F_c$	$\sigma F$	$h$	$k$	$l$	$F_o$	$F_c$	$\sigma F$
1	1	10	19.60	20.08	0.18	1	2	-9	5.19	4.92	0.16
1	3	5	19.76	20.31	0.18	2	1	-8	11.78	11.19	0.16
0	3	7	30.53	31.83	0.20	2	1	7	10.84	10.26	0.18
0	2	10	23.26	21.58	0.18	1	3	-6	13.56	14.32	0.16
2	2	-6	1.47	1.04	0.13	2	2	5	8.06	9.04	0.16
1	1	-11	14.52	14.08	0.18	1	2	9	27.96	28.91	0.20
0	0	-12	12.54	11.82	0.17	2	0	8	24.03	22.05	0.21
1	3	6	6.64	6.70	0.16	1	2	-10	3.07	3.47	0.10
1	3	-7	8.91	7.95	0.16	2	1	-9	11.10	11.67	0.17
2	2	-7	6.33	8.25	0.17	0	3	8	8.93	8.10	0.16
0	1	-12	3.79	2.48	0.13	2	2	6	14.51	14.81	0.18
2	1	8	10.19	10.50	0.18	1	1	11	1.56	1.70	0.16
1	0	-12	19.49	19.27	0.19	0	4	0	19.13	21.67	0.18
0	4	1	14.29	15.97	0.17	1	3	7	20.38	20.47	0.19
2	0	-10	56.93	54.82	0.31	0	2	-11	17.02	17.01	0.18
2	3	-1	36.25	35.17	0.23	2	3	0	7.00	7.08	0.19
3	0	0	16.45	15.12	0.18	3	0	-2	6.85	4.30	0.15
2	3	-2	18.96	19.46	0.18	1	2	10	6.36	6.47	0.18
0	4	2	14.07	13.11	0.17	2	3	1	7.35	6.35	0.17
1	1	-12	72.59	73.15	0.37	2	2	-8	13.70	14.35	0.18
2	3	-3	28.95	28.60	0.21	1	3	-8	6.03	5.94	0.17
2	3	2	27.59	28.24	0.20	0	4	-3	22.57	23.30	0.19
1	0	12	18.01	18.80	0.19	2	2	7	32.89	32.48	0.22
3	0	2	21.42	19.71	0.20	0	3	-9	11.16	11.23	0.18
2	1	-10	7.41	6.39	0.18	3	0	-4	9.49	10.32	0.17
3	1	-1	3.73	3.04	0.11	3	1	0	20.39	18.63	0.18
1	2	-11	12.95	12.11	0.18	3	1	-2	45.68	45.38	0.26
2	1	9	6.07	5.40	0.19	2	3	-4	4.09	5.38	0.13
2	3	3	35.32	33.92	0.23	0	4	4	11.58	9.91	0.17
3	1	-3	15.46	14.85	0.17	1	3	8	1.86	0.99	0.12
1	4	0	19.82	19.53	0.19	1	4	-1	5.64	4.74	0.17
1	1	12	44.32	42.59	0.26	0	1	-13	20.58	20.98	0.19
1	4	1	26.95	26.97	0.21	3	1	2	23.38	23.72	0.19
2	3	-5	2.42	1.93	0.12	3	1	-4	17.82	15.46	0.18
2	3	4	14.73	15.14	0.18	1	4	2	27.60	27.69	0.21
2	2	-9	11.11	9.71	0.18	2	0	10	13.89	14.35	0.19
1	3	-9	11.78	10.84	0.18	0	2	-12	4.90	3.59	0.13
0	4	5	7.70	6.07	0.17	1	4	-3	32.18	30.32	0.22
2	2	8	19.88	21.12	0.19	3	1	3	1.59	0.49	0.15
3	0	-6	8.51	5.76	0.17	1	4	3	56.45	54.72	0.31
3	1	-5	5.34	5.60	0.18	1	1	-13	9.46	10.43	0.18
0	3	10	14.82	15.52	0.17	2	1	-11	7.70	7.57	0.18
2	3	-6	14.01	13.05	0.18	1	4	-4	13.26	12.35	0.18
2	3	5	45.20	45.07	0.27	2	1	10	19.83	19.60	0.20
1	3	9	13.73	12.84	0.18	3	1	4	6.43	6.44	0.19
1	2	-12	9.83	10.06	0.18	0	4	-6	16.97	16.51	0.19
1	4	4	1.95	2.85	0.17	0	0	-14	25.75	26.12	0.21
3	1	-6	3.60	3.73	0.11	1	4	-5	8.21	9.20	0.17
2	2	-10	32.25	31.21	0.23	3	2	-1	21.66	20.61	0.19
3	2	0	19.88	20.26	0.19	1	3	-10	7.66	7.60	0.18
3	2	-2	6.59	6.31	0.17	2	0	-12	35.98	36.21	0.24
2	3	-7	5.82	5.53	0.19	2	2	9	15.26	13.52	0.19
1	1	13	2.51	2.08	0.13	2	3	6	4.59	6.50	0.14
3	2	1	11.83	13.05	0.17	3	1	5	7.68	7.82	0.19
1	4	5	6.46	5.26	0.19	3	2	-3	13.60	15.36	0.18
0	1	-14	16.68	16.72	0.19	1	0	-14	27.27	27.42	0.22
3	0	6	18.35	18.16	0.21	0	4	7	6.84	6.48	0.18
1	2	12	8.72	8.14	0.18	0	2	13	7.88	8.90	0.17

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<i>h</i>	<i>k</i>	<i>l</i>	$F_o$	$F_c$	$\sigma F$	<i>h</i>	<i>k</i>	<i>l</i>	$F_o$	$F_c$	$\sigma F$
3	2	2	21.91	21.09	0.19	3	1	-7	7.13	6.11	0.17
1	4	-6	14.46	15.07	0.19	0	3	-11	3.60	4.71	0.12
3	2	-4	4.34	4.48	0.14	3	0	-8	17.40	18.19	0.19
2	1	-12	5.92	4.64	0.13	1	3	10	6.15	4.34	0.19
2	1	11	10.31	8.34	0.19	3	2	3	11.62	11.06	0.18
1	1	-14	2.77	3.37	0.11	2	3	-8	12.57	11.36	0.18
3	1	6	5.35	4.63	0.14	3	2	-5	6.93	6.85	0.18
2	3	7	10.83	9.15	0.18	1	2	-13	16.42	16.14	0.20
2	2	-11	4.88	3.54	0.14	1	0	14	2.30	1.52	0.13
3	1	-8	35.94	34.57	0.24	1	3	-11	5.55	6.47	0.13
1	4	-7	2.60	2.05	0.13	2	2	10	4.32	4.50	0.12
0	4	-8	6.47	6.04	0.18	3	2	4	5.01	3.82	0.14
2	0	12	30.57	30.44	0.24	1	4	7	5.14	5.49	0.14
2	4	-1	9.63	9.85	0.18	2	4	0	7.00	8.06	0.19
1	1	14	18.47	19.53	0.20	2	3	-9	12.62	13.67	0.19
3	1	7	7.61	9.21	0.20	2	4	-2	8.82	8.93	0.18
0	3	12	7.30	7.98	0.18	2	4	1	7.66	8.90	0.20
1	2	13	14.89	15.14	0.19	0	1	-15	2.59	2.15	0.13
1	3	11	9.23	8.35	0.19	3	2	5	3.56	5.52	0.10
0	2	14	5.61	6.46	0.18	2	1	-13	12.22	11.27	0.19
1	4	-8	27.07	28.23	0.22	2	4	-3	6.22	7.33	0.19
3	1	-9	4.74	4.18	0.14	2	4	2	17.62	17.98	0.20
3	2	-7	1.69	2.42	0.15	3	0	8	11.93	10.65	0.21
2	1	12	9.00	9.33	0.21	0	4	-9	8.90	8.98	0.19
2	2	-12	5.39	5.56	0.14	2	4	-4	16.88	15.75	0.19
2	4	3	25.51	25.15	0.22	1	1	-15	8.60	8.42	0.21
1	3	-12	6.49	6.23	0.20	3	0	-10	24.00	21.87	0.21
2	2	11	11.18	10.02	0.20	1	2	-14	12.32	12.28	0.20
1	4	8	8.78	6.79	0.19	3	2	6	5.21	4.60	0.14
3	1	8	14.08	13.26	0.21	0	5	1	13.26	12.22	0.19
2	3	-10	17.93	17.39	0.20	2	4	-5	12.05	11.55	0.20
3	3	-1	11.20	12.15	0.18	3	3	0	12.92	13.06	0.19
2	4	4	32.13	34.12	0.23	2	0	-14	34.55	34.40	0.25
3	2	-8	13.32	14.41	0.20	3	3	-2	10.77	9.10	0.19
2	3	9	5.39	4.61	0.14	0	5	-2	8.32	9.10	0.19
1	4	-9	7.43	8.75	0.19	3	3	1	1.76	1.56	0.16
3	1	-10	13.49	12.45	0.19	0	0	-16	4.28	3.91	0.13
0	5	-3	2.12	2.54	0.14	1	3	12	17.07	16.67	0.20
0	3	13	14.49	15.00	0.18	3	3	2	2.29	3.20	0.13
0	4	-10	25.05	24.93	0.22	2	4	-6	6.09	6.38	0.14
3	3	-4	5.54	6.39	0.14	1	2	14	9.03	9.33	0.19
2	1	-14	2.83	2.65	0.12	2	4	5	15.68	15.61	0.20
1	4	9	25.68	23.86	0.22	1	0	-16	30.45	29.35	0.24
0	2	15	6.07	6.45	0.19	0	5	-4	4.90	4.13	0.15
2	1	13	10.10	11.33	0.21	3	3	3	14.00	14.61	0.19
0	1	-16	7.13	7.88	0.20	2	2	-13	3.16	3.08	0.12
3	2	-9	19.89	21.17	0.21	1	5	-1	4.38	3.37	0.15
3	1	9	3.13	2.63	0.13	3	3	-5	4.63	3.39	0.15
1	5	1	12.81	11.80	0.20	2	2	12	24.80	23.44	0.22
1	3	-13	9.83	9.54	0.20	1	5	-2	9.71	9.85	0.19
2	3	-11	2.50	1.69	0.13	1	4	-10	10.12	9.89	0.20
1	5	2	16.62	16.92	0.20	2	4	-7	3.34	3.73	0.13
2	3	10	13.97	12.40	0.20	0	5	-5	6.48	5.81	0.19
2	4	6	21.65	21.83	0.21	3	1	-11	2.82	3.33	0.12
1	5	-3	6.51	5.60	0.20	1	1	-16	15.30	15.48	0.21
3	3	-6	18.45	18.60	0.20	1	5	3	16.85	15.78	0.21
3	0	10	8.71	9.12	0.21	3	2	8	12.62	11.70	0.21
0	4	11	11.89	11.34	0.19	1	5	-4	17.85	17.53	0.20

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$h$	$k$	$l$	$F_o$	$F_c$	$\sigma F$	$h$	$k$	$l$	$F_o$	$F_c$	$\sigma F$
1	0	16	7.54	8.46	0.21	1	4	10	3.33	3.77	0.12
2	0	14	19.67	18.52	0.23	3	2	-10	16.61	15.53	0.20
0	5	6	12.80	11.91	0.19	3	3	5	9.56	9.08	0.20
1	5	4	4.12	4.68	0.14	3	0	-12	12.00	10.45	0.20
0	3	14	2.46	2.39	0.13	2	4	-8	2.39	2.95	0.17
4	0	-2	10.44	10.67	0.18	4	0	0	9.71	8.57	0.20
2	4	7	24.00	22.77	0.22	3	1	10	15.61	14.78	0.22
3	3	-7	4.00	3.49	0.13	1	5	-5	8.28	8.17	0.20
2	1	-15	9.90	9.63	0.20	1	2	15	6.79	6.00	0.20
2	2	-14	7.51	7.77	0.20	1	4	-11	4.91	5.39	0.15
2	3	-12	20.64	19.73	0.22	1	1	16	3.09	2.88	0.11
2	3	11	6.13	6.30	0.15	1	5	5	8.68	7.92	0.20
2	2	13	12.10	11.07	0.21	3	1	-12	5.50	5.07	0.15
0	2	16	14.50	14.03	0.19	1	3	-14	10.97	11.54	0.21
4	0	2	32.04	32.97	0.25	4	1	-1	12.48	13.92	0.19
3	3	6	12.35	12.31	0.20	4	1	0	13.90	14.23	0.19
3	2	9	15.53	15.60	0.21	0	5	7	13.91	13.49	0.20
0	1	17	2.62	2.30	0.13	1	5	-6	22.32	22.39	0.22
4	1	-3	15.20	14.62	0.20	4	1	1	3.63	3.41	0.11
3	3	-8	14.11	14.06	0.20	2	4	-9	7.39	6.45	0.21
3	2	-11	4.48	4.22	0.13	2	4	8	11.10	10.84	0.21
4	1	-4	11.39	12.04	0.20	1	2	-16	3.31	4.10	0.12
4	1	2	3.01	3.68	0.13	1	5	6	11.87	10.83	0.21
1	1	-17	7.09	6.73	0.21	2	0	-16	52.69	51.04	0.32
4	0	-6	12.73	11.78	0.20	3	1	11	4.65	4.49	0.14
4	1	-5	4.78	4.03	0.15	1	5	-7	13.54	12.73	0.21
3	3	7	2.22	2.25	0.15	4	0	4	5.49	6.80	0.16
0	5	8	11.60	10.73	0.20	4	1	3	5.37	5.32	0.15
0	3	15	15.52	15.97	0.20	1	4	-12	13.40	13.70	0.21
2	3	-13	3.31	2.43	0.13	3	3	-9	2.77	2.99	0.14
3	2	10	5.22	5.43	0.16	3	1	-13	6.87	6.97	0.20
2	3	12	8.69	9.66	0.21	2	2	-15	2.68	3.64	0.13
2	1	-16	2.57	2.82	0.15	1	5	7	20.17	18.84	0.22
2	4	-10	12.32	11.59	0.21	4	1	-6	2.03	2.66	0.16
3	4	-1	7.62	7.12	0.20	2	5	-1	8.19	8.37	0.22
2	5	0	2.25	2.12	0.15	3	4	0	9.41	9.60	0.20
3	4	-2	3.74	3.31	0.12	2	4	9	19.91	20.09	0.22
1	2	16	4.94	5.80	0.15	4	1	4	3.58	2.99	0.13
2	5	1	8.77	9.23	0.20	2	2	14	11.07	10.19	0.21
0	0	-18	15.84	15.79	0.22	1	3	-15	4.04	4.26	0.14
3	4	1	4.14	3.77	0.13	3	4	-3	2.38	2.88	0.14
3	0	12	23.24	21.93	0.24	4	2	-1	5.94	5.83	0.19
1	1	17	1.67	0.71	0.17	1	5	-8	6.53	6.37	0.22
2	5	-3	6.36	6.08	0.15	4	2	-2	3.98	3.35	0.13
2	5	2	11.29	11.41	0.21	4	2	0	2.83	2.18	0.12
3	4	2	6.13	6.05	0.20	3	3	8	9.41	10.25	0.21
0	5	9	2.41	1.62	0.13	4	1	-7	8.17	8.75	0.21
1	0	-18	16.33	16.77	0.23	2	5	-4	11.61	11.91	0.21
2	5	3	6.38	5.92	0.16	4	0	-8	20.97	20.69	0.22
0	1	18	4.28	4.50	0.14	4	1	5	13.83	14.00	0.22
3	3	-10	7.71	7.35	0.20	4	2	-4	3.42	2.85	0.13
3	4	3	2.58	2.41	0.13	1	5	8	4.82	4.38	0.14
3	1	12	9.76	10.58	0.23	4	2	2	13.90	14.17	0.20
4	0	6	8.52	8.40	0.22	1	2	-17	17.66	18.16	0.22
3	4	-5	6.70	7.47	0.21	1	4	-13	15.87	15.21	0.21
2	4	-11	12.00	11.26	0.21	2	5	-5	1.82	2.50	0.14
3	2	11	9.53	9.34	0.22	4	2	-5	5.15	4.90	0.15
2	5	4	5.25	5.56	0.15	1	1	-18	7.04	6.81	0.16

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$h$	$k$	$l$	$F_o$	$F_c$	$\sigma F$	$h$	$k$	$l$	$F_o$	$F_c$	$\sigma F$
1	5	-9	10.11	10.27	0.21	4	2	3	6.25	6.02	0.15
4	1	-8	2.72	2.04	0.13	3	4	4	17.13	17.01	0.21
3	1	-14	15.05	13.08	0.21	2	3	13	7.76	9.00	0.21
0	3	-16	4.49	5.19	0.14	2	0	16	2.51	3.32	0.15
3	4	-6	7.79	8.44	0.21	4	1	6	14.92	16.04	0.23
3	3	9	11.31	11.41	0.21	3	2	-13	17.91	17.74	0.22
0	5	10	3.03	4.05	0.13	2	2	-16	9.97	9.73	0.22
4	2	-6	11.55	11.69	0.21	2	1	-17	7.02	6.71	0.22
2	5	5	19.92	19.34	0.22	1	0	18	7.49	6.63	0.21
4	2	4	13.34	13.47	0.22	1	5	9	8.02	8.66	0.22
1	4	13	3.95	3.74	0.12	2	2	15	9.74	11.36	0.22
3	3	-11	5.43	5.39	0.16	1	3	-16	4.35	4.79	0.13
3	4	5	5.19	4.28	0.16	0	4	14	8.09	8.41	0.20
2	1	16	5.50	4.29	0.17	1	2	17	7.37	8.03	0.21
4	1	-9	4.88	4.86	0.13	3	4	-7	2.38	1.96	0.15
0	6	0	19.37	17.91	0.22	0	6	-1	3.62	3.91	0.13
4	2	-7	5.51	5.21	0.16	1	5	-10	5.94	5.63	0.16
1	1	18	11.68	11.50	0.22	2	4	-12	8.89	8.75	0.22
2	5	-7	1.48	1.50	0.24	0	6	2	1.77	1.38	0.17
3	1	13	7.36	7.05	0.24	0	2	-18	11.88	12.16	0.22
2	5	6	18.75	18.45	0.23	2	4	11	2.00	2.35	0.18
4	0	-10	21.49	20.88	0.22	1	4	-14	14.02	13.73	0.22
3	2	12	8.42	8.64	0.22	3	4	6	3.54	3.49	0.13
0	6	3	4.62	4.91	0.14	3	3	10	8.38	9.83	0.22
4	0	8	5.52	5.05	0.17	2	3	-15	1.38	0.88	0.20
0	5	-11	2.40	1.87	0.15	0	1	-19	3.69	4.46	0.14
3	1	-15	3.84	3.92	0.13	1	2	-18	3.80	3.99	0.13
3	4	-8	2.14	2.03	0.16	1	3	16	3.25	4.06	0.12
1	5	10	13.06	11.45	0.21	2	3	14	2.53	2.02	0.14
4	2	-8	9.95	9.67	0.22	3	2	-14	12.87	12.40	0.22
0	6	4	5.06	5.48	0.16	4	1	-10	9.39	9.79	0.21
3	3	-12	8.28	8.54	0.23	2	5	-8	5.38	5.57	0.16
4	3	-1	4.68	4.86	0.13	4	3	-2	4.60	4.31	0.14
1	6	-1	4.25	4.66	0.13	4	2	6	11.03	11.29	0.22
1	1	-19	4.41	4.45	0.14	0	3	-17	6.25	5.27	0.16
1	6	-2	14.30	14.51	0.22	4	1	8	8.77	8.80	0.23
4	3	-3	6.32	6.32	0.16	4	3	1	9.79	8.64	0.20
1	4	14	4.95	6.01	0.16	1	5	-11	4.45	4.04	0.14
1	6	2	13.21	13.36	0.22	3	4	7	2.70	2.90	0.14
0	6	5	9.50	9.17	0.22	1	6	-3	1.65	1.98	0.20
0	4	-15	11.18	10.64	0.22	2	4	-13	6.65	7.01	0.17
2	2	16	5.81	4.95	0.16	4	3	2	6.60	5.12	0.21
1	3	-17	9.43	9.84	0.23	3	4	-9	13.79	13.58	0.22
1	6	3	3.97	2.56	0.14	4	2	-9	7.93	7.82	0.23
2	1	17	6.72	6.91	0.21	1	6	-4	6.92	7.36	0.23
3	0	-16	9.94	9.56	0.22	4	3	-5	4.18	3.67	0.12
3	3	11	6.35	7.84	0.16	3	1	14	9.34	8.18	0.23
1	2	18	9.83	9.24	0.22	2	5	-9	1.86	2.19	0.17
4	2	7	10.69	9.88	0.23	4	3	3	2.24	3.05	0.14
2	5	8	6.72	6.16	0.17	4	1	-11	17.37	17.71	0.22
0	6	6	12.49	11.75	0.22	1	6	4	16.44	16.19	0.23
4	1	9	5.66	5.12	0.18	1	6	-5	2.58	2.30	0.15
1	1	19	1.97	1.60	0.15	2	3	-16	7.52	7.34	0.23
0	0	20	25.24	24.76	0.25	4	3	-6	4.13	3.93	0.13
0	2	19	6.24	6.61	0.16	3	1	-16	4.63	4.48	0.14
3	2	-15	15.57	16.93	0.22	4	3	4	3.43	3.55	0.12
2	3	15	3.18	3.75	0.14	1	5	-12	2.09	2.12	0.18
3	4	-10	8.15	8.21	0.22	1	6	5	5.14	5.35	0.15

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<i>h</i>	<i>k</i>	<i>l</i>	$F_o$	$F_c$	$\sigma F$	<i>h</i>	<i>k</i>	<i>l</i>	$F_o$	$F_c$	$\sigma F$
4	0	-12	11.73	13.64	0.22	4	2	-10	20.01	20.33	0.23
1	3	17	1.60	2.35	0.18	1	0	-20	5.68	5.01	0.18
1	2	-19	24.67	24.39	0.25	0	1	-20	10.85	10.37	0.23
4	2	8	1.69	2.06	0.21	2	5	-10	5.12	5.10	0.17
4	0	10	17.80	18.92	0.25	3	5	-1	16.41	15.63	0.22
1	4	15	1.35	0.13	0.20	4	3	-7	8.16	8.52	0.23
3	5	0	9.09	10.21	0.23	2	4	-14	7.40	7.26	0.22
3	5	-2	13.45	13.32	0.23	2	5	9	17.28	17.34	0.23
0	3	18	1.68	1.17	0.17	4	3	5	6.44	7.29	0.16
3	5	1	15.10	15.84	0.22	4	1	-12	11.16	10.09	0.22
2	4	13	7.01	7.99	0.17	3	5	-3	5.20	4.76	0.14
0	4	-16	10.69	10.19	0.23	2	2	-18	6.70	6.18	0.17
3	3	12	2.83	2.83	0.14	2	0	18	7.54	6.58	0.24
1	6	6	10.94	11.23	0.24	1	1	-20	17.75	16.81	0.24
3	4	9	8.36	10.04	0.23	1	5	12	9.55	10.31	0.23
3	5	2	7.59	8.95	0.23	4	1	10	4.09	4.65	0.14
3	5	-4	7.33	7.45	0.23	2	1	-19	7.61	7.07	0.22
1	3	-18	9.61	10.63	0.24	1	6	-7	4.25	4.56	0.13
3	1	15	5.10	5.84	0.15	0	6	-8	9.76	8.89	0.23
4	3	-8	7.55	7.64	0.22	3	4	-11	5.69	5.85	0.17
3	3	-14	11.05	11.40	0.22	2	1	18	2.75	1.66	0.16
4	3	6	4.72	3.75	0.15	3	5	-5	6.97	7.10	0.23
1	5	-13	10.63	10.73	0.24	1	0	20	10.71	10.70	0.24
1	2	19	11.58	10.88	0.23	1	6	7	13.25	13.11	0.24
2	5	-11	1.92	1.82	0.19	3	2	-16	7.48	7.48	0.17
2	6	-1	14.40	15.14	0.24	2	6	0	9.29	9.11	0.23
2	3	-17	13.44	13.20	0.23	3	1	-17	7.60	7.99	0.23
2	5	10	4.34	5.18	0.14	2	6	-2	4.53	4.64	0.14
3	5	4	7.34	7.50	0.17	2	3	16	5.24	5.94	0.16
1	6	-8	6.82	5.97	0.17	2	6	-3	21.60	21.67	0.24
2	6	2	10.38	9.39	0.23	3	5	-6	13.60	13.57	0.23
4	1	-13	7.47	8.27	0.24	4	3	-9	4.39	4.31	0.14
3	4	10	3.30	2.60	0.15	1	1	20	10.88	11.09	0.23
2	4	-15	6.25	6.24	0.17	0	2	20	16.07	16.44	0.22
1	3	18	6.71	6.87	0.16	2	6	-4	14.39	14.60	0.24
4	3	7	5.85	4.91	0.17	2	4	14	2.03	2.72	0.19
1	5	13	8.11	8.29	0.23	2	6	3	12.13	12.97	0.25
4	1	11	13.53	14.41	0.25	3	5	5	8.12	8.82	0.24
4	2	-12	6.82	7.86	0.23	3	0	16	14.03	12.66	0.24
3	4	-12	1.86	1.70	0.21	1	6	8	3.49	3.49	0.15
4	4	-1	9.61	9.10	0.22	1	2	-20	5.83	5.45	0.19
4	4	-2	5.95	5.62	0.17	4	4	0	2.52	1.16	0.16
5	0	-2	4.54	4.44	0.15	3	5	-7	16.43	15.71	0.24
2	0	-20	26.38	26.78	0.26	4	2	10	8.23	8.86	0.26
2	6	-5	5.63	5.38	0.19	0	3	19	2.44	3.08	0.15
0	1	-21	5.07	5.19	0.16	4	4	1	7.04	6.40	0.23
3	3	-15	5.94	5.71	0.18	2	6	4	26.02	24.69	0.26
2	5	-12	3.12	2.76	0.15	3	2	15	12.41	12.13	0.25
4	0	-14	17.22	18.02	0.23	1	6	-9	5.82	5.92	0.18
4	4	-4	13.91	13.82	0.23	2	5	11	13.35	14.06	0.24
5	0	-4	7.11	6.37	0.22	4	3	-10	2.63	3.25	0.18
3	0	-18	13.58	13.53	0.23	1	5	-14	7.75	6.95	0.24
2	2	18	5.14	6.03	0.15	1	4	-17	2.24	1.74	0.17
1	1	-21	11.58	10.93	0.24	3	5	6	12.34	11.36	0.24
5	1	-1	11.68	12.26	0.22	5	1	-2	13.93	13.83	0.22
0	6	10	8.28	7.74	0.22	4	0	12	9.26	9.65	0.25
2	1	-20	5.78	5.91	0.18	5	0	2	9.40	8.99	0.23
5	1	0	2.42	3.43	0.17	4	3	8	5.32	5.62	0.18

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<i>h</i>	<i>k</i>	<i>l</i>	$F_o$	$F_c$	$\sigma F$	<i>h</i>	<i>k</i>	<i>l</i>	$F_o$	$F_c$	$\sigma F$
5	1	-3	6.38	6.19	0.17	3	4	11	15.48	15.24	0.24
4	4	-5	16.09	15.77	0.24	2	6	5	29.99	30.70	0.27
3	5	-8	3.42	3.24	0.15	3	2	-17	4.52	4.75	0.15
4	1	-14	7.35	8.57	0.23	1	6	9	5.87	5.72	0.19
5	1	1	7.74	7.65	0.24	2	1	19	4.84	4.16	0.16
5	1	-4	8.57	7.99	0.23	3	1	-18	6.35	5.51	0.17
2	3	-18	6.66	7.22	0.18	4	2	-13	15.26	14.68	0.24
3	4	-13	15.03	14.63	0.24	4	1	12	9.78	9.46	0.26
1	2	20	6.68	6.69	0.17	5	0	-6	11.62	11.43	0.23
2	4	-16	21.28	21.46	0.25	5	1	2	5.52	4.86	0.15
2	3	17	6.29	6.92	0.17	1	5	14	12.50	12.50	0.23
1	6	-10	3.43	3.69	0.14	3	3	14	10.16	10.68	0.25
2	6	-7	9.31	9.71	0.24	3	5	7	19.12	19.82	0.25
4	4	4	3.13	2.18	0.15	2	4	15	11.13	10.98	0.24
2	6	6	12.89	13.10	0.25	4	3	-11	17.38	17.21	0.24
0	5	-15	6.91	6.69	0.17	2	5	-13	3.87	4.10	0.14
1	4	17	6.60	6.01	0.17	5	0	4	18.17	17.66	0.25
3	5	-9	8.09	7.17	0.24	5	1	3	8.14	8.12	0.24
5	1	-6	4.10	3.90	0.14	4	3	9	12.17	11.02	0.24
1	3	19	7.67	7.18	0.24	0	8	-11	10.36	10.81	0.24
3	3	-16	7.25	7.76	0.18	0	2	21	8.54	8.58	0.24
4	4	-7	12.37	12.14	0.25	1	6	10	10.26	10.79	0.24
4	4	5	2.62	1.80	0.16	0	0	-22	25.26	23.36	0.27
1	5	-15	2.43	2.69	0.19	3	2	16	6.17	6.23	0.19
3	4	12	6.16	6.78	0.19	2	6	-8	3.77	3.51	0.14
5	1	4	12.07	12.48	0.25	2	6	7	4.00	2.70	0.17
5	2	-1	15.90	14.86	0.23	5	2	-2	2.81	2.92	0.17
3	5	8	31.57	31.44	0.27	4	1	-15	5.78	5.26	0.16
2	2	-20	6.88	7.08	0.18	5	1	-7	5.23	5.99	0.16
1	0	-22	7.57	7.78	0.19	5	2	0	2.53	2.55	0.17
0	7	1	7.52	7.77	0.23	0	3	-20	8.12	7.18	0.25
5	2	-3	4.35	4.37	0.14	1	4	-18	8.89	8.75	0.25
5	0	-8	8.42	9.30	0.24	1	6	-11	5.02	4.75	0.15
4	2	-14	12.54	12.68	0.24	0	7	2	7.26	6.71	0.17
3	4	-14	10.48	9.50	0.25	5	2	1	5.03	4.61	0.14
0	1	-22	7.48	7.22	0.19	2	2	19	6.94	7.51	0.18
3	5	-10	4.98	4.96	0.14	4	3	-12	12.80	12.47	0.25
2	0	20	5.44	4.52	0.18	3	2	-18	5.77	6.02	0.18
4	1	13	5.46	4.87	0.18	1	3	-20	7.23	6.65	0.18
0	7	3	5.54	5.62	0.18	4	2	12	16.23	17.39	0.26
5	1	5	11.66	11.04	0.26	5	2	2	4.82	4.40	0.15
2	1	-21	11.42	12.51	0.26	1	1	-22	10.28	10.75	0.26
4	3	10	4.89	5.84	0.15	1	5	15	9.20	8.13	0.23
5	2	-5	2.84	2.05	0.17	3	1	-19	8.72	9.45	0.25
2	4	-17	3.67	3.80	0.15	2	5	-14	6.96	7.10	0.18
5	1	-8	21.25	21.08	0.25	2	6	-9	9.87	9.66	0.24
3	3	15	7.01	7.93	0.19	5	0	6	8.04	8.47	0.25
0	6	12	5.25	4.82	0.18	2	6	8	13.49	14.36	0.25
1	6	11	6.35	6.25	0.19	2	1	20	4.44	3.80	0.14
0	7	4	4.75	4.50	0.15	0	5	16	5.56	4.66	0.16
2	4	16	2.25	2.07	0.18	1	7	0	5.17	6.32	0.16
1	7	-1	4.12	3.46	0.14	3	5	9	3.92	4.94	0.18
5	2	3	5.58	3.98	0.18	4	0	-16	8.06	8.35	0.23
4	4	-9	4.64	4.92	0.14	5	2	-6	8.29	8.19	0.26
1	7	-2	1.75	1.74	0.20	1	2	21	5.17	4.42	0.16
1	4	18	2.69	3.06	0.15	1	7	2	6.65	6.76	0.18
3	3	-17	8.12	9.09	0.25	5	1	6	3.14	4.53	0.18
0	7	5	7.81	7.99	0.24	1	7	-3	5.46	4.96	0.16

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$h$	$k$	$l$	$F_o$	$F_c$	$\sigma F$	$h$	$k$	$l$	$F_o$	$F_c$	$\sigma F$
1	0	22	14.64	13.16	0.25	1	6	-12	3.92	3.26	0.14
1	5	-16	9.72	10.16	0.25	4	0	14	2.22	1.94	0.24
5	1	-9	7.14	7.18	0.19	3	0	18	16.28	17.50	0.26
5	2	4	5.15	4.24	0.15	4	3	-13	17.76	17.89	0.25
5	2	-7	12.02	11.43	0.25	4	2	-15	2.26	1.58	0.19
1	3	20	2.62	2.95	0.16	3	2	17	3.85	4.71	0.14
2	6	-10	7.49	7.23	0.25	3	6	-1	16.53	15.39	0.24
1	7	-4	12.59	12.45	0.25	0	4	19	8.60	8.28	0.22
3	6	0	4.41	3.73	0.15	3	4	-15	12.89	13.03	0.25
5	0	-10	15.08	14.49	0.23	3	6	-2	3.04	3.23	0.17
2	6	9	8.12	8.69	0.19	3	6	1	8.25	7.58	0.26
4	3	11	12.96	13.33	0.25	0	2	-22	9.94	9.35	0.25
1	1	22	11.90	11.79	0.24	0	7	6	8.17	7.93	0.25
1	7	4	4.50	4.62	0.15	3	6	-3	9.59	9.96	0.24
4	4	-10	2.06	2.60	0.23	4	1	14	19.08	20.70	0.27
3	1	18	6.94	6.61	0.20	1	6	12	4.52	4.53	0.15
1	4	-19	22.48	22.45	0.26	0	6	-13	12.18	11.41	0.25
3	6	2	7.06	6.23	0.24	5	1	7	5.18	5.24	0.17
1	7	-5	4.47	3.98	0.14	5	2	5	5.24	5.51	0.18
2	5	-15	7.47	6.51	0.25	4	4	8	3.69	3.97	0.16
1	2	-22	6.45	5.71	0.18	3	6	-4	4.19	3.61	0.15
0	3	21	13.08	13.38	0.23	5	2	-8	1.78	2.52	0.26
2	0	-22	29.37	30.15	0.28	5	1	-10	25.52	26.90	0.26
1	5	16	9.93	10.87	0.25	2	5	14	10.90	11.09	0.26
1	7	5	5.79	5.78	0.19	3	3	16	3.31	3.48	0.16
3	6	3	4.77	3.64	0.15	3	5	-12	15.03	14.41	0.25
2	4	-18	12.47	12.61	0.25	4	5	-1	8.33	8.27	0.23
5	0	8	12.35	10.99	0.26	1	3	-21	6.58	6.47	0.19
4	5	0	17.09	16.70	0.25	3	6	-5	4.22	3.17	0.15
5	3	-1	9.68	10.12	0.24	3	1	-20	21.68	21.88	0.26
0	5	17	2.68	2.80	0.14	1	6	-13	2.60	2.13	0.17
2	3	-20	8.08	8.02	0.25	1	7	-6	11.14	11.27	0.25
4	5	-3	4.28	4.29	0.15	5	3	0	10.39	10.22	0.24
2	4	17	2.71	0.68	0.17	5	3	-3	4.54	3.95	0.14
4	5	1	12.02	11.17	0.25	2	1	-22	13.19	13.95	0.26
3	4	14	6.23	6.01	0.18	4	3	-14	2.33	0.81	0.20
5	3	1	12.44	11.51	0.23	4	4	-11	9.37	9.87	0.27
3	6	4	16.46	14.78	0.25	1	1	-23	6.23	6.48	0.19
4	5	-4	9.20	9.16	0.25	5	2	-9	6.36	7.00	0.20
4	5	2	14.24	14.07	0.25	1	7	6	1.95	1.66	0.22
5	1	8	1.94	1.79	0.23	1	5	-17	9.39	9.00	0.27
2	1	21	3.58	3.37	0.14	4	4	9	8.33	8.84	0.25
4	3	12	3.38	3.13	0.17	4	1	-17	8.27	8.51	0.26
5	3	2	2.78	2.55	0.16	1	4	19	2.39	2.74	0.18
5	1	-11	2.92	1.97	0.16	5	3	-5	5.65	6.09	0.18
3	4	-16	4.21	4.42	0.16	3	5	11	7.29	7.89	0.19
4	5	-5	12.63	12.65	0.25	1	7	-7	5.90	6.26	0.19
0	7	-8	13.59	14.12	0.26	1	6	13	19.20	19.15	0.26
1	2	22	12.01	11.65	0.24	3	6	5	3.60	3.08	0.18
0	6	14	10.86	11.79	0.23	4	2	14	3.49	3.98	0.17
3	2	18	4.98	6.00	0.16	4	1	15	3.85	3.42	0.17
5	3	3	5.29	4.77	0.15	3	6	-7	9.12	8.68	0.26
5	2	7	4.89	6.08	0.16	3	5	-13	3.03	3.01	0.20
1	7	7	9.16	9.56	0.26	0	4	20	2.21	2.21	0.19
4	5	-6	11.82	12.26	0.24	5	0	-12	9.69	11.23	0.24
2	7	0	12.85	12.27	0.25	1	3	21	1.72	1.84	0.23
2	7	-1	3.81	4.23	0.16	2	6	-12	8.73	8.27	0.26
5	2	-10	3.93	4.22	0.16	2	7	-2	7.93	7.21	0.27

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$h$	$k$	$l$	$F_o$	$F_c$	$\sigma F$	$h$	$k$	$l$	$F_o$	$F_c$	$\sigma F$
2	7	1	5.20	3.78	0.16	2	5	15	13.66	13.77	0.26
2	6	11	10.77	10.16	0.26	4	4	-12	11.59	12.23	0.26
3	1	19	8.52	8.52	0.26	1	5	17	7.80	7.58	0.25
2	7	-3	2.76	2.10	0.18	1	7	-8	1.75	2.34	0.23
5	3	4	2.48	3.14	0.19	3	2	-20	5.91	5.90	0.19
0	2	-23	5.97	5.78	0.17	4	3	-15	4.79	5.28	0.16
5	3	-7	3.72	4.55	0.17	3	3	17	7.79	7.69	0.20
0	7	-9	5.44	5.17	0.17	1	1	23	2.53	1.83	0.21
4	4	10	6.77	6.33	0.18	5	1	-12	3.90	3.56	0.14
4	5	-7	4.53	4.76	0.15	2	2	-22	8.27	9.02	0.28
2	4	-19	6.18	6.35	0.19	3	6	-8	3.34	2.50	0.18
4	0	-18	7.25	5.99	0.24	3	4	15	4.22	4.11	0.15
2	7	-4	3.18	3.43	0.18	0	5	-18	7.52	7.70	0.19
4	5	5	2.73	2.31	0.20	1	2	-23	2.30	2.71	0.19
1	7	8	4.61	4.51	0.15	3	5	12	2.05	1.14	0.22
2	4	18	6.25	6.60	0.19	0	0	-24	11.20	10.61	0.27
2	2	21	4.82	4.28	0.14	5	2	8	9.27	8.78	0.27
3	1	-21	2.58	3.07	0.20	5	0	10	3.36	3.98	0.17
4	2	-17	5.72	5.80	0.19	5	3	5	8.37	7.38	0.25
2	3	-21	7.17	7.32	0.19	1	3	-22	6.93	6.69	0.18
2	7	-5	5.89	5.90	0.16	4	0	16	3.28	2.17	0.18
1	0	-24	9.60	10.42	0.27	2	0	22	10.51	8.65	0.26
3	3	-19	6.51	7.34	0.19	5	3	-8	9.11	9.17	0.26
1	6	14	3.92	4.30	0.16	1	5	-18	3.28	3.50	0.16
2	7	4	4.44	4.23	0.15	4	1	-18	3.15	3.12	0.16
3	6	7	13.45	13.85	0.26	3	4	-17	7.28	7.56	0.19
1	7	-9	4.07	3.81	0.15	4	5	-8	13.33	13.05	0.26
3	5	-14	19.04	19.43	0.27	0	6	15	5.32	5.11	0.17
2	3	20	2.25	1.99	0.18	2	1	-23	1.96	1.81	0.23
0	1	24	6.61	6.12	0.19	4	2	15	2.71	3.33	0.18
4	5	6	6.23	6.31	0.16	3	6	-9	5.51	6.16	0.17
4	4	-13	18.36	18.24	0.27	5	1	10	7.29	5.78	0.20
2	6	12	3.79	3.17	0.16	1	4	20	1.83	1.04	0.22
2	7	-6	10.81	10.59	0.26	4	1	16	7.58	7.81	0.21
2	5	-17	6.15	6.08	0.20	2	7	5	2.88	1.79	0.18
5	3	6	7.76	8.17	0.19	1	7	9	4.79	4.05	0.16
1	6	-15	6.51	6.36	0.17	3	2	19	5.66	5.11	0.16
2	5	16	15.78	15.61	0.26	5	3	-9	2.77	2.97	0.19
3	0	20	7.03	6.50	0.20	5	2	9	6.16	6.10	0.20
4	3	-16	3.05	2.11	0.17	4	5	-9	3.81	2.99	0.16
3	6	8	3.20	2.17	0.19	1	2	23	5.29	5.69	0.17
5	2	-12	8.37	9.65	0.27	1	7	-10	3.46	4.19	0.17
2	7	-7	1.89	1.79	0.25	4	5	7	3.43	3.58	0.18
3	5	13	4.40	4.08	0.14	2	7	6	2.37	3.07	0.20
3	6	-10	4.51	4.68	0.16	1	3	22	3.94	4.08	0.14
3	4	16	2.86	2.83	0.18	4	3	14	4.58	4.62	0.16
3	1	20	2.29	1.32	0.23	1	4	-21	2.59	2.37	0.20
5	0	-14	6.80	7.80	0.18	1	0	24	2.80	3.29	0.18
5	4	-1	7.21	7.11	0.20	5	4	-2	3.39	2.72	0.16
3	0	-22	2.15	1.62	0.18	5	4	-3	5.64	6.00	0.16
0	5	19	4.99	4.62	0.14	1	6	15	9.95	9.12	0.26
3	5	-15	10.24	10.92	0.28	4	2	-18	6.75	5.79	0.19
2	6	-14	8.38	8.45	0.26	5	3	-10	8.92	9.68	0.27
1	7	10	8.75	8.51	0.27	5	4	1	6.61	6.90	0.19
2	4	19	3.24	3.01	0.16	2	6	13	4.81	4.32	0.15
2	2	-23	2.23	2.22	0.20	0	6	16	3.40	3.92	0.15
2	7	-8	11.03	10.82	0.26	0	2	24	11.86	11.47	0.24
4	1	-19	3.44	3.53	0.14	5	1	-14	4.45	3.80	0.14

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$h$	$k$	$l$	$F_o$	$F_c$	$\sigma F$	$h$	$k$	$l$	$F_o$	$F_c$	$\sigma F$
3	6	9	9.58	9.13	0.26	2	7	7	4.49	4.28	0.16
1	1	24	16.72	15.80	0.26	5	2	10	3.00	2.64	0.17
0	3	-23	3.07	3.75	0.17	4	4	12	8.70	8.16	0.25
3	1	-22	6.43	7.67	0.18	4	5	8	2.35	1.35	0.18
5	4	2	2.50	2.11	0.23	4	2	16	3.21	3.59	0.18
5	4	-5	4.95	5.33	0.15	2	2	22	4.42	3.92	0.15
1	7	-11	2.92	2.82	0.19	5	2	-13	3.34	4.14	0.17
3	6	-11	6.77	6.83	0.21	1	6	-16	1.79	1.85	0.22
1	3	-23	5.16	5.55	0.16	2	5	-18	7.39	7.31	0.20
4	1	17	3.49	3.26	0.19	5	3	8	4.56	4.88	0.15
5	4	3	9.42	8.94	0.25	5	0	12	9.83	12.46	0.29
4	3	-17	6.82	6.20	0.20	5	4	-6	4.35	4.64	0.16
2	5	17	8.53	8.54	0.27	5	3	-11	6.34	7.32	0.21
1	4	21	8.90	7.47	0.25	2	1	-24	5.80	5.64	0.16
2	7	-9	5.88	5.08	0.17	0	7	12	7.65	8.11	0.24
4	5	-11	9.16	9.85	0.27	2	7	8	4.76	5.42	0.15
0	1	25	3.75	3.20	0.17	4	3	15	3.09	2.88	0.18
2	1	23	4.77	4.43	0.15	5	1	12	15.21	14.84	0.29
5	4	-7	4.29	4.84	0.16	4	5	9	2.38	2.36	0.23
4	4	-15	3.06	1.92	0.18	1	1	-25	3.45	3.22	0.17
1	5	19	4.20	3.49	0.16	2	6	-15	4.08	3.97	0.17
3	4	17	8.51	8.78	0.27	3	5	-16	5.78	5.96	0.17
5	2	11	5.64	5.85	0.18	0	8	-2	2.36	2.03	0.19
4	0	-20	2.54	2.99	0.17	2	6	14	1.58	1.47	0.26
0	4	22	4.07	3.06	0.13	3	6	-12	10.80	11.26	0.27
3	3	19	5.55	5.60	0.16	6	0	-2	2.59	3.20	0.21
4	4	13	5.46	5.68	0.17	4	6	-2	4.85	4.80	0.14
1	2	24	6.52	7.57	0.19	0	6	-17	9.35	8.86	0.26
6	0	0	3.80	2.72	0.18	5	4	5	8.34	7.10	0.26
3	1	21	6.45	5.86	0.20	3	2	-22	9.46	8.99	0.27
1	4	-22	6.59	5.53	0.20	4	6	-3	1.87	1.71	0.23
2	7	-10	5.23	5.52	0.15	1	3	23	5.52	4.42	0.16
3	7	-1	5.20	5.83	0.17	5	3	-12	2.53	2.01	0.22
4	6	1	2.29	2.19	0.17	6	0	-4	2.89	1.82	0.18
3	4	-19	2.01	2.48	0.25	3	7	0	6.22	6.24	0.19
5	4	-8	2.40	3.16	0.21	2	7	9	6.59	6.81	0.19
4	1	-20	7.59	5.84	0.18	3	7	1	2.84	3.72	0.19
4	6	-4	10.13	10.68	0.27	2	4	20	2.32	3.14	0.19
4	5	-12	7.58	7.88	0.20	3	7	-3	7.43	6.98	0.20
6	1	-2	6.69	7.12	0.19	4	2	17	5.39	5.86	0.15
4	6	2	3.20	2.86	0.18	6	1	-1	5.51	5.56	0.17
1	5	-20	7.29	6.52	0.20	1	6	-17	2.90	2.10	0.17
6	1	-3	4.08	3.67	0.17	3	3	-21	3.30	2.57	0.15
1	7	12	4.20	4.37	0.15	6	1	0	11.29	10.40	0.26
1	8	1	5.50	4.46	0.16	3	7	2	2.77	2.06	0.18
6	0	2	9.77	8.09	0.28	1	8	-2	8.93	9.27	0.28
4	5	10	6.36	6.03	0.20	3	7	-4	10.55	11.08	0.27
3	6	11	5.95	5.69	0.18	6	1	-4	7.96	7.83	0.21
2	5	-19	4.84	4.82	0.15	4	6	-5	6.89	6.66	0.21
2	2	-24	3.20	3.77	0.17	4	3	-18	4.03	3.51	0.16
4	1	18	5.81	6.63	0.18	6	0	-6	7.19	7.93	0.19
1	8	-3	4.81	4.81	0.16	2	3	-23	10.66	10.14	0.28
5	4	-9	3.75	4.69	0.18	0	3	24	4.08	3.82	0.14
2	5	18	1.76	1.77	0.28	5	1	13	3.75	4.11	0.18
6	1	-5	6.56	6.34	0.18	2	2	23	5.14	4.42	0.17
1	8	3	5.36	4.39	0.18	4	4	-16	2.56	1.69	0.20
5	2	12	3.38	3.82	0.20	3	6	-13	3.87	4.96	0.17
1	7	-13	4.78	4.61	0.16	6	1	2	4.12	2.99	0.17

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$h$	$k$	$l$	$F_o$	$F_c$	$\sigma F$	$h$	$k$	$l$	$F_o$	$F_c$	$\sigma F$
1	2	-25	8.57	9.19	0.28	2	6	-16	17.64	17.96	0.27
2	7	-11	4.15	3.97	0.16	1	8	-4	1.94	1.85	0.23
1	3	-24	3.67	2.67	0.16	3	5	-17	2.00	2.54	0.24
5	3	-13	4.49	3.28	0.16	5	2	-15	7.94	6.25	0.19
3	7	4	2.73	3.63	0.23	6	1	-6	8.34	9.76	0.22
0	8	-6	6.04	5.70	0.19	1	8	4	8.75	9.60	0.20
2	0	24	8.05	8.27	0.19	4	4	14	4.80	4.87	0.16
3	4	18	2.17	2.51	0.23	3	7	-6	3.03	3.95	0.20
5	4	7	4.08	3.92	0.17	1	8	-5	4.88	4.95	0.16
1	5	20	6.63	6.88	0.20	1	0	-26	4.06	4.29	0.17
5	4	-10	3.89	4.69	0.18	1	7	13	7.91	7.60	0.20
4	5	11	2.57	2.53	0.21	6	1	-7	8.61	8.18	0.22
1	8	5	8.77	9.36	0.20	0	7	-14	5.24	5.37	0.15
6	0	-8	11.71	13.74	0.26	3	6	12	5.95	5.43	0.18
2	1	24	8.53	7.40	0.28	6	2	-2	4.23	3.27	0.16
5	0	14	4.30	4.14	0.17	6	2	-1	2.53	2.37	0.21
3	3	20	6.16	5.84	0.19	0	1	-26	7.93	7.11	0.20
6	2	-3	4.83	4.96	0.17	0	8	7	3.81	4.23	0.16
6	1	4	9.70	8.05	0.30	3	7	-7	12.64	11.89	0.27
6	2	0	6.14	5.81	0.20	0	4	23	3.80	3.67	0.13
1	8	-6	5.60	5.60	0.16	6	2	-4	2.66	3.14	0.25
0	5	-21	4.55	4.74	0.15	1	6	-18	7.31	6.52	0.20
2	7	-12	3.48	3.20	0.17	5	3	11	4.70	3.96	0.15
3	2	-23	1.75	0.63	0.21	6	2	1	9.92	10.10	0.28
4	2	18	4.32	4.77	0.16	4	6	-8	4.82	5.63	0.16
3	1	22	5.36	6.42	0.17	3	6	-14	3.08	2.75	0.18
1	4	-23	3.02	2.40	0.17	2	7	11	6.99	6.07	0.20
3	5	16	5.41	5.36	0.17	6	1	-8	12.87	12.77	0.28
5	1	14	10.70	11.68	0.30	1	8	6	6.90	7.46	0.20
5	2	13	3.08	3.05	0.20	4	3	-19	13.29	13.94	0.27
6	2	-5	5.07	5.70	0.17	2	4	21	5.96	5.27	0.17
4	6	6	5.60	5.18	0.17	3	7	6	11.91	13.06	0.27
1	2	25	6.14	7.30	0.20	3	0	-24	6.81	7.13	0.19
1	3	24	6.57	6.47	0.19	5	5	-1	3.61	3.26	0.17
4	4	-17	7.07	7.92	0.21	3	3	-22	1.59	2.52	0.26
6	2	2	8.20	7.62	0.21	2	5	-20	3.99	3.48	0.17
5	5	0	5.30	5.24	0.17	5	4	-11	4.35	3.22	0.16
5	5	-3	7.55	7.70	0.21	2	6	-17	9.33	9.09	0.29
5	2	-16	2.34	3.23	0.21	5	1	-17	2.33	2.61	0.18
3	7	-8	5.10	5.65	0.17	4	5	-14	6.43	4.97	0.20
4	1	19	2.34	2.64	0.21	0	8	8	5.69	6.46	0.19
5	5	1	6.07	6.37	0.17	6	2	-6	4.87	5.19	0.18
5	5	-4	7.40	8.83	0.21	6	0	6	7.06	6.00	0.22
3	5	-18	4.55	4.29	0.15	2	6	16	2.60	2.90	0.21
4	4	15	3.49	4.35	0.18	6	2	3	5.48	6.28	0.16
3	1	-24	3.83	3.50	0.16	4	6	-9	5.41	5.16	0.17
4	5	12	6.54	6.86	0.20	1	0	26	7.51	6.34	0.20
6	1	-9	3.90	4.22	0.19	5	5	2	6.20	4.97	0.17
2	2	-25	4.27	3.92	0.16	1	8	7	4.30	4.60	0.16
5	5	-5	4.71	4.48	0.17	2	8	-1	3.90	3.51	0.16
2	8	0	4.31	4.01	0.16	2	3	-24	8.36	8.33	0.27
1	6	18	4.20	4.51	0.18	3	7	7	10.10	10.66	0.29
4	6	7	1.82	1.21	0.26	3	6	13	6.05	6.09	0.18
6	2	-7	5.78	4.89	0.17	0	7	-15	2.24	1.40	0.23
6	1	6	5.40	4.57	0.17	6	0	-10	2.75	2.57	0.20
3	4	19	4.59	5.06	0.15	0	3	25	4.99	4.92	0.16
1	8	-8	4.27	4.26	0.17	0	2	-26	1.87	1.42	0.29
2	8	-3	3.50	3.18	0.18	3	7	-9	5.03	5.45	0.17

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<i>h</i>	<i>k</i>	<i>l</i>	$F_o$	$F_c$	$\sigma F$	<i>h</i>	<i>k</i>	<i>l</i>	$F_o$	$F_c$	$\sigma F$
2	3	23	7.44	6.65	0.19	2	8	2	3.12	3.02	0.18
6	2	4	2.96	3.03	0.20	5	3	12	3.27	3.44	0.16
2	7	12	3.47	4.06	0.17	1	1	26	2.31	1.97	0.21
5	5	-6	2.94	3.18	0.23	2	0	-26	3.69	4.50	0.15
1	3	-25	4.16	3.88	0.17	1	2	-26	4.18	4.33	0.17
1	4	23	3.93	3.22	0.15	5	4	-12	4.49	2.62	0.17
0	6	19	10.57	11.51	0.25	1	5	21	3.75	4.21	0.16
3	6	-15	4.85	4.15	0.16	2	8	-4	3.59	4.83	0.17
4	2	-21	2.83	3.28	0.19	5	3	-15	6.11	6.30	0.17
2	8	3	4.20	3.06	0.17	6	2	-8	15.26	15.49	0.29
5	1	15	3.29	3.21	0.20	3	3	21	5.88	5.31	0.17
3	7	8	12.14	13.02	0.29	2	1	-26	6.43	7.50	0.21
4	6	8	5.35	7.39	0.16	3	5	17	4.66	5.46	0.16
2	8	-5	4.51	4.19	0.16	6	2	5	3.72	2.81	0.20
6	1	7	5.20	4.64	0.17	2	8	4	7.48	7.61	0.21
4	4	-18	2.45	2.25	0.22	5	2	-17	5.56	6.05	0.17
4	2	19	1.86	2.13	0.26	4	3	-20	5.96	5.76	0.18
4	0	20	4.00	5.23	0.17	0	5	-22	2.75	1.48	0.20
5	1	-18	3.02	2.98	0.17	3	7	-10	1.71	1.74	0.24
2	6	-18	12.76	12.09	0.28	4	5	13	4.92	4.12	0.16
6	3	-3	2.01	1.59	0.24	5	4	10	4.03	4.29	0.16
6	2	-9	6.16	4.93	0.20	0	8	-10	3.36	3.77	0.17
6	0	8	4.72	3.49	0.17	1	5	-22	2.91	2.44	0.17
2	8	-6	4.79	5.12	0.16	4	4	16	7.07	6.06	0.22
1	7	15	2.74	2.52	0.21	3	5	-19	3.15	3.66	0.16
6	3	-4	3.97	4.61	0.20	1	4	-24	2.62	3.16	0.21
2	4	22	2.32	1.53	0.21	3	6	14	4.76	5.79	0.16
2	7	-14	10.92	11.32	0.29	2	8	5	6.42	6.50	0.18
5	5	-8	5.54	5.22	0.17	5	4	-13	1.63	0.31	0.22
3	3	-23	3.73	5.08	0.17	1	1	-27	4.26	4.58	0.17
6	1	-11	7.03	7.11	0.20	4	3	18	3.32	2.97	0.18
4	1	20	11.96	12.57	0.30	4	6	-11	8.27	8.14	0.20
2	5	20	4.93	4.89	0.16	0	7	16	3.12	2.79	0.17
6	3	-5	8.20	8.00	0.22	1	3	25	2.10	2.18	0.22
3	7	9	6.07	5.08	0.17	4	6	9	3.41	3.17	0.18
1	2	26	2.48	1.71	0.21	1	6	19	9.38	8.86	0.27
3	6	-16	10.26	11.14	0.30	5	0	16	7.09	8.92	0.22
5	5	6	6.10	7.52	0.18	2	8	6	5.74	6.08	0.18
1	7	-16	3.48	4.20	0.18	6	2	-10	4.25	3.63	0.19
3	1	-25	3.69	4.57	0.17	5	5	-9	8.18	8.22	0.21
3	4	20	2.77	2.06	0.20	6	3	3	7.12	6.27	0.20
5	2	15	3.59	3.95	0.17	4	5	-16	4.87	5.15	0.17
0	6	20	7.42	6.87	0.20	0	8	11	1.91	1.85	0.25
6	2	7	2.79	3.85	0.22	6	1	-12	2.62	3.03	0.23
5	4	11	3.04	3.66	0.21	1	8	10	7.11	7.08	0.22
4	2	-22	3.42	4.54	0.19	6	3	-7	9.82	8.68	0.30
1	5	22	2.52	2.76	0.21	4	6	-12	4.56	5.64	0.19
4	5	14	2.73	0.99	0.22	2	3	24	3.05	2.96	0.20
3	5	18	4.35	2.81	0.17	4	4	-19	3.82	3.55	0.20
1	6	-20	5.56	6.38	0.16	5	4	-14	4.27	3.50	0.19
5	1	-19	3.51	3.49	0.18	3	4	-22	4.80	4.71	0.17
0	2	27	5.89	6.09	0.17	2	7	-15	7.32	7.02	0.22
6	1	9	3.15	3.20	0.20	1	3	-26	3.33	3.78	0.21
4	6	10	5.67	6.35	0.19	5	5	-10	2.86	1.56	0.24
1	8	-11	3.01	3.45	0.21	4	3	-21	2.90	3.27	0.21
1	7	16	10.92	10.98	0.28	6	2	-11	3.17	2.08	0.22
1	1	27	2.03	0.70	0.23	2	7	14	2.52	1.21	0.22
3	7	-12	9.70	9.47	0.29	5	3	14	10.11	9.38	0.31

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$h$	$k$	$l$	$F_o$	$F_c$	$\sigma F$	$h$	$k$	$l$	$F_o$	$F_c$	$\sigma F$
2	6	18	4.30	4.47	0.17	4	7	-1	3.52	2.93	0.18
4	7	0	4.97	4.91	0.16	3	5	-20	5.34	4.88	0.18
0	5	23	2.75	1.76	0.16	3	0	24	11.10	8.87	0.29
4	7	-3	3.52	3.75	0.18	6	2	8	3.68	3.31	0.20
6	3	5	2.76	3.30	0.19	2	4	-24	2.03	2.59	0.26
2	1	-27	4.25	5.02	0.17	2	5	-22	7.74	7.37	0.20
5	3	-17	5.80	4.34	0.17	6	0	10	2.67	3.00	0.22
1	8	11	4.36	3.83	0.17	2	8	8	6.41	6.60	0.19
1	5	-23	4.73	5.30	0.17	0	0	28	4.84	4.30	0.17
4	7	2	3.12	4.30	0.20	5	5	8	2.25	2.87	0.26
1	7	-17	2.25	2.66	0.26	2	5	21	3.44	3.20	0.19
1	0	-28	2.22	2.66	0.23	4	1	21	2.92	2.59	0.24
4	6	-13	3.41	3.99	0.20	3	3	-24	1.86	2.02	0.23
2	1	26	2.37	0.85	0.23	6	3	-9	3.17	2.09	0.22
1	6	20	3.78	2.85	0.20	3	1	24	4.83	4.29	0.17
1	4	-25	9.85	10.99	0.30	5	5	-11	5.15	4.96	0.18
3	7	11	5.94	4.65	0.18	4	7	-5	4.25	3.88	0.17
5	2	16	6.01	6.09	0.20	6	1	10	4.78	3.96	0.19
4	6	11	5.40	4.16	0.16	1	8	-12	1.92	1.88	0.27
1	1	-28	3.98	4.56	0.18	6	0	-14	7.43	7.69	0.20
5	2	-19	1.77	0.66	0.26	3	4	21	5.01	4.55	0.16
1	3	26	2.94	2.10	0.21	2	7	-16	3.10	3.71	0.23
6	2	9	2.67	1.55	0.26	3	8	-1	4.12	3.77	0.17
0	6	-21	6.73	7.38	0.22	3	8	-2	2.77	2.53	0.21
2	8	9	2.37	2.50	0.25	4	7	4	3.36	3.16	0.18
1	2	27	2.93	3.19	0.19	4	4	-20	3.22	3.02	0.20
2	7	15	4.95	4.69	0.18	5	1	-20	3.05	3.58	0.18
3	1	-26	7.73	7.69	0.21	6	3	-10	3.26	4.25	0.23
6	4	-1	3.63	4.59	0.17	6	4	-3	4.83	4.24	0.17
5	3	15	2.67	2.44	0.27	5	6	-2	1.97	3.04	0.26
0	9	1	3.39	3.20	0.22	1	5	23	2.98	3.64	0.21
5	5	-12	4.42	4.88	0.20	6	3	7	4.18	3.72	0.18
0	9	2	2.39	2.89	0.22	4	3	-22	2.63	1.75	0.22
6	2	-13	4.10	3.02	0.19	4	7	5	3.61	4.21	0.19
3	6	-18	6.47	6.11	0.18	2	3	25	7.84	7.38	0.21
4	2	21	3.23	2.86	0.21	3	8	-5	6.32	5.83	0.19
0	9	-3	4.94	5.95	0.17	1	4	25	3.38	4.36	0.17
2	2	26	6.55	6.07	0.21	1	0	28	4.18	5.12	0.17
1	8	-13	2.13	1.89	0.26	3	2	24	2.34	1.80	0.24
6	4	2	2.86	3.88	0.22	2	8	-11	2.24	1.67	0.23
5	6	-5	2.18	3.16	0.26	4	1	-24	4.42	2.99	0.17
1	7	-18	5.55	6.45	0.17	1	3	-27	3.98	4.49	0.18
6	3	-11	5.54	5.90	0.18	4	0	22	7.32	7.37	0.23
6	2	10	1.95	1.67	0.31	3	8	4	5.43	5.99	0.17
3	7	-14	4.29	5.24	0.21	6	4	-6	3.36	3.12	0.19
0	9	4	3.78	4.32	0.20	2	5	-23	4.80	5.02	0.18
5	0	18	3.25	3.55	0.21	2	0	-28	9.41	9.30	0.32
1	9	0	2.32	1.86	0.24	3	8	-6	4.51	4.38	0.16
6	4	3	2.04	3.14	0.25	1	9	1	6.81	6.43	0.22
1	1	28	3.51	2.38	0.18	6	3	8	2.69	3.26	0.21
1	5	-24	11.06	10.02	0.29	1	6	21	10.18	10.26	0.29
2	5	22	4.33	4.55	0.17	6	1	-15	3.42	3.59	0.18
6	4	-7	2.94	3.25	0.25	0	9	-5	6.12	6.43	0.19
1	9	-3	2.90	3.30	0.23	3	8	5	8.89	7.65	0.30
3	2	-26	5.08	5.06	0.17	0	8	14	7.21	8.37	0.20
2	1	-28	7.20	8.63	0.21	2	7	16	5.46	5.83	0.17
3	3	-25	3.07	4.86	0.20	2	4	24	2.24	2.39	0.26
0	4	-26	3.76	3.28	0.19	6	2	-14	5.78	5.81	0.19

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<i>h</i>	<i>k</i>	<i>l</i>	$F_o$	$F_c$	$\sigma F$	<i>h</i>	<i>k</i>	<i>l</i>	$F_o$	$F_c$	$\sigma F$
4	7	-9	2.17	1.63	0.24	4	6	-15	4.97	5.71	0.18
5	6	-7	4.47	4.36	0.17	1	4	-26	2.56	1.43	0.22
3	1	25	4.55	4.35	0.16	1	9	-4	4.10	4.11	0.18
2	1	27	4.80	4.92	0.18	4	7	7	4.06	3.99	0.19
6	1	12	4.72	4.59	0.20	0	6	22	1.78	1.24	0.25
1	9	4	5.34	5.38	0.18	6	4	-8	5.25	5.33	0.19
1	8	-14	3.07	2.66	0.21	4	6	13	3.49	3.53	0.19
3	5	20	3.01	3.28	0.19	5	6	5	4.16	4.17	0.18
1	6	-22	2.98	1.49	0.19	6	3	9	3.93	4.77	0.19
0	7	19	4.32	4.27	0.15	6	0	-16	2.28	3.02	0.21
4	2	-24	3.19	2.17	0.20	3	7	-15	7.15	7.86	0.24
5	6	-8	2.81	2.22	0.19	5	4	-17	3.88	4.51	0.21
5	5	11	2.24	2.52	0.26	4	4	19	2.58	3.63	0.23
2	6	20	5.79	5.31	0.19	4	7	-10	3.50	3.89	0.19
3	1	-27	5.30	4.81	0.18	4	5	-19	4.50	5.44	0.19
5	5	-14	8.98	9.98	0.23	0	9	7	2.66	3.22	0.23
1	7	-19	4.05	3.46	0.19	3	4	-24	2.98	1.69	0.18
4	7	8	2.80	3.36	0.24	1	8	14	3.70	3.79	0.18
3	8	7	3.09	2.14	0.22	4	2	22	3.68	4.18	0.20
5	6	6	3.86	3.43	0.17	6	2	-15	3.50	4.90	0.20
2	7	-18	4.49	5.61	0.19	5	6	-9	2.11	1.42	0.23
1	9	6	3.47	3.87	0.20	4	1	-25	3.51	2.56	0.16
4	6	-16	3.51	2.61	0.22	3	3	24	2.69	2.55	0.22
1	4	26	2.49	2.69	0.21	0	9	-8	5.80	6.92	0.19
5	2	-21	3.57	3.42	0.18	5	0	-22	5.06	4.20	0.16
1	8	-15	5.56	5.15	0.16	0	5	-25	5.98	6.75	0.19
4	6	14	3.83	3.87	0.19	2	5	23	5.84	6.10	0.17
5	3	17	2.20	3.84	0.27	5	6	7	3.04	4.42	0.21
4	7	9	3.36	2.70	0.23	3	8	8	3.03	3.95	0.23
1	5	-25	2.99	2.55	0.20	1	7	19	2.58	2.96	0.23
3	7	-16	10.34	10.89	0.31	0	2	-29	3.72	4.88	0.18
5	6	-10	2.91	2.74	0.21	5	5	-15	10.11	10.53	0.33
3	0	26	9.34	9.00	0.29	5	1	-22	6.61	4.77	0.21
7	0	-4	3.00	4.57	0.19	5	4	-18	6.53	6.13	0.19
3	8	-10	2.55	3.29	0.25	5	3	-20	4.19	4.58	0.18
2	9	-3	5.76	5.57	0.19	6	3	-14	3.79	5.16	0.21
7	1	-2	5.19	5.17	0.15	0	7	-20	2.14	1.44	0.22
0	9	9	4.27	4.90	0.19	7	1	-1	2.94	2.38	0.19
3	4	23	4.40	4.40	0.17	6	1	-17	6.07	5.15	0.17
1	8	15	2.08	1.47	0.25	6	2	-16	4.24	2.83	0.18
2	1	-29	3.96	4.49	0.19	6	0	14	6.63	6.44	0.22
4	5	-20	2.47	2.91	0.23	4	4	20	2.32	3.42	0.24
4	7	-12	2.50	2.81	0.26	2	8	13	2.69	2.13	0.23
1	9	8	4.15	4.06	0.18	6	5	-2	2.89	5.31	0.22
5	6	8	1.95	2.88	0.27	6	5	0	2.45	1.60	0.23
2	1	28	7.38	6.39	0.22	4	6	-17	8.26	9.22	0.22
3	0	-28	6.71	7.32	0.20	6	4	8	4.82	5.16	0.17
4	7	10	3.73	4.69	0.19	2	7	-19	2.95	2.55	0.21
2	9	4	3.25	3.75	0.21	1	0	-30	4.03	5.59	0.20
3	5	-23	2.38	3.30	0.25	1	8	-16	1.83	2.04	0.29
7	1	2	2.76	2.20	0.21	4	0	-26	3.35	3.28	0.18
5	0	20	2.50	2.47	0.22	2	9	-6	2.88	3.04	0.22
5	4	16	2.71	1.82	0.25	2	9	5	2.36	2.56	0.26
6	0	-18	6.44	6.86	0.19	1	1	-30	3.34	2.55	0.21
6	4	-12	4.60	4.97	0.19	3	7	-17	3.09	2.05	0.23
4	3	22	2.31	2.11	0.26	6	5	-6	1.83	0.45	0.27
7	0	4	4.03	3.42	0.20	7	0	-8	2.21	5.03	0.23
5	3	18	4.02	2.72	0.18	5	1	20	3.43	3.52	0.20