

LSFM (1.3) 02/14/96 16:12:56 Elapsed time = 0.1 min

FEKINO Demonstration Copy - Not for Resale

The space group is number 12 -- C12/m1

Refinement cycle no. 1. 750 observations. 59 variables.

Anisotropic
3.2%

Esd of an observation of unit weight = 1.012

Unweighted R factor = 0.032 Weighted R factor = 0.036

$\bar{a}^3 Fo^3 = 2.81306E+04$

$\bar{a}^3 Fo^3 - \bar{a}^3 Fc^3 = 8.94628E+02$

$\bar{a} W*DELy = 7.07633E+02$

$\bar{a} W*Fo_y = 5.45704E+05$

Scale factor:	New	Old	Shift	Error	SHFT/ERR
	1.80813	1.80794	0.00019	0.00137	0.14

Extinction coefficient:	New =	Old =	Shift =	Error =	SHFT/ERR =
	2.63928E-06	2.65255E-06	-1.32678E-08	1.21468E-07	-0.10923

Atom no. 1	FE1				
Parameter	New	Old	Shift	Error	SHFT/ERR
Mult.	0.25000				
x	0.00000				
y	0.00000				
z	0.50000				
5 B(1,1)	0.00701	0.00701	0.00000	0.00030	0.00
6 B(2,2)	0.00133	0.00133	0.00000	0.00010	0.03
7 B(3,3)	0.00341	0.00341	0.00000	0.00010	0.01
B(1,2)	0.00000				
9 B(1,3)	0.00283	0.00283	0.00000	0.00028	0.01
B(2,3)	0.00000				
Total shift = 0.0000					

Atom no. 2	MG				
Parameter	New	Old	Shift	Error	SHFT/ERR
Mult.	0.50000				
x	0.00000				
12 y	0.33306	0.33305	0.00001 (0.0001 %)	0.00010 (0.0009 %)	0.11
z	0.50000				
14 B(1,1)	0.00548	0.00549	-0.00001	0.00021	-0.04
15 B(2,2)	0.00202	0.00202	0.00000	0.00008	-0.03
16 B(3,3)	0.00324	0.00323	0.00001	0.00007	0.08
B(1,2)	0.00000				
18 B(1,3)	0.00122	0.00123	-0.00001	0.00020	-0.03
B(2,3)	0.00000				
Total shift = 0.0001					

Atom no. 3	K				
Parameter	New	Old	Shift	Error	SHFT/ERR
Mult.	0.25000				
x	0.00000				

	J	0.00000					
23	B(1,1)	0.01404	0.01404	0.00000		0.00019	-0.02
24	B(2,2)	0.00386	0.00386	0.00000		0.00006	0.01
25	B(3,3)	0.00671	0.00671	0.00000		0.00007	0.01
	B(1,2)	0.00000					
27	B(1,3)	0.00380	0.00381	-0.00001		0.00018	-0.03
	B(2,3)	0.00000					
Total shift =		0.00000					

Atom no.	4	SI					
Parameter	New	Old	Shift		Error		SHFT/ERR
	Mult.	1.00000					
29	x	0.07450	0.07458	-0.00008 (0.0004 %)	0.00018 (0.0010 %)		-0.45
30	y	0.16644	0.16647	-0.00003 (0.0003 %)	0.00011 (0.0010 %)		-0.26
31	z	0.21994	0.21991	0.00003 (0.0003 %)	0.00010 (0.0010 %)		0.33
32	B(1,1)	0.00762	0.00762	0.00000	0.00025		0.01
33	B(2,2)	0.00193	0.00193	0.00000	0.00009		-0.04
34	B(3,3)	0.00303	0.00303	0.00000	0.00008		-0.02
35	B(1,2)	-0.00003	-0.00003	0.00000	0.00027		-0.01
36	B(1,3)	0.00174	0.00174	0.00000	0.00024		0.02
37	B(2,3)	-0.00016	-0.00015	-0.00001	0.00015		-0.04
Total shift =		0.00060					

Atom no.	5	F					
Parameter	New	Old	Shift		Error		SHFT/ERR
	Mult.	0.50000					
38	x	0.12294	0.12299	-0.00005 (0.0003 %)	0.00068 (0.0037 %)		-0.08
	y	0.50000					
40	z	0.38709	0.38706	0.00003 (0.0003 %)	0.00042 (0.0042 %)		0.07
41	B(1,1)	0.00972	0.00971	0.00001	0.00100		0.01
42	B(2,2)	0.00278	0.00279	-0.00001	0.00034		-0.02
43	B(3,3)	0.00633	0.00632	0.00001	0.00037		0.02
	B(1,2)	0.00000					
45	B(1,3)	0.00398	0.00396	0.00002	0.00100		0.02
	B(2,3)	0.00000					
Total shift =		0.00040					

Atom no.	6	O1					
Parameter	New	Old	Shift		Error		SHFT/ERR
	Mult.	0.50000					
47	x	0.03330	0.03295	0.00035 (0.0019 %)	0.00090 (0.0048 %)		0.39
	y	0.00000					
49	z	0.15784	0.15777	0.00007 (0.0007 %)	0.00041 (0.0041 %)		0.17
50	B(1,1)	0.02672	0.02670	0.00002	0.00155		0.01
51	B(2,2)	0.00337	0.00338	-0.00001	0.00038		-0.02
52	B(3,3)	0.00273	0.00273	0.00000	0.00032		0.01
	B(1,2)	0.00000					
54	B(1,3)	0.00061	0.00056	0.00005	0.00121		0.04
	B(2,3)	0.00000					
Total shift =		0.00190					

Atom no.	7	O2					
Parameter	New	Old	Shift		Error		SHFT/ERR
	Mult.	1.00000					
56	x	0.31342	0.31339	0.00003 (0.0002 %)	0.00055 (0.0030 %)		0.06
57	y	0.24000	0.24001	-0.00001 (0.0001 %)	0.00036 (0.0033 %)		-0.04
58	z	0.15862	0.15853	0.00009 (0.0009 %)	0.00029 (0.0029 %)		0.30
59	B(1,1)	0.01596	0.01596	0.00000	0.00085		0.00
60	B(2,2)	0.00636	0.00636	0.00000	0.00032		0.01
61	B(3,3)	0.00386	0.00387	-0.00001	0.00023		-0.03
62	B(1,2)	-0.00768	-0.00768	0.00000	0.00095		0.00
63	B(1,3)	0.00279	0.00280	-0.00001	0.00074		-0.01

Total shift = 0.0009%

Atom no.	8	O3						
Parameter		New	Old	Shift		Error		SHFT/ERR
	Mult.	1.00000						
65	x	0.13191	0.13193	-0.00002 (0.0001 %)		0.00047 (0.0025 %)		-0.05
66	y	0.16591	0.16590	0.00001 (0.0001 %)		0.00029 (0.0027 %)		0.04
67	z	0.38831	0.38835	-0.00004 (0.0004 %)		0.00026 (0.0026 %)		-0.17
68	B(1,1)	0.00989	0.00990	-0.00001		0.00069		-0.02
69	B(2,2)	0.00302	0.00302	0.00000		0.00024		-0.01
70	B(3,3)	0.00362	0.00362	0.00000		0.00022		0.00
71	B(1,2)	-0.00002	-0.00002	0.00000		0.00078		0.00
72	B(1,3)	0.00257	0.00257	0.00000		0.00064		0.00
73	B(2,3)	-0.00054	-0.00054	0.00000		0.00042		0.00
Total shift =		0.0004%						

Largest parameter shift/error = 0.45

Average parameter shift/error = 0.06

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LSFM (1.3) 02/14/96 16:12:58 Elapsed time = 0.0 min

FEKINO Demonstration Copy - Not for Resale

The space group is number 12 -- C12/m1

Refinement cycle no. 2. 750 observations. 59 variables.

Esd of an observation of unit weight = 1.011

Unweighted R factor = 0.032 Weighted R factor = 0.036

$\ddot{a}^3 Fo^3 = 2.81336E+04$

$\ddot{a}^3 Fo^3 -^3 Fc^3 = 8.94929E+02$

$\ddot{a} W*DELY = 7.06883E+02$

$\ddot{a} W*FOY = 5.45704E+05$

Scale factor:	New	Old	Shift	Error	SHFT/ERR
	1.80812	1.80813	-0.00001	0.00137	-0.01

Extinction coefficient:	New =	2.63840E-06
	Old =	2.63928E-06
	Shift =	-8.83755E-10
	Error =	1.21432E-07
	SHFT/ERR =	-0.00728

Atom no.	1	FE1					
Parameter		New	Old	Shift		Error	SHFT/ERR
	Mult.	0.25000					
	x	0.00000					
	y	0.00000					
	z	0.50000					
5	B(1,1)	0.00701	0.00701	0.00000		0.00030	0.00
6	B(2,2)	0.00133	0.00133	0.00000		0.00010	0.00
7	B(3,3)	0.00341	0.00341	0.00000		0.00010	0.01
	B(1,2)	0.00000					
9	B(1,3)	0.00283	0.00283	0.00000		0.00028	-0.01
	B(2,3)	0.00000					
Total shift =		0.0000%					

Parameter	New	Old	Shift	Error	SHFT/ERR
Mult.	0.50000				
x	0.00000				
12 y	0.33306	0.33306	0.00000 (0.0000 ✖)	0.00010 (0.0009 ✖)	0.00
z	0.50000				
14 B(1,1)	0.00548	0.00548	0.00000	0.00021	0.00
15 B(2,2)	0.00202	0.00202	0.00000	0.00008	0.00
16 B(3,3)	0.00324	0.00324	0.00000	0.00007	0.00
B(1,2)	0.00000				
18 B(1,3)	0.00123	0.00122	0.00000	0.00020	0.00
B(2,3)	0.00000				
Total shift = 0.0000✖					

Atom no.	3	K	Parameter	New	Old	Shift	Error	SHFT/ERR
			Mult.	0.25000				
			x	0.00000				
			y	0.50000				
			z	0.00000				
23			B(1,1)	0.01404	0.01404	0.00000	0.00019	0.00
24			B(2,2)	0.00386	0.00386	0.00000	0.00006	0.00
25			B(3,3)	0.00671	0.00671	0.00000	0.00007	0.00
			B(1,2)	0.00000				
27			B(1,3)	0.00380	0.00380	0.00000	0.00018	-0.01
			B(2,3)	0.00000				
Total shift = 0.0000✖								

Atom no.	4	SI	Parameter	New	Old	Shift	Error	SHFT/ERR
			Mult.	1.00000				
29			x	0.07450	0.07450	0.00000 (0.0000 ✖)	0.00018 (0.0010 ✖)	-0.01
30			y	0.16644	0.16644	0.00000 (0.0000 ✖)	0.00011 (0.0010 ✖)	-0.01
31			z	0.21994	0.21994	0.00000 (0.0000 ✖)	0.00010 (0.0010 ✖)	0.01
32			B(1,1)	0.00762	0.00762	0.00000	0.00025	0.00
33			B(2,2)	0.00193	0.00193	0.00000	0.00009	0.00
34			B(3,3)	0.00303	0.00303	0.00000	0.00008	-0.01
35			B(1,2)	-0.00003	-0.00003	0.00000	0.00027	0.00
36			B(1,3)	0.00175	0.00174	0.00000	0.00024	0.01
37			B(2,3)	-0.00016	-0.00016	0.00000	0.00015	0.00
Total shift = 0.0000✖								

Atom no.	5	F	Parameter	New	Old	Shift	Error	SHFT/ERR
			Mult.	0.50000				
38			x	0.12293	0.12294	0.00000 (0.0000 ✖)	0.00068 (0.0037 ✖)	-0.01
			y	0.50000				
40			z	0.38709	0.38709	0.00000 (0.0000 ✖)	0.00042 (0.0042 ✖)	0.01
41			B(1,1)	0.00972	0.00972	0.00000	0.00100	0.00
42			B(2,2)	0.00279	0.00278	0.00000	0.00034	0.00
43			B(3,3)	0.00633	0.00633	0.00000	0.00037	-0.01
			B(1,2)	0.00000				
45			B(1,3)	0.00398	0.00398	0.00000	0.00100	0.00
			B(2,3)	0.00000				
Total shift = 0.0000✖								

Atom no.	6	O1	Parameter	New	Old	Shift	Error	SHFT/ERR
			Mult.	0.50000				
47			x	0.03330	0.03330	0.00000 (0.0000 ✖)	0.00090 (0.0048 ✖)	0.00
			y	0.00000				
49			z	0.15785	0.15784	0.00000 (0.0000 ✖)	0.00041 (0.0041 ✖)	0.01
50			B(1,1)	0.02674	0.02672	0.00001	0.00155	0.01

52	B(3,3)	0.00273	0.00273	0.00000		0.00032		0.00
	B(1,2)	0.00000						
54	B(1,3)	0.00062	0.00061	0.00002		0.00121		0.01
	B(2,3)	0.00000						
Total shift =		0.0000*						

Atom no.	7	O2							
Parameter	New	Old	Shift	Error		SHFT/ERR			
Mult.	1.00000								
56	x	0.31342	0.31342	0.00000	(0.0000 *)	0.00055	(0.0030 *)	0.00	
57	y	0.24000	0.24000	0.00000	(0.0000 *)	0.00036	(0.0033 *)	0.00	
58	z	0.15863	0.15862	0.00001	(0.0001 *)	0.00029	(0.0029 *)	0.02	
59	B(1,1)	0.01596	0.01596	0.00000		0.00085		0.00	
60	B(2,2)	0.00636	0.00636	0.00000		0.00032		0.00	
61	B(3,3)	0.00386	0.00386	0.00000		0.00023		0.00	
62	B(1,2)	-0.00768	-0.00768	0.00000		0.00095		0.00	
63	B(1,3)	0.00280	0.00279	0.00001		0.00074		0.01	
64	B(2,3)	-0.00096	-0.00096	0.00000		0.00050		0.00	
Total shift =		0.0001*							

Atom no.	8	O3							
Parameter	New	Old	Shift	Error		SHFT/ERR			
Mult.	1.00000								
65	x	0.13191	0.13191	0.00000	(0.0000 *)	0.00047	(0.0025 *)	0.00	
66	y	0.16591	0.16591	0.00000	(0.0000 *)	0.00029	(0.0027 *)	0.00	
67	z	0.38830	0.38831	0.00000	(0.0000 *)	0.00026	(0.0026 *)	-0.01	
68	B(1,1)	0.00989	0.00989	0.00000		0.00069		0.00	
69	B(2,2)	0.00302	0.00302	0.00000		0.00024		0.00	
70	B(3,3)	0.00362	0.00362	0.00000		0.00022		0.01	
71	B(1,2)	-0.00002	-0.00002	0.00000		0.00078		0.00	
72	B(1,3)	0.00256	0.00257	0.00000		0.00064		-0.01	
73	B(2,3)	-0.00054	-0.00054	0.00000		0.00042		0.00	
Total shift =		0.0000*							

Largest parameter shift/error = 0.02
Average parameter shift/error = 0.00

The calculations have converged with a shift/error less than 0.100

No.	h	k	l	Fo	Fc	sin ϵ /l	Fo-Fc	w(Fo-Fc)	Flag
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1	0	0	1	41.135	47.137	0.05058	-6.002	-3.320	*
2	0	0	2	80.027	85.925	0.10117	-5.898	-3.262	*
3	0	0	3	111.000	111.063	0.15175	-0.063	-0.035	
4	0	0	4	96.807	101.049	0.20233	-4.243	-2.346	*
5	0	0	5	80.769	79.837	0.25292	0.931	0.515	
6	0	0	6	119.679	113.072	0.30350	6.608	3.654	*
7	0	0	7	59.867	58.713	0.35408	1.154	0.638	
8	0	0	8	107.926	108.366	0.40467	-0.440	-0.243	
9	0	0	9	23.072	24.465	0.45525	-1.394	-0.771	
10	0	0	10	72.252	70.535	0.50583	1.717	0.950	
11	0	0	11	49.759	47.003	0.55642	2.757	1.525	
12	0	0	12	34.535	32.543	0.60700	1.992	1.102	
13	0	0	13	22.475	20.891	0.65758	1.584	0.876	
14	0	2	0	11.482	10.528	0.10710	0.954	0.528	
15	0	2	1	41.912	45.781	0.11845	-3.869	-2.140	*
16	0	2	2	111.290	112.861	0.14733	-1.572	-0.869	
17	0	2	3	102.900	99.569	0.18574	3.331	1.842	
18	0	2	4	43.214	43.599	0.22893	-0.386	-0.213	
19	0	2	5	19.365	17.708	0.27466	1.657	0.916	
20	0	2	6	45.402	44.288	0.32184	1.114	0.616	
21	0	2	7	52.544	51.875	0.36993	0.668	0.370	

23	0	2	9	12.277	11.972	0.46768	0.306	0.169	
24	0	2	10	21.643	19.680	0.51705	1.963	1.086	
25	0	2	11	30.015	30.028	0.56663	-0.013	-0.007	
26	0	2	12	21.354	20.256	0.61637	1.098	0.607	
27	0	4	0	94.402	85.183	0.21420	9.218	5.098	**
28	0	4	1	75.091	79.444	0.22009	-4.353	-2.408	*
29	0	4	2	67.985	69.217	0.23689	-1.231	-0.681	
30	0	4	3	21.734	20.792	0.26251	0.941	0.521	
31	0	4	4	4.502	1.996	0.29465	2.506	1.386	
32	0	4	5	29.436	26.419	0.33143	3.017	1.669	
33	0	4	6	83.969	80.626	0.37148	3.343	1.849	
34	0	4	7	72.813	73.496	0.41383	-0.683	-0.378	
35	0	4	8	25.060	25.056	0.45786	0.004	0.002	
36	0	4	9	11.825	11.920	0.50312	-0.095	-0.053	
37	0	4	11	26.724	27.401	0.59622	-0.677	-0.374	
38	0	4	12	32.655	31.287	0.64368	1.367	0.756	
39	0	4	13	12.060	11.929	0.69159	0.131	0.073	
40	0	6	0	217.173	203.948	0.32130	13.225	5.785	**
41	0	6	1	59.668	53.919	0.32526	5.749	3.179	*
42	0	6	2	85.741	74.477	0.33685	11.264	6.230	**
43	0	6	3	34.535	30.220	0.35534	4.315	2.386	*
44	0	6	4	121.252	114.187	0.37970	7.065	3.907	*
45	0	6	5	40.845	40.594	0.40890	0.251	0.139	
46	0	6	6	51.332	49.979	0.44198	1.354	0.749	
47	0	6	7	68.690	67.957	0.47813	0.734	0.406	
48	0	6	8	83.408	84.178	0.51671	-0.770	-0.426	
49	0	6	10	74.205	71.206	0.59925	2.999	1.659	
50	0	6	11	39.923	37.950	0.64252	1.973	1.091	
51	0	6	12	17.105	16.376	0.68679	0.729	0.403	
52	0	8	0	40.086	38.332	0.42840	1.754	0.970	
53	0	8	1	40.032	41.026	0.43138	-0.994	-0.550	
54	0	8	2	50.627	50.050	0.44019	0.578	0.319	
55	0	8	3	28.044	24.776	0.45449	3.268	1.808	
56	0	8	4	6.021	4.486	0.47378	1.535	0.849	
57	0	8	5	15.080	15.807	0.49749	-0.728	-0.402	
58	0	8	6	49.814	48.923	0.52502	0.891	0.493	
59	0	8	7	48.729	48.649	0.55579	0.080	0.044	
60	0	8	8	19.238	18.848	0.58931	0.391	0.216	
61	0	8	9	6.582	6.885	0.62512	-0.303	-0.168	
62	0	8	10	3.218	1.970	0.66287	1.248	0.690	
63	0	8	11	18.352	19.261	0.70223	-0.909	-0.503	
64	0	10	0	11.048	10.130	0.53550	0.918	0.508	
65	0	10	1	21.354	21.032	0.53789	0.322	0.178	

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No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
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66	0	10	2	45.781	47.263	0.54498	-1.481	-0.819	
67	0	10	3	36.126	34.221	0.55659	1.905	1.053	
68	0	10	4	16.779	14.540	0.57245	2.239	1.238	
69	0	10	5	5.189	6.324	0.59223	-1.135	-0.628	
70	0	10	6	30.955	28.633	0.61553	2.322	1.284	
71	0	10	7	29.364	28.430	0.64198	0.934	0.516	
72	0	10	8	14.808	15.906	0.67121	-1.097	-0.607	
73	0	12	0	106.914	108.466	0.64260	-1.552	-0.859	
74	0	12	1	16.273	15.995	0.64459	0.278	0.154	
75	0	12	2	25.910	28.117	0.65052	-2.207	-1.221	
76	0	12	3	31.425	30.519	0.66028	0.906	0.501	
77	0	12	4	54.497	51.646	0.67371	2.850	1.576	
78	0	12	5	20.197	18.831	0.69058	1.365	0.755	
79	1	1	-14	3.237	2.279	0.69918	0.957	0.529	
80	1	1	-13	6.979	4.363	0.64924	2.617	1.447	
81	1	1	-12	26.670	25.029	0.59940	1.641	0.908	

83	1	1	-10	16.309	15.304	0.50019	1.005	0.556	
84	1	1	-9	16.924	17.338	0.45091	-0.415	-0.229	
85	1	1	-8	35.620	36.752	0.40196	-1.132	-0.626	
86	1	1	-7	51.477	54.719	0.35346	-3.242	-1.793	
87	1	1	-6	31.606	30.195	0.30564	1.411	0.780	
88	1	1	-5	21.408	22.922	0.25888	-1.513	-0.837	
89	1	1	-4	56.160	59.615	0.21385	-3.455	-1.911	
90	1	1	-3	110.006	115.756	0.17195	-5.750	-3.180	*
91	1	1	-2	88.941	92.834	0.13608	-3.893	-2.153	*
92	1	1	-1	26.344	27.844	0.11219	-1.499	-0.829	
93	1	1	0	11.988	10.751	0.10851	1.236	0.684	
94	1	1	1	73.229	75.569	0.12679	-2.340	-1.294	
95	1	1	2	110.964	113.970	0.15968	-3.006	-1.663	
96	1	1	3	83.047	86.183	0.20009	-3.136	-1.734	
97	1	1	4	23.885	25.156	0.24432	-1.271	-0.703	
98	1	1	5	26.959	26.763	0.29063	0.196	0.109	
99	1	1	6	47.770	49.204	0.33816	-1.433	-0.793	
100	1	1	7	44.606	46.780	0.38647	-2.174	-1.202	
101	1	1	8	21.480	21.316	0.43530	0.164	0.091	
102	1	1	9	14.338	14.154	0.48449	0.185	0.102	
103	1	1	10	26.109	25.034	0.53393	1.075	0.595	
104	1	1	11	31.859	31.149	0.58358	0.710	0.392	
105	1	1	12	13.199	10.427	0.63337	2.772	1.533	
106	1	1	13	3.779	2.286	0.68328	1.493	0.825	
107	1	3	-13	50.971	46.536	0.66667	4.435	2.453	*
108	1	3	-12	57.932	55.592	0.61824	2.340	1.294	
109	1	3	-11	44.443	44.733	0.57019	-0.289	-0.160	
110	1	3	-10	13.181	11.281	0.52262	1.900	1.051	
111	1	3	-9	98.452	97.747	0.47567	0.705	0.390	
112	1	3	-8	14.375	14.214	0.42955	0.160	0.089	
113	1	3	-7	14.736	13.639	0.38455	1.097	0.607	
114	1	3	-6	29.527	28.549	0.34111	0.977	0.541	
115	1	3	-5	181.481	183.369	0.29993	-1.888	-0.989	
116	1	3	-4	44.299	45.169	0.26206	-0.870	-0.481	
117	1	3	-3	157.234	160.130	0.22915	-2.897	-1.602	
118	1	3	-2	111.054	108.312	0.20362	2.742	1.517	
119	1	3	-1	180.305	177.842	0.18849	2.463	1.298	
120	1	3	0	55.383	51.502	0.18632	3.881	2.146	*
121	1	3	1	57.082	58.754	0.19753	-1.672	-0.925	
122	1	3	2	44.624	47.027	0.22009	-2.403	-1.329	
123	1	3	3	133.312	136.282	0.25095	-2.970	-1.643	
124	1	3	4	19.708	21.247	0.28746	-1.539	-0.851	
125	1	3	5	166.943	166.887	0.32773	0.057	0.031	
126	1	3	6	103.515	109.230	0.37053	-5.715	-3.161	*
127	1	3	7	55.979	58.707	0.41509	-2.727	-1.508	
128	1	3	9	96.409	92.581	0.50761	3.828	2.117	*
129	1	3	11	10.397	10.765	0.60291	-0.368	-0.204	
130	1	3	12	20.432	21.914	0.65123	-1.482	-0.820	

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No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
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131	1	3	13	55.943	50.988	0.69986	4.955	2.740	*
132	1	5	-13	6.346	4.117	0.70024	2.229	1.233	
133	1	5	-12	23.939	22.707	0.65430	1.232	0.681	
134	1	5	-11	27.501	26.925	0.60910	0.576	0.319	
135	1	5	-10	13.416	13.229	0.56482	0.187	0.104	
136	1	5	-9	11.337	11.840	0.52168	-0.504	-0.278	
137	1	5	-8	26.652	28.217	0.47999	-1.565	-0.866	
138	1	5	-7	40.484	44.572	0.44018	-4.088	-2.261	*
139	1	5	-6	27.610	27.741	0.40279	-0.131	-0.073	
140	1	5	-5	21.679	21.764	0.36857	-0.084	-0.047	
141	1	5	-4	43.105	43.974	0.33846	-0.869	-0.481	

143	1	5	-2	62.434	61.777	0.29554	0.657	0.364	
144	1	5	-1	19.455	18.371	0.28533	1.085	0.600	
145	1	5	0	14.881	13.202	0.28390	1.679	0.928	
146	1	5	1	64.206	62.111	0.29138	2.095	1.159	
147	1	5	2	90.713	88.885	0.30712	1.829	1.011	
148	1	5	3	59.415	59.722	0.32994	-0.307	-0.170	
149	1	5	4	12.259	12.361	0.35849	-0.102	-0.057	
150	1	5	5	19.003	18.777	0.39152	0.226	0.125	
151	1	5	6	37.753	41.763	0.42799	-4.009	-2.217	*
152	1	5	7	41.062	43.083	0.46710	-2.021	-1.118	
153	1	5	8	18.732	19.550	0.50824	-0.818	-0.452	
154	1	5	9	11.735	11.094	0.55095	0.640	0.354	
155	1	5	10	19.256	19.067	0.59490	0.189	0.105	
156	1	5	11	25.386	24.736	0.63983	0.650	0.360	
157	1	5	12	11.283	9.515	0.68555	1.768	0.978	
158	1	7	-11	18.913	19.624	0.66319	-0.711	-0.393	
159	1	7	-10	9.167	9.025	0.62277	0.142	0.078	
160	1	7	-9	14.754	15.447	0.58393	-0.692	-0.383	
161	1	7	-8	27.429	29.577	0.54701	-2.148	-1.188	
162	1	7	-7	37.356	41.999	0.51243	-4.643	-2.568	*
163	1	7	-6	16.436	16.653	0.48069	-0.218	-0.120	
164	1	7	-5	5.949	5.904	0.45240	0.045	0.025	
165	1	7	-4	29.472	29.177	0.42823	0.295	0.163	
166	1	7	-3	74.693	74.395	0.40892	0.299	0.165	
167	1	7	-2	65.689	63.584	0.39518	2.104	1.164	
168	1	7	-1	24.916	22.867	0.38760	2.048	1.133	
169	1	7	0	3.942	1.831	0.38655	2.111	1.167	
170	1	7	1	40.285	38.317	0.39208	1.968	1.089	
171	1	7	2	63.664	62.366	0.40391	1.298	0.718	
172	1	7	3	54.189	53.312	0.42152	0.877	0.485	
173	1	7	4	18.841	18.667	0.44423	0.173	0.096	
174	1	7	5	22.131	22.764	0.47129	-0.632	-0.350	
175	1	7	6	30.919	33.500	0.50200	-2.581	-1.428	
176	1	7	7	26.905	28.863	0.53573	-1.958	-1.083	
177	1	7	8	9.890	10.279	0.57195	-0.389	-0.215	
178	1	7	9	11.301	10.699	0.61022	0.602	0.333	
179	1	7	10	20.631	20.937	0.65018	-0.307	-0.170	
180	1	7	11	26.995	26.636	0.69153	0.359	0.198	
181	1	9	-10	8.155	5.935	0.69253	2.220	1.228	
182	1	9	-9	57.968	59.295	0.65783	-1.326	-0.734	
183	1	9	-8	15.514	17.419	0.62529	-1.906	-1.054	
184	1	9	-7	7.576	9.093	0.59527	-1.517	-0.839	
185	1	9	-6	12.060	12.475	0.56818	-0.415	-0.230	
186	1	9	-5	110.205	114.637	0.54445	-4.433	-2.452	*
187	1	9	-4	16.056	16.055	0.52454	0.001	0.001	
188	1	9	-3	68.274	66.843	0.50890	1.431	0.791	
189	1	9	-2	67.967	64.441	0.49793	3.526	1.950	
190	1	9	-1	102.954	97.890	0.49193	5.064	2.800	*
191	1	9	0	31.335	29.691	0.49111	1.644	0.909	
192	1	9	1	53.122	51.019	0.49547	2.103	1.163	
193	1	9	2	35.945	34.226	0.50489	1.720	0.951	
194	1	9	3	71.475	70.172	0.51908	1.302	0.720	
195	1	9	4	7.468	7.195	0.53768	0.272	0.151	

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
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196	1	9	5	88.254	90.787	0.56025	-2.533	-1.401	
197	1	9	6	56.214	60.812	0.58631	-4.598	-2.543	*
198	1	9	7	39.670	40.815	0.61544	-1.145	-0.633	
199	1	9	8	3.797	3.508	0.64722	0.289	0.160	
200	1	9	9	61.476	59.664	0.68128	1.812	1.002	
201	1	11	-7	22.348	25.994	0.68487	-3.646	-2.016	*

203	1	11	-4	16.237	16.090	0.62438	0.147	0.081	
204	1	11	-3	43.142	44.536	0.61130	-1.394	-0.771	
205	1	11	-2	37.374	36.854	0.60219	0.520	0.287	
206	1	11	-1	13.706	13.975	0.59725	-0.270	-0.149	
207	1	11	0	2.911	2.006	0.59657	0.905	0.501	
208	1	11	1	21.697	21.968	0.60016	-0.271	-0.150	
209	1	11	2	36.651	36.992	0.60796	-0.342	-0.189	
210	1	11	3	31.534	31.002	0.61980	0.531	0.294	
211	1	11	4	11.048	11.333	0.63546	-0.286	-0.158	
212	1	11	5	12.801	14.618	0.65466	-1.816	-1.005	
213	1	11	6	18.877	19.580	0.67710	-0.704	-0.389	
214	1	11	7	17.304	18.582	0.70248	-1.278	-0.707	
215	1	13	-1	7.522	7.738	0.70310	-0.216	-0.120	
216	2	0	-14	54.949	51.405	0.69876	3.544	1.960	
217	2	0	-13	21.245	20.924	0.65014	0.322	0.178	
218	2	0	-12	9.691	10.279	0.60183	-0.588	-0.325	
219	2	0	-10	84.584	90.070	0.50655	-5.486	-3.034	*
220	2	0	-8	58.348	58.607	0.41408	-0.259	-0.143	
221	2	0	-7	105.268	107.250	0.36956	-1.981	-1.096	
222	2	0	-6	162.296	166.854	0.32680	-4.557	-2.520	*
223	2	0	-5	18.587	19.665	0.28661	-1.077	-0.596	
224	2	0	-4	128.358	132.932	0.25021	-4.574	-2.530	*
225	2	0	-3	43.250	46.836	0.21951	-3.586	-1.983	
226	2	0	-2	56.576	60.025	0.19718	-3.449	-1.908	
227	2	0	-1	54.840	51.286	0.18626	3.554	1.966	
228	2	0	0	175.586	177.144	0.18874	-1.558	-0.843	
229	2	0	1	112.248	109.314	0.20414	2.933	1.622	
230	2	0	2	163.544	160.820	0.22986	2.725	1.507	
231	2	0	3	43.666	44.243	0.26291	-0.577	-0.319	
232	2	0	4	178.371	182.343	0.30086	-3.973	-2.116	*
233	2	0	5	29.942	29.610	0.34211	0.333	0.184	
234	2	0	6	16.852	15.088	0.38558	1.764	0.976	
235	2	0	7	13.253	12.679	0.43061	0.575	0.318	
236	2	0	8	93.787	98.795	0.47675	-5.008	-2.770	*
237	2	0	9	11.608	9.459	0.52372	2.149	1.188	
238	2	0	10	44.624	43.648	0.57130	0.977	0.540	
239	2	0	11	58.456	55.267	0.61936	3.189	1.764	
240	2	0	12	53.538	48.784	0.66779	4.754	2.629	*
241	2	2	-13	27.104	24.620	0.65890	2.484	1.374	
242	2	2	-12	33.577	32.776	0.61129	0.801	0.443	
243	2	2	-11	8.444	7.863	0.56419	0.581	0.321	
244	2	2	-10	8.498	10.567	0.51775	-2.069	-1.144	
245	2	2	-9	6.383	5.992	0.47217	0.390	0.216	
246	2	2	-8	60.373	61.958	0.42771	-1.585	-0.877	
247	2	2	-7	77.821	81.469	0.38476	-3.648	-2.018	*
248	2	2	-6	46.921	47.668	0.34390	-0.748	-0.414	
249	2	2	-5	5.461	1.858	0.30596	3.602	1.992	
250	2	2	-4	9.239	9.821	0.27217	-0.582	-0.322	
251	2	2	-3	50.446	53.384	0.24424	-2.937	-1.625	
252	2	2	-2	78.653	80.518	0.22439	-1.865	-1.031	
253	2	2	-1	82.107	78.885	0.21486	3.222	1.782	
254	2	2	0	88.688	86.255	0.21701	2.433	1.346	
255	2	2	1	68.256	70.467	0.23053	-2.211	-1.223	
256	2	2	2	39.634	41.178	0.25359	-1.544	-0.854	
257	2	2	3	3.490	2.110	0.28388	1.380	0.763	
258	2	2	4	13.199	13.252	0.31936	-0.053	-0.029	
259	2	2	5	64.749	65.289	0.35848	-0.540	-0.299	
260	2	2	6	80.045	83.210	0.40018	-3.165	-1.750	
No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
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261	2	2	7	41.424	41.484	0.44373	-0.060	-0.033	

263	2	2	9	6.744	8.482	0.53456	-1.737	-0.961	
264	2	2	10	21.987	20.070	0.58125	1.916	1.060	
265	2	2	11	34.481	33.381	0.62855	1.100	0.608	
266	2	2	12	21.119	18.443	0.67632	2.675	1.480	
267	2	4	-13	11.915	10.015	0.68451	1.900	1.051	
268	2	4	-12	29.111	28.596	0.63881	0.515	0.285	
269	2	4	-11	20.757	20.108	0.59390	0.649	0.359	
270	2	4	-10	12.114	10.745	0.54998	1.369	0.757	
271	2	4	-9	11.988	12.769	0.50730	-0.782	-0.432	
272	2	4	-8	37.374	38.707	0.46620	-1.333	-0.737	
273	2	4	-7	38.314	40.840	0.42715	-2.526	-1.397	
274	2	4	-6	24.301	24.346	0.39074	-0.045	-0.025	
275	2	4	-5	21.245	21.494	0.35781	-0.248	-0.137	
276	2	4	-4	60.138	61.247	0.32937	-1.109	-0.614	
277	2	4	-3	80.298	80.053	0.30670	0.245	0.136	
278	2	4	-2	49.090	50.533	0.29114	-1.442	-0.798	
279	2	4	-1	5.768	4.313	0.28386	1.455	0.805	
280	2	4	0	30.919	29.946	0.28549	0.973	0.538	
281	2	4	1	74.874	73.973	0.29589	0.901	0.499	
282	2	4	2	89.104	87.921	0.31420	1.183	0.654	
283	2	4	3	39.200	38.879	0.33912	0.320	0.177	
284	2	4	4	8.335	8.791	0.36933	-0.456	-0.252	
285	2	4	5	26.254	26.115	0.40363	0.139	0.077	
286	2	4	6	47.626	48.621	0.44108	-0.996	-0.551	
287	2	4	7	33.721	34.341	0.48094	-0.620	-0.343	
288	2	4	8	14.049	15.567	0.52266	-1.518	-0.839	
289	2	4	9	11.102	10.323	0.56583	0.779	0.431	
290	2	4	10	23.994	23.366	0.61014	0.627	0.347	
291	2	4	11	21.860	21.089	0.65535	0.771	0.426	
292	2	4	12	5.424	4.576	0.70130	0.848	0.469	
293	2	6	-12	9.637	11.220	0.68223	-1.583	-0.875	
294	2	6	-11	13.217	13.435	0.64037	-0.217	-0.120	
295	2	6	-10	49.235	55.534	0.59986	-6.299	-3.484	*
296	2	6	-9	6.455	6.582	0.56099	-0.127	-0.070	
297	2	6	-8	56.431	57.542	0.52412	-1.111	-0.614	
298	2	6	-7	52.435	53.301	0.48970	-0.865	-0.479	
299	2	6	-6	131.034	135.043	0.45830	-4.009	-2.217	*
300	2	6	-4	61.729	59.785	0.40723	1.944	1.075	
301	2	6	-3	69.052	67.899	0.38913	1.153	0.638	
302	2	6	-2	68.871	66.462	0.37698	2.409	1.332	
303	2	6	-1	73.319	72.472	0.37139	0.847	0.468	
304	2	6	0	160.217	157.849	0.37264	2.368	1.310	
305	2	6	1	87.043	82.837	0.38067	4.205	2.326	*
306	2	6	2	71.384	67.261	0.39506	4.123	2.280	*
307	2	6	3	53.303	52.717	0.41516	0.586	0.324	
308	2	6	4	136.838	138.708	0.44018	-1.870	-1.034	
309	2	6	6	34.246	34.293	0.50190	-0.048	-0.026	
310	2	6	7	9.999	10.107	0.53727	-0.108	-0.060	
311	2	6	8	59.812	63.920	0.57492	-4.107	-2.272	*
312	2	6	9	7.341	9.119	0.61442	-1.778	-0.983	
313	2	6	10	31.118	31.931	0.65545	-0.814	-0.450	
314	2	6	11	40.520	37.642	0.69774	2.878	1.592	
315	2	8	-11	13.434	13.609	0.70026	-0.174	-0.096	
316	2	8	-10	6.021	6.393	0.66342	-0.372	-0.206	
317	2	8	-9	7.359	8.621	0.62849	-1.262	-0.698	
318	2	8	-8	27.646	30.126	0.59581	-2.480	-1.372	
319	2	8	-7	29.237	30.336	0.56578	-1.098	-0.607	
320	2	8	-6	17.665	17.872	0.53882	-0.207	-0.114	
321	2	8	-5	10.921	11.749	0.51543	-0.828	-0.458	
322	2	8	-4	37.627	36.638	0.49612	0.989	0.547	
323	2	8	-3	52.670	52.533	0.48137	0.137	0.076	
324	2	8	-2	35.548	35.179	0.47160	0.368	0.204	

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
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326	2	8	0	22.276	21.111	0.46814	1.165	0.644	
327	2	8	1	47.101	46.651	0.47455	0.451	0.249	
328	2	8	2	55.708	55.268	0.48617	0.440	0.243	
329	2	8	3	23.270	22.687	0.50264	0.584	0.323	
330	2	8	4	7.052	7.526	0.52350	-0.474	-0.262	
331	2	8	5	20.269	20.467	0.54824	-0.198	-0.110	
332	2	8	6	36.072	35.884	0.57637	0.188	0.104	
333	2	8	7	23.325	24.922	0.60741	-1.597	-0.883	
334	2	8	8	8.697	9.287	0.64095	-0.590	-0.326	
335	2	8	9	7.468	6.502	0.67662	0.965	0.534	
336	2	10	-8	28.098	30.301	0.67693	-2.203	-1.218	
337	2	10	-7	34.246	35.826	0.65064	-1.581	-0.874	
338	2	10	-6	18.443	20.462	0.62735	-2.019	-1.117	
339	2	10	-5	3.182	1.513	0.60738	1.669	0.923	
340	2	10	-4	17.503	16.327	0.59107	1.176	0.650	
341	2	10	-3	29.942	30.663	0.57875	-0.720	-0.398	
342	2	10	-2	35.150	34.012	0.57065	1.138	0.629	
343	2	10	-1	17.195	17.539	0.56697	-0.343	-0.190	
344	2	10	0	28.858	28.075	0.56779	0.783	0.433	
345	2	10	1	33.956	34.196	0.57309	-0.240	-0.133	
346	2	10	2	30.810	31.134	0.58275	-0.324	-0.179	
347	2	10	3	5.967	5.288	0.59656	0.678	0.375	
348	2	10	4	5.027	5.017	0.61423	0.010	0.005	
349	2	10	5	24.572	25.395	0.63545	-0.823	-0.455	
350	2	10	6	41.026	40.635	0.65988	0.392	0.217	
351	2	10	7	18.334	20.271	0.68716	-1.936	-1.071	
352	2	12	-4	41.334	42.877	0.68960	-1.543	-0.854	
353	2	12	-3	29.906	29.791	0.67906	0.116	0.064	
354	2	12	-2	30.087	31.470	0.67218	-1.383	-0.765	
355	2	12	-1	19.419	18.288	0.66905	1.132	0.626	
356	2	12	0	67.370	68.291	0.66975	-0.921	-0.509	
357	2	12	1	39.742	39.825	0.67425	-0.083	-0.046	
358	2	12	2	40.773	42.277	0.68248	-1.504	-0.832	
359	2	12	3	16.165	16.666	0.69431	-0.501	-0.277	
360	3	1	-13	18.696	16.538	0.66887	2.158	1.193	
361	3	1	-12	20.775	22.507	0.62343	-1.732	-0.958	
362	3	1	-11	16.996	15.959	0.57883	1.037	0.574	
363	3	1	-10	9.691	9.830	0.53530	-0.139	-0.077	
364	3	1	-9	26.597	27.530	0.49312	-0.933	-0.516	
365	3	1	-8	45.980	45.177	0.45266	0.803	0.444	
366	3	1	-7	34.336	34.421	0.41444	-0.085	-0.047	
367	3	1	-6	9.294	8.414	0.37911	0.880	0.487	
368	3	1	-5	25.404	27.346	0.34759	-1.942	-1.074	
369	3	1	-4	70.589	69.799	0.32097	0.790	0.437	
370	3	1	-3	89.954	89.878	0.30058	0.076	0.042	
371	3	1	-2	37.916	37.565	0.28773	0.351	0.194	
372	3	1	-1	10.089	8.843	0.28345	1.246	0.689	
373	3	1	0	31.588	31.949	0.28813	-0.361	-0.200	
374	3	1	1	74.368	74.817	0.30135	-0.449	-0.249	
375	3	1	2	73.283	72.268	0.32206	1.015	0.561	
376	3	1	3	31.859	32.558	0.34893	-0.699	-0.386	
377	3	1	4	18.497	17.859	0.38065	0.638	0.353	
378	3	1	5	38.585	39.703	0.41612	-1.117	-0.618	
379	3	1	6	40.520	39.936	0.45446	0.584	0.323	
380	3	1	7	21.408	21.813	0.49501	-0.405	-0.224	
381	3	1	8	9.113	9.372	0.53726	-0.259	-0.143	
382	3	1	9	18.208	17.823	0.58084	0.384	0.213	
383	3	1	10	27.104	29.690	0.62548	-2.586	-1.430	
384	3	1	11	18.678	16.779	0.67096	1.898	1.050	

386	3	3	-12	36.217	36.981	0.64156	-0.765	-0.423
387	3	3	-11	73.301	71.412	0.59832	1.889	1.045
388	3	3	-9	81.040	81.760	0.51586	-0.720	-0.398
389	3	3	-8	67.732	68.236	0.47733	-0.504	-0.279
390	3	3	-7	49.814	49.442	0.44125	0.372	0.206

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No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
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391	3	3	-6	38.549	40.430	0.40825	-1.881	-1.040	
392	3	3	-5	111.778	111.855	0.37915	-0.078	-0.043	
393	3	3	-4	30.955	31.928	0.35491	-0.973	-0.538	
394	3	3	-3	75.145	74.255	0.33658	0.891	0.493	
395	3	3	-2	56.124	53.245	0.32516	2.879	1.592	
396	3	3	-1	206.342	202.604	0.32138	3.738	1.721	
397	3	3	0	57.263	54.852	0.32552	2.411	1.333	
398	3	3	1	75.326	73.203	0.33727	2.123	1.174	
399	3	3	2	28.568	29.710	0.35590	-1.142	-0.631	
400	3	3	3	115.159	114.269	0.38038	0.890	0.492	
401	3	3	4	37.699	39.174	0.40968	-1.475	-0.816	
402	3	3	5	49.741	49.608	0.44283	0.134	0.074	
403	3	3	6	67.135	68.054	0.47904	-0.919	-0.508	
404	3	3	7	83.933	84.513	0.51766	-0.580	-0.321	
405	3	3	9	70.263	71.445	0.60027	-1.182	-0.654	
406	3	3	10	36.506	37.712	0.64356	-1.206	-0.667	
407	3	3	11	19.654	16.935	0.68785	2.720	1.504	
408	3	5	-12	16.092	17.355	0.67638	-1.262	-0.698	
409	3	5	-11	13.525	13.513	0.63551	0.012	0.007	
410	3	5	-10	9.728	9.565	0.59613	0.163	0.090	
411	3	5	-9	24.536	25.719	0.55856	-1.183	-0.654	
412	3	5	-8	38.115	38.859	0.52319	-0.744	-0.412	
413	3	5	-7	26.489	26.490	0.49049	-0.001	-0.001	
414	3	5	-6	5.334	4.213	0.46103	1.121	0.620	
415	3	5	-5	19.618	19.834	0.43548	-0.216	-0.119	
416	3	5	-4	57.824	58.033	0.41454	-0.210	-0.116	
417	3	5	-3	75.272	75.708	0.39896	-0.436	-0.241	
418	3	5	-2	31.805	31.585	0.38937	0.220	0.122	
419	3	5	-1	8.064	5.734	0.38622	2.331	1.289	
420	3	5	0	21.191	21.239	0.38967	-0.048	-0.026	
421	3	5	1	57.986	58.297	0.39954	-0.310	-0.172	
422	3	5	2	59.632	59.075	0.41539	0.557	0.308	
423	3	5	3	28.405	28.782	0.43655	-0.377	-0.208	
424	3	5	4	16.924	17.050	0.46230	-0.126	-0.069	
425	3	5	5	32.365	31.823	0.49191	0.542	0.300	
426	3	5	6	30.503	31.265	0.52475	-0.762	-0.422	
427	3	5	7	15.911	16.806	0.56023	-0.894	-0.495	
428	3	5	8	7.829	8.076	0.59789	-0.247	-0.137	
429	3	5	9	16.996	17.190	0.63734	-0.194	-0.107	
430	3	5	10	23.506	26.583	0.67827	-3.078	-1.702	
431	3	7	-11	12.096	12.470	0.68753	-0.373	-0.206	
432	3	7	-9	15.279	16.271	0.61710	-0.993	-0.549	
433	3	7	-8	30.196	30.719	0.58528	-0.523	-0.289	
434	3	7	-7	29.725	29.562	0.55624	0.163	0.090	
435	3	7	-6	9.438	9.630	0.53045	-0.192	-0.106	
436	3	7	-5	20.341	20.191	0.50839	0.150	0.083	
437	3	7	-4	41.098	41.336	0.49058	-0.237	-0.131	
438	3	7	-3	52.996	53.497	0.47749	-0.501	-0.277	
439	3	7	-2	20.992	20.810	0.46950	0.182	0.101	
440	3	7	-1	10.216	9.519	0.46690	0.696	0.385	
441	3	7	0	28.369	28.254	0.46975	0.115	0.064	
442	3	7	1	55.708	55.863	0.47797	-0.155	-0.086	
443	3	7	2	44.263	43.847	0.49129	0.416	0.230	
444	3	7	3	15.062	14.954	0.50931	0.108	0.060	

446	3	7	5	31.009	31.084	0.55750	-0.074	-0.041
447	3	7	6	33.649	33.019	0.58667	0.630	0.349
448	3	7	7	17.955	19.151	0.61861	-1.196	-0.662
449	3	7	8	4.737	5.246	0.65291	-0.509	-0.281
450	3	7	9	9.601	10.231	0.68922	-0.630	-0.348
451	3	9	-9	54.171	57.593	0.68744	-3.422	-1.892
452	3	9	-8	41.424	43.364	0.65903	-1.940	-1.073
453	3	9	-7	26.941	28.476	0.63338	-1.535	-0.849
454	3	9	-6	15.622	16.099	0.61085	-0.477	-0.264
455	3	9	-5	68.166	68.130	0.59180	0.036	0.020

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No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
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456	3	9	-4	18.497	19.438	0.57657	-0.941	-0.520	
457	3	9	-3	46.812	46.826	0.56547	-0.014	-0.008	
458	3	9	-2	23.379	22.849	0.55875	0.530	0.293	
459	3	9	-1	116.533	115.515	0.55656	1.018	0.563	
460	3	9	0	35.457	34.464	0.55896	0.993	0.549	
461	3	9	1	35.023	35.460	0.56588	-0.437	-0.242	
462	3	9	2	18.786	19.349	0.57718	-0.563	-0.311	
463	3	9	3	78.888	78.313	0.59259	0.576	0.318	
464	3	9	4	25.476	25.143	0.61181	0.333	0.184	
465	3	9	5	29.508	30.558	0.63448	-1.049	-0.580	
466	3	9	6	47.499	49.685	0.66026	-2.186	-1.209	
467	3	9	7	47.915	51.542	0.68880	-3.627	-2.006	*
468	3	11	-6	6.455	6.986	0.69846	-0.531	-0.294	
469	3	11	-5	12.349	12.659	0.68186	-0.309	-0.171	
470	3	11	-4	24.500	25.072	0.66869	-0.572	-0.317	
471	3	11	-3	30.684	32.369	0.65914	-1.685	-0.932	
472	3	11	-2	11.861	11.572	0.65338	0.289	0.160	
473	3	11	-1	5.949	7.029	0.65151	-1.081	-0.598	
474	3	11	0	17.286	17.115	0.65356	0.171	0.095	
475	3	11	1	33.812	34.844	0.65949	-1.032	-0.571	
476	3	11	2	26.706	26.803	0.66921	-0.097	-0.054	
477	3	11	3	8.317	8.482	0.68254	-0.165	-0.091	
478	3	11	4	3.490	4.073	0.69929	-0.583	-0.322	
479	4	0	-13	39.037	37.430	0.69583	1.608	0.889	
480	4	0	-12	31.967	31.976	0.65360	-0.009	-0.005	
481	4	0	-11	6.907	8.351	0.61264	-1.444	-0.799	
482	4	0	-10	63.176	60.768	0.57321	2.408	1.332	
483	4	0	-9	11.482	11.569	0.53567	-0.087	-0.048	
484	4	0	-8	35.096	33.032	0.50042	2.064	1.141	
485	4	0	-7	2.622	2.554	0.46799	0.068	0.038	
486	4	0	-6	136.495	136.051	0.43901	0.443	0.245	
487	4	0	-5	55.256	55.153	0.41421	0.103	0.057	
488	4	0	-4	69.269	65.921	0.39436	3.348	1.852	
489	4	0	-3	82.486	79.723	0.38024	2.764	1.528	
490	4	0	-2	158.481	156.584	0.37252	1.897	1.049	
491	4	0	-1	67.678	69.013	0.37158	-1.335	-0.739	
492	4	0	0	64.893	62.998	0.37748	1.895	1.048	
493	4	0	1	68.365	67.857	0.38991	0.508	0.281	
494	4	0	2	66.322	63.286	0.40827	3.036	1.679	
495	4	0	4	130.745	133.060	0.45972	-2.315	-1.280	
496	4	0	5	53.701	54.693	0.49128	-0.992	-0.548	
497	4	0	6	59.071	58.506	0.52581	0.565	0.313	
498	4	0	7	5.858	5.703	0.56278	0.155	0.086	
499	4	0	8	59.107	56.324	0.60173	2.783	1.539	
500	4	0	9	15.568	14.711	0.64230	0.857	0.474	
501	4	0	10	9.927	12.077	0.68421	-2.151	-1.190	
502	4	2	-12	23.885	23.113	0.66232	0.772	0.427	
503	4	2	-11	12.548	10.832	0.62193	1.716	0.949	
504	4	2	-10	8.552	8.128	0.58313	0.424	0.234	

506	4	2	-8	36.723	36.099	0.51175	0.624	0.345
507	4	2	-7	21.896	21.410	0.48009	0.486	0.269
508	4	2	-6	19.672	19.506	0.45189	0.166	0.092
509	4	2	-5	34.517	35.866	0.42783	-1.349	-0.746
510	4	2	-4	62.669	64.055	0.40864	-1.385	-0.766
511	4	2	-3	45.944	47.081	0.39504	-1.137	-0.629
512	4	2	-2	9.221	8.134	0.38761	1.087	0.601
513	4	2	-1	12.747	10.665	0.38671	2.082	1.151
514	4	2	0	51.586	51.664	0.39238	-0.078	-0.043
515	4	2	1	71.258	72.975	0.40435	-1.717	-0.950
516	4	2	2	46.559	47.694	0.42208	-1.135	-0.628
517	4	2	3	5.298	5.875	0.44489	-0.578	-0.319
518	4	2	4	11.952	11.979	0.47203	-0.028	-0.015
519	4	2	5	35.132	35.533	0.50282	-0.401	-0.222
520	4	2	6	35.963	35.857	0.53661	0.106	0.059

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
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521	4	2	7	19.311	19.867	0.57288	-0.557	-0.308	
522	4	2	8	11.337	8.779	0.61119	2.558	1.415	
523	4	2	9	16.128	15.475	0.65117	0.654	0.362	
524	4	2	10	18.533	19.132	0.69254	-0.599	-0.331	
525	4	4	-12	13.832	14.634	0.68781	-0.802	-0.444	
526	4	4	-11	5.135	5.117	0.64901	0.018	0.010	
527	4	4	-10	3.345	1.061	0.61193	2.284	1.263	
528	4	4	-9	27.158	26.860	0.57691	0.298	0.165	
529	4	4	-8	54.732	54.506	0.54434	0.226	0.125	
530	4	4	-7	33.089	33.972	0.51468	-0.884	-0.489	
531	4	4	-6	8.806	9.537	0.48848	-0.731	-0.404	
532	4	4	-5	6.925	5.700	0.46631	1.225	0.678	
533	4	4	-4	37.898	36.940	0.44878	0.958	0.530	
534	4	4	-3	47.318	47.816	0.43643	-0.498	-0.275	
535	4	4	-2	36.831	36.891	0.42971	-0.059	-0.033	
536	4	4	-1	35.783	34.723	0.42890	1.059	0.586	
537	4	4	0	47.608	47.563	0.43402	0.045	0.025	
538	4	4	1	41.496	40.753	0.44487	0.743	0.411	
539	4	4	2	18.967	18.389	0.46105	0.579	0.320	
540	4	4	3	2.549	1.485	0.48202	1.064	0.589	
541	4	4	4	27.863	28.767	0.50718	-0.904	-0.500	
542	4	4	5	53.791	53.257	0.53594	0.535	0.296	
543	4	4	6	38.531	38.750	0.56777	-0.219	-0.121	
544	4	4	7	6.780	7.163	0.60216	-0.382	-0.211	
545	4	4	8	7.359	6.659	0.63872	0.700	0.387	
546	4	4	9	8.173	8.365	0.67708	-0.192	-0.106	
547	4	6	-11	6.925	4.716	0.69178	2.209	1.222	
548	4	6	-10	56.974	56.861	0.65712	0.113	0.063	
549	4	6	-9	17.973	17.504	0.62464	0.469	0.259	
550	4	6	-8	9.475	9.573	0.59469	-0.098	-0.054	
551	4	6	-7	12.024	12.127	0.56767	-0.103	-0.057	
552	4	6	-6	111.073	112.021	0.54403	-0.949	-0.525	
553	4	6	-5	17.430	17.991	0.52422	-0.561	-0.310	
554	4	6	-4	65.418	65.650	0.50868	-0.232	-0.128	
555	4	6	-3	64.550	62.879	0.49782	1.671	0.924	
556	4	6	-2	97.530	96.654	0.49194	0.876	0.485	
557	4	6	-1	28.677	27.548	0.49123	1.128	0.624	
558	4	6	0	49.687	49.263	0.49571	0.424	0.235	
559	4	6	1	34.752	34.091	0.50524	0.661	0.365	
560	4	6	2	71.710	70.767	0.51954	0.943	0.521	
561	4	6	3	6.310	6.361	0.53823	-0.051	-0.028	
562	4	6	4	88.580	89.044	0.56088	-0.465	-0.257	
563	4	6	5	60.952	60.894	0.58702	0.058	0.032	
564	4	6	6	41.117	41.393	0.61621	-0.276	-0.153	

566	4	6	8	59.143	59.030	0.68214	0.114	0.063
567	4	8	-9	18.352	19.343	0.68591	-0.991	-0.548
568	4	8	-8	37.392	37.786	0.65875	-0.394	-0.218
569	4	8	-7	22.258	23.032	0.63447	-0.775	-0.428
570	4	8	-6	7.594	8.426	0.61340	-0.832	-0.460
571	4	8	-5	6.274	6.228	0.59590	0.046	0.026
572	4	8	-4	28.659	28.712	0.58228	-0.054	-0.030
573	4	8	-3	31.859	32.346	0.57281	-0.487	-0.269
574	4	8	-2	22.909	22.606	0.56771	0.302	0.167
575	4	8	-1	22.149	21.933	0.56710	0.217	0.120
576	4	8	0	33.830	33.349	0.57098	0.480	0.266
577	4	8	1	31.805	32.060	0.57928	-0.255	-0.141
578	4	8	2	15.622	15.072	0.59179	0.550	0.304
579	4	8	4	18.497	19.014	0.62839	-0.517	-0.286
580	4	8	5	36.289	36.555	0.65183	-0.266	-0.147
581	4	8	6	28.351	29.166	0.67824	-0.814	-0.450
582	4	10	-6	7.486	8.153	0.69246	-0.667	-0.369
583	4	10	-5	14.049	13.694	0.67700	0.355	0.196
584	4	10	-4	31.063	32.502	0.66504	-1.438	-0.796
585	4	10	-3	24.066	25.281	0.65677	-1.215	-0.672

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
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586	4	10	-2	9.185	8.931	0.65233	0.255	0.141	
587	4	10	-1	4.339	4.847	0.65180	-0.507	-0.281	
588	4	10	0	26.832	26.602	0.65518	0.231	0.128	
589	4	10	1	31.371	32.776	0.66242	-1.406	-0.777	
590	4	10	2	23.451	23.292	0.67339	0.160	0.088	
591	5	1	-12	11.463	11.053	0.69949	0.411	0.227	
592	5	1	-11	7.504	6.805	0.66269	0.699	0.386	
593	5	1	-10	9.493	10.045	0.62781	-0.553	-0.306	
594	5	1	-9	31.588	31.444	0.59519	0.144	0.080	
595	5	1	-8	30.991	29.642	0.56523	1.349	0.746	
596	5	1	-7	13.687	12.628	0.53835	1.060	0.586	
597	5	1	-6	8.137	8.355	0.51506	-0.218	-0.121	
598	5	1	-5	34.228	33.229	0.49585	0.998	0.552	
599	5	1	-4	53.900	54.363	0.48121	-0.463	-0.256	
600	5	1	-3	38.567	38.312	0.47156	0.255	0.141	
601	5	1	-2	8.444	7.686	0.46723	0.758	0.419	
602	5	1	-1	18.804	18.452	0.46835	0.352	0.195	
603	5	1	0	40.845	41.147	0.47488	-0.302	-0.167	
604	5	1	1	50.049	49.902	0.48662	0.147	0.081	
605	5	1	2	26.308	25.169	0.50318	1.139	0.630	
606	5	1	3	8.390	8.713	0.52413	-0.323	-0.179	
607	5	1	4	25.350	24.656	0.54895	0.694	0.384	
608	5	1	5	32.980	32.960	0.57714	0.020	0.011	
609	5	1	6	20.142	20.881	0.60825	-0.738	-0.408	
610	5	1	7	6.328	6.767	0.64183	-0.439	-0.243	
611	5	1	8	7.992	7.410	0.67754	0.581	0.322	
612	5	3	-11	60.355	56.944	0.67978	3.411	1.886	
613	5	3	-9	38.838	38.597	0.61416	0.241	0.133	
614	5	3	-8	58.131	59.225	0.58517	-1.094	-0.605	
615	5	3	-7	88.037	88.905	0.55925	-0.867	-0.480	
616	5	3	-6	5.406	5.318	0.53687	0.088	0.049	
617	5	3	-5	67.443	66.100	0.51846	1.343	0.743	
618	5	3	-4	34.517	34.055	0.50448	0.462	0.255	
619	5	3	-3	51.875	50.785	0.49529	1.090	0.603	
620	5	3	-2	28.008	27.421	0.49116	0.587	0.325	
621	5	3	-1	97.964	94.697	0.49223	3.267	1.807	
622	5	3	0	67.099	64.963	0.49845	2.136	1.182	
623	5	3	1	68.799	67.332	0.50964	1.467	0.811	
624	5	3	2	15.098	15.634	0.52549	-0.536	-0.296	

626	5	3	4	14.555	14.534	0.56946	0.021	0.012
627	5	3	5	9.330	10.103	0.59669	-0.773	-0.427
628	5	3	6	16.852	16.468	0.62682	0.383	0.212
629	5	3	7	59.849	59.577	0.65946	0.272	0.150
630	5	3	8	5.533	4.010	0.69426	1.523	0.842
631	5	5	-10	6.328	6.942	0.68042	-0.613	-0.339
632	5	5	-9	26.652	26.813	0.65045	-0.162	-0.090
633	5	5	-8	26.923	26.165	0.62314	0.758	0.419
634	5	5	-7	13.109	13.043	0.59887	0.066	0.036
635	5	5	-6	6.997	8.006	0.57802	-1.008	-0.558
636	5	5	-5	27.194	26.388	0.56097	0.806	0.446
637	5	5	-4	41.731	43.165	0.54807	-1.433	-0.793
638	5	5	-3	30.159	30.398	0.53962	-0.239	-0.132
639	5	5	-2	8.390	8.077	0.53584	0.313	0.173
640	5	5	-1	19.275	18.382	0.53682	0.893	0.494
641	5	5	0	35.638	36.145	0.54253	-0.507	-0.280
642	5	5	1	40.393	41.217	0.55283	-0.824	-0.456
643	5	5	2	18.244	18.322	0.56747	-0.078	-0.043
644	5	5	3	5.605	5.914	0.58612	-0.308	-0.171
645	5	5	4	21.553	21.349	0.60841	0.203	0.112
646	5	5	5	30.521	30.014	0.63397	0.507	0.280
647	5	5	6	18.515	19.703	0.66241	-1.188	-0.657
648	5	5	7	4.936	5.459	0.69338	-0.523	-0.289
649	5	7	-9	23.958	24.574	0.70136	-0.617	-0.341
650	5	7	-8	19.708	19.490	0.67611	0.218	0.121

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No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
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651	5	7	-7	5.605	5.986	0.65381	-0.381	-0.211	
652	5	7	-5	27.881	27.017	0.61928	0.864	0.478	
653	5	7	-4	43.214	42.596	0.60762	0.618	0.342	
654	5	7	-3	31.190	30.590	0.60002	0.600	0.332	
655	5	7	-2	2.947	2.188	0.59661	0.759	0.420	
656	5	7	-1	8.896	9.051	0.59749	-0.156	-0.086	
657	5	7	0	26.055	26.709	0.60263	-0.654	-0.362	
658	5	7	1	37.681	38.164	0.61192	-0.483	-0.267	
659	5	7	2	22.041	21.409	0.62517	0.632	0.349	
660	5	7	3	7.920	8.978	0.64215	-1.059	-0.586	
661	5	7	4	16.327	16.568	0.66256	-0.241	-0.133	
662	5	7	5	21.697	21.873	0.68611	-0.176	-0.097	
663	5	9	-6	3.924	3.206	0.70335	0.718	0.397	
664	5	9	-5	39.327	40.903	0.68940	-1.577	-0.872	
665	5	9	-4	29.617	29.799	0.67895	-0.182	-0.101	
666	5	9	-3	29.563	31.241	0.67215	-1.678	-0.928	
667	5	9	-2	18.461	17.515	0.66911	0.946	0.523	
668	5	9	-1	64.839	66.918	0.66990	-2.079	-1.150	
669	5	9	0	38.838	39.945	0.67448	-1.107	-0.612	
670	5	9	1	38.115	41.706	0.68279	-3.590	-1.986	
671	5	9	2	15.134	17.088	0.69470	-1.954	-1.081	
672	6	0	-10	47.101	47.627	0.68687	-0.526	-0.291	
673	6	0	-9	49.018	47.846	0.65852	1.172	0.648	
674	6	0	-8	30.883	30.757	0.63295	0.126	0.069	
675	6	0	-7	24.410	24.160	0.61050	0.249	0.138	
676	6	0	-6	74.097	72.689	0.59154	1.408	0.779	
677	6	0	-5	21.715	22.238	0.57640	-0.522	-0.289	
678	6	0	-4	35.837	35.923	0.56540	-0.086	-0.048	
679	6	0	-3	34.155	32.706	0.55878	1.449	0.802	
680	6	0	-2	113.170	112.386	0.55669	0.784	0.434	
681	6	0	-1	25.006	25.416	0.55920	-0.410	-0.227	
682	6	0	0	44.986	45.043	0.56622	-0.057	-0.031	
683	6	0	1	16.996	18.023	0.57761	-1.027	-0.568	
684	6	0	2	68.835	68.216	0.59311	0.619	0.343	

686	6	0	4	27.158	27.997	0.63515	-0.839	-0.464
687	6	0	5	42.310	42.527	0.66100	-0.217	-0.120
688	6	0	6	58.908	59.171	0.68959	-0.263	-0.145
689	6	2	-10	12.783	13.023	0.69517	-0.240	-0.132
690	6	2	-9	34.137	33.477	0.66717	0.660	0.365
691	6	2	-8	30.973	29.376	0.64194	1.597	0.883
692	6	2	-7	6.943	8.044	0.61982	-1.100	-0.609
693	6	2	-6	4.448	4.210	0.60115	0.238	0.131
694	6	2	-5	18.804	18.799	0.58627	0.006	0.003
695	6	2	-4	37.518	37.027	0.57545	0.492	0.272
696	6	2	-3	25.440	24.916	0.56895	0.524	0.290
697	6	2	-2	20.088	19.262	0.56690	0.826	0.457
698	6	2	-1	27.212	26.959	0.56936	0.254	0.140
699	6	2	0	30.593	31.327	0.57626	-0.734	-0.406
700	6	2	1	21.480	21.659	0.58746	-0.179	-0.099
701	6	2	2	3.327	3.638	0.60270	-0.311	-0.172
702	6	2	3	10.415	11.436	0.62170	-1.021	-0.565
703	6	2	4	34.065	33.170	0.64412	0.894	0.495
704	6	2	5	32.546	31.813	0.66962	0.733	0.405
705	6	2	6	11.102	11.364	0.69785	-0.262	-0.145
706	6	4	-9	19.365	19.461	0.69248	-0.096	-0.053
707	6	4	-8	17.991	17.847	0.66821	0.144	0.080
708	6	4	-7	7.775	8.109	0.64699	-0.334	-0.185
709	6	4	-6	17.720	17.212	0.62912	0.507	0.280
710	6	4	-5	31.371	30.486	0.61491	0.884	0.489
711	6	4	-4	34.553	35.527	0.60461	-0.974	-0.539
712	6	4	-3	9.366	9.618	0.59843	-0.252	-0.139
713	6	4	-2	3.056	2.385	0.59648	0.671	0.371
714	6	4	-1	21.679	21.329	0.59882	0.351	0.194
715	6	4	0	40.429	40.814	0.60539	-0.384	-0.213

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No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
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716	6	4	1	35.023	34.696	0.61605	0.327	0.181	
717	6	4	2	8.480	8.664	0.63060	-0.184	-0.102	
718	6	4	4	17.973	18.644	0.67030	-0.671	-0.371	
719	6	4	5	23.795	23.575	0.69484	0.220	0.121	
720	6	6	-7	17.014	17.198	0.68989	-0.184	-0.102	
721	6	6	-6	47.861	48.271	0.67316	-0.410	-0.227	
722	6	6	-5	30.557	30.887	0.65990	-0.330	-0.182	
723	6	6	-4	27.013	28.472	0.65032	-1.458	-0.807	
724	6	6	-3	15.622	16.002	0.64457	-0.379	-0.210	
725	6	6	-2	104.021	103.693	0.64276	0.327	0.181	
726	6	6	-1	17.575	18.380	0.64493	-0.805	-0.445	
727	6	6	0	25.892	27.155	0.65103	-1.263	-0.698	
728	6	6	1	28.116	28.878	0.66096	-0.762	-0.421	
729	6	6	2	49.850	51.236	0.67455	-1.386	-0.766	
730	6	6	3	16.418	16.265	0.69158	0.153	0.085	
731	7	1	-7	3.490	4.395	0.69220	-0.905	-0.501	
732	7	1	-6	11.988	11.990	0.67682	-0.003	-0.001	
733	7	1	-5	30.666	30.572	0.66495	0.094	0.052	
734	7	1	-4	28.659	28.519	0.65677	0.140	0.077	
735	7	1	-3	8.390	8.306	0.65241	0.084	0.046	
736	7	1	-2	6.346	6.056	0.65197	0.290	0.161	
737	7	1	-1	19.907	20.227	0.65544	-0.320	-0.177	
738	7	1	0	28.821	29.286	0.66276	-0.465	-0.257	
739	7	1	1	21.282	21.246	0.67381	0.035	0.020	
740	7	1	2	4.918	5.551	0.68841	-0.632	-0.350	
741	7	3	-6	18.479	19.457	0.69356	-0.978	-0.541	
742	7	3	-5	38.567	39.577	0.68198	-1.009	-0.558	
743	7	3	-4	37.772	37.694	0.67400	0.078	0.043	
744	7	3	-3	66.087	65.924	0.66976	0.163	0.090	

746	7	1	0	28.821	29.286	0.66276	-0.465	-0.257
747	7	1	1	21.282	21.246	0.67381	0.035	0.020
748	7	1	2	4.918	5.551	0.68841	-0.632	-0.350
749	7	3	-6	18.479	19.457	0.69356	-0.978	-0.541
750	7	3	-5	38.567	39.577	0.68198	-1.009	-0.558

LSFM (1.3) 02/14/96 16:12:59 Elapsed time = 0.0 min

FEKINO Demonstration Copy - Not for Resale

The space group is number 12 -- C12/m1

After refinement cycle no. 2. 750 observations. 74 variables.

Esd of an observation of unit weight = 1.023

Unweighted R factor = 0.032 Weighted R factor = 0.036

$\bar{a}^3 Fo^3 = 2.81334E+04$

$\bar{a}^3 Fo^3 - \bar{a}^3 Fc^3 = 8.95032E+02$

$\bar{a} W * DEL Y = 7.06883E+02$

$\bar{a} W * Fo Y = 5.45704E+05$

Largest parameter shift/error = 0.02

Average parameter shift/error = 0.00

The calculations have converged with a shift/error less than 0.100

Cycle	Error	R1	R2	Max.shift	Av.shift
1	1.012	0.032	0.036	0.45	0.06
2	1.023	0.032	0.036	0.02	0.00
3	0.000	0.000	0.000	0.00	0.00
4	0.000	0.000	0.000	0.00	0.00