Supplementary material

1. Data statistics

Summary of observation redundancies

Shell		% of reflections with given No. of observations										
Lower limit	Upper limit	0	1	2	3	4	5-6	7-8	9-12	13-19	>19	Total
30.00	7.50	24.9	19.0	26.5	12.2	10.4	4.4	1.4	1.2	0.0	0.0	75.1
7.50	5.97	18.6	21.5	23.9	16.1	9.4	5.3	2.9	2.2	0.1	0.0	81.4
5.97	5.22	13.4	26.3	22.4	18.5	8.6	6.5	1.6	2.6	0.0	0.0	86.6
5.22	4.75	12.8	27.1	28.6	17.1	5.6	5.7	1.7	1.4	0.0	0.0	87.2
4.75	4.41	11.7	27.5	30.0	16.3	5.0	6.0	2.4	1.2	0.0	0.0	88.3
4.41	4.15	7.8	28.8	30.5	18.5	5.7	4.9	2.7	1.1	0.0	0.0	92.2
4.15	3.94	7.7	28.0	35.2	16.2	6.6	3.1	3.0	0.3	0.0	0.0	92.3
3.94	3.77	6.4	30.0	37.5	14.4	4.9	4.7	2.0	0.1	0.0	0.0	93.6
3.77	3.62	6.5	33.0	37.7	11.9	4.9	4.9	0.9	0.0	0.0	0.0	93.5
3.62	3.50	6.5	35.6	34.9	12.4	5.1	4.4	1.1	0.0	0.0	0.0	93.5
All *hkl*		11.7	27.6	30.7	15.4	6.6	5.0	2.0	1.0	0.0	0.0	88.3

***I*/σ in resolution shells**:

Shell		% of reflections with *I*/σ less than								
Lower limit	Upper limit	0	1	2	3	5	10	20	>20	Total
30.00	7.50	1.0	2.4	3.7	5.3	7.5	14.1	33.9	41.2	75.1
7.50	5.97	2.1	5.6	8.4	11.4	18.2	37.9	71.2	10.2	81.4
5.97	5.22	2.8	7.9	13.4	18.7	29.4	51.8	80.8	5.8	86.6
5.22	4.75	2.9	8.7	13.9	19.7	30.2	53.1	80.9	6.3	87.2
4.75	4.41	3.4	10.2	16.1	21.4	33.3	59.2	84.6	3.7	88.3
4.41	4.15	5.2	15.4	23.6	31.8	45.1	69.5	90.1	2.1	92.2
4.15	3.94	6.2	20.3	30.0	40.2	56.5	79.0	91.7	0.6	92.3
3.94	3.77	9.4	24.7	38.9	49.1	66.8	86.3	93.4	0.3	93.6
3.77	3.62	10.5	31.0	48.3	59.8	74.3	90.3	93.5	0.0	93.5
3.62	3.50	11.8	34.7	54.9	67.0	80.4	91.4	93.5	0.0	93.5
All *hkl*		5.5	15.9	24.9	32.2	43.8	62.9	81.0	7.2	88.3

Summary of reflections intensities and *R* factors by shells

R linear = $\Sigma[\mathrm{ABS}(I - \langle I \rangle)] / \Sigma(I)$.
R square = $\Sigma[(I - \langle I \rangle)^2] / \Sigma(I^2)$.
$\chi^2 = \Sigma[(I - \langle I \rangle)^2] / [\mathrm{Error}^2 * N/(N - 1)]$.
In all sums single measurements are excluded.

Shell limit		I	Average error	Average stat.	Norm. χ^2	R linear	R square
Lower	Upper						
30.00	7.50	1230.8	51.1	33.8	1.498	0.042	0.048
7.50	5.97	479.3	38.8	28.3	1.053	0.074	0.082
5.97	5.22	432.6	46.6	37.5	0.935	0.093	0.097
5.22	4.75	577.4	61.8	49.1	1.057	0.095	0.102
4.75	4.41	588.7	72.3	57.6	1.091	0.108	0.117
4.41	4.15	478.8	77.8	67.4	0.944	0.130	0.140
4.15	3.94	385.1	83.6	76.9	0.903	0.170	0.180
3.94	3.77	315.9	95.2	90.8	0.797	0.210	0.226
3.77	3.62	265.0	103.8	100.5	0.856	0.294	0.324
3.62	3.50	236.4	116.9	114.4	0.853	0.344	0.369
All reflections		487.7	75.8	66.8	1.007	0.118	0.112

Intensities of systematic absences

h	*k*	*l*	Intensity	σ	*I*/σ
0	0	16	-9.5	6.3	-1.5
0	0	17	-2.5	4.8	-0.5
0	0	19	-0.9	5.3	-0.2
0	0	20	-1.1	5.7	-0.2
0	0	22	4.8	9.0	0.5
0	0	26	3.6	8.1	0.4
0	0	29	2.7	8.7	0.3
0	0	31	-2.3	9.5	-0.2
0	0	32	0.3	13.4	0.0
0	0	34	-16.7	10.9	-1.5
0	0	41	-15.7	13.9	-1.1
0	0	43	-1.8	14.3	-0.1
0	0	44	-14.0	14.9	-0.9
0	0	46	0.0	19.5	0.0
0	0	47	-9.5	15.1	-0.6
0	0	49	-6.8	16.8	-0.4
0	0	50	15.4	17.7	0.9
0	0	52	-10.8	18.4	-0.6
0	0	53	-6.2	18.9	-0.3
0	0	55	-1.7	20.2	-0.1
0	0	59	-2.3	21.9	-0.1
0	0	61	-11.6	28.1	-0.4
0	0	62	20.5	23.9	0.9
0	0	64	18.7	24.7	0.8
0	0	65	-23.2	25.3	-0.9
0	0	67	23.2	27.2	0.9
0	0	68	-21.0	27.7	-0.8
0	0	70	-1.8	29.9	-0.1
0	0	74	-23.2	32.1	-0.7
0	0	76	18.5	33.2	0.6
0	0	77	-29.3	33.9	-0.9
0	0	79	25.4	36.6	0.7
0	0	80	-20.2	37.0	-0.5
0	0	82	20.3	41.1	0.5
0	0	83	-6.4	42.9	-0.1
0	0	85	-4.6	46.1	-0.1
0	0	86	180.6	67.9	2.7
0	0	92	-70.1	58.4	-1.2
0	0	106	-102.2	70.6	-1.4
0	0	107	-138.9	72.0	-1.9
0	0	109	-49.3	76.0	-0.6
0	0	110	32.9	76.9	0.4
0	0	112	-10.8	75.5	-0.1
0	0	113	-5.0	76.5	-0.1
0	0	115	87.1	81.3	1.1

2. Refinement statistics

R value by resolution for test set

Bin No.	Resolution range		# refl.	*R*
1	7.35	8.00	49	0.2518
2	6.87	7.35	46	0.2625
3	6.50	6.87	40	0.3065
4	6.20	6.50	44	0.2227
5	5.94	6.20	39	0.2664
6	5.73	5.94	46	0.3403
7	5.54	5.73	48	0.3815
8	5.37	5.54	47	0.3261
9	5.22	5.37	43	0.3026
10	5.09	5.22	60	0.3343
11	4.97	5.09	66	0.2201
12	4.86	4.97	54	0.2809
13	4.76	4.86	50	0.2197
14	4.67	4.76	48	0.2484
15	4.58	4.67	65	0.2324
16	4.50	4.58	41	0.2280
17	4.43	4.50	40	0.3110
18	4.36	4.43	59	0.2144
19	4.29	4.36	49	0.3225
20	4.23	4.29	52	0.2212
21	4.17	4.23	56	0.3175
22	4.12	4.17	62	0.2708
23	4.06	4.12	49	0.2785
24	4.02	4.06	57	0.2848
25	3.97	4.02	54	0.2695
26	3.92	3.97	47	0.2567
27	3.88	3.92	38	0.2970
28	3.84	3.88	55	0.3682
29	3.80	3.84	49	0.2764
30	3.76	3.80	49	0.3276
31	3.72	3.76	53	0.2372
32	3.69	3.72	48	0.3243
33	3.65	3.69	51	0.3527
34	3.62	3.65	53	0.2501
35	3.59	3.62	41	0.4389
36	3.56	3.59	57	0.3833
37	3.53	3.56	42	0.4164
38	3.50	3.53	68	0.3965
1	3.50	8.00	1915	0.2872

Overall *R* value for test set: 0.28717

R value by resolution for working set

Bin No.	Resolution range		# refl.	*R*
1	7.35	8.00	435	0.2181
2	6.87	7.35	443	0.2346
3	6.50	6.87	422	0.2196
4	6.20	6.50	416	0.2037
5	5.94	6.20	445	0.2429
6	5.73	5.94	448	0.2304
7	5.54	5.73	450	0.2635
8	5.37	5.54	460	0.2578
9	5.22	5.37	458	0.2326
10	5.09	5.22	453	0.2026
11	4.97	5.09	409	0.1822
12	4.86	4.97	464	0.1803
13	4.76	4.86	452	0.1564
14	4.67	4.76	440	0.1935
15	4.58	4.67	460	0.1665
16	4.50	4.58	460	0.1685
17	4.43	4.50	456	0.1967
18	4.36	4.43	462	0.1535
19	4.29	4.36	455	0.1732
20	4.23	4.29	476	0.1778
21	4.17	4.23	481	0.1839
22	4.12	4.17	478	0.1989
23	4.06	4.12	424	0.2060
24	4.02	4.06	500	0.1966
25	3.97	4.02	466	0.1928
26	3.92	3.97	504	0.1904
27	3.88	3.92	448	0.1984
28	3.84	3.88	519	0.2204
29	3.80	3.84	493	0.2249
30	3.76	3.80	446	0.2536
31	3.72	3.76	461	0.2115
32	3.69	3.72	492	0.2327
33	3.65	3.69	504	0.2423
34	3.62	3.65	471	0.2744
35	3.59	3.62	459	0.2590
36	3.56	3.59	498	0.2520
37	3.53	3.56	476	0.2715
38	3.50	3.53	483	0.3220
1	3.50	8.00	17567	0.2114

Overall *R* value for working set: 0.211351

```
CNSsolve>display======== geometry ==============
CNSsolve> display
CNSsolve> set print=&list_outfile end
CNSsolve>
CNSsolve> display =======> bond violations
CNSsolve> display
CNSsolve> print threshold=&bond_thresh bond
Number of violations greater 0.050: 5
RMS deviation= 0.008
CNSsolve>
CNSsolve> display
CNSsolve> display =======> angle violations
CNSsolve> display
CNSsolve>
CNSsolve> print threshold=&angle_thresh angle
Number of violations greater 8.000: 27
RMS deviation= 1.337
CNSsolve>
CNSsolve> display
CNSsolve> display =======> improper angle violations
CNSsolve> display
CNSsolve>
CNSsolve> print threshold=&impr_thresh improper
Number of violations greater 3.000: 37
RMS deviation= 0.834
CNSsolve>
CNSsolve> display
CNSsolve> display =======> dihedral angle violations
CNSsolve> display
CNSsolve>
CNSsolve> print threshold=&dihe_thresh dihedral
Number of violations greater 60.000: 4
RMS deviation= 22.678
CNSsolve>
CNSsolve> set print=OUTPUT end
CNSsolve>
CNSsolve> display
```