

D9 data refined without extinction correction:

Most Disagreeable Reflections (* if suppressed or used for Rfree)

h	k	l	Fo ²	Fc ²	Delta(F ²)/esd	Fc/Fc(max)	Resolution(A)
0	3	0	11415.35	11608.42	6.82	0.610	2.58
2	0	9	14191.57	15906.59	6.47	0.714	1.65
4	0	4	14108.96	15754.26	6.41	0.711	2.25
2	0	7	10028.82	11382.23	6.18	0.604	2.06
1	1	1	431.01	108.10	5.86	0.059	5.87
8	0	4	22539.49	24530.33	5.79	0.887	1.30
13	9	2	730.98	1240.57	5.43	0.199	0.60
0	1	14	21298.65	23306.97	5.42	0.865	1.10
1	5	11	20383.09	22452.18	5.26	0.849	1.04
5	1	12	15599.43	17248.83	5.10	0.744	1.11
4	11	12	287.17	710.74	5.09	0.151	0.60
7	2	1	15746.81	17167.79	4.98	0.742	1.46
10	0	4	21642.24	23581.71	4.90	0.870	1.06
6	4	0	14863.35	16222.71	4.82	0.721	1.33
7	4	21	199.52	554.08	4.66	0.133	0.63
3	2	0	2068.51	1612.38	4.40	0.227	2.67
8	2	-5	13157.54	14361.41	4.37	0.679	1.20
0	4	8	6099.59	5272.17	4.29	0.411	1.37
1	1	3	6213.25	6778.88	4.22	0.466	4.01
1	2	4	5707.33	5076.44	4.09	0.404	2.66
1	3	1	8193.42	8926.25	3.98	0.535	2.48
2	6	6	2812.49	2527.81	3.89	0.285	1.13
1	3	2	1641.21	1299.05	3.85	0.204	2.39
2	4	1	5194.17	4550.30	3.79	0.382	1.81
7	1	7	12652.09	13658.85	3.76	0.662	1.27
2	7	0	2228.23	1603.55	3.73	0.227	1.08
0	6	0	10587.72	9797.85	3.70	0.561	1.29
9	4	21	44.96	289.16	3.70	0.096	0.60
4	6	2	3958.89	3592.45	3.65	0.339	1.15
0	2	2	7071.53	7953.32	3.56	0.505	3.46
0	2	6	4009.87	3482.04	3.55	0.334	2.15
8	3	-4	16100.02	17149.99	3.47	0.742	1.16
4	2	0	1217.32	923.22	3.46	0.172	2.25
8	3	3	10824.20	11385.77	3.43	0.604	1.19
3	5	22	287.69	649.70	3.42	0.144	0.63
0	0	8	7409.37	8079.62	3.40	0.509	1.94
3	2	4	5845.09	5289.23	3.29	0.412	2.20
3	5	2	3629.72	3103.06	3.25	0.315	1.40
0	3	4	1341.59	1066.99	3.24	0.185	2.15
1	5	5	3214.64	2722.42	3.21	0.295	1.37
4	9	0	14752.58	16275.23	3.15	0.722	0.82
1	1	0	209.55	75.25	3.15	0.049	6.33
6	2	11	10255.97	11129.21	3.10	0.597	1.08
3	1	12	1604.49	1441.91	3.09	0.215	1.21
1	4	6	2964.66	2510.67	3.09	0.284	1.53
2	0	16	12333.63	13475.90	3.08	0.657	0.96
15	6	5	2935.33	3769.40	3.07	0.348	0.63
1	6	4	4376.83	4066.82	3.07	0.361	1.22
2	5	0	2082.07	1665.05	3.07	0.231	1.49
0	2	10	2628.08	2198.74	2.98	0.266	1.44

D9 data post-refined extinction correction:

Most Disagreeable Reflections (* if suppressed)

	h	k	l	Fo ²	Fc ²	Delta(F ²)/esd	Fc/Fc(max)	
Resolution(A)								
*	3	9	16	585.75	2344.32	36.40	0.221	0.63
*	14	7	4	250.82	834.84	27.58	0.132	0.63
*	13	8	3	887.59	2339.54	27.51	0.221	0.63
*	18	0	5	728.86	2346.69	26.49	0.221	0.60
*	2	1	0	4545.54	3123.32	18.66	0.255	4.50
*	0	0	12	42825.04	48106.94	17.39	1.000	1.30
*	1	12	4	142.95	617.17	16.15	0.113	0.63
*	8	11	7	539.67	1476.14	15.47	0.175	0.60
*	10	10	0	1685.78	3459.55	13.84	0.268	0.63
*	18	2	3	191.87	634.43	13.48	0.115	0.60
	1	1	1	378.56	109.77	7.90	0.048	5.87
	4	11	12	251.87	606.18	6.90	0.112	0.60
	13	9	2	643.49	1041.75	6.86	0.147	0.60
	7	4	21	174.81	473.73	6.38	0.099	0.63
	0	5	6	17147.19	15859.19	5.96	0.574	1.33
	0	0	4	9410.63	10305.90	5.92	0.463	3.89
	1	2	4	5631.64	5087.87	5.08	0.325	2.66
	2	1	1	11134.08	10488.63	4.95	0.467	4.32
	1	1	12	7286.99	7951.27	4.58	0.407	1.27
	1	1	0	183.62	65.42	4.49	0.037	6.33
	3	5	22	252.20	539.15	4.40	0.106	0.63
	9	4	21	39.30	214.84	4.32	0.067	0.60
	2	0	7	10672.42	11378.64	4.31	0.486	2.06
	6	1	2	13999.83	13182.94	4.30	0.523	1.75
	15	3	11	45.00	124.42	4.21	0.051	0.63
	10	1	2	8884.73	8126.95	4.19	0.411	1.08
	2	2	0	6641.70	6061.31	4.05	0.355	3.17
	0	3	0	12959.26	13049.81	4.00	0.521	2.58
	15	6	5	2632.81	3303.21	3.92	0.262	0.63
	0	3	8	45291.81	43848.26	3.85	0.955	1.55
	3	4	1	2533.06	2875.94	3.80	0.245	1.70
	10	7	10	2637.94	3462.64	3.74	0.268	0.70
	3	1	1	9054.69	8581.08	3.68	0.422	3.25
	8	0	4	25568.21	24666.08	3.29	0.716	1.30
	0	5	22	2630.39	3182.30	3.27	0.257	0.64
	6	7	17	2922.74	3549.73	3.25	0.272	0.66
	4	9	15	425.16	743.42	3.18	0.124	0.64
	1	12	3	735.90	1162.76	3.17	0.155	0.64
	3	6	21	672.86	1023.21	3.14	0.146	0.63
	3	2	4	5685.47	5323.92	3.13	0.333	2.20
	2	0	3	12310.16	11861.18	3.05	0.497	3.78
	3	2	0	1886.60	1683.86	3.05	0.187	2.67
	17	1	9	568.35	341.38	3.01	0.084	0.61
	9	1	-5	10812.59	11372.84	3.00	0.486	1.13
	11	9	11	1383.76	1036.92	3.00	0.147	0.59
	3	7	1	10825.16	10215.58	2.99	0.461	1.05
	6	2	8	1951.11	2221.57	2.97	0.215	1.26
	6	2	11	10012.63	10586.63	2.97	0.469	1.08
	3	3	0	2173.22	2297.36	2.90	0.219	2.11
	0	0	6	5208.41	5301.42	2.89	0.332	2.59

LADI data without extinction correction:

(NB. The resolution given in the last column is non-sensical here, since SHELXL requires a wavelength entry, and uses this to calculate the resolution - but given the polychromatic nature of this data, a dummy wavelength was given)

Most Disagreeable Reflections (* if suppressed)

	h	k	l	Fo ²	Fc ²	Delta(F ²)/esd	Fc/Fc(max)	Resolution(A)
*	4	6	6	7568.88	71.65	33.41	0.040	1.06
*	6	4	6	9316.59	454.60	31.85	0.102	1.19
*	6	4	8	5821.73	639.39	24.10	0.121	1.10
*	4	2	12	4370.71	367.40	21.04	0.091	1.12
*	8	2	10	4270.11	198.28	20.97	0.067	1.00
*	2	4	12	4254.76	599.23	17.91	0.117	1.06
*	10	2	2	11478.08	3759.51	16.12	0.293	1.05
*	8	0	10	11769.08	4805.50	12.16	0.331	1.03
*	10	4	2	3508.50	767.32	12.14	0.132	0.95
*	10	2	6	5804.68	2469.89	11.13	0.237	0.98
*	8	2	8	3018.00	1513.65	8.49	0.186	1.08
*	2	4	10	1753.97	821.60	8.01	0.137	1.18
*	6	2	12	14113.00	9653.33	5.21	0.469	1.02
*	0	3	8	29287.14	43930.45	5.03	1.000	1.55
	7	7	6	4267.26	2782.55	3.72	0.252	0.85
	2	6	6	4534.39	3412.43	3.71	0.279	1.13
	8	2	6	2736.66	2028.77	3.60	0.215	1.16
	1	1	12	10504.47	8185.49	3.30	0.432	1.27
	3	2	18	2463.85	984.44	3.25	0.150	0.82
	8	4	6	14050.48	11168.81	3.14	0.504	1.03
	6	1	17	341.02	968.21	3.12	0.148	0.82
	4	6	4	14062.99	11185.83	3.11	0.505	1.12
	1	5	11	16833.75	21348.44	3.05	0.697	1.04
	2	1	4	913.93	730.06	2.99	0.129	2.94
	10	2	0	2231.39	1626.29	2.98	0.192	1.06
	1	1	13	3657.41	2447.90	2.96	0.236	1.18
	2	1	2	206.88	158.85	2.77	0.060	3.89
	6	3	1	268.84	427.29	2.76	0.099	1.49
	7	3	11	277.36	32.24	2.66	0.027	0.98
	13	3	1	876.98	135.33	2.63	0.056	0.81
	9	2	3	9737.18	11928.01	2.62	0.521	1.14
	9	7	1	6030.89	7438.29	2.58	0.411	0.82
	8	0	3	5033.98	6151.52	2.55	0.374	1.34
	10	0	11	2275.72	2907.48	2.54	0.257	0.87
	6	1	8	8597.62	10433.50	2.50	0.487	1.32
	10	2	4	5003.86	4154.52	2.46	0.308	1.03
	7	7	3	2555.93	1955.20	2.42	0.211	0.89
	4	0	5	8859.63	7447.70	2.36	0.412	2.07
	5	2	7	2707.68	3252.11	2.35	0.272	1.45
	9	4	5	269.97	140.66	2.33	0.057	0.98
	3	1	6	5824.58	4922.41	2.30	0.335	2.05
	2	8	3	1245.85	894.62	2.28	0.143	0.94
	6	1	10	214.84	317.73	2.28	0.085	1.18
	1	7	4	1210.04	970.05	2.28	0.149	1.06
	0	5	6	13378.11	15898.65	2.24	0.602	1.33
	13	1	6	1096.94	726.66	2.24	0.129	0.80
	9	4	12	1503.32	1927.84	2.20	0.209	0.81
	3	5	6	2503.07	2107.24	2.18	0.219	1.25
	8	7	0	308.05	4.42	2.17	0.010	0.86
	0	5	8	366.03	177.34	2.17	0.064	1.21

