

Shell		Average Redundancy Per Shell
Lower limit	Upper limit	
50.00	4.74	4.3
4.74	3.76	4.5
3.76	3.29	4.4
3.29	2.99	4.1
2.99	2.77	3.8
2.77	2.61	3.6
2.61	2.48	3.4
2.48	2.37	3.2
2.37	2.28	2.7
2.28	2.20	2.5
All hkl		3.7

Shell		Summary of observation redundancies:										
Lower limit	Upper limit	% of reflections with given No. of observations										total
		0	1	2	3	4	5-6	7-8	9-12	13-19	>19	
50.00	4.74	2.5	6.2	11.4	13.2	23.9	34.4	8.4	0.0	0.0	0.0	97.5
4.74	3.76	1.8	4.3	9.1	13.1	22.8	39.3	9.5	0.0	0.0	0.0	98.2
3.76	3.29	2.1	5.3	9.7	12.8	22.5	38.3	9.2	0.0	0.0	0.0	97.9
3.29	2.99	2.8	6.9	12.3	15.3	22.3	33.1	7.2	0.0	0.0	0.0	97.2
2.99	2.77	3.3	9.0	14.6	17.4	21.6	28.6	5.4	0.0	0.0	0.0	96.7
2.77	2.61	3.7	10.5	16.6	19.3	20.5	25.2	4.2	0.0	0.0	0.0	96.3
2.61	2.48	4.2	12.0	19.0	20.3	19.9	21.1	3.5	0.0	0.0	0.0	95.8
2.48	2.37	5.9	15.2	21.3	21.0	17.5	16.8	2.4	0.0	0.0	0.0	94.1
2.37	2.28	13.0	22.0	23.1	17.2	12.8	10.5	1.4	0.0	0.0	0.0	87.0
2.28	2.20	28.1	23.7	18.7	12.2	9.2	7.4	0.7	0.0	0.0	0.0	71.9
All hkl		6.7	11.5	15.5	16.2	19.3	25.5	5.2	0.0	0.0	0.0	93.3

Shell		I/Sigma in resolution shells:									
Lower limit	Upper limit	No. of reflections with I / Sigma less than									total
		0	1	2	3	5	10	20	>20		
50.00	4.74	0	1809	4974	7054	9633	12601	14844	11004	25848	
4.74	3.76	0	1127	3086	4680	7057	11069	15049	10318	25367	
3.76	3.29	0	1372	3883	5969	8679	12941	16860	8247	25107	
3.29	2.99	0	1996	5542	8335	11598	15727	19583	5192	24775	
2.99	2.77	0	2774	7437	10823	14407	18420	21860	2928	24788	
2.77	2.61	0	3317	9040	12777	16555	20265	22930	1564	24494	
2.61	2.48	0	4001	10606	14745	18391	21527	23427	949	24376	
2.48	2.37	0	4758	12060	16295	19476	21930	23269	660	23929	
2.37	2.28	0	5581	12709	16185	18734	20500	21570	545	22115	
2.28	2.20	0	5261	10931	13552	15510	17000	17867	396	18263	
All hkl		0	31996	80268	110415	140040	171980	197259	41803	239062	

Shell		I/Sigma in resolution shells:								
Lower limit	Upper limit	% of reflections with I / Sigma less than								total
		0	1	2	3	5	10	20	>20	
50.00	4.74	0.0	6.8	18.8	26.6	36.3	47.5	56.0	41.5	97.5
4.74	3.76	0.0	4.4	11.9	18.1	27.3	42.8	58.2	39.9	98.2
3.76	3.29	0.0	5.3	15.1	23.3	33.8	50.4	65.7	32.1	97.9
3.29	2.99	0.0	7.8	21.7	32.7	45.5	61.7	76.8	20.4	97.2
2.99	2.77	0.0	10.8	29.0	42.2	56.2	71.9	85.3	11.4	96.7
2.77	2.61	0.0	13.0	35.5	50.2	65.1	79.6	90.1	6.1	96.3
2.61	2.48	0.0	15.7	41.7	57.9	72.3	84.6	92.1	3.7	95.8
2.48	2.37	0.0	18.7	47.4	64.1	76.6	86.2	91.5	2.6	94.1
2.37	2.28	0.0	21.9	50.0	63.6	73.7	80.6	84.8	2.1	87.0
2.28	2.20	0.0	20.7	43.0	53.4	61.1	66.9	70.4	1.6	71.9
All hkl		0.0	12.5	31.3	43.1	54.6	67.1	77.0	16.3	93.3

Summary of reflections intensities and R-factors by intensity bins

$$R \text{ linear} = \text{SUM} ( \text{ABS}(I - \langle I \rangle) ) / \text{SUM} ( I )$$

$$R \text{ square} = \text{SUM} ( ( I - \langle I \rangle ) ** 2 ) / \text{SUM} ( I ** 2 )$$

$$\text{Chi}^{**2} = \text{SUM} ( ( I - \langle I \rangle ) ** 2 ) / ( \text{Error} ** 2 * N / ( N - 1 ) )$$

In all sums single measurements are excluded

Number	Average I	Average error	Average stat.	Norm. Chi**2	Linear R-fac	Square R-fac	nonunf
255947	66.4	67.1	67.1	0.460	0.451	0.620	0.000
163601	146.2	74.3	74.2	0.678	0.286	0.373	0.000
125536	288.9	81.6	81.1	0.810	0.176	0.225	0.000
93919	571.8	92.8	91.1	0.975	0.110	0.139	0.000
68100	1144.1	111.3	105.6	1.381	0.078	0.100	0.000
53608	2295.7	151.1	134.0	1.900	0.063	0.081	0.000
42326	4562.4	237.4	193.1	2.281	0.055	0.070	0.000
27185	8958.0	405.0	300.9	2.524	0.050	0.064	0.000
13779	17608.8	724.4	492.5	2.520	0.046	0.058	0.000
6200	35560.5	1354.1	834.9	2.522	0.042	0.053	0.000
2536	69954.9	2502.9	1372.3	2.486	0.040	0.050	0.000
788	136703.5	4618.2	2176.8	2.737	0.039	0.049	0.000
106	263532.6	8457.5	3258.3	2.422	0.035	0.044	0.000
8	602218.6	18210.4	5146.1	4.788	0.051	0.055	0.000

Summary of reflections intensities and R-factors by shells

R linear =  $\text{SUM} ( \text{ABS}(I - \langle I \rangle) ) / \text{SUM} (I)$

R square =  $\text{SUM} ( (I - \langle I \rangle) ** 2) / \text{SUM} (I ** 2)$

Chi\*\*2 =  $\text{SUM} ( (I - \langle I \rangle) ** 2) / (\text{Error} ** 2 * N / (N-1) )$

In all sums single measurements are excluded

Shell limit	Lower Angstrom	Upper Angstrom	Average I	Average error	Average stat.	Norm. Chi**2	Linear R-fac	Square R-fac
50.00	4.74		102.3	2.8	2.2	1.324	0.052	0.056
	4.74	3.76	113.2	3.5	2.8	1.636	0.063	0.062
	3.76	3.29	68.8	3.0	2.6	1.221	0.071	0.067
	3.29	2.99	34.0	2.6	2.4	0.936	0.093	0.078
	2.99	2.77	19.9	2.5	2.4	0.830	0.129	0.107
	2.77	2.61	13.7	2.5	2.5	0.741	0.171	0.142
	2.61	2.48	10.8	2.7	2.7	0.679	0.203	0.168
	2.48	2.37	9.1	2.9	2.9	0.641	0.227	0.188
	2.37	2.28	8.8	3.2	3.2	0.637	0.217	0.170
	2.28	2.20	8.5	3.3	3.3	0.690	0.213	0.175
All reflections			40.8	2.9	2.7	1.014	0.081	0.064