

Summary of reflections intensities and R factors by shells

$R_{\text{linear}} = \text{SUM} (\text{ABS}(I - \langle I \rangle)) / \text{SUM} (I)$
 In all sums single measurements are excluded

Shell limit		Average intensity	Average error	Linear R factor
lower	upper			
20.00	7.42	1278.7	53.9	0.067
7.42	5.94	666.0	42.3	0.094
5.94	5.21	570.0	42.3	0.118
5.21	4.74	645.7	58.6	0.120
4.74	4.40	672.9	64.5	0.129
4.40	4.14	605.1	69.1	0.149
4.14	3.94	483.7	72.1	0.200
3.94	3.77	424.7	74.1	0.242
3.77	3.62	363.4	79.4	0.303
3.62	3.50	281.7	82.5	0.391
All reflections		587.9	64.6	0.150

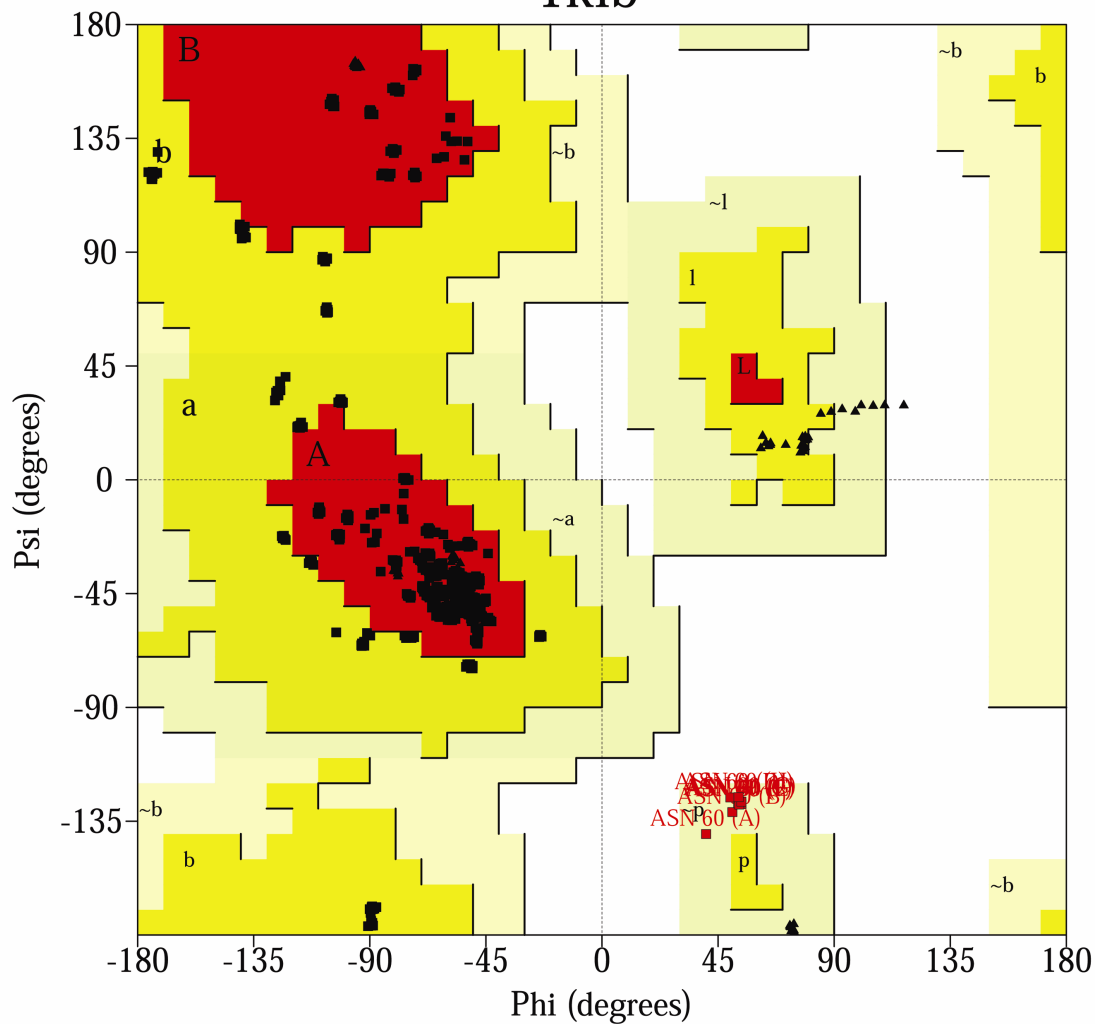
R_{work} and R_{free} by shells

Shell limit		R_{work}	R_{free}
Lower	Upper		
20.00	8.23	18.8	21.1
8.23	6.53	21.3	22.4
6.53	5.71	22.1	29.1
5.71	5.18	18.4	19.8
5.18	4.81	19.3	23.8
4.81	4.53	18.3	21.6
4.53	4.30	18.3	18.9
4.30	4.11	18.9	17.0
4.11	3.96	19.7	22.7
3.96	3.82	20.9	23.9
3.82	3.70	21.4	21.1
3.70	3.59	22.9	24.4
3.59	3.50	24.9	29.4
All reflections		20.2	22.3

PROCHECK

Ramachandran Plot

1kib



Plot statistics

Residues in most favoured regions [A,B,L]	481	78.1%
Residues in additional allowed regions [a,b,l,p]	127	20.6%
Residues in generously allowed regions [~a,~b,~l,~p]	8	1.3%
Residues in disallowed regions	0	0.0%

Number of non-glycine and non-proline residues	616	100.0%
Number of end-residues (excl. Gly and Pro)	8	
Number of glycine residues (shown as triangles)	72	
Number of proline residues	16	

Total number of residues	712	

Based on an analysis of 118 structures of resolution of at least 2.0 Angstroms and R-factor no greater than 20%, a good quality model would be expected to have over 90% in the most favoured regions.