Table 3a. Interatomic distances between TTR and PBP molecule in the primary mode.

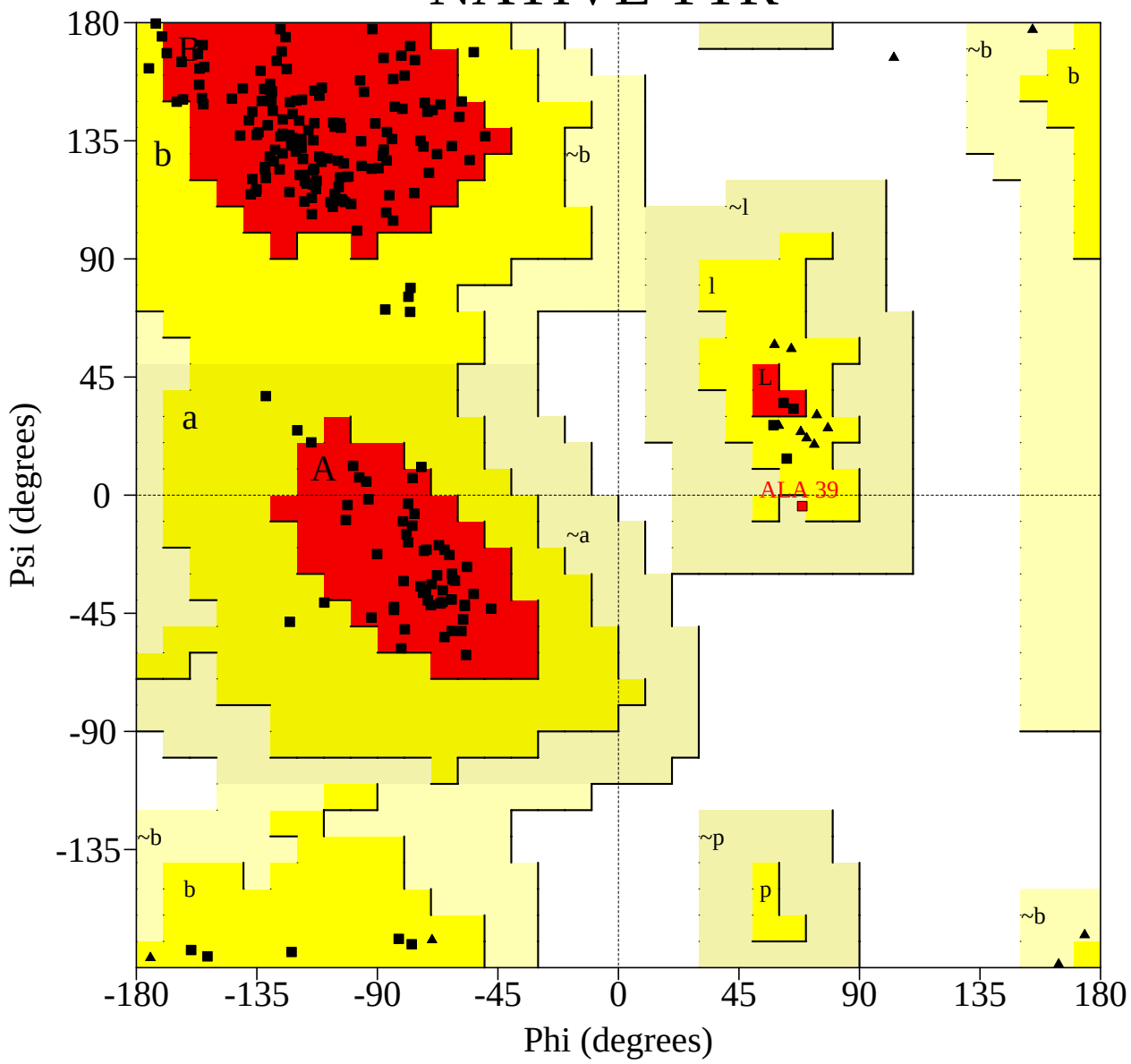
	PBP primary binding site at AC			BD		
Ligand atom	Protein atom		Distance (Å)	Protein atom		Distance (Å)
Br2	Wat-V217	O	3.5	Wat-V229	O	3.6
	Val-A121	$C^{\gamma 2}$	4.0	Val-B121	$C^{\gamma 2}$	3.9
	Lys-C15	C^{ε}	3.7	Lys-D15	$C^{\gamma 1}$	3.9
				Lys-D15	N^{z}	3.6
				Leu-D17	$C^{\delta 1}$	3.1
Br3	Thr-A119	C^{β}	3.5	Thr-B119	C^{β}	3.6
	Thr-A119	$C^{\gamma 2}$	3.8	Thr-B119	$C^{\gamma 2}$	3.9
	Thr-A119	$O^{\gamma 1}$	3.7	Thr-B119	$O^{\gamma 1}$	3.7
	Ala-A108	C^{β}	3.8	Ala-B108	C^{β}	3.7
				Leu-D17	$C^{\delta 1}$	3.2
Br4	Wat-W9	O	3.5	Wat-W5	O	3.6
	Wat-V9	O	3.5	Wat-V5	O	3.6
Br5	Ala-C108	C^{β}	3.8	Ala-D108	C^{β}	3.8
	Thr-C119	C^{β}	3.5	Thr-D119	C^{β}	3.6
	Thr-C119	$O^{\gamma 1}$	3.7	Thr-D119	$O^{\gamma 1}$	3.7
	Thr-C119	$C^{\gamma 2}$	3.8	Thr-D119	$C^{\gamma 2}$	3.9
				Leu-B17	$C^{\delta 1}$	3.2
Br6	Wat-W217	O	3.5	Wat-W229	O	3.6
	Val-C121	$C^{\gamma 2}$	4.0	Val-D121	$C^{\gamma 2}$	3.9
	Lys-A15	C^{ε}	3.7	Lys-B15	C^{ε}	3.9
				Lys-B15	N^{ζ}	3.6
				Leu-B17	$C^{\delta 1}$	3.1
O1	Lys-C15	C^{δ}	3.5	Lys-D15	C^{δ}	3.8
	Lys-C15	C^{ε}	3.4	Lys-D15	C^{ε}	3.6
				Lys-D15	N^{ζ}	2.9
	Lys-A15	C^{δ}	3.5	Lys-B15	C^{δ}	3.8
	Lys-A15	C^{ε}	3.4	Lys-B15	C^{ε}	3.6
				Lys-B15	N^{ζ}	2.9
C1				Lys-B15	N^{ζ}	4.0
				Lys-D15	N^{ζ}	4.0
C2				Ala-B108	C^{β}	3.9
				Leu-D17	$C^{\delta 1}$	3.3
C3	Ala-A108	C^{β}	3.9	Ala-B108	C^{β}	3.8
				Leu-D17	$C^{\delta 1}$	3.3
C5	Ala-C108	C^{β}	3.9	Ala-D108	C^{β}	3.8
				Leu-B17	$C^{\delta 1}$	3.3
C6				Ala-D108	C^{β}	3.9
				Leu-B17	$C^{\delta 1}$	3.3

H-bonds are underlined.

PROCHECK

Ramachandran Plot

NATIVE TTR



Plot statistics

Residues in most favoured regions [A,B,L]	179	89.1%
Residues in additional allowed regions [a,b,l,p]	21	10.4%
Residues in generously allowed regions [~a,~b,~l,~p]	1	0.5%
Residues in disallowed regions	0	0.0%
	----	------
Number of non-glycine and non-proline residues	201	100.0%
Number of end-residues (excl. Gly and Pro)	91	
Number of glycine residues (shown as triangles)	14	
Number of proline residues	13	

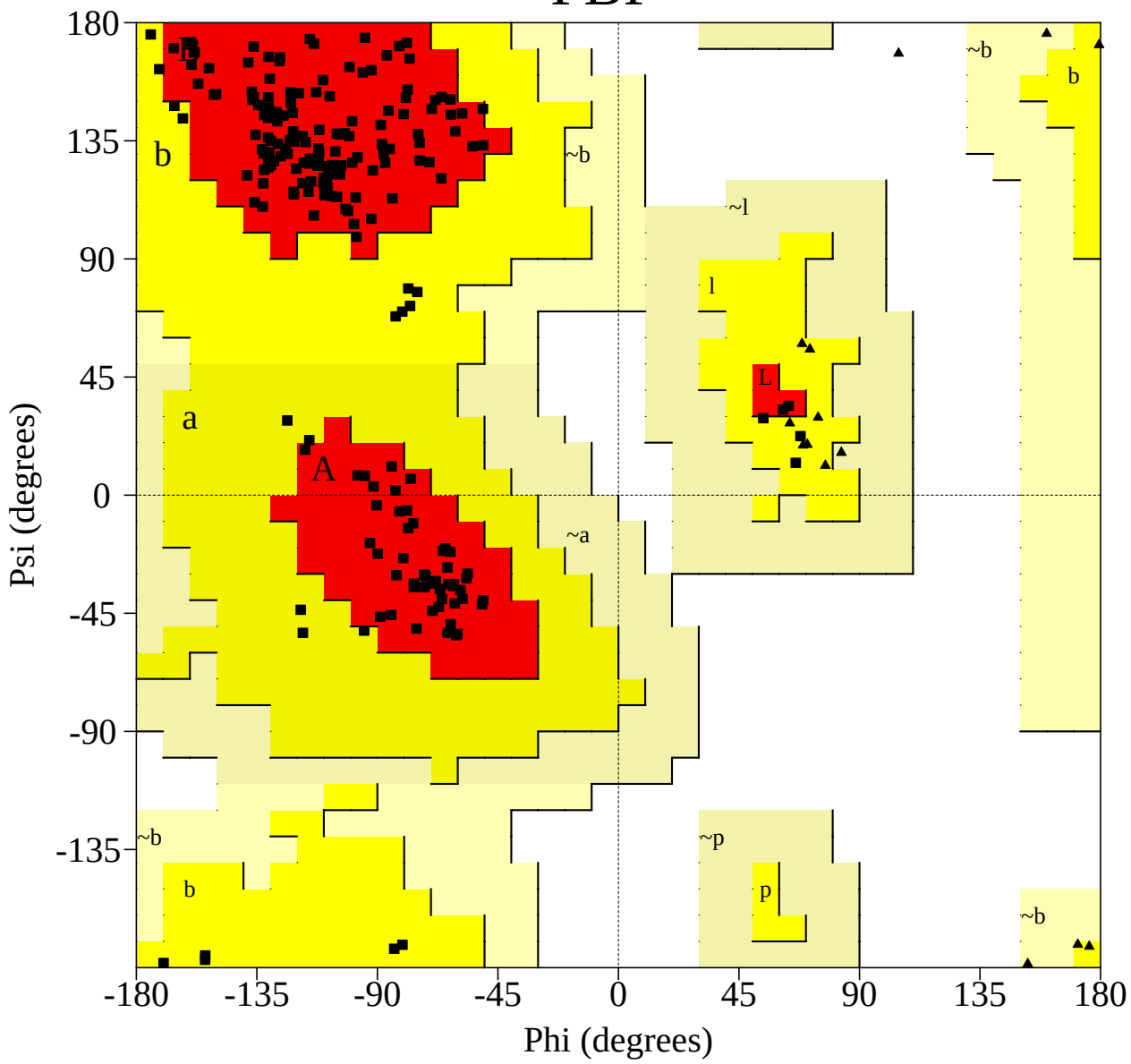
Total number of residues	319	

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.

SLOW_6C2_01.ps

Ramachandran Plot

PBP



Plot statistics

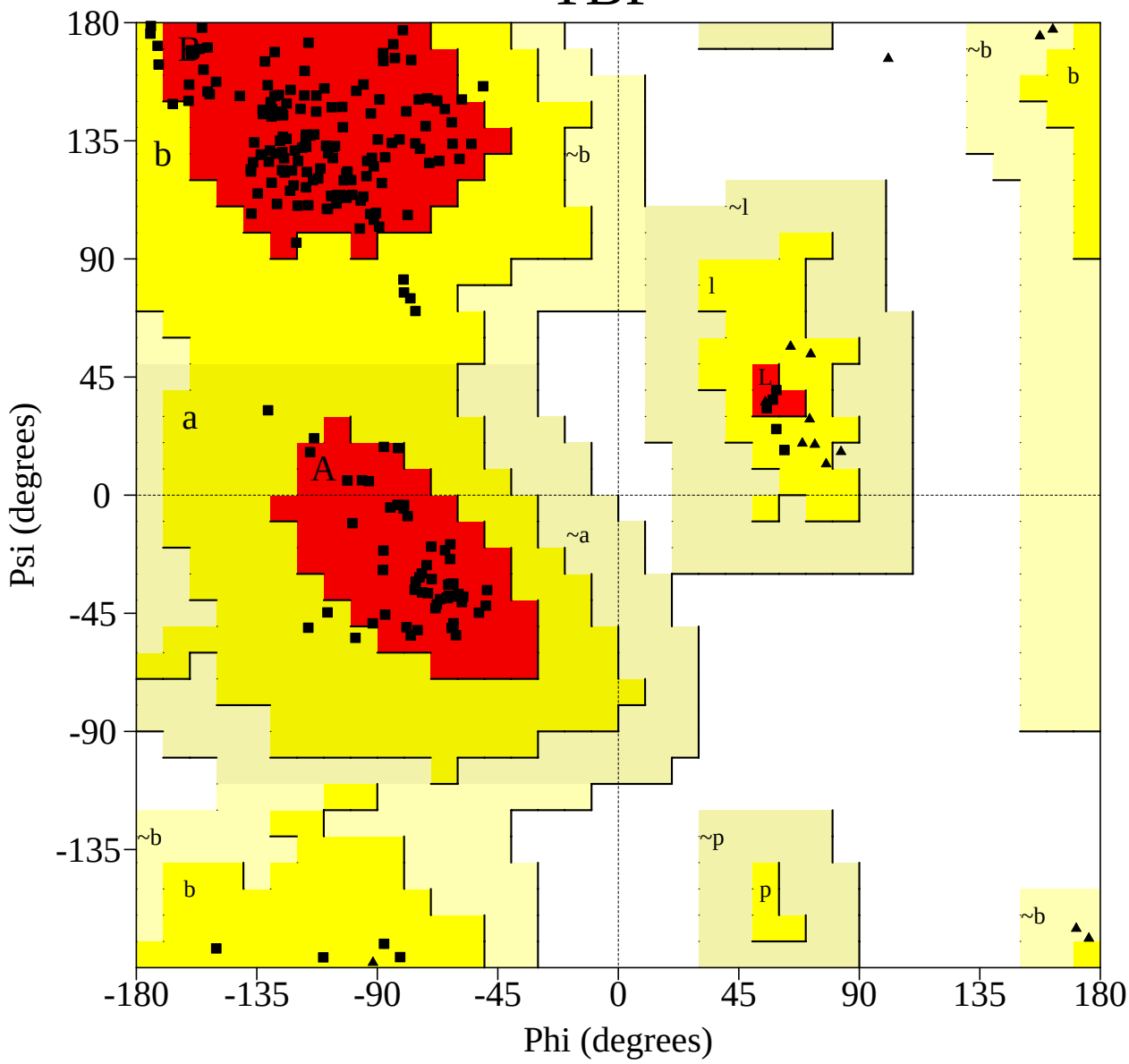
Residues in most favoured regions [A,B,L]	180	89.1%
Residues in additional allowed regions [a,b,l,p]	22	10.9%
Residues in generously allowed regions [~a,~b,~l,~p]	0	0.0%
Residues in disallowed regions	0	0.0%
	----	------
Number of non-glycine and non-proline residues	202	100.0%
Number of end-residues (excl. Gly and Pro)	165	
Number of glycine residues (shown as triangles)	14	
Number of proline residues	13	

Total number of residues	394	

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.

Ramachandran Plot

TBP



Plot statistics

Residues in most favoured regions [A,B,L]	181	89.6%
Residues in additional allowed regions [a,b,l,p]	21	10.4%
Residues in generously allowed regions [~a,~b,~l,~p]	0	0.0%
Residues in disallowed regions	0	0.0%
	----	------
Number of non-glycine and non-proline residues	202	100.0%
Number of end-residues (excl. Gly and Pro)	151	
Number of glycine residues (shown as triangles)	14	
Number of proline residues	14	

Total number of residues	381	

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.