Viewing pde6b_sm_52-221.pdb_4_1FH_reg-multi.table

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All-Atom Contacts	Clashscore, all atoms:	1.85		99th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	3	1.95%	Goal: <1%
	Ramachandran outliers	3	1.79%	Goal: <0.05%
	Ramachandran favored	150	89.29%	Goal: >98%
	MolProbity score^	1.73		88th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	2	1.21%	Goal: 0
	Bad backbone bonds:	0 / 1367	0.00%	Goal: 0%
	Bad backbone angles:	15 / 1853	0.81%	Goal: <0.1%

In the two column results, the left column gives the raw count, right column gives the percentage.

* 100th percentile is the best among structures of comparable resolution; 0th percentile is the worst. For clashscore the comparative set of structures was selected in 2004, for MolProbity score in 2006.

^ MolProbity score combines the clashscore, rotamer, and Ramachandran evaluations into a single score, normalized to be on the same scale as X-ray resolution.

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.00	Clashscore: 1.85	Outliers: 3 of 168	Poor rotamers: 3 of 154	Outliers: 2 of 165	Outliers: 0 of 170	Outliers: 14 of 170
B 52		GLN	50	-	-	93.7% (*mm-40*) chi angles: 291.2,303.3,318.1	0.155Å	-	-
B 53		VAL	50	-	Favored (42.01%) Isoleucine or valine / -72.5,-49.4	64.6% (*t*) chi angles: 171.3	0.103Å	-	OUTLIER(S) worst is C-N-CA: 4.667 σ
B 54		GLU	50	-	Allowed (0.45%) General / -67.7,7.8	2.4% (*pm0*) chi angles: 75,310.6,336.1	0.095Å	-	OUTLIER(S) worst is CB-CG-CD: 4.201 σ
B 55		GLU	50	0.482Å OE1 with B 78 LYS NZ	Favored (97.37%) General / -62.9,-40.4	9.7% (*mm-40*) chi angles: 271.6,273.6,309.5	0.105Å	-	-
B		SER	50	-	Favored (78.65%)	74.9% (*m*)	0.105Å	-	-

56				General / -69.1,-37.8	chi angles: 294.3			
B 57	THR	50	-	Favored (32.12%) General / -81.5,-32.9	31.7% (*p*) chi angles: 51.5	0.112Å	-	-
B 58	ALA	50	-	Favored (78.87%) General / -66.4,-34.9	-	0.108Å	-	-
B 59	LEU	50	-	Favored (45.62%) General / -78.6,-26.9	75.2% (*mt*) chi angles: 299.9,171.2	0.136Å	-	-
B 60	LEU	50	-	Favored (36.61%) General / -68.0,-52.4	10.4% (*tp*) chi angles: 180.8,43.3	0.067Å	-	-
B 61	GLU	50	-	Favored (87.93%) General / -61.7,-38.5	0.5% chi angles: 283,63,279.5	0.118Å	-	-
B 62	LEU	50	-	Favored (68.32%) General / -53.2,-48.1	20.7% (*tp*) chi angles: 178.4,76.1	0.048Å	-	-
B 63	VAL	50	-	Favored (10.4%) Isoleucine or valine / -81.7,-21.3	3.3% (*p*) chi angles: 79.9	0.193Å	-	-
B 64	GLN	50	-	Favored (12.98%) General / -95.0,-32.8	11.7% (*pt20*) chi angles: 72.8,193.8,15.1	0.176Å	-	-
B 65	ASP	50	-	Favored (67.25%) General / -72.0,-32.4	23.7% (*m-20*) chi angles: 298.8,3.5	0.1Å	-	-
B 66	MET	99.99	-	Favored (3.99%) General / -135.7,98.7	21.9% (*ptp*) chi angles: 55.3,174.6,68.1	0.069Å	-	-
B 67	GLN	99.99	-	Favored (13.88%) General / -117.5,11.4	15.3% (*pt20*) chi angles: 61.6,178.2,15.7	0.107Å	-	OUTLIER(S) worst is C-N- CA: 4.052 σ
B 68	GLU	99.99	-	OUTLIER (0.04%) General /	15.3% (*pm0*) chi angles: 63.5,271.1,39.2	0.084Å	-	OUTLIER(S) worst is C-N- CA: 5.365 σ

-70.9,32.1

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
B 69		SER	99.99	-	OUTLIER (0%) General / 137.1,-174.0	26.8% (*t*) chi angles: 185.6	0.116Å	-	OUTLIER(S) worst is C-N-CA: 5.192 σ
B 70		ILE	50	-	OUTLIER (0%) Isoleucine or valine / 106.1,0.4	0.3% chi angles: 83.9,211.9	0.405Å	-	-
B 71		ASN	99.99	-	Allowed (0.06%) General / 70.4,102.1	35.1% (*m120*) chi angles: 300.4,110.8	0.127Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.00	Clashscore: 1.85	Outliers: 3 of 168	Poor rotamers: 3 of 154	Outliers: 2 of 165	Outliers: 0 of 170	Outliers: 14 of 170
B 72		MET	50	-	Favored (81.28%) General / -60.3,-37.7	16.8% (*mmt*) chi angles: 283.6,285.4,181.9	0.074Å	-	-
B 73		GLU	50	-	Allowed (0.26%) General / -44.1,-26.0	39% (*mp0*) chi angles: 291,65.8,11.1	0.097Å	-	OUTLIER(S) worst is CB-CG-CD: 5.767 σ
B 74		ARG	99.99	-	Favored (98.65%) General / -62.5,-41.2	80.2% (*mtm-85*) chi angles: 291.9,201.9,289.6,287.5	0.136Å	-	-
B 75		VAL	99.99	0.542Å HB with B 219 TYR CZ	Favored (12.32%) Isoleucine or valine / -81.2,-32.6	86.3% (*t*) chi angles: 175	0.097Å	-	-
B 76		VAL	50	-	Favored (54.67%) Isoleucine or valine / -53.1,-47.9	93.4% (*t*) chi angles: 175.7	0.096Å	-	-
B 77		PHE	50	-	Favored (83.09%) General / -59.0,-48.0	77.5% (*t80*) chi angles: 183,70.7	0.066Å	-	-
B 78		LYS	50	0.482Å NZ with B 55 GLU OE1	Favored (83.37%) General / -57.4,-43.0	69% (*mttt*) chi angles: 285.5,199.3,161.8,184.3	0.152Å	-	-
B 79		VAL	50	-	Favored (51.36%) Isoleucine or valine / -72.9,-36.4	16.9% (*m*) chi angles: 305.2	0.258Å	-	-

B 80	LEU	50	-	Favored (76.82%) General / -63.7,-34.0	53% (*mt*) chi angles: 290.2,182.6	0.141Å	-	-
B 81	ARG	99.99	-	Favored (91.92%) General / -64.8,-38.7	41% (*mtm105*) chi angles: 292.9,186.7,301.8,97.5	0.059Å	-	-
B 82	ARG	50	-	Favored (60.98%) General / -74.5,-28.4	4.1% (*mmt-85*) chi angles: 294.5,292.4,138.1,264.5	0.138Å	-	-
B 83	LEU	50	-	Favored (83.34%) General / -63.6,-47.0	26.7% (*tp*) chi angles: 186.9,53.9	0.04Å	-	-
B 84	CYS	50	-	Favored (92.4%) General / -61.3,-39.9	74% (*m*) chi angles: 296.8	0.139Å	-	-
B 85	THR	50	-	Favored (80.13%) General / -61.9,-36.0	7% (*p*) chi angles: 42.8	0.163Å	-	-
B 86	LEU	50	-	Favored (20.38%) General / -95.5,-18.7	70% (*mt*) chi angles: 304.8,179.5	0.176Å	-	-
B 87	LEU	50	-	Favored (23.54%) General / -88.3,-23.1	95.2% (*mt*) chi angles: 295,177.4	0.079Å	-	-
B 88	GLN	50	-	Favored (18.8%) General / 51.9,50.3	2.8% (*pt20*) chi angles: 74.7,186.1,190	0.231Å	-	-
B 89	ALA	50	-	Favored (25.5%) General / -89.7,145.0	-	0.101Å	-	-
B 90	ASP	50	-	Favored (95.14%) General / -62.3,-45.0	38.4% (*t70*) chi angles: 186.9,62.8	0.122Å	-	-
B 91	ARG	50	-	Favored (44.32%) General / -149.0,158.6	65.5% (*mtt180*) chi angles: 304.1,170.3,195.1,203.1	0.061Å	-	-

High   **Clash >**   **Cβ**   **Bond**   **Bond**

# Alt Res	B	0.4Å	Ramachandran	Rotamer	deviation	lengths	angles
	Avg: 55.00	Clashscore: 1.85	Outliers: 3 of 168	Poor rotamers: 3 of 154	Outliers: 2 of 165	Outliers: 0 of 170	Outliers: 14 of 170
B 92	CYS 50	-	Favored (16.85%) General / -120.7,164.3	41.5% (*m*) chi angles: 282.9	0.033Å	-	-
B 93	SER 50	-	Favored (41.21%) General / -150.6,162.1	96% (*p*) chi angles: 66.7	0.039Å	-	-
B 94	LEU 50	-	Favored (51.36%) General / -126.7,131.5	8% (*tt*) chi angles: 185.5,142.7	0.04Å	-	-
B 95	PHE 50	-	Favored (55.08%) General / -111.3,126.6	25.5% (*m-85*) chi angles: 289.9,69.6	0.058Å	-	-
B 96	MET 50	-	Favored (37.56%) General / -78.3,134.3	62.1% (*tpp*) chi angles: 182.3,60.7,72	0.092Å	-	-
B 97	TYR 50	-	Favored (49.94%) General / -103.1,131.7	52.7% (*t80*) chi angles: 181.9,94.1	0.078Å	-	-
B 98	ARG 50	-	Favored (3.85%) General / -142.6,-173.4	83.8% (*mtm180*) chi angles: 291.2,185.7,293.5,184.4	0.082Å	-	-
B 99	GLN 99.99	-	Favored (4.87%) General / -142.8,107.5	64% (*tt0*) chi angles: 187.9,181.7,16.4	0.081Å	-	-
B 100	ARG 50	-	Favored (4.69%) General / -138.9,103.0	5% (*tmm_?*) chi angles: 181.3,255.8,293.6,190.3	0.065Å	-	OUTLIER(S) worst is C-N-CA: 4.099 σ
B 101	ASN 50	-	Allowed (1.78%) General / -114.8,82.8	36.1% (*m120*) chi angles: 297,116	0.042Å	-	-
B 102	GLY 50	-	Favored (5.36%) Glycine / 129.4,-19.6	-	-	-	-
B			Favored (36.31%)	28% (*m*)			

# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
103 VAL	50	-	Isoleucine or valine / -112.6,139.7	chi angles: 296.6	0.051Å	-	-
B 104 ALA	50	-	Favored (44.52%) General / -73.3,136.6	-	0.047Å	-	-
B 105 GLU	50	-	Favored (16.65%) General / -146.6,170.6	21.4% (*pt-20*) chi angles: 71.2,173.6,27.5	0.025Å	-	-
B 106 LEU	50	-	Favored (15.89%) General / -143.4,126.0	6.3% (*tt*) chi angles: 175.6,142.1	0.156Å	-	-
B 107 ALA	50	-	Favored (35.48%) General / -122.4,155.7	-	0.136Å	-	-
B 108 THR	50	-	Favored (28.11%) General / -66.0,158.5	2.9% (*p*) chi angles: 39.6	0.122Å	-	-
B 109 ARG	50	-	Allowed (0.17%) General / -148.6,-51.6	1.5% (*tpm_?*) chi angles: 202.4,75,273.8,268.7	0.042Å	-	-
B 110 LEU	50	-	Favored (44.76%) General / -127.2,127.6	78.8% (*mt*) chi angles: 288.4,169.6	0.061Å	-	-
B 111 PHE	99.99	-	Favored (51.4%) General / -133.2,153.6	87.3% (*t80*) chi angles: 181.2,75.2	0.082Å	-	-
# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
	Avg: 55.00	Clashscore: 1.85	Outliers: 3 of 168	Poor rotamers: 3 of 154	Outliers: 2 of 165	Outliers: 0 of 170	Outliers: 14 of 170
B 112 SER	50	-	Favored (22.81%) General / 59.3,39.2	16.5% (*m*) chi angles: 283.4	0.132Å	-	-
B 113 VAL	50	-	Favored (32.56%) Isoleucine or valine / -76.2,123.5	47.5% (*t*) chi angles: 183	0.052Å	-	-
			Allowed				

B 114	GLN	50	-	(0.54%) Pre-proline / -120.4,-178.1	71.7% (*mt-30*) chi angles: 287.8,192.6,329.5	0.111Å	-	-
B 115	PRO	50	-	Favored (89.9%) Trans-proline / -54.8,-36.0	0.2% chi angles: 319.3	0.028Å	-	-
B 116	ASP	99.99	-	Favored (2.38%) General / -140.5,17.8	57.7% (*m-20*) chi angles: 303.4,324.3	0.068Å	-	-
B 117	SER	50	-	Favored (37.23%) General / -66.3,155.5	2.9% (*p*) chi angles: 39.1	0.133Å	-	-
B 118	VAL	50	-	Favored (2.15%) Isoleucine or valine / -87.6,165.2	33.5% (*m*) chi angles: 299.7	0.202Å	-	-
B 119	LEU	50	-	Favored (78.25%) General / -65.9,-46.5	29.7% (*tp*) chi angles: 167.9,67.5	0.06Å	-	OUTLIER(S) worst is C-N-CA: 4.461 σ
B 120	GLU	50	-	Favored (85.55%) General / -66.6,-43.2	31.1% (*mp0*) chi angles: 302.5,70,355.8	0.126Å	-	OUTLIER(S) worst is CB-CG-CD: 6.735 σ
B 121	ASP	50	-	Favored (68.21%) General / -56.4,-35.8	4.3% (*m-20*) chi angles: 305.4,10.1	0.072Å	-	-
B 122	CYS	50	-	Favored (21.16%) General / -87.8,-29.3	67.1% (*m*) chi angles: 302.1	0.068Å	-	-
B 123	LEU	50	-	Favored (12.25%) General / -80.6,106.0	60.3% (*tp*) chi angles: 176.1,60.2	0.035Å	-	-
B 124	VAL	50	-	Favored (67.56%) Pre-proline / -80.9,117.3	12.1% (*p*) chi angles: 62.1	0.132Å	-	-
B 125	PRO	50	-	Favored (28.63%) Trans-proline / -78.5,161.0	73.6% (*Cg_endo*) chi angles: 33.4	0.043Å	-	-
B	PRO	50	-	Favored (7.12%)	38.8% (*Cg_exo*)	0.075Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
					Trans-proline / -52.4,-17.9	chi angles: 325.8			
B 127		ASP	50	-	Favored (55.39%) General / -55.1,-28.8	11.8% (*m-20*) chi angles: 312.6,288.8	0.065Å	-	-
B 128		SER	50	-	Allowed (0.48%) General / -153.3,37.5	38.6% (*t*) chi angles: 181.8	0.069Å	-	-
B 129		GLU	50	-	Favored (36.23%) General / -76.8,149.2	19.7% (*pt-20*) chi angles: 63.3,173.3,33.7	0.04Å	-	-
B 130		ILE	50	-	Favored (12.83%) Isoleucine or valine / -104.6,145.7	23.2% (*pt*) chi angles: 67.2,180.4	0.109Å	-	-
B 131		VAL	50	-	Favored (50.33%) Isoleucine or valine / -136.1,134.8	48% (*t*) chi angles: 182.9	0.078Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.00	Clashscore: 1.85	Outliers: 3 of 168	Poor rotamers: 3 of 154	Outliers: 2 of 165	Outliers: 0 of 170	Outliers: 14 of 170
B 132		PHE	50	-	Favored (23.8%) Pre-proline / -118.1,136.3	72.1% (*m-85*) chi angles: 292.9,290.1	0.087Å	-	-
B 133		PRO	50	-	Favored (56.04%) Trans-proline / -65.8,158.0	82.6% (*Cg_exo*) chi angles: 330.8	0.064Å	-	-
B 134		LEU	50	-	Favored (60.65%) General / -73.3,-21.0	22.2% (*mt*) chi angles: 309,189.3	0.167Å	-	-
B 135		ASP	50	-	Favored (67.83%) General / -71.2,-43.3	21.2% (*p-10*) chi angles: 52.9,340.3	0.066Å	-	OUTLIER(S) worst is CA-CB-CG: 4.1 σ
B 136		ILE	50	-	Favored (13.89%) Isoleucine or valine / -74.6,114.0	60.4% (*mt*) chi angles: 301.3,180	0.049Å	-	-

B 137	GLY	50	-	Favored (19.93%) Glycine / 99.5,146.4	-	-	-	-
B 138	VAL	50	-	Favored (63.61%) Isoleucine or valine / -53.9,-45.5	2.1% (*m*) chi angles: 279.1	0.157Å	-	-
B 139	VAL	50	-	Favored (95.14%) Isoleucine or valine / -61.3,-42.9	13.9% (*p*) chi angles: 64.8	0.184Å	-	-
B 140	GLY	50	-	Favored (97.26%) Glycine / -64.8,-40.2	-	-	-	-
B 141	HIS	99.99	-	Favored (76.98%) General / -61.3,-35.3	84.2% (*t60*) chi angles: 182.9,63.9	0.061Å	-	-
B 142	VAL	50	-	Favored (85.74%) Isoleucine or valine / -68.0,-42.8	50.1% (*t*) chi angles: 168.6	0.105Å	-	-
B 143	ALA	50	-	Favored (90.02%) General / -65.8,-43.0	-	0.066Å	-	-
B 144	GLN	50	-	Favored (86.56%) General / -61.6,-47.2	40.9% (*tt0*) chi angles: 175.1,185.8,75.8	0.043Å	-	-
B 145	THR	50	-	Favored (50.33%) General / -77.5,-25.4	48.1% (*p*) chi angles: 55.5	0.155Å	-	-
B 146	LYS	50	-	Favored (20.98%) General / 60.2,36.4	51.9% (*mtpt*) chi angles: 296.4,186.4,68.5,183.4	0.179Å	-	-
B 147	LYS	50	-	Favored (50.59%) General / -127.9,146.5	48.1% (*tttm*) chi angles: 185.2,189.2,168.4,294.3	0.053Å	-	-
B 148	MET	99.99	-	Favored (38.2%) General /	75.6% (*mtm*) chi angles:	0.084Å	-	-

-77.0,145.0   299.8,183.9,288.9

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
B 149		VAL	50	-	Favored (23.63%) Isoleucine or valine / -140.4,147.1	8.8% (*p*) chi angles: 73.2	0.093Å	-	-
B 150		ASN	50	-	Favored (53.1%) General / -118.8,127.0	61% (*t-20*) chi angles: 181.2,349.6	0.123Å	-	-
B 151		VAL	50	-	Favored (19.82%) Isoleucine or valine / -124.5,108.1	95.1% (*t*) chi angles: 176.8	0.046Å	-	OUTLIER(S) worst is C-N-CA: 4.487 σ

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.00	Clashscore: 1.85	Outliers: 3 of 168	Poor rotamers: 3 of 154	Outliers: 2 of 165	Outliers: 0 of 170	Outliers: 14 of 170
B 152		GLU	50	-	Favored (47.48%) General / -81.7,-17.5	22.4% (*mp0*) chi angles: 305.8,79.3,337.1	0.066Å	-	OUTLIER(S) worst is CB-CG-CD: 4.462 σ
B 153		ASP	50	-	Favored (2.05%) General / -157.5,105.5	10.4% (*t0*) chi angles: 206.3,332	0.03Å	-	-
B 154		VAL	50	-	Favored (2.48%) Isoleucine or valine / -65.3,162.6	33.5% (*m*) chi angles: 299.7	0.129Å	-	-
B 155		ALA	50	-	Allowed (0.1%) General / 81.9,-31.2	-	0.219Å	-	-
B 156		GLU	50	-	Favored (60.13%) General / -70.0,-47.9	8.6% (*tm-20*) chi angles: 179.2,294,332.5	0.068Å	-	-
B 157		CYS	50	-	Favored (39.54%) Pre-proline / -58.5,119.8	49.6% (*t*) chi angles: 186.3	0.082Å	-	-
B 158		PRO	50	-	Favored (7.3%) Trans-proline / -79.1,3.6	44.4% (*Cg_endo*) chi angles: 35.7	0.03Å	-	-

B 159	HIS	50	-	Favored (21.29%) General / -96.2,-16.7	90% (*m-70*) chi angles: 306,288.5	0.069Å	-	-
B 160	PHE	50	-	Favored (48.58%) General / -55.3,136.8	54.8% (*t80*) chi angles: 179.7,62.2	0.048Å	-	-
B 161	SER	50	-	Favored (56%) General / -117.5,129.8	39.9% (*t*) chi angles: 176.5	0.062Å	-	-
B 162	SER	50	-	Favored (56.64%) General / -93.6,0.6	59.4% (*p*) chi angles: 55.9	0.061Å	-	-
B 163	PHE	50	-	Favored (42.37%) General / -49.1,-44.2	68.8% (*t80*) chi angles: 184,86.5	0.088Å	-	-
B 164	ALA	50	-	Favored (72.82%) General / -71.0,-38.9	-	0.101Å	-	-
B 165	ASP	50	-	Favored (93.93%) General / -62.8,-39.4	8.1% (*m-20*) chi angles: 291.5,21.1	0.053Å	-	-
B 166	GLU	50	-	Favored (66.6%) General / -73.1,-36.0	34.4% (*mt-10*) chi angles: 294.6,166.8,274.4	0.049Å	-	-
B 167	LEU	50	-	Favored (56.89%) General / -76.6,-37.2	7.8% (*tt*) chi angles: 192.6,148	0.079Å	-	-
B 168	THR	50	-	Favored (16.41%) General / -102.8,-15.0	31.5% (*p*) chi angles: 69.4	0.135Å	-	-
B 169	ASP	50	-	Allowed (0.1%) General / 85.6,-26.2	34.1% (*t0*) chi angles: 198.5,1.5	0.108Å	-	-
B 170	TYR	50	-	Favored (2.84%) General / -51.4,151.9	31.8% (*t80*) chi angles: 195.1,69.7	0.033Å	-	-
B 171	LYS	50	-	Favored (11.95%) General / -126.6,109.3	41.9% (*mmtm*) chi angles: 300,299,170.8,284.4	0.031Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.00	Clashscore: 1.85	Outliers: 3 of 168	Poor rotamers: 3 of 154	Outliers: 2 of 165	Outliers: 0 of 170	Outliers: 14 of 170
B 172		THR	50	-	Favored (38.92%) General / -76.8,135.1	96.3% (*m*) chi angles: 299.6	0.096Å	-	-
B 173		LYS	50	-	Allowed (1.17%) General / -129.4,-55.0	56% (*tptt*) chi angles: 187.4,62,176.4,173.5	0.071Å	-	-
B 174		ASN	50	-	Favored (47.38%) General / -115.8,142.0	31.8% (*m-20*) chi angles: 308.7,332.7	0.124Å	-	-
B 175		MET	50	-	Favored (11.75%) General / -154.1,132.2	42.8% (*ttm*) chi angles: 175.7,192.8,289.9	0.064Å	-	-
B 176		LEU	50	-	Favored (52.4%) General / -104.5,131.0	8.7% (*mp*) chi angles: 268.9,55.1	0.082Å	-	-
B 177		ALA	50	-	Favored (22%) General / -142.4,130.5	-	0.05Å	-	-
B 178		THR	99.99	-	Favored (27.56%) Pre-proline / -135.4,137.9	7.9% (*m*) chi angles: 286.1	0.087Å	-	-
B 179		PRO	50	-	Allowed (0.81%) Trans-proline / -92.5,127.3	19.7% (*Cg_endo*) chi angles: 38.7	0.063Å	-	-
B 180		ILE	50	-	Favored (36.41%) Isoleucine or valine / -76.8,125.2	45% (*mt*) chi angles: 297.2,184	0.053Å	-	-
B 181		MET	50	-	Favored (34.62%) General / -131.9,126.7	20.1% (*ptp*) chi angles: 59.1,181.1,84	0.028Å	-	-
B 182		ASN	50	-	Allowed (1.85%) General / -99.3,72.8	80.9% (*m-20*) chi angles: 289.2,353.1	0.094Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
B 183		GLY	50	-	Allowed (0.22%) Glycine / 66.9,-93.4	-	-	-	-
B 184		LYS	50	0.461Å NZ with B 185 ASP OD2	Favored (69.82%) General / -65.2,-49.5	19.6% (*ttpp*) chi angles: 181.3,194.9,66.4,60	0.077Å	-	-
B 185		ASP	50	0.461Å OD2 with B 184 LYS NZ	Favored (14.39%) General / -119.5,165.4	4.5% (*t0*) chi angles: 217.8,332.6	0.14Å	-	-
B 186		VAL	50	-	Favored (15.62%) Isoleucine or valine / -94.5,141.0	70.1% (*t*) chi angles: 173.6	0.105Å	-	-
B 187		VAL	50	-	Favored (2.9%) Isoleucine or valine / -103.7,-29.5	8.5% (*p*) chi angles: 68.5	0.199Å	-	-
B 188		ALA	50	-	Favored (14.05%) General / -167.4,167.2	-	0.103Å	-	-
B 189		VAL	50	-	Favored (73.23%) Isoleucine or valine / -124.6,127.9	95.3% (*t*) chi angles: 175.9	0.048Å	-	-
B 190		ILE	99.99	-	Favored (8.95%) Isoleucine or valine / -105.1,148.9	47.5% (*mt*) chi angles: 291.9,182.6	0.061Å	-	-
B 191		MET	50	-	Favored (43.04%) General / -144.9,159.4	16.2% (*ptp*) chi angles: 70.7,194.3,61.9	0.026Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.00	Clashscore: 1.85	Outliers: 3 of 168	Poor rotamers: 3 of 154	Outliers: 2 of 165	Outliers: 0 of 170	Outliers: 14 of 170
B 192		ALA	50	-	Favored (55.18%) General / -120.5,135.1	-	0.1Å	-	-
B		VAL	50	-	Favored (26.7%) Isoleucine or	12.4% (*p*) chi angles: 65.8	0.113Å	-	OUTLIER(S) worst is C-N-

193				valine / -122.2,146.9				CA: 4.121 σ
B 194	ASN	50	-	Allowed (0.07%) General / 51.2,81.8	76.9% (*m-20*) chi angles: 295.2,350.3	0.092Å	-	-
B 195	LYS	50	-	Favored (5.78%) General / -47.1,123.8	54.1% (*tptt*) chi angles: 182.7,67.8,165.1,180.7	0.111Å	-	-
B 196	LEU	50	-	Favored (28.1%) General / -87.3,142.2	66.4% (*mt*) chi angles: 300.1,169.7	0.073Å	-	-
B 197	ASN	50	-	Favored (18.66%) General / 61.6,30.4	32.7% (*m-20*) chi angles: 313.1,313.2	0.06Å	-	-
B 198	GLY	50	-	Favored (32.85%) Glycine / -164.0,160.0	-	-	-	-
B 199	PRO	50	-	Allowed (1.14%) Trans-proline / -81.8,-31.2	96.7% (*Cg_endo*) chi angles: 30.6	0.09Å	-	-
B 200	PHE	50	-	Favored (21.47%) General / -151.6,169.7	44.5% (*p90*) chi angles: 63.1,97.5	0.049Å	-	-
B 201	PHE	50	-	Favored (34.47%) General / -80.5,129.4	77% (*m-85*) chi angles: 287.8,276.7	0.103Å	-	-
B 202	THR	50	-	Favored (8.04%) General / -78.6,178.2	29.8% (*p*) chi angles: 70.5	0.066Å	-	-
B 203	SER	50	-	Favored (89.51%) General / -62.9,-38.1	49.9% (*m*) chi angles: 301	0.079Å	-	-
B 204	GLU	50	-	Favored (86.24%) General / -60.5,-39.0	28.2% (*mp0*) chi angles: 308.2,74.1,356.6	0.129Å	-	OUTLIER(S) worst is CB-CG-CD: 5.106 σ
				Favored				

B 205	ASP	50	-	(95.12%) General / -60.3,-44.8	79.6% (*m-20*) chi angles: 291.2,326.5	0.137Å	-	-
B 206	GLU	50	-	Favored (72.38%) General / -54.9,-48.9	57.6% (*mt-10*) chi angles: 292.8,183.8,35.6	0.101Å	-	-
B 207	ASP	50	0.43Å HB3 with B 211 LYS NZ	Favored (70%) General / -60.5,-30.8	8.6% (*m-20*) chi angles: 286.6,274.5	0.168Å	-	-
B 208	VAL	50	-	Favored (26.3%) Isoleucine or valine / -78.4,-42.4	72.4% (*t*) chi angles: 173.8	0.07Å	-	-
B 209	PHE	50	-	Favored (87.07%) General / -59.0,-46.9	71.4% (*t80*) chi angles: 184.3,69.9	0.066Å	-	-
B 210	LEU	50	-	Favored (95.43%) General / -61.7,-40.5	10.1% (*mp*) chi angles: 273.9,55.7	0.084Å	-	-
B 211	LYS	50	0.43Å NZ with B 207 ASP HB3	Favored (81.14%) General / -63.8,-47.4	40.4% (*mttp*) chi angles: 285.3,164.5,192.3,72.2	0.101Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.00	Clashscore: 1.85	Outliers: 3 of 168	Poor rotamers: 3 of 154	Outliers: 2 of 165	Outliers: 0 of 170	Outliers: 14 of 170
B 212		TYR	50	-	Favored (85.2%) General / -65.8,-37.0	11.9% (*m-85*) chi angles: 270.2,274.1	0.099Å	-	-
B 213		LEU	50	-	Favored (67.11%) General / -68.3,-28.4	1.8% (*mp*) chi angles: 260.7,84.7	0.224Å	-	-
B 214		ASN	50	-	Favored (71.39%) General / -60.2,-32.7	88.6% (*m-20*) chi angles: 296.1,325.9	0.114Å	-	-
B 215		PHE	50	-	Favored (39%) General / -74.4,-46.6	60.4% (*t80*) chi angles: 181.2,91.5	0.067Å	-	-
B 216		ALA	50	-	Favored (72.12%) General / -63.5,-31.1	-	0.112Å	-	-

B 217	THR	50	-	Favored (57.81%) General / -68.7,-49.6	23% (*p*) chi angles: 49.5	0.114Å	-	-
B 218	LEU	50	-	Favored (71.4%) General / -57.6,-36.2	90.4% (*mt*) chi angles: 297.6,171.9	0.073Å	-	-
B 219	TYR	99.99	0.542Å CZ with B 75 VAL HB	Favored (85.95%) General / -66.1,-37.5	65.5% (*t80*) chi angles: 187.8,79.4	0.112Å	-	-
B 220	LEU	50	-	Favored (6.96%) General / -87.8,62.4	82.8% (*mt*) chi angles: 294.1,179.9	0.074Å	-	-
B 221	LYS	99.99	0.445Å HG2 with B 221 LYS O	-	11.4% (*ttpp*) chi angles: 192.8,197.5,57.6,48.5	0.085Å	-	-

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