Viewing pde6b_sm_52-221H-multi.table

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All-Atom Contacts	Clashscore, all atoms:	25.22		21st percentile[*] (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	5	3.25%	Goal: <1%
	Ramachandran outliers	6	3.57%	Goal: <0.05%
	Ramachandran favored	151	89.88%	Goal: >98%
	MolProbity score[^]	2.83		30th percentile[*] (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	2	1.21%	Goal: 0
	Bad backbone bonds:	4 / 1367	0.29%	Goal: 0%
	Bad backbone angles:	11 / 1853	0.59%	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: 25.22	Outliers: 6 of 168	Poor rotamers: 5 of 154	Outliers: 2 of 165	Outliers: 2 of 170	Outliers: 9 of 170
B 52		GLN	50	-	-	53.8% (*tt0*) chi angles: 185.4,179.9,57	0.041Å	-	-
B 53		VAL	50	-	Favored (60.25%) Isoleucine or valine / -66.5,-32.9	11.5% (*p*) chi angles: 61.7	0.078Å	-	-
B 54		GLU	50	-	Favored (53.15%) General / -90.9,4.0	0.1% chi angles: 82.4,136.3,331.3	0.064Å	-	-
B 55		GLU	50	-	Favored (82.66%) General / -57.1,-46.2	49.4% (*mm-40*) chi angles: 276.5,294.5,313.9	0.011Å	-	-
B 56		SER	50	-	Favored (82.43%) General / -60.2,-38.1	32.1% (*t*) chi angles: 184.4	0.009Å	-	-

B 57	THR	50	-	Favored (28.43%) General / -78.7,-42.4	73.2% (*p*) chi angles: 59.9	0.03Å	-	-
B 58	ALA	50	-	Favored (85.07%) General / -58.6,-41.1	-	0.019Å	-	-
B 59	LEU	50	0.436Å O with B 62 LEU HB3	Favored (70.04%) General / -71.7,-35.0	98.2% (*mt*) chi angles: 297,176.9	0.009Å	-	-
B 60	LEU	50	0.53Å HD13 with B 219 TYR HD1	Favored (66.79%) General / -71.0,-44.0	47.8% (*tp*) chi angles: 182.2,57.2	0.059Å	-	-
B 61	GLU	50	0.482Å HA with B 64 GLN HG2	Favored (77.26%) General / -67.0,-34.2	0% chi angles: 256.8,66.5,315.1	0.02Å	-	-
B 62	LEU	50	0.436Å HB3 with B 59 LEU O	Favored (40.58%) General / -57.8,-55.0	20.3% (*tp*) chi angles: 171.9,75.2	0.083Å	-	-
B 63	VAL	50	0.72Å HA with B 70 ILE HD11	Favored (35.67%) Isoleucine or valine / -69.7,-28.0	8.7% (*p*) chi angles: 70.6	0.151Å	-	-
B 64	GLN	50	0.482Å HG2 with B 61 GLU HA	Favored (21.3%) General / -89.7,-25.4	18.4% (*pt20*) chi angles: 66.3,180.8,56.9	0.087Å	-	-
B 65	ASP	50	-	Favored (48.69%) General / -77.8,-37.5	31.1% (*t70*) chi angles: 188.7,49.8	0.049Å	-	-
B 66	MET	99.99	0.497Å HG3 with B 66 MET O	Favored (4.46%) General / -131.2,98.1	23.6% (*ptp*) chi angles: 62.2,172.2,68.6	0.039Å	-	-
B 67	GLN	99.99	0.447Å C with B 69 SER H	Favored (13.17%) General / -117.4,21.3	9.8% (*pm0*) chi angles: 68.5,289,356.1	0.01Å	-	OUTLIER(S) worst is OE1-CD-NE2: 4.246 σ
B 68	GLU	99.99	-	OUTLIER (0.04%) General / -70.5,29.1	17.2% (*pm0*) chi angles: 58.8,279.9,2.8	0.075Å	-	OUTLIER(S) worst is C-N-CA: 4.715 σ
B			0.545Å	OUTLIER (0%)	12% (*p*)			

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
69		SER	99.99	O with B 70 ILE HG12	General / 141.8,163.9	chi angles: 47.4	0.149Å	-	-
B 70		ILE	50	0.72Å HD11 with B 63 VAL HA	OUTLIER (0%) Isoleucine or valine / 132.3,27.5	3.2% (pt) chi angles: 72.6,196.8	0.252Å	-	-
B 71		ASN	99.99	-	OUTLIER (0.02%) General / 54.7,94.4	81.2% (m-20) chi angles: 298.5,332.4	0.089Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.00	Clashscore: 25.22	Outliers: 6 of 168	Poor rotamers: 5 of 154	Outliers: 2 of 165	Outliers: 2 of 170	Outliers: 9 of 170
B 72		MET	50	0.844Å HA with B 219 TYR OH	Favored (36.52%) General / -64.8,-11.4	18.8% (mmt) chi angles: 285.8,289.5,186.8	0.287Å	-	OUTLIER(S) worst is CA-C-O: 5.709 σ
B 73		GLU	50	-	Favored (56.29%) General / -75.8,-25.3	16.1% (mp0) chi angles: 282.9,58.7,38.5	0.133Å	-	-
B 74		ARG	99.99	0.507Å HG2 with B 119 LEU HD21	Favored (82.38%) General / -68.2,-40.5	93.2% (mtm-85) chi angles: 295.6,196.8,290.1,276.4	0.067Å	-	-
B 75		VAL	99.99	0.763Å HB with B 219 TYR CZ	Favored (65.1%) Isoleucine or valine / -71.4,-37.4	89.1% (t) chi angles: 175.2	0.111Å	-	-
B 76		VAL	50	0.596Å HA with B 79 VAL HG22	Favored (81.01%) Isoleucine or valine / -63.1,-38.0	89.6% (t) chi angles: 177.9	0.039Å	-	-
B 77		PHE	50	0.418Å HE1 with B 122 CYS SG	Favored (35.24%) General / -65.8,-53.8	84.6% (t80) chi angles: 182.6,79.9	0.083Å	-	OUTLIER(S) worst is CA-CB-CG: 4.63 σ
B 78		LYS	50	0.778Å HG2 with B 81 ARG HH21	Favored (62.11%) General / -52.0,-41.4	53.3% (mttt) chi angles: 277.5,202,162.5,173.8	0.044Å	-	-
B 79		VAL	50	0.596Å HG22 with B 76 VAL HA	Favored (76.13%) Isoleucine or valine / -70.5,-39.4	24.4% (m) chi angles: 302.3	0.178Å	-	-
B		LEU	50	-	Favored (68.93%)	24.6% (mt)	0.101Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
80					General / -65.4,-28.0	chi angles: 282.5,182.1			
B 81		ARG	99.99	0.778Å HH21 with B 78 LYS HG2	Favored (52.69%) General / -64.2,-53.2	47.4% (*mtm105*) chi angles: 293,182.8,296.9,104.3	0.031Å	-	-
B 82		ARG	50	-	Favored (74.13%) General / -61.2,-33.8	1.1% (*mmt-85*) chi angles: 294.7,295.1,136.5,246.3	0.038Å	-	-
B 83		LEU	50	0.519Å HD22 with B 87 LEU HG	Favored (94%) General / -63.8,-39.3	0% chi angles: 214.8,217.5	0.028Å	-	-
B 84		CYS	50	0.469Å SG with B 92 CYS SG	Favored (89.86%) General / -63.9,-45.3	74.2% (*m*) chi angles: 298.5	0.077Å	-	-
B 85		THR	50	-	Favored (84.62%) General / -58.1,-46.9	70.5% (*p*) chi angles: 64	0.035Å	-	-
B 86		LEU	50	-	Favored (41.78%) General / -81.8,-19.2	78.6% (*mt*) chi angles: 300.5,182.5	0.098Å	-	-
B 87		LEU	50	0.629Å O with B 88 GLN HG2	Favored (20.72%) General / -89.0,-27.6	25.7% (*mt*) chi angles: 283.5,183.3	0.09Å	-	-
B 88		GLN	50	0.629Å HG2 with B 87 LEU O	Favored (23.21%) General / 55.1,34.7	13.1% (*pt20*) chi angles: 71.7,190,42.7	0.179Å	-	-
B 89		ALA	50	-	Favored (40.51%) General / -76.9,140.3	-	0.09Å	-	-
B 90		ASP	50	-	Favored (98.5%) General / -61.5,-43.6	26.3% (*t0*) chi angles: 190.5,37.2	0.023Å	-	-
B 91		ARG	50	0.412Å O with B 193 VAL HG12	Favored (30.89%) General / -151.9,151.2	98.5% (*mtt180*) chi angles: 302.2,176.4,185.2,184.2	0.024Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.00	Clashscore: 25.22	Outliers: 6 of 168	Poor rotamers: 5 of 154	Outliers: 2 of 165	Outliers: 2 of 170	Outliers: 9 of 170

Favored

B 92	CYS	50	0.469Å SG with B 84 CYS SG	(48.16%) General / -125.9,150.2	74.7% (*m*) chi angles: 296.6	0.019Å	-	-
B 93	SER	50	-	Favored (44.82%) General / -143.0,156.2	90.9% (*p*) chi angles: 62.7	0.043Å	-	-
B 94	LEU	50	0.587Å HD13 with B 76 VAL HG11	Favored (52.33%) General / -125.5,133.4	9.7% (*tt*) chi angles: 185.2,155.7	0.049Å	-	-
B 95	PHE	50	0.555Å CD2 with B 106 LEU HD21	Favored (32.62%) General / -111.5,117.3	26.2% (*m-85*) chi angles: 281.4,70.7	0.076Å	-	-
B 96	MET	50	-	Favored (56.08%) General / -66.8,144.8	61.1% (*tpp*) chi angles: 187.3,59.5,72.6	0.039Å	-	-
B 97	TYR	50	0.427Å CD2 with B 186 VAL O	Favored (29.43%) General / -119.8,117.9	75.4% (*t80*) chi angles: 183.6,83.6	0.059Å	-	-
B 98	ARG	50	-	Favored (19.28%) General / -137.2,168.6	99.5% (*mtt180*) chi angles: 287.6,180.8,174.8,177.8	0.003Å	-	-
B 99	GLN	99.99	0.646Å HE21 with B 102 GLY HA2	Favored (53.56%) General / -116.2,126.4	64.8% (*tt0*) chi angles: 186.2,179.1,356.9	0.147Å	-	-
B 100	ARG	50	0.456Å HA with B 101 ASN HA	Favored (2.06%) General / -150.8,94.3	6.9% (*tmm_?*) chi angles: 181.9,258.7,284.5,180.6	0.09Å	-	-
B 101	ASN	50	0.456Å HA with B 100 ARG HA	Allowed (1.94%) General / -122.2,82.2	64.3% (*t30*) chi angles: 188.8,31.5	0.045Å	-	-
B 102	GLY	50	0.646Å HA2 with B 99 GLN HE21	Favored (7.37%) Glycine / 126.5,0.2	-	-	-	-
B 103	VAL	50	-	Favored (32.55%) Isoleucine or valine / -137.2,125.2	34.7% (*m*) chi angles: 298.5	0.079Å	-	-
B 104	ALA	50	-	Favored (57.31%) General / -65.2,144.3	-	0.039Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
B 105		GLU	50	-	Favored (32.31%) General / -159.2,158.2	16.3% (*pt-20*) chi angles: 65.8,173.3,41.9	0.042Å	-	-
B 106		LEU	50	0.555Å HD21 with B 95 PHE CD2	Favored (47.72%) General / -126.1,128.7	9.9% (*tt*) chi angles: 181,150.9	0.234Å	-	OUTLIER(S) worst is N-CA-CB: 4.693 σ
B 107		ALA	50	-	Favored (18.14%) General / -121.7,164.0	-	0.065Å	-	-
B 108		THR	50	-	Favored (31.25%) General / -82.4,143.4	32.1% (*p*) chi angles: 51.6	0.015Å	-	-
B 109		ARG	50	-	Allowed (0.7%) General / -137.3,-58.0	0.8% chi angles: 195.3,90.7,262.7,283.4	0.071Å	-	-
B 110		LEU	50	-	Favored (45.27%) General / -121.0,124.6	44.6% (*mt*) chi angles: 283.2,174.1	0.039Å	-	-
B 111		PHE	99.99	-	Favored (47.7%) General / -129.4,153.7	82.4% (*t80*) chi angles: 183.6,78.5	0.047Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.00	Clashscore: 25.22	Outliers: 6 of 168	Poor rotamers: 5 of 154	Outliers: 2 of 165	Outliers: 2 of 170	Outliers: 9 of 170
B 112		SER	50	-	Favored (20.17%) General / 59.3,41.2	13.2% (*m*) chi angles: 282.4	0.059Å	-	-
B 113		VAL	50	-	Favored (28.57%) Isoleucine or valine / -78.2,120.2	89.5% (*t*) chi angles: 177.9	0.078Å	-	-
B 114		GLN	50	0.582Å HG2 with B 117 SER HB3	Favored (5.24%) Pre-proline / -119.1,171.5	17.4% (*pt20*) chi angles: 69.7,179.5,56.4	0.115Å	-	-
B 115		PRO	50	-	Favored (14.4%) Trans-proline / -47.4,-32.1	33.6% (*Cg_exo*) chi angles: 325.4	0.05Å	-	-

B 116	ASP	99.99	-	Favored (7.94%) General / -124.6,-2.0	83.7% (*m-20*) chi angles: 296.3,336.3	0.083Å	-	-
B 117	SER	50	0.582Å HB3 with B 114 GLN HG2	Favored (56.26%) General / -57.6,134.6	22.2% (*p*) chi angles: 50.6	0.07Å	-	-
B 118	VAL	50	-	Favored (7.89%) Isoleucine or valine / -73.0,151.1	9.4% (*p*) chi angles: 60.6	0.143Å	-	-
B 119	LEU	50	0.507Å HD21 with B 74 ARG HG2	Favored (74.95%) General / -55.3,-47.9	58.7% (*tp*) chi angles: 179.4,65.3	0.036Å	-	-
B 120	GLU	50	-	Favored (76.3%) General / -61.7,-34.7	86.6% (*mt-10*) chi angles: 297.7,185.8,333.9	0.036Å	-	-
B 121	ASP	50	-	Favored (63.21%) General / -70.0,-24.0	4.4% (*m-20*) chi angles: 291.2,28.6	0.059Å	-	-
B 122	CYS	50	0.418Å SG with B 77 PHE HE1	Favored (12.08%) General / -97.9,-31.7	74.6% (*m*) chi angles: 296.6	0.027Å	-	-
B 123	LEU	50	-	Favored (18.19%) General / -70.3,121.7	55.7% (*tp*) chi angles: 181.4,59.8	0.038Å	-	-
B 124	VAL	50	-	Favored (44.13%) Pre-proline / -100.5,106.7	9.1% (*p*) chi angles: 60.3	0.153Å	-	-
B 125	PRO	50	-	Favored (69.37%) Trans-proline / -64.7,155.0	87.5% (*Cg_endo*) chi angles: 30.1	0.048Å	-	-
B 126	PRO	50	-	Favored (3.58%) Trans-proline / -52.8,-14.7	83.3% (*Cg_exo*) chi angles: 328.7	0.062Å	-	-
B 127	ASP	50	-	Favored (39.08%) General / -52.7,-31.8	22.7% (*m-20*) chi angles: 276.6,325.3	0.037Å	-	-
B 128	SER	50	-	Allowed (0.43%) General /	62.1% (*p*) chi angles: 56.5	0.028Å	-	-

-161.2,72.3

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
B 129		GLU	50	-	Favored (18.99%) General / -111.8,158.8	20.2% (*pt-20*) chi angles: 56.5,170.2,19.1	0.013Å	-	-
B 130		ILE	50	-	Favored (70.87%) Isoleucine or valine / -114.8,123.9	12.8% (*pt*) chi angles: 74.7,178.5	0.131Å	-	-
B 131		VAL	50	-	Favored (28.07%) Isoleucine or valine / -110.8,140.9	53.5% (*t*) chi angles: 182.2	0.071Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.00	Clashscore: 25.22	Outliers: 6 of 168	Poor rotamers: 5 of 154	Outliers: 2 of 165	Outliers: 2 of 170	Outliers: 9 of 170
B 132		PHE	50	-	Favored (24.97%) Pre-proline / -123.4,134.1	90.4% (*m-85*) chi angles: 291.6,278.9	0.044Å	-	-
B 133		PRO	50	-	Favored (78.46%) Trans-proline / -64.2,153.1	81.4% (*Cg_exo*) chi angles: 331.9	0.102Å	-	-
B 134		LEU	50	-	Favored (66.82%) General / -65.7,-23.7	19.8% (*mt*) chi angles: 301.3,193.8	0.156Å	-	-
B 135		ASP	50	-	Favored (59.59%) General / -76.0,-33.4	20.4% (*p-10*) chi angles: 62.5,318.2	0.112Å	-	-
B 136		ILE	50	-	Favored (36.6%) Isoleucine or valine / -85.1,121.1	72.8% (*mt*) chi angles: 302.5,174.5	0.025Å	-	-
B 137		GLY	50	-	Favored (20.13%) Glycine / 95.0,146.1	-	-	-	-
B 138		VAL	50	0.67Å HG13 with B 160 PHE HA	Favored (65.64%) Isoleucine or valine / -64.7,-33.8	4.5% (*m*) chi angles: 284.3	0.086Å	-	-

B 139	VAL	50	0.457Å HG22 with B 106 LEU CD1	Favored (95.35%) Isoleucine or valine / -61.5,-42.8	7.5% (*p*) chi angles: 59	0.109Å	-	-
B 140	GLY	50	-	Favored (97.9%) Glycine / -63.6,-39.7	-	-	-	-
B 141	HIS	99.99	-	Favored (91.03%) General / -60.8,-40.0	83% (*t60*) chi angles: 185.2,65	0.008Å	OUTLIER(S) worst is CG--ND1: 4.329 σ	OUTLIER(S) worst is CB-CG-CD2: 4.084 σ
B 142	VAL	50	-	Favored (96.89%) Isoleucine or valine / -64.5,-43.3	96.3% (*t*) chi angles: 176.7	0.063Å	-	-
B 143	ALA	50	-	Favored (99.6%) General / -62.6,-42.5	-	0.039Å	-	-
B 144	GLN	50	-	Favored (2.75%) General / -64.6,-60.8	53.7% (*tt0*) chi angles: 185.5,179.7,56.7	0.037Å	-	-
B 145	THR	50	-	Favored (67.48%) General / -67.5,-28.1	67.1% (*p*) chi angles: 64.6	0.045Å	-	-
B 146	LYS	50	-	Favored (18.85%) General / 61.3,33.6	36.5% (*mtpt*) chi angles: 300.9,147.6,65.9,180.5	0.058Å	-	-
B 147	LYS	50	-	Favored (42.28%) General / -119.3,149.2	21.7% (*ttmm*) chi angles: 194.1,188.5,296.3,292	0.088Å	-	-
B 148	MET	99.99	0.603Å HG2 with B 178 THR HG23	Favored (29.07%) General / -79.3,154.5	76.3% (*mtm*) chi angles: 296.2,180.7,289.3	0.03Å	-	-
B 149	VAL	50	-	Favored (3.95%) Isoleucine or valine / -150.2,130.2	7.2% (*p*) chi angles: 69.4	0.112Å	-	-
B 150	ASN	50	-	Favored (16.95%) General / -111.3,107.6	54.9% (*t-20*) chi angles: 181.4,341.8	0.055Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
B 151		VAL	50	0.471Å CG2 with B 175 MET HB3	Favored (29.29%) Isoleucine or valine / -103.8,110.2	17.2% (*m*) chi angles: 305	0.124Å	-	-
			Avg: 55.00	Clashscore: 25.22	Outliers: 6 of 168	Poor rotamers: 5 of 154	Outliers: 2 of 165	Outliers: 2 of 170	Outliers: 9 of 170
B 152		GLU	50	-	Favored (58.97%) General / -75.3,-20.6	12.2% (*pt-20*) chi angles: 62.9,178.1,62.6	0.073Å	-	-
B 153		ASP	50	-	Allowed (0.66%) General / -164.3,92.9	50.6% (*t0*) chi angles: 185.3,16.3	0.042Å	-	-
B 154		VAL	50	0.4Å HB with B 160 PHE CD1	Allowed (0.81%) Isoleucine or valine / -57.5,161.4	35% (*m*) chi angles: 298.3	0.023Å	-	-
B 155		ALA	50	-	Allowed (0.1%) General / 81.7,-32.4	-	0.146Å	-	-
B 156		GLU	50	-	Favored (60.3%) General / -75.8,-14.1	57.2% (*mt-10*) chi angles: 294.8,186.3,304.6	0.026Å	-	-
B 157		CYS	50	-	Favored (65.62%) Pre-proline / -98.0,116.8	45.1% (*t*) chi angles: 183	0.026Å	-	-
B 158		PRO	50	-	Favored (60.93%) Trans-proline / -64.8,-25.1	98.1% (*Cg_endo*) chi angles: 30.6	0.066Å	-	-
B 159		HIS	50	-	Favored (54.62%) General / -76.2,-24.2	93.5% (*m-70*) chi angles: 301,296.5	0.038Å	OUTLIER(S) worst is CG--ND1: 4.369 σ	OUTLIER(S) worst is CB-CG-CD2: 4.283 σ
B 160		PHE	50	0.67Å HA with B 138 VAL HG13	Favored (4.3%) General / -49.8,120.4	74.4% (*t80*) chi angles: 185.4,73.7	0.066Å	-	-
B 161		SER	50	-	Favored (29.96%) General / -100.1,143.8	28.9% (*t*) chi angles: 172.2	0.074Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
B 162		SER 50	-		Favored (8.47%) General / -120.8,27.5	89.1% (*p*) chi angles: 62.1	0.024Å	-	-
B 163		PHE 50	-		Favored (88.81%) General / -66.5,-39.8	81.8% (*t80*) chi angles: 182.5,82.2	0.019Å	-	-
B 164		ALA 50	-		Favored (41.77%) General / -79.2,-35.5	-	0.014Å	-	-
B 165		ASP 50	-		Favored (81.06%) General / -63.0,-35.7	17.6% (*m-20*) chi angles: 277.2,16.1	0.006Å	-	-
B 166		GLU 50	-		Favored (60.6%) General / -75.0,-40.6	53% (*mt-10*) chi angles: 297.9,181.3,293.7	0.03Å	-	-
B 167		LEU 50	-		Favored (60.84%) General / -74.8,-40.9	9.8% (*tt*) chi angles: 186.9,155.1	0.067Å	-	-
B 168		THR 50	-		Favored (15.04%) General / -90.5,-35.5	69.9% (*p*) chi angles: 63.3	0.076Å	-	-
B 169		ASP 50	-		OUTLIER (0.01%) General / 109.5,-13.6	42% (*t0*) chi angles: 189.9,328.8	0.056Å	-	OUTLIER(S) worst is CA-CB-CG: 8.695 σ
B 170		TYR 50	-		Favored (44.7%) General / -68.1,153.0	28.6% (*t80*) chi angles: 196.9,74.7	0.051Å	-	-
B 171		LYS 50	-		Favored (19.24%) General / -118.8,112.0	28.3% (*tptp*) chi angles: 184,63,181.5,66.8	0.008Å	-	-
			Avg: 55.00	Clashscore: 25.22	Outliers: 6 of 168	Poor rotamers: 5 of 154	Outliers: 2 of 165	Outliers: 2 of 170	Outliers: 9 of 170
B 172		THR 50	-		Favored (34.95%) General / -86.0,129.1	69% (*m*) chi angles: 303.3	0.078Å	-	-
B		LYS 50	-		Allowed (1.91%)	59.7% (*tptt*) chi angles:	0.031Å	-	-

173				General / -122.6,-52.6	185.8,64.8,174.3,178.9			
B 174	ASN	50	-	Favored (19.21%) General / -109.2,157.0	84.2% (*m-20*) chi angles: 298.5,326.2	0.085Å	-	-
B 175	MET	50	0.471Å HB3 with B 151 VAL CG2	Allowed (0.69%) General / -171.5,129.8	41.6% (*ttm*) chi angles: 172.9,189.2,296.6	0.035Å	-	-
B 176	LEU	50	0.659Å HD13 with B 201 PHE CD2	Favored (54.14%) General / -111.1,125.8	10.1% (*mp*) chi angles: 271.9,56.3	0.072Å	-	-
B 177	ALA	50	-	Favored (51.23%) General / -127.0,143.7	-	0.031Å	-	-
B 178	THR	99.99	0.603Å HG23 with B 148 MET HG2	Favored (12.85%) Pre-proline / -149.7,138.9	93.3% (*m*) chi angles: 300.2	0.061Å	-	-
B 179	PRO	50	-	Allowed (0.74%) Trans-proline / -93.7,130.9	40.1% (*Cg_endo*) chi angles: 36.5	0.044Å	-	-
B 180	ILE	50	0.452Å HD11 with B 190 ILE HD11	Favored (30.54%) Isoleucine or valine / -81.9,118.9	64.7% (*mt*) chi angles: 302.1,178.2	0.025Å	-	-
B 181	MET	50	-	Favored (44.86%) General / -122.4,125.0	25.4% (*ptp*) chi angles: 61.7,181.2,72.4	0.032Å	-	-
B 182	ASN	50	-	Favored (3.59%) General / -100.2,88.0	29.1% (*t-20*) chi angles: 184.8,302.6	0.041Å	-	-
B 183	GLY	50	-	Allowed (0.31%) Glycine / 57.2,-103.5	-	-	-	-
B 184	LYS	50	-	Favored (2.91%) General / -55.7,-60.8	49.3% (*mttm*) chi angles: 299.5,168.6,184.2,279	0.046Å	-	-
B 185	ASP	50	-	Favored (12.82%) General / -103.6,162.7	38.4% (*t70*) chi angles: 182.9,59.7	0.078Å	-	-

						Cβ deviation	Bond lengths	Bond angles
B 186	VAL	50	0.427Å O with B 97 TYR CD2	Favored (33.4%) Isoleucine or valine / -91.3,133.3	88.2% (*t*) chi angles: 175.2	0.089Å	-	-
B 187	VAL	50	-	Favored (4.33%) Isoleucine or valine / -94.1,-31.0	11.9% (*p*) chi angles: 62	0.125Å	-	-
B 188	ALA	50	-	Favored (8.1%) General / -169.0,157.6	-	0.051Å	-	-
B 189	VAL	50	-	Favored (73.12%) Isoleucine or valine / -118.7,124.4	98.8% (*t*) chi angles: 178.5	0.051Å	-	-
B 190	ILE	99.99	0.452Å HD11 with B 180 ILE HD11	Favored (9.56%) Isoleucine or valine / -105.8,149.0	69.5% (*mt*) chi angles: 301.3,177.3	0.042Å	-	-
B 191	MET	50	-	Favored (23.51%) General / -156.3,148.7	12% (*ptp*) chi angles: 62.8,184.5,94.1	0.059Å	-	OUTLIER(S) worst is CG-SD-CE: 4.61 σ

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.00	Clashscore: 25.22	Outliers: 6 of 168	Poor rotamers: 5 of 154	Outliers: 2 of 165	Outliers: 2 of 170	Outliers: 9 of 170
B 192	ALA	50		0.422Å O with B 175 MET HA	Favored (46.32%) General / -110.2,138.6	-	0.097Å	-	-
B 193	VAL	50		0.412Å HG12 with B 91 ARG O	Favored (29.8%) Isoleucine or valine / -120.9,144.5	13.9% (*p*) chi angles: 64.8	0.084Å	-	-
B 194	ASN	50		-	OUTLIER (0.03%) General / 52.0,87.7	88% (*m-20*) chi angles: 295.4,339.4	0.053Å	-	-
B 195	LYS	50		0.586Å HE3 with B 88 GLN NE2	Favored (42.82%) General / -55.8,140.3	49.4% (*tptt*) chi angles: 179,71.5,161.1,176.1	0.145Å	-	-
B 196	LEU	50		-	Favored (27.88%) General /	98% (*mt*) chi angles: 293.4,172.2	0.07Å	-	-

				-97.4,143.7				
B 197	ASN	50	-	Favored (16.64%) General / 61.1,26.8	55.5% (*m-20*) chi angles: 307.1,323.5	0.031Å	-	-
B 198	GLY	50	-	Favored (15.1%) Glycine / -164.9,149.0	-	-	-	-
B 199	PRO	50	-	Favored (8.93%) Trans-proline / -72.8,-32.7	88.1% (*Cg_endo*) chi angles: 31.2	0.083Å	-	-
B 200	PHE	50	-	Favored (39.25%) General / -153.5,163.8	51.1% (*p90*) chi angles: 64.8,87.2	0.032Å	-	-
B 201	PHE	50	0.659Å CD2 with B 176 LEU HD13	Favored (35.97%) General / -73.8,128.6	91.4% (*m-85*) chi angles: 294.4,282.4	0.039Å	-	-
B 202	THR	50	-	Favored (9.64%) General / -76.8,175.2	44.2% (*p*) chi angles: 66.9	0.052Å	-	-
B 203	SER	50	-	Favored (85.25%) General / -62.6,-37.2	49.4% (*m*) chi angles: 301.8	0.052Å	-	-
B 204	GLU	50	-	Favored (89.05%) General / -63.1,-37.9	14.9% (*mm-40*) chi angles: 287.5,284.3,23.8	0.011Å	-	-
B 205	ASP	50	-	Favored (72.47%) General / -65.4,-31.4	84.1% (*m-20*) chi angles: 294.7,332	0.041Å	-	-
B 206	GLU	50	0.448Å O with B 210 LEU HD13	Favored (73.19%) General / -65.7,-48.1	76.7% (*mt-10*) chi angles: 292.6,179.9,23.1	0.02Å	-	-
B 207	ASP	50	-	Favored (78.1%) General / -61.6,-35.5	61.5% (*m-20*) chi angles: 295.3,302	0.033Å	-	-
B 208	VAL	50	-	Favored (67.77%) Isoleucine or valine / -70.9,-46.5	60% (*t*) chi angles: 181.7	0.039Å	-	-

			High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
B 209		PHE	50	0.415Å CD1 with B 83 LEU HD11	Favored (91.76%) General / -59.0,-44.9	66.3% (t80) chi angles: 186.8,71	0.05Å	-	-
B 210		LEU	50	0.448Å HD13 with B 206 GLU O	Favored (95.46%) General / -62.7,-39.9	11.2% (mp) chi angles: 275.2,62.1	0.023Å	-	-
B 211		LYS	50	-	Favored (93.84%) General / -62.7,-45.2	55.3% (tttp) chi angles: 192.2,169.9,180.8,60.2	0.054Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.00	Clashscore: 25.22	Outliers: 6 of 168	Poor rotamers: 5 of 154	Outliers: 2 of 165	Outliers: 2 of 170	Outliers: 9 of 170
B 212		TYR	50	-	Favored (73.79%) General / -70.6,-36.7	13.3% (m-85) chi angles: 271,273.7	0.066Å	-	-
B 213		LEU	50	0.503Å O with B 217 THR HG23	Favored (69.31%) General / -66.3,-29.1	0.7% chi angles: 254.3,85.7	0.146Å	-	-
B 214		ASN	50	-	Favored (76.35%) General / -59.9,-36.1	97.6% (m-20) chi angles: 290.1,343.3	0.048Å	-	-
B 215		PHE	50	-	Favored (33.62%) General / -75.9,-45.8	76.5% (t80) chi angles: 176.9,86.4	0.06Å	-	-
B 216		ALA	50	-	Favored (83.77%) General / -61.6,-37.4	-	0.018Å	-	-
B 217		THR	50	0.503Å HG23 with B 213 LEU O	Favored (98.11%) General / -62.6,-40.8	68.8% (p) chi angles: 57.5	0.06Å	-	-
B 218		LEU	50	-	Favored (84.46%) General / -67.7,-39.7	87.2% (mt) chi angles: 290.9,175.3	0.051Å	-	-
B 219		TYR	99.99	0.844Å OH with B 72 MET HA	Favored (85.94%) General / -61.5,-38.1	88.2% (t80) chi angles: 181.1,75.9	0.123Å	-	-
B 220		LEU	50	-	Allowed (0.4%) General /	63.3% (mt) chi angles: 292.3,182.8	0.076Å	-	-

B 221	LYS	99.99	-	-	-78.2,42.1 98.6% (*mttt*) chi angles: 296.4,178.8,180.3,182.7	0.028Å	-	-

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