Viewing TPK1_FFX1FH_reg-multi.table

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All-Atom Contacts	Clashscore, all atoms:	1.18		100th percentile* (N=63, 2.82Å - 9999Å)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	12	2.15%	Goal: <1%
	Ramachandran outliers	7	1.13%	Goal: <0.05%
	Ramachandran favored	572	92.26%	Goal: >98%
	MolProbity score^	1.56		100th percentile* (N=2114, 3.07Å ± 0.25Å)
	Cβ deviations >0.25Å	14	2.37%	Goal: 0
	Bad backbone bonds:	0 / 5170	0.00%	Goal: 0%
	Bad backbone angles:	59 / 6984	0.84%	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: 138.32	Clashscore: 1.18	Outliers: 7 of 620	Poor rotamers: 12 of 557	Outliers: 14 of 591	Outliers: 0 of 628	Outliers: 57 of 628
A -1		ALA	137.51	-	-	-	0.154Å	-	-
A 0		MET	171.28	-	Favored (21.48%) General / -109.3,155.2	17% (*mmt*) chi angles: 293.2,292.3,196	0.06Å	-	-
A 1		GLY	112.33	-	Favored (17.09%) Glycine / -142.0,-177.4	-	-	-	-
A 2		GLN	131.7	-	Favored (14.65%) General / -133.1,171.0	55.5% (*mt-30*) chi angles: 279.9,192.8,322.6	0.052Å	-	-
A 3		SER	117	-	Favored (7.57%) General /	92% (*p*) chi angles: 65.9	0.094Å	-	-

			-151.0,-179.8			
A 4	THR 113.01	-	Favored (2.36%) General / -135.7,-169.2	26.9% (*p*) chi angles: 71.4	0.073Å	-	-
A 5	SER 119.29	-	Favored (60.15%) General / -50.8,-46.8	45.3% (*t*) chi angles: 180.7	0.026Å	-	-
A 6	ASN 108.07	0.426Å O with A 28 HIS HD2	Favored (9.37%) General / -120.7,-9.2	18.8% (*m-20*) chi angles: 316.7,308.2	0.033Å	-	-
A 7	HIS 99.63	-	Favored (36.9%) General / -139.9,161.7	71.6% (*m80*) chi angles: 299.6,80.5	0.042Å	-	-
A 8	LEU 105.83	-	Favored (41.02%) General / -154.4,159.2	2.3% (*pp*) chi angles: 49.6,69.3	0.047Å	-	-
A 9	TRP 96	-	Favored (34.4%) General / -160.0,162.6	39% (*p90*) chi angles: 54.4,96	0.093Å	-	-
A 10	LEU 116.62	-	Favored (22.37%) General / -89.8,150.1	87.9% (*mt*) chi angles: 300.7,178.7	0.045Å	-	-
A 11	LEU 122.11	-	Favored (57.05%) General / -78.6,-6.9	56.8% (*mt*) chi angles: 304.1,184.6	0.195Å	-	-
A 12	SER 100.98	-	Favored (54.79%) General / -77.0,-27.7	24.3% (*p*) chi angles: 51.1	0.077Å	-	-
A 13	ASP 102.44	-	Favored (5.72%) General / -85.7,59.6	50.7% (*m-20*) chi angles: 303.8,337.4	0.091Å	-	-
A 14	ILE 124.9	-	Favored (14.95%) Isoleucine or valine / -80.1,141.7	10.4% (*tp*) chi angles: 197.5,65.3	0.108Å	-	-
A 15	LEU 126.94	-	Allowed (1.84%) General / -129.7,-33.3	19.9% (*mt*) chi angles: 312.6,170.4	0.037Å	-	-
			Favored			

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 16		GLY	135.44	-	(8.12%) Glycine / -143.0,138.1	-	-	-	-
A 17		GLN	166.63	-	Favored (2.26%) General / -139.4,88.4	17.9% (*tp60*) chi angles: 200.2,54.7,9.1	0.133Å	-	-
A 18		GLY	138.22	-	Favored (12.24%) Glycine / -114.1,167.1	-	-	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 138.32	Clashscore: 1.18	Outliers: 7 of 620	Poor rotamers: 12 of 557	Outliers: 14 of 591	Outliers: 0 of 628	Outliers: 57 of 628
A 19		ALA	139.69	-	Favored (75.34%) General / -61.0,-34.8	-	0.118Å	-	-
A 20		THR	141.64	-	Favored (20.52%) General / -100.4,-11.1	19.1% (*p*) chi angles: 47.9	0.091Å	-	-
A 21		ALA	111.94	-	Favored (2.38%) General / -172.2,150.1	-	0.095Å	-	-
A 22		ASN	129.67	-	Favored (52.84%) General / -128.0,139.0	8.2% (*m120*) chi angles: 305.1,156.8	0.105Å	-	OUTLIER(S) worst is CA-CB-CG: 6.46 σ
A 23		VAL	109.42	0.441Å HA with A 37 ILE O	Favored (64.42%) Isoleucine or valine / -107.9,125.2	85.2% (*t*) chi angles: 177.6	0.034Å	-	-
A 24		PHE	111.69	-	Favored (36.01%) General / -117.6,152.0	94.3% (*m-85*) chi angles: 298.9,92.5	0.08Å	-	-
A 25		ARG	114.3	-	Favored (23.07%) General / -71.9,123.6	31.5% (*ttt180*) chi angles: 189.6,202.2,196.1,182.8	0.129Å	-	-
A 26		GLY	93.98	-	Favored (16.51%) Glycine / -128.5,179.6	-	-	-	-
					Favored				OUTLIER(S)

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 27		ARG 97.53		-	(45.43%) General / -135.8,143.7	9.4% (*mtp180*) chi angles: 307.3,193.4,85.6,137.2	0.051Å	-	worst is CD-NE-CZ: 4.328 σ
A 28		HIS 116.79		0.426Å HD2 with A 6 ASN O	Favored (58.3%) General / -65.3,142.4	19.5% (*t-160*) chi angles: 182.9,206	0.098Å	-	-
A 29		LYS 132.41		-	Favored (59.03%) General / -75.7,-29.9	46% (*mtpt*) chi angles: 289.3,165.6,49.6,166.4	0.093Å	-	-
A 30		LYS 146.94		-	Favored (32.86%) General / -79.8,-38.6	41.1% (*mmtt*) chi angles: 316.9,290.2,172.5,157.4	0.12Å	-	-
A 31		THR 105.52		-	Favored (12.29%) General / -114.0,-15.6	60.7% (*p*) chi angles: 56.6	0.111Å	-	-
A 32		GLY 80.84		-	Favored (57.37%) Glycine / 69.1,7.8	-	-	-	-
A 33		ASP 80.27		-	Favored (37.25%) General / -71.4,128.9	84.8% (*m-20*) chi angles: 295,333.6	0.037Å	-	-
A 34		LEU 81.09		-	Favored (49.92%) General / -68.5,134.3	21.1% (*mt*) chi angles: 296.5,158.1	0.063Å	-	-
A 35		PHE 84.89		-	Favored (13.59%) General / -133.7,171.8	45.6% (*m-85*) chi angles: 295.4,75	0.057Å	-	-
A 36		ALA 95.25		0.569Å HB3 with A 86 MET HB2	Favored (45.13%) General / -104.0,135.6	-	0.05Å	-	-
A 37		ILE 97.52		0.441Å O with A 23 VAL HA	Favored (25.79%) Isoleucine or valine / -113.5,108.5	10.1% (*mm*) chi angles: 317.3,293.2	0.06Å	-	-
A 38		LYS 115.03		-	Favored (7.41%) General / -94.7,93.2	51.8% (*tttt*) chi angles: 198.6,153.5,180.5,169.1	0.054Å	-	-

		Avg: 138.32	Clashscore: 1.18	Outliers: 7 of 620	Poor rotamers: 12 of 557	Outliers: 14 of 591	Outliers: 0 of 628	Outliers: 57 of 628
A 39	VAL	125.83	-	Favored (8.52%) Isoleucine or valine / -86.8,99.6	46.3% (*t*) chi angles: 183.4	0.036Å	-	-
A 40	PHE	153.29	-	Favored (6.67%) General / -61.4,118.2	19.9% (*m-85*) chi angles: 274.1,281.1	0.061Å	-	-
A 41	ASN	171.95	-	Favored (56.43%) General / -116.0,129.6	2.8% (*t-20*) chi angles: 223.8,352.5	0.054Å	-	-
A 42	ASN	173.84	-	Allowed (0.98%) General / 76.5,25.1	1.7% (*t30*) chi angles: 217,90.1	0.151Å	-	-
A 43	ILE	195.92	-	Favored (2.42%) Isoleucine or valine / -85.8,86.5	12.6% (*tt*) chi angles: 194.5,157.5	0.225Å	-	-
A 44	SER	198.7	-	Allowed (0.4%) General / -140.5,-69.3	27.4% (*p*) chi angles: 51.7	0.083Å	-	-
A 45	PHE	215.02	-	Favored (60.78%) General / -74.5,-17.4	14.1% (*p90*) chi angles: 59.9,253.1	0.114Å	-	-
A 46	LEU	233.02	-	OUTLIER (0%) General / -58.0,-142.6	9.5% (*mt*) chi angles: 310.3,197.7	0.088Å	-	-
A 47	ARG	243.17	-	OUTLIER (0.07%) Pre-proline / 80.9,50.0	24.1% (*mmt180*) chi angles: 301.9,267,177.3,179.9	0.165Å	-	-
A 48	PRO	246.55	0.489Å HD3 with A 163 GLU OE2	Favored (8.09%) Trans-proline / -82.2,67.4	0.2% chi angles: 44.3	0.092Å	-	-
A 49	VAL	228.33	-	Allowed (1.05%) Isoleucine or valine / -42.5,-49.8	5.6% (*m*) chi angles: 285.4	0.352Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 50		ASP 216.1	-		Favored (39.7%) General / -80.0,-30.6	2.1% (*m-20*) chi angles: 311.4,250.4	0.108Å	-	-
A 51		VAL 204.85	-		Favored (88.04%) Isoleucine or valine / -66.7,-41.3	43.4% (*t*) chi angles: 167.5	0.15Å	-	-
A 52		GLN 205.13	-		Favored (61.07%) General / -75.0,-30.0	78.7% (*mt-30*) chi angles: 285.6,166.6,356.9	0.133Å	-	-
A 53		MET 192.63	-		Favored (13.6%) General / -50.9,-56.2	2.8% (*ttm*) chi angles: 184.8,238.8,286.2	0.032Å	-	-
A 54		ARG 209.99	-		Favored (60.06%) General / -75.2,-39.5	25% (*ptt180*) chi angles: 81.6,197.8,181.5,194.5	0.132Å	-	-
A 55		GLU 211.94	-		Favored (31.87%) General / -81.9,-30.2	62.3% (*mt-10*) chi angles: 293.7,193.5,18.9	0.154Å	-	-
A 56		PHE 181.28	-		Favored (62.97%) General / -72.0,-27.9	17.7% (*m-30*) chi angles: 299,345.2	0.156Å	-	OUTLIER(S) worst is CA-CB-CG: 4.119 σ
A 57		GLU 172.39	-		Favored (76.69%) General / -66.7,-33.9	33.3% (*tp10*) chi angles: 183,59.2,37.3	0.104Å	-	-
A 58		VAL 141.56	-		Favored (95%) Isoleucine or valine / -65.2,-42.7	28.9% (*t*) chi angles: 164.8	0.132Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 138.32	Clashscore: 1.18	Outliers: 7 of 620	Poor rotamers: 12 of 557	Outliers: 14 of 591	Outliers: 0 of 628	Outliers: 57 of 628
A 59		LEU 147.57	-		Favored (71.26%) General / -62.7,-30.2	21.8% (*mt*) chi angles: 301.9,192.5	0.176Å	-	-
A 60		LYS 158.59	-		Favored (83.35%) General / -65.7,-45.3	28.8% (*ttmt*) chi angles: 183,198.7,284.6,164.4	0.079Å	-	-

A 61	LYS 154.27	-	Favored (61.08%) General / -73.9,-16.9	61.8% (*mttp*) chi angles: 300.5,186,176.4,71.1	0.144Å	-	-
A 62	LEU 140.49	-	Favored (2.64%) General / -75.6,83.9	1.1% (*tt*) chi angles: 211.6,150.3	0.08Å	-	-
A 63	ASN 162.35	-	Favored (22.1%) General / -101.2,151.2	42.2% (*t-20*) chi angles: 195.7,349.9	0.037Å	-	-
A 64	HIS 157.54	-	Allowed (0.75%) General / -176.2,147.9	5.1% (*t60*) chi angles: 216,63.6	0.073Å	-	-
A 65	LYS 139.63	-	Favored (64.39%) General / -55.5,-34.3	65.7% (*tttm*) chi angles: 186,178.5,185.1,291.2	0.055Å	-	-
A 66	ASN 121.8	-	Favored (18.66%) General / -110.5,19.6	23.3% (*m120*) chi angles: 309.1,117.1	0.025Å	-	-
A 67	ILE 109.49	-	Favored (44.7%) Isoleucine or valine / -130.4,142.1	21% (*mt*) chi angles: 282.7,156.1	0.122Å	-	-
A 68	VAL 92.28	-	Favored (34.41%) Isoleucine or valine / -73.8,126.4	97.8% (*t*) chi angles: 176.3	0.09Å	-	-
A 69	LYS 115.62	-	Favored (21.84%) General / -76.7,120.4	7.1% (*tptp*) chi angles: 196.3,69.5,223.9,75.7	0.047Å	-	-
A 70	LEU 107	-	Favored (37.29%) General / -77.7,130.8	40.2% (*tp*) chi angles: 181.6,55.2	0.094Å	-	-
A 71	PHE 113.38	-	Favored (4.86%) General / -107.7,-42.0	40.1% (*m-85*) chi angles: 295.1,254	0.081Å	-	-
A 72	ALA 118.5	-	Favored (36.49%) General / -155.8,157.5	-	0.065Å	-	-

A 73		ILE 145.48	-	Favored (63.61%) Isoleucine or valine / -109.6,129.9	4.3% (*mp*) chi angles: 292.6,88.3	0.083Å	-	-
A 74		GLU 159.67	-	Favored (13.91%) General / -135.4,171.8	93.7% (*mt-10*) chi angles: 299.3,178.6,338.6	0.088Å	-	-
A 75		GLU 178.39	-	Favored (52.42%) General / -122.9,130.1	40.2% (*mt-10*) chi angles: 284.3,203.5,353.3	0.107Å	-	OUTLIER(S) worst is C-N-CA: 4.215 σ
A 76		GLU 152.75	-	Favored (57.58%) General / -64.5,137.0	8.2% (*tm-20*) chi angles: 180.5,293.2,320.9	0.133Å	-	-
A 77		THR 141.03	-	Favored (61.26%) General / -61.8,-53.0	1.6% (*p*) chi angles: 37	0.122Å	-	-
A 78		THR 155.95	-	Favored (29.2%) General / -84.0,-26.4	51.4% (*p*) chi angles: 65.7	0.161Å	-	-
#	Alt	Res High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 138.32	Clashscore: 1.18	Outliers: 7 of 620	Poor rotamers: 12 of 557	Outliers: 14 of 591	Outliers: 0 of 628	Outliers: 57 of 628
A 79		THR 163.86	-	Favored (5.1%) General / -129.4,1.8	19.1% (*p*) chi angles: 73.7	0.111Å	-	-
A 80		ARG 154.32	-	Favored (18.36%) General / 61.0,37.0	76.6% (*mtp180*) chi angles: 301.2,175.8,71.1,179.2	0.149Å	-	-
A 81		HIS 170.12	-	Favored (33.21%) General / -83.9,138.4	6.9% (*m80*) chi angles: 283.9,49.3	0.12Å	-	-
A 82		LYS 171.9	-	Favored (58.9%) General / -64.3,140.8	81.6% (*mttt*) chi angles: 304.9,192.7,191.1,180.6	0.088Å	-	-
A 83		VAL 129.21	-	Favored (53.02%) Isoleucine or valine / -134.7,135.9	2.2% (*t*) chi angles: 150.5	0.124Å	-	-

A 84	LEU 120.38	-	Favored (48.91%) General / -105.5,134.3	22.1% (*mt*) chi angles: 305.9,191.4	0.059Å	-	-
A 85	ILE 102.5	-	Favored (24.78%) Isoleucine or valine / -100.4,109.3	35.2% (*mm*) chi angles: 302,308.3	0.099Å	-	-
A 86	MET 111.76	0.569Å HB2 with A 36 ALA HB3	Favored (18.68%) General / -111.0,158.5	2.3% (*mmm*) chi angles: 313.3,277.5,339.6	0.104Å	-	-
A 87	GLU 110.69	-	Favored (56.35%) General / -65.5,136.4	14.2% (*pt-20*) chi angles: 64.7,180.1,283.4	0.067Å	-	-
A 88	PHE 81.96	-	Favored (35.77%) General / -80.5,133.3	29.7% (*t80*) chi angles: 177.3,52.6	0.043Å	-	-
A 89	CYS 78.3	-	Favored (9.17%) Pre-proline / -110.3,89.9	74.5% (*m*) chi angles: 301.2	0.052Å	-	-
A 90	PRO 60.77	-	Favored (20.31%) Trans-proline / -47.7,-34.2	58.8% (*Cg_exo*) chi angles: 327.1	0.066Å	-	-
A 91	CYS 103.12	-	Favored (59.75%) General / -81.7,-8.9	19.8% (*m*) chi angles: 312.2	0.072Å	-	-
A 92	GLY 85.41	-	Favored (18.98%) Glycine / 91.2,-147.7	-	-	-	-
A 93	SER 97.41	-	Favored (4.75%) General / -119.2,177.8	99.2% (*p*) chi angles: 64.4	0.073Å	-	-
A 94	LEU 92.14	-	Favored (73.33%) General / -62.9,-32.1	50% (*tp*) chi angles: 175.5,57.3	0.067Å	-	-
A 95	TYR 131.09	-	Favored (95.96%) General / -62.2,-44.7	71% (*t80*) chi angles: 174.3,69.8	0.115Å	-	-

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A 96		THR	85.13	-	Favored (63.73%) General / -51.8,-45.0	5.9% (*m*) chi angles: 316	0.101Å	-	-
A 97		VAL	77.58	-	Favored (96.05%) Isoleucine or valine / -63.2,-46.3	97.3% (*t*) chi angles: 178.3	0.07Å	-	-
A 98		LEU	97.61	-	Favored (65.7%) General / -67.3,-24.2	35.2% (*mt*) chi angles: 300.4,164	0.154Å	-	OUTLIER(S) worst is C-N-CA: 4.303 σ

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A 99		GLU	135.73	-	Favored (66.89%) General / -66.1,-25.2	6.2% (*mm-40*) chi angles: 279.6,272.4,34.9	0.071Å	-	-
A 100		GLU	89.74	-	Favored (97.68%) Pre-proline / -64.5,139.2	51.5% (*mt-10*) chi angles: 289.9,171.4,225.3	0.064Å	-	-
A 101		PRO	101.37	-	Favored (29.02%) Trans-proline / -70.5,-22.2	85% (*Cg_exo*) chi angles: 330.2	0.067Å	-	-
A 102		SER	120.52	-	Favored (65.43%) General / -55.8,-34.5	71.1% (*m*) chi angles: 295.8	0.065Å	-	-
A 103		ASN	77.24	-	Favored (8.15%) General / -108.3,28.6	61.9% (*m-20*) chi angles: 308.5,311.5	0.075Å	-	-
A 104		ALA	92.23	-	Favored (75.77%) General / -61.5,-34.6	-	0.093Å	-	-
A 105		TYR	114.12	-	Allowed (1.71%) General / -115.3,45.1	72.2% (*m-85*) chi angles: 302.4,289	0.093Å	-	-
A 106		GLY	83.2	-	Favored (10.81%) Glycine / 77.6,159.0	-	-	-	-

A 107	LEU 87.69	-	Favored (69.03%) Pre-proline / -64.2,157.6	10.9% (*mt*) chi angles: 309.6,196.7	0.051Å	-	-
A 108	PRO 106.26	-	Favored (39.94%) Trans-proline / -50.4,136.8	26.6% (*Cg_exo*) chi angles: 324.8	0.056Å	-	-
A 109	GLU 116.03	-	Favored (5.33%) General / -42.6,-47.6	16.6% (*tt0*) chi angles: 172.9,155.1,243.6	0.072Å	-	-
A 110	SER 96.1	-	Favored (85.99%) General / -58.4,-46.6	24.6% (*p*) chi angles: 51.2	0.099Å	-	-
A 111	GLU 96.65	-	Favored (75.2%) General / -67.3,-33.4	16.6% (*tp10*) chi angles: 197.3,72.9,171.7	0.089Å	-	-
A 112	PHE 107.81	-	Favored (84.35%) General / -60.7,-47.9	70.7% (*t80*) chi angles: 177.6,88.5	0.125Å	-	-
A 113	LEU 100.31	-	Favored (84.3%) General / -59.9,-39.2	21.4% (*mt*) chi angles: 287.1,156.6	0.142Å	-	-
A 114	ILE 98.15	-	Favored (87.73%) Isoleucine or valine / -61.1,-48.7	67.1% (*mt*) chi angles: 296.4,179.5	0.134Å	-	-
A 115	VAL 94.75	-	Favored (77.18%) Isoleucine or valine / -57.6,-50.5	49.8% (*t*) chi angles: 168.6	0.088Å	-	-
A 116	LEU 101.38	-	Favored (72.41%) General / -55.1,-49.2	60.7% (*tp*) chi angles: 178.6,59.8	0.056Å	-	-
A 117	ARG 108.68	-	Favored (80.35%) General / -59.4,-48.8	9.8% (*ttm180*) chi angles: 181.7,239.3,298,147.9	0.07Å	-	-
A 118	ASP 105.66	-	Favored (43.64%) General / -79.3,-32.6	97.5% (*m-20*) chi angles: 289.7,341.3	0.109Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 138.32	Clashscore: 1.18	Outliers: 7 of 620	Poor rotamers: 12 of 557	Outliers: 14 of 591	Outliers: 0 of 628	Outliers: 57 of 628
A 119		VAL	114.59	-	Favored (87.65%) Isoleucine or valine / -67.2,-42.0	69.2% (*t*) chi angles: 171.7	0.096Å	-	-
A 120		VAL	122.91	-	Favored (75.8%) Isoleucine or valine / -69.7,-38.2	72.8% (*t*) chi angles: 172	0.169Å	-	-
A 121		GLY	148.09	-	Favored (71.9%) Glycine / -69.3,-29.6	-	-	-	-
A 122		GLY	138.9	-	Favored (10.91%) Glycine / -80.2,-42.2	-	-	-	-
A 123		MET	179.96	-	Favored (84.39%) General / -66.5,-43.7	21.9% (*ttt*) chi angles: 181.9,181,191.9	0.061Å	-	-
A 124		ASN	137.64	-	Favored (77.82%) General / -60.1,-36.6	5.2% (*p-10*) chi angles: 83.6,320.8	0.226Å	-	-
A 125		HIS	143.48	-	Favored (74.72%) General / -64.2,-32.9	37.7% (*t60*) chi angles: 199,72.1	0.172Å	-	OUTLIER(S) worst is CA-CB-CG: 5.614 σ
A 126		LEU	156.7	-	Favored (83.32%) General / -66.4,-44.3	50.4% (*mt*) chi angles: 300,186.9	0.088Å	-	-
A 127		ARG	157.59	-	Favored (74.49%) General / -68.2,-33.5	13.3% (*ttp180*) chi angles: 194.2,217.8,63.7,177	0.129Å	-	-
A 128		GLU	169.81	-	Favored (46.31%) General / -55.0,-27.7	43.7% (*mt-10*) chi angles: 284.8,169.4,44.6	0.112Å	-	-
A					Favored (9.18%)	11.7% (*m120*)			OUTLIER(S)

# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
129	ASN 152.65	-	General / -122.1,25.1	chi angles: 302.3,150.8	0.068Å	-	worst is CA-CB-CG: 4.8 σ
A 130	GLY 155.48	-	Favored (15.54%) Glycine / 79.8,-15.2	-	-	-	-
A 131	ILE 162.36	-	Favored (24.45%) Isoleucine or valine / -84.3,114.3	9.8% (pt) chi angles: 52.4,185.5	0.17Å	-	-
A 132	VAL 165.47	-	OUTLIER (0.04%) Isoleucine or valine / -72.0,-163.8	26.9% (m) chi angles: 296.4	0.265Å	-	-
A 133	HIS 142.47	-	Allowed (0.27%) General / -147.8,-61.5	15.2% (t-160) chi angles: 192.6,179.3	0.126Å	-	-
A 134	ARG 185.33	-	Favored (16.16%) General / 57.0,29.3	93.2% (mtt180) chi angles: 306.5,171.5,188.7,176.7	0.087Å	-	-
A 135	ASP 175.92	-	Allowed (0.3%) General / -160.9,56.0	23% (t70) chi angles: 196.5,60.9	0.077Å	-	-
A 136	ILE 135.71	-	Favored (3.5%) Isoleucine or valine / -89.0,90.9	2.7% (mm) chi angles: 296.1,267.6	0.066Å	-	-
A 137	LYS 115.96	-	Favored (35.01%) Pre-proline / -94.4,158.8	53.6% (tttt) chi angles: 200.5,168.8,193.2,161.9	0.049Å	-	-
A 138	PRO 95.63	-	Favored (46.78%) Trans-proline / -67.8,-16.8	33.1% (Cg_endo) chi angles: 21.9	0.117Å	-	-

# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
	Avg: 138.32	Clashscore: 1.18	Outliers: 7 of 620	Poor rotamers: 12 of 557	Outliers: 14 of 591	Outliers: 0 of 628	Outliers: 57 of 628
A 139	GLY 88.66	-	Favored (80.91%) Glycine / -76.0,-16.1	-	-	-	-

A 140	ASN 95.81	-	Favored (16.18%) General / -115.3,11.4	35.4% (*p30*) chi angles: 53.5,10.5	0.203Å	-	OUTLIER(S) worst is CA-CB-CG: 5.22 σ
A 141	ILE 96.01	-	Favored (15.63%) Isoleucine or valine / -97.2,104.2	87.1% (*mt*) chi angles: 297.8,166.3	0.044Å	-	-
A 142	MET 85.24	-	Favored (24.24%) General / -88.2,148.7	42.4% (*mmm*) chi angles: 306.7,323.5,292	0.03Å	-	-
A 143	ARG 78.25	-	Favored (44.18%) General / -114.3,121.6	23.6% (*ttt180*) chi angles: 184.9,196.8,171.4,234.3	0.102Å	-	-
A 144	VAL 85.96	-	Favored (5.41%) Isoleucine or valine / -111.8,167.4	34% (*m*) chi angles: 299.2	0.143Å	-	-
A 145	ILE 75.44	-	Favored (54.59%) Isoleucine or valine / -107.8,118.0	15.1% (*mt*) chi angles: 278.1,173.7	0.064Å	-	-
A 146	GLY 69.59	-	Favored (28.71%) Glycine / -67.2,173.3	-	-	-	-
A 147	GLU 123.24	-	Favored (63%) General / -54.5,-35.2	5.2% (*mm-40*) chi angles: 288.5,268.4,50.7	0.049Å	-	-
A 148	ASP 94.17	-	Favored (55.1%) General / -89.5,2.0	6.1% (*p-10*) chi angles: 69.9,284	0.036Å	-	-
A 149	GLY 95	-	Favored (12.49%) Glycine / 91.8,-26.5	-	-	-	-
A 150	GLN 124.21	-	Favored (52.62%) General / -70.2,141.3	85.6% (*mt-30*) chi angles: 287.2,177.8,2.8	0.113Å	-	-
A 151	SER 84.81	-	Allowed (0.19%) General / -52.5,166.3	24.2% (*m*) chi angles: 304.8	0.069Å	-	-

A 152	VAL 75.67	-	Favored (10.67%) Isoleucine or valine / -144.8,127.5	35% (*t*) chi angles: 185.8	0.074Å	-	-	
A 153	TYR 103.03	-	Favored (21.52%) General / -97.5,150.1	74.4% (*m-85*) chi angles: 293.2,260.2	0.14Å	-	-	
A 154	LYS 102.56	-	Favored (20.89%) General / -148.9,137.1	29% (*mttm*) chi angles: 288.2,166.1,153.7,281	0.141Å	-	-	
A 155	LEU 100.29	-	Favored (33.49%) General / -87.3,134.9	20.9% (*mt*) chi angles: 312.7,184.8	0.039Å	-	-	
A 156	THR 125.5	-	Favored (6.22%) General / -124.5,-16.8	2.3% (*t*) chi angles: 202	0.132Å	-	-	
A 157	ASP 103.01	-	Favored (2.64%) General / -139.6,93.2	36.5% (*t70*) chi angles: 187.6,54.3	0.07Å	-	-	
A 158	PHE 138.89	-	Favored (48%) General / -139.1,153.5	1.6% (*p90*) chi angles: 42.1,63.8	0.051Å	-	-	

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 138.32	Clashscore: 1.18	Outliers: 7 of 620	Poor rotamers: 12 of 557	Outliers: 14 of 591	Outliers: 0 of 628	Outliers: 57 of 628
A 159		GLY 167.55	-		Favored (71.82%) Glycine / 69.2,30.7	-	-	-	-
A 160		ALA 173.71	-		Favored (56.71%) General / -76.3,-27.8	-	0.124Å	-	-
A 161		ALA 190.14	-		Favored (9.85%) General / -84.0,77.9	-	0.043Å	-	-
A 162		ARG 195.28	-		Allowed (0.21%) General / -161.5,49.2	22.7% (*ttt85*) chi angles: 184.7,155.8,186.5,64.9	0.135Å	-	OUTLIER(S) worst is C-N-CA: 5.39 σ

A 163	GLU 209.28	0.489Å OE2 with A 48 PRO HD3	OUTLIER (0%) General / 170.7,-41.1	42.9% (*tt0*) chi angles: 184.1,164.2,32.5	0.173Å	-	-
A 164	LEU 187.96	-	-	4.3% (*mt*) chi angles: 322.8,191.2	0.122Å	-	-
A 175	GLY 151.52	-	-	-	-	-	-
A 176	THR 163.32	-	Favored (2.55%) General / -47.8,146.1	8.4% (*t*) chi angles: 179.6	0.13Å	-	OUTLIER(S) worst is C-N-CA: 5.534 σ
A 177	GLU 158.48	-	Allowed (0.43%) General / -44.0,-28.1	17.7% (*pm0*) chi angles: 62.1,285.9,4	0.123Å	-	OUTLIER(S) worst is CB-CG-CD: 5.167 σ
A 178	GLU 161.74	-	Favored (3.01%) General / -136.8,8.2	1.2% (*pm0*) chi angles: 74.5,306,28.7	0.079Å	-	OUTLIER(S) worst is CB-CG-CD: 8.023 σ
A 179	TYR 124.82	-	Favored (13.03%) General / -114.3,-4.2	0.5% chi angles: 301.4,54.4	0.176Å	-	-
A 180	LEU 158.27	-	Allowed (1.98%) General / -52.1,155.1	44.4% (*mt*) chi angles: 289.4,161.8	0.057Å	-	-
A 181	HIS 166.24	-	Favored (34.55%) Pre-proline / -106.7,157.7	23.2% (*t-80*) chi angles: 170.2,274.5	0.124Å	-	-
A 182	PRO 168.8	-	Allowed (0.15%) Trans-proline / -37.4,-65.6	0.3% chi angles: 319.6	0.132Å	-	-
A 183	ASP 168.75	-	Favored (33.79%) General / -67.8,127.7	0% chi angles: 332.9,22.3	0.105Å	-	OUTLIER(S) worst is CA-CB-CG: 10.502 σ
A 184	MET 187	-	OUTLIER (0.03%) General / 77.3,55.1	46% (*mtt*) chi angles: 302.5,169.6,196.6	0.212Å	-	OUTLIER(S) worst is C-N-CA: 4.629 σ
A 185	TYR 163.54	-	Allowed (0.15%) General / -149.4,-51.4	9% (*t80*) chi angles: 170.6,282.8	0.087Å	-	-
A	GLU 173.49	-	-	15.1% (*tt0*) chi angles:	0.102Å	-	-

# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 199	GLY 180.07	0.771Å N with A 289 GLN HE21	-	-	-	-	-
A 200	ALA 192.66	-	Favored (41.61%) General / -92.3,7.7	-	0.067Å	-	OUTLIER(S) worst is C-N-CA: 4.813 σ

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 138.32	Clashscore: 1.18	Outliers: 7 of 620	Poor rotamers: 12 of 557	Outliers: 14 of 591	Outliers: 0 of 628	Outliers: 57 of 628
A 201		THR	193.08	-	Favored (4.4%) General / -41.8,-50.1	7.5% (*m*) chi angles: 314.5	0.097Å	-	-
A 202		VAL	181.49	-	Favored (12.85%) Isoleucine or valine / -48.1,-45.9	17.6% (*m*) chi angles: 291.6	0.151Å	-	-
A 203		ASP	182.01	-	Favored (92.41%) General / -65.7,-40.5	4.8% (*m-20*) chi angles: 293,260.4	0.049Å	-	-
A 204		LEU	146.69	-	Favored (47.96%) General / -79.4,-20.3	45.3% (*mt*) chi angles: 296.6,163.7	0.109Å	-	-
A 205		TRP	135.03	-	Favored (70.73%) General / -70.5,-42.9	9.2% (*t-105*) chi angles: 174.8,287.6	0.143Å	-	-
A 206		SER	120.79	-	Favored (87.4%) General / -58.8,-41.8	11.2% (*m*) chi angles: 311.1	0.125Å	-	-
A 207		ILE	100.51	-	Favored (16.19%) Isoleucine or valine / -52.2,-54.0	18% (*mm*) chi angles: 288.5,290.1	0.042Å	-	-
A 208		GLY	96.34	-	Favored (96.46%) Glycine / -59.1,-44.3	-	-	-	-
A					Favored (78.61%)	89.6% (*t*)			

# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
209 VAL 117.07	-		Isoleucine or valine / -61.3,-37.9	chi angles: 177.1	0.131Å	-	-
A 210 THR 100.62	-		Favored (72.65%) General / -60.0,-50.7	92% (*m*) chi angles: 298	0.048Å	-	-
A 211 PHE 95.72	-		Favored (74.95%) General / -70.3,-38.1	22.9% (*m-30*) chi angles: 296.3,337.7	0.129Å	-	-
A 212 TYR 119.86	-		Favored (95.66%) General / -62.6,-40.0	40.2% (*t80*) chi angles: 182.8,277.9	0.042Å	-	-
A 213 HIS 99.08	-		Favored (99.42%) General / -62.4,-43.2	2.1% (*t-160*) chi angles: 208.7,141.2	0.156Å	-	-
A 214 ALA 74	-		Favored (71.06%) General / -71.5,-38.1	-	0.133Å	-	-
A 215 ALA 88.01	-		Favored (25.78%) General / -73.5,-49.6	-	0.024Å	-	-
A 216 THR 115.34	-		Favored (7.02%) General / -79.7,-53.2	69.8% (*m*) chi angles: 296.7	0.032Å	-	-
A 217 GLY 123.56	-		Favored (9.87%) Glycine / 113.3,-26.9	-	-	-	-
A 218 SER 100.92	-		Favored (8.3%) General / -112.4,170.3	58.5% (*m*) chi angles: 290.8	0.06Å	-	-
A 219 LEU 104.78	-		Favored (86.19%) Pre-proline / -75.1,155.6	20.2% (*mt*) chi angles: 285.6,156.6	0.035Å	-	-
A 220 PRO 110.62	-		Allowed (1.07%) Trans-proline / -77.5,-36.9	0.8% chi angles: 0.9	0.08Å	-	-
	Avg: 138.32	Clashscore: 1.18	Outliers: 7 of 620	Poor rotamers: 12 of 557	Outliers: 14 of	Outliers: 0 of 628	Outliers: 57 of 628

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A 221	PHE 106.66	-	Favored (32.81%) General / -111.0,117.2	33.5% (*m-85*) chi angles: 310.8,296.4	0.097Å	-	OUTLIER(S) worst is CA-CB-CG: 5.228 σ
A 222	ARG 119.95	-	Favored (6.94%) Pre-proline / -142.4,118.6	80.8% (*mtm-85*) chi angles: 306.2,196.5,302.2,264.6	0.063Å	-	-
A 223	PRO 139.98	-	Allowed (0.82%) Trans-proline / -63.2,179.5	60% (*Cg_exo*) chi angles: 327.2	0.093Å	-	-
A 224	PHE 174.28	-	Favored (68.75%) General / -71.8,-33.8	70.3% (*t80*) chi angles: 184.2,69.1	0.099Å	-	-
A 225	GLU 179.13	-	Allowed (0.17%) General / -91.0,-89.4	4.1% (*tp10*) chi angles: 165.7,46,288.1	0.174Å	-	-
A 226	GLY 189.86	-	Favored (23.67%) Glycine / 150.5,-151.7	-	-	-	-
A 227	PRO 200.74	-	Favored (5.9%) Trans-proline / -80.4,73.7	3.5% (*Cg_endo*) chi angles: 41.5	0.06Å	-	-
A 228	ARG 211.51	-	Allowed (0.36%) General / -129.5,-148.2	85.8% (*mtt180*) chi angles: 285.2,165.1,160.8,174.6	0.164Å	-	-
A 229	ARG 204.18	-	Allowed (0.78%) General / -72.2,10.4	4.4% (*ptm-85*) chi angles: 70.4,168.3,313.2,297.2	0.179Å	-	-
A 230	ASN 195.46	-	Favored (11.33%) General / -121.1,21.2	8.2% (*m-20*) chi angles: 298.3,13.4	0.05Å	-	-
A 231	LYS 196.42	-	Favored (14.53%) General / -66.5,-6.4	65.7% (*tttt*) chi angles: 203.6,187,179.3,191	0.088Å	-	-
A 232	GLU 191.74	-	Favored (69.63%) General / -67.1,-29.8	60.8% (*tt0*) chi angles: 197.4,183.4,5.9	0.161Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 233		VAL 148.39	-		Favored (51.55%) Isoleucine or valine / -70.4,-32.8	67.5% (*t*) chi angles: 179.6	0.241Å	-	-
A 234		MET 163.47	-		Favored (90.23%) General / -59.0,-42.5	29.5% (*tpp*) chi angles: 171.8,69.6,94.9	0.09Å	-	-
A 235		TYR 193.06	-		Favored (87.95%) General / -59.1,-46.6	1.3% (*t80*) chi angles: 188,8.8	0.027Å	-	-
A 236		LYS 167.8	-		Favored (53.29%) General / -78.0,-20.1	44% (*mmtm*) chi angles: 307.8,303.4,180.3,285.2	0.176Å	-	-
A 237		ILE 128.29	-		Favored (16.84%) Isoleucine or valine / -66.7,-55.8	72.1% (*mt*) chi angles: 290.4,163.7	0.054Å	-	-
A 238		ILE 159.53	-		Favored (78.19%) Isoleucine or valine / -62.6,-37.1	44% (*mt*) chi angles: 285.9,177.7	0.181Å	-	-
A 239		THR 150.39	-		Favored (36.32%) General / -81.6,-24.7	20.2% (*p*) chi angles: 48.3	0.128Å	-	-
A 240		GLY 177.8	-		Favored (68.12%) Glycine / -65.8,-20.2	-	-	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 138.32	Clashscore: 1.18	Outliers: 7 of 620	Poor rotamers: 12 of 557	Outliers: 14 of 591	Outliers: 0 of 628	Outliers: 57 of 628
A 241		LYS 170.51	-		Allowed (0.68%) Pre-proline / 29.3,67.4	0.9% chi angles: 62,176.1,134.1,290.1	0.14Å	-	-
A 242		PRO 160.71	-		Favored (2.54%) Trans-proline / -76.9,81.7	53.3% (*Cg_endo*) chi angles: 25.3	0.094Å	-	OUTLIER(S) worst is C-N-CA: 4.49 σ
A					Allowed	44.1% (*p*)			OUTLIER(S) worst is C-

243	SER 159.31	-	(0.08%) General / 33.5,-122.2	chi angles: 76.1	0.327Å	-	CA-CB: 4.697 σ
A 244	GLY 150.93	-	Allowed (1.5%) Glycine / -75.1,22.8	-	-	-	-
A 245	ALA 154.05	-	Favored (15.08%) General / -80.1,110.0	-	0.022Å	-	-
A 246	ILE 142.75	-	Favored (13.15%) Isoleucine or valine / -79.2,-11.9	31.7% (*pt*) chi angles: 65.7,177.5	0.173Å	-	-
A 247	SER 115.32	-	Favored (16.59%) General / -153.9,138.2	59.8% (*p*) chi angles: 56	0.05Å	-	-
A 248	GLY 95.39	0.438Å HA2 with A 258 ASP O	Favored (2.44%) Glycine / -125.0,115.4	-	-	-	-
A 249	VAL 121.23	-	Allowed (1.16%) Isoleucine or valine / -143.5,107.1	84.2% (*t*) chi angles: 174.8	0.072Å	-	-
A 250	GLN 153.72	-	Favored (35.11%) General / -82.8,134.5	4.6% (*pt20*) chi angles: 52.5,151.7,349.7	0.147Å	-	-
A 251	LYS 129.33	-	Favored (19.73%) General / -112.6,16.5	41.4% (*mtmt*) chi angles: 301.1,170.2,299,194.8	0.072Å	-	-
A 252	ALA 134.61	-	Allowed (0.98%) General / -167.1,120.5	-	0.071Å	-	-
A 253	GLU 174.15	-	Favored (51.99%) General / -59.1,142.2	6% (*tp10*) chi angles: 186,53.7,291.1	0.061Å	-	-
A 254	ASN 165.48	-	Favored (4.4%) General / 71.6,21.5	7.8% (*m-80*) chi angles: 316.9,278.6	0.1Å	-	-
A	GLY 134.12	-	Favored (15.71%)	-	-	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
255					Glycine / -115.3,-169.1				
A 256		PRO	135.55	-	Favored (6.31%) Trans-proline / -83.9,134.6	31.2% (*Cg_endo*) chi angles: 37.3	0.047Å	-	-
A 257		ILE	119.61	-	Favored (20.38%) Isoleucine or valine / -83.0,112.2	53.9% (*mt*) chi angles: 295.9,157.7	0.104Å	-	-
A 258		ASP	124.54	0.438Å O with A 248 GLY HA2	Favored (16.91%) General / -53.2,143.9	43.3% (*m-20*) chi angles: 276.8,184.4	0.205Å	-	OUTLIER(S) worst is CA-CB-CG: 7.379 σ
A 259		TRP	154.88	-	Favored (23.31%) General / -133.3,122.0	93.4% (*m95*) chi angles: 286.4,104.1	0.05Å	-	OUTLIER(S) worst is CE3-CD2-CG: 4.977 σ
A 260		SER	132.23	-	Favored (51.61%) General / -124.4,142.0	36.1% (*t*) chi angles: 182.5	0.072Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 138.32	Clashscore: 1.18	Outliers: 7 of 620	Poor rotamers: 12 of 557	Outliers: 14 of 591	Outliers: 0 of 628	Outliers: 57 of 628
A 261		GLY	128.06	-	Favored (13.36%) Glycine / -101.9,29.0	-	-	-	-
A 262		ASP	128.81	-	Favored (25.44%) General / -161.3,157.5	5% (*t0*) chi angles: 218,341.6	0.058Å	-	-
A 263		MET	129.12	-	Favored (70.1%) Pre-proline / -65.3,158.9	17.4% (*mmt*) chi angles: 307.2,296.2,158	0.099Å	-	-
A 264		PRO	112.08	-	Favored (32.34%) Trans-proline / -77.2,161.4	68.6% (*Cg_endo*) chi angles: 28	0.013Å	-	-
A 265		VAL	130.17	-	Favored (48.05%) Isoleucine or valine / -67.2,-30.1	75.5% (*t*) chi angles: 174.1	0.133Å	-	-

A 266	SER 129.29	-	Favored (68.65%) General / -58.0,-33.2	87.4% (*p*) chi angles: 61.5	0.066Å	-	-
A 267	CYS 110.09	-	Favored (2.2%) General / -41.4,134.8	43.8% (*t*) chi angles: 176.3	0.095Å	-	-
A 268	SER 121.21	-	Favored (60.77%) General / -72.5,-11.7	72.6% (*m*) chi angles: 295.5	0.057Å	-	-
A 269	LEU 117.23	-	Favored (28.21%) General / -82.2,148.8	34.4% (*mt*) chi angles: 302.8,189.6	0.048Å	-	-
A 270	SER 122.67	-	Favored (43.49%) General / -71.9,151.2	35.4% (*p*) chi angles: 76.9	0.026Å	-	-
A 271	ARG 200.7	-	Favored (71.85%) General / -60.7,-32.6	28.8% (*tpt180*) chi angles: 189.3,55.6,180.2,175.3	0.194Å	-	-
A 272	GLY 111.45	-	Favored (94.92%) Glycine / -66.2,-40.5	-	-	-	-
A 273	LEU 107.41	-	Favored (87.8%) General / -65.6,-44.0	24.1% (*tp*) chi angles: 184,51.1	0.058Å	-	-
A 274	GLN 109.59	-	Favored (77.29%) General / -56.9,-41.0	80.2% (*mt-30*) chi angles: 293.3,185.7,13.2	0.103Å	-	-
A 275	VAL 124.18	-	Favored (52.42%) Isoleucine or valine / -61.9,-31.9	39.3% (*t*) chi angles: 166.2	0.153Å	-	-
A 276	LEU 134.63	-	Favored (24.4%) General / -84.0,-34.4	36.5% (*mt*) chi angles: 310.3,175.1	0.074Å	-	-
A 277	LEU 112.54	-	Favored (61.14%) General / -73.6,-42.7	43.9% (*tp*) chi angles: 184.5,58.6	0.089Å	-	-
A	THR 146.02	-	Favored (99.15%)	53.2% (*m*)	0.205Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
	278				Pre-proline / -54.7,-44.4	chi angles: 294.3			
A 279		PRO 148.36		-	Favored (36.34%) Trans-proline / -64.2,-38.4	74.4% (*Cg_exo*) chi angles: 333.7	0.098Å	-	-
A 280		VAL 121.89		-	Favored (30.4%) Isoleucine or valine / -55.8,-54.1	77.6% (*t*) chi angles: 172.7	0.081Å	-	-
			Avg: 138.32	Clashscore: 1.18	Outliers: 7 of 620	Poor rotamers: 12 of 557	Outliers: 14 of 591	Outliers: 0 of 628	Outliers: 57 of 628
A 281		LEU 111.53		-	Favored (92.78%) General / -64.0,-38.9	14.2% (*mt*) chi angles: 315.1,187.8	0.151Å	-	-
A 282		ALA 131.92		-	Favored (73.71%) General / -61.8,-33.2	-	0.084Å	-	-
A 283		ASN 153.57		-	Favored (50.58%) General / -95.5,-1.5	1.8% (*m-80*) chi angles: 291.3,235.6	0.105Å	-	OUTLIER(S) worst is CA-CB-CG: 4.72 σ
A 284		ILE 142.66		-	Favored (12.19%) Isoleucine or valine / -114.9,-10.8	29% (*pt*) chi angles: 62.4,180.3	0.241Å	-	-
A 285		LEU 149.67		-	Allowed (0.88%) General / -102.0,61.6	95.8% (*mt*) chi angles: 296.4,174.2	0.089Å	-	-
A 286		GLU 186.33		-	Favored (51.98%) General / -134.5,152.7	5.1% (*tp10*) chi angles: 171,61,297.7	0.078Å	-	OUTLIER(S) worst is C-N-CA: 4.11 σ
A 287		ALA 181.96		-	Favored (4.91%) General / -79.9,-55.5	-	0.051Å	-	OUTLIER(S) worst is C-N-CA: 4.912 σ
A 288		ASP 192.17		-	Favored (25.69%) General / -68.0,125.2	6.7% (*m-20*) chi angles: 303.3,8.5	0.071Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 289		GLN	200.46	0.771Å HE21 with A 199 GLY N	Favored (59.15%) General / -81.1,-12.9	1% chi angles: 276.8,123.3,286.6	0.157Å	-	OUTLIER(S) worst is C-N-CA: 4.044 σ
A 290		GLU	197.74	-	Favored (52.48%) General / -77.7,-31.7	21.5% (pm0) chi angles: 60.1,280,201.8	0.113Å	-	OUTLIER(S) worst is CB-CG-CD: 4.19 σ
A 291		LYS	170.39	-	Favored (18.34%) General / -89.7,-30.0	6.2% (mptt) chi angles: 303,95.3,182.6,168.3	0.134Å	-	-
A 292		CYS	176.16	-	Favored (8.18%) General / -45.6,132.9	50.2% (t) chi angles: 179.5	0.111Å	-	-
A 293		TRP	160.91	-	Favored (12.52%) General / -62.2,121.2	26% (m0) chi angles: 278.5,4.4	0.09Å	-	OUTLIER(S) worst is CE3-CD2-CG: 4.518 σ
A 294		GLY	155.57	-	Favored (27.53%) Glycine / -58.6,153.9	-	-	-	-
A 295		PHE	161.96	-	Favored (83.44%) General / -60.5,-38.2	3.3% (p90) chi angles: 39.5,72.3	0.301Å	-	-
A 296		ASP	125.76	-	Favored (83.01%) General / -65.2,-36.0	3.1% (m-20) chi angles: 294.7,252.2	0.214Å	-	-
A 297		GLN	153.53	-	Favored (83.18%) General / -66.1,-44.8	3% (tp60) chi angles: 171.5,70.2,108.6	0.033Å	-	-
A 298		PHE	128.13	-	Favored (94.44%) General / -59.8,-43.0	19.8% (t80) chi angles: 160.1,81	0.09Å	-	-
A 299		PHE	139.76	-	Favored (95.61%) General / -63.1,-39.8	22.4% (m-30) chi angles: 296.3,329.8	0.102Å	-	-
A 300		ALA	106.6	-	Favored (45.92%) General / -62.0,-54.1	-	0.083Å	-	-

		Avg: 138.32	Clashscore: 1.18	Outliers: 7 of 620	Poor rotamers: 12 of 557	Outliers: 14 of 591	Outliers: 0 of 628	Outliers: 57 of 628
A 301	GLU 151.14		-	Favored (35.7%) General / -80.8,-30.6	36.9% (*mm-40*) chi angles: 278,299.8,288.4	0.181Å	-	-
A 302	THR 129.92		-	Favored (95.51%) General / -64.2,-43.2	43.4% (*p*) chi angles: 54.8	0.13Å	-	-
A 303	SER 112.1		-	Favored (85.42%) General / -59.0,-40.7	1.3% (*p*) chi angles: 95.5	0.246Å	-	-
A 304	ASP 118.69		-	Favored (87.02%) General / -58.0,-45.3	16.2% (*t70*) chi angles: 183.9,272.7	0.117Å	-	-
A 305	ILE 122.89		-	Favored (68.95%) Isoleucine or valine / -54.4,-48.2	42.2% (*mt*) chi angles: 300.2,184.3	0.056Å	-	-
A 306	LEU 113.48		-	Favored (63.24%) General / -70.0,-24.3	33.5% (*mt*) chi angles: 302.8,165.5	0.093Å	-	-
A 307	HIS 139.1		-	Favored (59.09%) General / -86.1,-4.1	19.6% (*m-70*) chi angles: 316.4,308.3	0.124Å	-	OUTLIER(S) worst is CA-CB-CG: 4.796 σ
A 308	ARG 123.34		-	Favored (4.34%) General / -77.7,-176.4	54.3% (*mtt180*) chi angles: 288.5,175.5,184.7,237.9	0.142Å	-	OUTLIER(S) worst is CD-NE-CZ: 4.456 σ
A 309	MET 138.74		-	Favored (19.32%) General / -146.2,132.3	3.3% (*ptp*) chi angles: 44.9,150.9,59.3	0.065Å	-	-
A 310	VAL 143.92		-	Favored (17.11%) Isoleucine or valine / -73.0,117.8	14.1% (*t*) chi angles: 161.4	0.08Å	-	-
A 311	ILE 137.21		-	Favored (50.23%) Isoleucine or valine / -97.2,125.4	32.2% (*mm*) chi angles: 302.8,309.4	0.035Å	-	-

A 312	HIS 140.55	-	Favored (37.63%) General / -94.4,133.8	79.9% (*m80*) chi angles: 297.2,87.7	0.093Å	-	OUTLIER(S) worst is CA-CB-CG: 4.818 σ
A 313	VAL 138.42	0.508Å HA with A 379 ILE O	Favored (33.56%) Isoleucine or valine / -132.5,146.0	2.2% (*t*) chi angles: 149.7	0.125Å	-	-
A 314	PHE 133.98	-	Favored (11.47%) General / -134.2,112.9	68.1% (*t80*) chi angles: 187.5,76.7	0.02Å	-	-
A 315	SER 132.9	-	Favored (21.38%) General / -82.9,114.7	29.2% (*t*) chi angles: 172.5	0.083Å	-	-
A 316	LEU 126.09	-	Favored (82.32%) General / -66.8,-44.0	78.1% (*mt*) chi angles: 289.2,167.9	0.133Å	-	-
A 317	GLN 155.02	-	Favored (8.76%) General / -44.1,-49.9	14.1% (*mm100*) chi angles: 285,302.3,147.2	0.096Å	-	-
A 318	GLN 133.85	-	Favored (25.43%) General / -102.7,-4.2	52.3% (*mt-30*) chi angles: 299.3,161.1,292.2	0.116Å	-	-
A 319	MET 107.6	-	Favored (22.12%) General / 48.9,46.2	12.4% (*ttt*) chi angles: 188.8,149.8,180.6	0.166Å	-	-
A 320	THR 96.08	-	Favored (52.53%) General / -132.0,149.0	22.5% (*p*) chi angles: 49.3	0.059Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 138.32	Clashscore: 1.18	Outliers: 7 of 620	Poor rotamers: 12 of 557	Outliers: 14 of 591	Outliers: 0 of 628	Outliers: 57 of 628
A 321		ALA 111.54		-	Favored (16.82%) General / -100.0,157.1	-	0.026Å	-	-
A 322		HIS 103.95		-	Favored (27.26%) General /	97.2% (*m-70*) chi angles: 296.4,277.8	0.131Å	-	-

-150.4,147.2

A 323	LYS 144.32	-	Favored (14.1%) General / -129.6,112.8	77.7% (*mttt*) chi angles: 292.1,176,173.7,156	0.043Å	-	-
A 324	ILE 129.96	-	Favored (54.37%) Isoleucine or valine / -105.0,119.7	4.4% (*mp*) chi angles: 293.1,90.2	0.106Å	-	-
A 325	TYR 139.57	-	Favored (11.55%) General / -90.9,98.1	23.5% (*m-85*) chi angles: 282,69	0.071Å	-	-
A 326	ILE 146.67	-	Favored (4%) Isoleucine or valine / -105.0,164.2	4.7% (*mt*) chi angles: 303.3,199.9	0.151Å	-	-
A 327	HIS 131.19	-	Favored (18.41%) General / -96.9,152.7	81.6% (*m-70*) chi angles: 289.5,301.9	0.056Å	-	-
A 328	SER 156.49	-	Favored (62.99%) General / -52.9,-39.7	23.4% (*p*) chi angles: 50.9	0.044Å	-	-
A 329	TYR 135.41	-	Favored (53.49%) General / -76.6,-24.9	12.9% (*p90*) chi angles: 50.4,74.1	0.107Å	-	-
A 330	ASN 132.94	-	Favored (17.59%) General / -56.4,149.1	14% (*m-20*) chi angles: 290.8,15.6	0.076Å	-	-
A 331	THR 125.06	-	Favored (13.22%) General / -88.9,167.5	39.9% (*p*) chi angles: 53.5	0.049Å	-	-
A 332	ALA 120.37	-	Favored (71.51%) General / -63.2,-30.4	-	0.165Å	-	-
A 333	THR 137.26	-	Favored (61.82%) General / -51.9,-50.1	20.4% (*m*) chi angles: 310.3	0.086Å	-	-
A 334	ILE 133.02	-	Favored (82.14%) Isoleucine or valine / -67.2,-39.0	60.1% (*mt*) chi angles: 303,179	0.152Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 335		PHE 126.32	-		Favored (34.72%) General / -52.6,-54.3	14% (*t80*) chi angles: 160.6,87.8	0.093Å	-	-
A 336		HIS 160.91	-		Favored (92.23%) General / -60.2,-41.1	96.9% (*m-70*) chi angles: 295.5,293.8	0.081Å	-	-
A 337		GLU 147.31	-		Favored (97.02%) General / -64.2,-41.6	21.2% (*tp10*) chi angles: 175.4,46.6,33.5	0.079Å	-	-
A 338		LEU 132.14	-		Favored (67.97%) General / -72.5,-35.0	26.3% (*mt*) chi angles: 301.1,162.5	0.129Å	-	-
A 339		VAL 111.2	-		Favored (87.85%) Isoleucine or valine / -59.3,-42.7	53.9% (*t*) chi angles: 169.2	0.125Å	-	-
A 340		TYR 150.11	-		Favored (75.1%) General / -55.5,-42.9	2.9% (*t80*) chi angles: 151.3,65.8	0.143Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 138.32	Clashscore: 1.18	Outliers: 7 of 620	Poor rotamers: 12 of 557	Outliers: 14 of 591	Outliers: 0 of 628	Outliers: 57 of 628
A 341		LYS 136.51	-		Favored (77.99%) General / -57.6,-40.0	10.2% (*mptt*) chi angles: 275.6,92.8,171.6,182.8	0.164Å	-	-
A 342		GLN 162.23	-		Favored (17.77%) General / -89.7,-30.9	60.6% (*mt-30*) chi angles: 305.4,190.1,8.7	0.145Å	-	-
A 343		THR 136.36	-		Favored (12.41%) General / -110.7,-20.7	40.1% (*p*) chi angles: 53.6	0.106Å	-	-
A 344		LYS 140.42	-		Favored (5.32%) General / 66.2,36.9	73.3% (*mmtt*) chi angles: 297.7,303.1,176.1,188.1	0.211Å	-	-
A					Favored (30.66%)	87.4% (*mt*)			

345	ILE 131.62	-	Isoleucine or valine / -99.0,136.3	chi angles: 294.7,174.6	0.064Å	-	-
A 346	ILE 163.4	-	Favored (17.79%) Isoleucine or valine / -58.9,140.1	14.3% (*mt*) chi angles: 277.2,169.1	0.112Å	-	-
A 347	SER 140.71	-	Favored (67.19%) General / -56.6,-34.4	2.9% (*m*) chi angles: 272.9	0.165Å	-	-
A 348	SER 167.48	-	Favored (59.67%) General / -80.9,-8.1	71.6% (*p*) chi angles: 57.8	0.073Å	-	-
A 349	ASN 188.58	-	Favored (17.92%) General / -114.4,14.6	7.3% (*m-20*) chi angles: 297.5,16.1	0.058Å	-	-
A 350	GLN 141.66	-	Favored (3.34%) General / -95.4,75.5	71.4% (*mt-30*) chi angles: 296.4,163.4,8.3	0.045Å	-	-
A 351	GLU 159.22	-	Favored (20.16%) General / -71.7,122.2	81.3% (*mt-10*) chi angles: 287.4,174.6,326.2	0.036Å	-	-
A 352	LEU 135.15	-	Favored (35.14%) General / -106.2,142.9	34.7% (*mt*) chi angles: 310.9,181.2	0.039Å	-	-
A 353	ILE 139.4	-	Favored (32.46%) Isoleucine or valine / -133.8,146.0	25.7% (*mt*) chi angles: 311.2,179.8	0.051Å	-	-
A 354	TYR 168.25	-	Favored (2.94%) General / -164.6,130.8	87.1% (*t80*) chi angles: 176.5,74	0.11Å	-	-
A 355	GLU 140.91	-	Favored (18.74%) General / 48.3,43.0	29.5% (*mt-10*) chi angles: 280.6,190.2,73	0.135Å	-	-
A 356	GLY 136.02	-	Favored (88.9%) Glycine / 85.0,0.6	-	-	-	-
A			Favored	89.3% (*mtt-85*)			

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
357		ARG	155.51	-	(23.06%) General / -131.4,165.6	chi angles: 295.2,168.7,177.9,269.9	0.095Å	-	-
A 358		ARG	157.5	-	Favored (22.39%) General / -74.6,167.1	19.3% (*ptp180*) chi angles: 66.2,196.5,71.7,200.2	0.133Å	-	-
A 359		LEU	172.77	-	Favored (4.27%) General / -143.5,104.9	6.8% (*tp*) chi angles: 182.6,88.6	0.093Å	-	-
A 360		VAL	171.96	-	Favored (11.57%) Isoleucine or valine / -68.2,149.0	9.6% (*p*) chi angles: 71.2	0.094Å	-	-
			Avg: 138.32	Clashscore: 1.18	Outliers: 7 of 620	Poor rotamers: 12 of 557	Outliers: 14 of 591	Outliers: 0 of 628	Outliers: 57 of 628
A 361		LEU	160.52	-	Allowed (1.86%) General / -141.6,83.4	1.4% (*tp*) chi angles: 229.3,69.3	0.099Å	-	-
A 362		GLU	136.78	-	Favored (30.5%) Pre-proline / -51.0,131.7	1% chi angles: 327.2,83.7,269.4	0.128Å	-	-
A 363		PRO	157.75	-	Favored (11.28%) Trans-proline / -43.6,-42.0	3.5% (*Cg_exo*) chi angles: 321.8	0.083Å	-	-
A 364		GLY	142.14	-	Favored (87.63%) Glycine / -84.7,-4.1	-	-	-	-
A 365		ARG	172.1	-	Favored (5.86%) General / -63.4,116.8	45.2% (*ttt85*) chi angles: 191.7,173.6,195.8,85.5	0.049Å	-	-
A 366		LEU	131.38	-	Favored (52.94%) General / -69.9,142.8	3.9% (*mt*) chi angles: 323.9,189.6	0.145Å	-	-
A 367		ALA	115.1	-	Favored (65.25%) General /	-	0.17Å	-	-

				-58.1,-29.2			
A 368	GLN 160.33	-	Allowed (0.08%) General / -34.1,-40.1	80.6% (*mt-30*) chi angles: 282.4,174.4,358.7	0.113Å	-	-
A 369	HIS 147.44	-	Favored (19.03%) General / -113.3,13.3	1.6% (*m80*) chi angles: 330.7,87.2	0.089Å	-	-
A 370	PHE 154.53	-	Favored (2.57%) Pre-proline / -68.5,174.4	10.6% (*m-30*) chi angles: 287.7,5.5	0.029Å	-	-
A 371	PRO 145.44	-	Favored (24.87%) Trans-proline / -78.3,166.0	57.3% (*Cg_endo*) chi angles: 26.2	0.036Å	-	-
A 372	LYS 152.32	-	Favored (48.62%) General / -63.8,131.7	63.3% (*tttt*) chi angles: 206.6,172.6,186.7,172.7	0.12Å	-	-
A 373	THR 132.3	-	Favored (3.77%) General / -147.0,105.3	5% (*t*) chi angles: 175.8	0.155Å	-	-
A 374	THR 124.54	-	Allowed (0.58%) General / -91.0,-158.8	32.5% (*p*) chi angles: 69.1	0.16Å	-	-
A 375	GLU 170.6	-	Favored (16.92%) General / -104.7,-11.4	0.5% chi angles: 34.4,219.8,103.9	0.309Å	-	-
A 376	GLU 170.36	-	Favored (30.1%) General / -78.7,-41.8	6% (*tm-20*) chi angles: 188.1,299.8,318.3	0.04Å	-	-
A 377	ASN 140.54	-	Favored (54.18%) Pre-proline / -123.5,75.8	13% (*t30*) chi angles: 213.1,46.3	0.07Å	-	-
A 378	PRO 129.46	-	Allowed (1.85%) Trans-proline / -91.7,177.4	7.8% (*Cg_endo*) chi angles: 40.7	0.074Å	-	-
A 379	ILE 131.87	0.508Å O with A 313 VAL HA	Favored (27.07%) Isoleucine or valine / -82.8,116.5	97% (*mt*) chi angles: 296,170.3	0.072Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 380		PHE	128.79	-	Favored (29.79%) General / -80.8,148.9	31.6% (*m-85*) chi angles: 289.5,71.3	0.035Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 138.32	Clashscore: 1.18	Outliers: 7 of 620	Poor rotamers: 12 of 557	Outliers: 14 of 591	Outliers: 0 of 628	Outliers: 57 of 628
A 381		VAL	124.7	-	Favored (75.97%) Isoleucine or valine / -120.5,128.0	23.1% (*t*) chi angles: 163.3	0.057Å	-	OUTLIER(S) worst is C-N-CA: 5.614 σ
A 382		VAL	154.04	-	Favored (18.93%) Isoleucine or valine / -122.6,165.2	15.6% (*t*) chi angles: 161.8	0.183Å	-	-
A 383		SER	160.54	-	Favored (24.39%) General / -149.1,168.0	35.9% (*t*) chi angles: 182.5	0.13Å	-	-
A 384		ARG	165.01	-	Favored (13.16%) General / -113.5,-11.0	8.1% (*mmm-85*) chi angles: 320.2,299.1,275.6,253.2	0.12Å	-	OUTLIER(S) worst is C-N-CA: 4.892 σ
A 385		GLU	166.14	-	Favored (61.66%) Pre-proline / -102.3,117.2	16% (*pt-20*) chi angles: 54.9,182.6,39.3	0.043Å	-	-
A 386		PRO	165.59	-	Favored (88.1%) Trans-proline / -56.9,144.5	0.7% chi angles: 320.6	0.067Å	-	-
A 387		LEU	154.97	-	Favored (22.01%) General / -151.7,141.6	10.5% (*mt*) chi angles: 268.5,168.7	0.045Å	-	-
A 388		ASN	133.59	-	Favored (46.47%) General / -72.9,145.9	5.2% (*m120*) chi angles: 310.4,68.6	0.098Å	-	-
A 389		THR	148.68	-	Favored (8.98%) General / -76.2,108.3	22% (*p*) chi angles: 49.1	0.049Å	-	-
A					Favored (12.43%)	51.1% (*mm*)			

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
390		ILE	131.94	-	Isoleucine or valine / -84.2,-36.9	chi angles: 301.9,301.4	0.062Å	-	-
A 391		GLY	112.11	-	Favored (32.19%) Glycine / 62.5,-160.6	-	-	-	-
A 392		LEU	113.67	-	Favored (18.5%) General / -80.9,112.7	47.3% (*tp*) chi angles: 181.3,56.8	0.048Å	-	-
A 393		ILE	111.39	-	Favored (18.5%) Isoleucine or valine / -72.5,119.1	40.1% (*mm*) chi angles: 297.4,304.1	0.041Å	-	-
A 394		TYR	109.5	-	Favored (33.21%) General / -141.8,142.3	55.5% (*p90*) chi angles: 62.1,90.8	0.049Å	-	-
A 395		GLU	110.23	-	Favored (46.01%) General / -66.9,131.5	6.4% (*tp10*) chi angles: 185.6,49.7,106.1	0.072Å	-	-
A 396		LYS	134	-	Allowed (1.35%) General / -102.9,74.8	78% (*mttt*) chi angles: 275.4,193.2,177.6,181.3	0.167Å	-	-
A 397		ILE	103.16	-	Favored (19.89%) Isoleucine or valine / -85.2,138.0	20% (*mt*) chi angles: 309.9,159.6	0.057Å	-	-
A 398		SER	116.68	-	Favored (5.87%) General / -110.6,174.4	7.2% (*t*) chi angles: 196.6	0.06Å	-	-
A 399		LEU	104.83	-	Favored (92.92%) Pre-proline / -72.0,152.3	61.2% (*mt*) chi angles: 304.5,173.3	0.03Å	-	-
A 400		PRO	110.38	-	Favored (11.59%) Trans-proline / -84.9,156.0	18.3% (*Cg_endo*) chi angles: 38.9	0.073Å	-	-
#	**Alt**	**Res**	**High B**	**Clash > 0.4Å**	**Ramachandran**	**Rotamer**	**Cβ deviation**	**Bond lengths**	**Bond angles**
			Avg: 138.32	Clashscore: 1.18	Outliers: 7 of 620	Poor rotamers: 12 of 557	Outliers: 14 of 591	Outliers: 0 of 628	Outliers: 57 of 628

A 401	LYS 149.81	-	Favored (8%) General / -74.5,109.5	22.8% (*tptp*) chi angles: 187.7,72.2,181.8,82.1	0.068Å	-	-
A 402	VAL 133.22	0.436Å HG22 with A 414 MET SD	Favored (24.24%) Isoleucine or valine / -63.6,137.7	60.6% (*t*) chi angles: 181.2	0.055Å	-	-
A 403	HIS 156.25	-	Favored (43.33%) Pre-proline / -111.5,155.2	50% (*m80*) chi angles: 284.7,70.8	0.063Å	-	-
A 404	PRO 154.09	-	Favored (10.72%) Trans-proline / -80.3,-16.8	55.5% (*Cg_endo*) chi angles: 34.8	0.034Å	-	-
A 405	ARG 144.28	-	Allowed (1.57%) General / -48.1,116.6	10.2% (*tpt180*) chi angles: 188.3,77.9,211.1,164.9	0.103Å	-	-
A 406	TYR 127.66	-	Favored (55.5%) General / -65.8,145.8	70.1% (*t80*) chi angles: 178.7,67.1	0.032Å	-	-
A 407	ASP 122.84	-	Favored (2.22%) General / -177.5,167.9	50% (*t0*) chi angles: 182.4,16.2	0.084Å	-	OUTLIER(S) worst is CA-CB-CG: 4.148 σ
A 408	LEU 132.08	-	Favored (2.29%) General / -123.7,-40.9	86.6% (*mt*) chi angles: 301,179	0.109Å	-	-
A 409	ASP 133.36	-	Favored (81.09%) General / -68.2,-41.6	3.3% (*m-20*) chi angles: 302.9,71.5	0.133Å	-	-
A 410	GLY 122.38	-	Favored (36.45%) Glycine / -85.6,-26.2	-	-	-	-
A 411	ASP 109.03	-	Favored (75.2%) General / -69.0,-34.4	64.6% (*m-20*) chi angles: 279.8,360	0.174Å	-	-
A 412	ALA 114.46	-	Favored (73.06%) General / -70.1,-42.1	-	0.087Å	-	-
			Favored				

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 413		SER	107.38	-	(73.75%) General / -59.6,-50.5	67.6% (*m*) chi angles: 292.8	0.084Å	-	-
A 414		MET	102.22	0.436Å SD with A 402 VAL HG22	Favored (90.08%) General / -63.9,-38.2	12.1% (*tmm?*) chi angles: 176.5,286.2,301.8	0.108Å	-	-
A 415		ALA	97.55	0.438Å HA with A 590 LEU HD21	Favored (92.07%) General / -59.5,-45.3	-	0.057Å	-	-
A 416		LYS	125.89	-	Favored (98.09%) General / -62.1,-41.3	55.2% (*tttp*) chi angles: 186.9,179.1,164.5,50.1	0.078Å	-	-
A 417		ALA	110.37	-	Favored (35.66%) General / -68.0,-52.4	-	0.07Å	-	-
A 418		ILE	79.06	-	Favored (93.33%) Isoleucine or valine / -62.6,-41.8	14.3% (*tt*) chi angles: 194.4,159.8	0.224Å	-	-
A 419		THR	94.3	-	Favored (91.76%) General / -65.8,-40.4	32.1% (*m*) chi angles: 306.8	0.171Å	-	-
A 420		GLY	87.95	-	Favored (96.99%) Glycine / -59.4,-41.4	-	-	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 138.32	Clashscore: 1.18	Outliers: 7 of 620	Poor rotamers: 12 of 557	Outliers: 14 of 591	Outliers: 0 of 628	Outliers: 57 of 628
A 421		VAL	100.97	-	Favored (91.1%) Isoleucine or valine / -63.9,-47.4	74.3% (*t*) chi angles: 172.1	0.121Å	-	-
A 422		VAL	87.19	-	Favored (71.53%) Isoleucine or valine / -68.0,-35.4	60.2% (*t*) chi angles: 181.1	0.134Å	-	-
					Favored				

A 423	CYS 99.35	-	(59.91%) General / -53.4,-52.3	35.3% (*m*) chi angles: 282.2	0.118Å	-	-
A 424	TYR 128.46	-	Favored (98.15%) General / -63.7,-41.2	42.2% (*t80*) chi angles: 172.3,92.6	0.076Å	-	-
A 425	ALA 81.41	-	Favored (70.15%) General / -55.0,-40.3	-	0.064Å	-	-
A 426	CYS 85.19	-	Favored (88.76%) General / -66.5,-41.4	2.4% (*t*) chi angles: 207.8	0.137Å	-	-
A 427	ARG 153.93	-	Favored (69.28%) General / -56.0,-51.0	59.4% (*ttm-85*) chi angles: 181.3,182.6,293.9,270.9	0.04Å	-	-
A 428	ILE 99.33	-	Favored (80.69%) Isoleucine or valine / -60.8,-50.4	11.3% (*mm*) chi angles: 295.5,316.9	0.1Å	-	-
A 429	ALA 88.73	-	Favored (72.67%) General / -57.9,-36.7	-	0.069Å	-	-
A 430	SER 121.43	-	Favored (94.57%) General / -62.9,-45.0	8.4% (*t*) chi angles: 194.5	0.045Å	-	-
A 431	THR 109.88	-	Favored (80.27%) General / -68.1,-42.4	22.3% (*m*) chi angles: 309.8	0.087Å	-	-
A 432	LEU 116.39	-	Favored (91.03%) General / -60.1,-40.8	62.5% (*mt*) chi angles: 306.8,177.8	0.162Å	-	-
A 433	LEU 115.33	-	Favored (80.67%) General / -67.1,-44.1	33.2% (*tp*) chi angles: 182.6,53.6	0.073Å	-	-
A 434	LEU 106.28	-	Favored (60.29%) General / -53.0,-51.8	52.6% (*tp*) chi angles: 173.9,66.2	0.046Å	-	-
A			Favored (84.96%)	9.2% (*m-30*)			

# Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
435	TYR	101.86	-	General / -60.0,-39.2	chi angles: 290.9,5.9	0.086Å	-	-
A 436	GLN	105.92	-	Favored (61.62%) General / -72.8,-15.9	47.8% (*mt-30*) chi angles: 287.4,167.1,77	0.07Å	-	-
A 437	GLU	102.22	-	Favored (13.96%) General / -93.3,-33.3	49.1% (*mm-40*) chi angles: 279.9,290.3,300.3	0.072Å	-	-
A 438	LEU	109.84	-	Favored (61.95%) General / -69.6,-47.9	80.5% (*mt*) chi angles: 288.4,173.5	0.097Å	-	-
A 439	MET	113.14	-	Favored (77.61%) General / -56.1,-47.6	75.3% (*mmm*) chi angles: 299.1,291,272.3	0.122Å	-	-
A 440	ARG	118.13	-	Favored (63.83%) General / -54.4,-36.3	54.1% (*mtt180*) chi angles: 285.9,166.3,190.5,130.9	0.138Å	-	-

# Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 138.32	Clashscore: 1.18	Outliers: 7 of 620	Poor rotamers: 12 of 557	Outliers: 14 of 591	Outliers: 0 of 628	Outliers: 57 of 628
A 441	LYS	143.92	-	Favored (3.42%) General / -73.4,-58.3	53.1% (*mtpt*) chi angles: 280.3,170.7,64.7,185.8	0.109Å	-	-
A 442	GLY	127.51	-	Favored (66.25%) Glycine / -70.8,-34.2	-	-	-	-
A 443	ILE	127.69	-	Favored (70.29%) Isoleucine or valine / -54.5,-48.1	8.8% (*mt*) chi angles: 286.1,190.8	0.107Å	-	-
A 444	ARG	164.74	-	Favored (68.71%) General / -71.2,-32.3	21.6% (*ttm105*) chi angles: 194,186.4,306.3,89.4	0.112Å	-	-
A 445	TRP	146.06	-	Favored (96%) General / -63.6,-40.1	48.6% (*m0*) chi angles: 301.8,345.1	0.144Å	-	-
A				Favored	13.7% (*tp*)			

446	LEU 108.67	-	(79.52%) General / -68.8,-40.5	chi angles: 186.8,46.3	0.087Å	-	-
A 447	ILE 131.68	-	Favored (54.57%) Isoleucine or valine / -71.5,-34.8	11.7% (*pt*) chi angles: 73.5,182.1	0.362Å	-	OUTLIER(S) worst is N-CA-CB: 4.407 σ
A 448	GLU 144.79	-	Favored (54.35%) General / -76.3,-24.6	16% (*mm-40*) chi angles: 305.8,311.5,281.9	0.198Å	-	-
A 449	LEU 143.01	-	Favored (69.16%) General / -70.8,-32.2	9.3% (*tp*) chi angles: 202.4,76.4	0.063Å	-	-
A 450	ILE 144.08	-	Favored (81.26%) Isoleucine or valine / -68.1,-39.3	66.5% (*mt*) chi angles: 295.6,161	0.098Å	-	-
A 451	LYS 156.49	-	Favored (74.66%) General / -58.9,-36.5	10.5% (*mttt*) chi angles: 279.9,132.7,157.1,167.9	0.18Å	-	-
A 452	ASP 153.9	-	Favored (86.62%) General / -62.8,-46.7	5.5% (*m-20*) chi angles: 315.5,335.1	0.169Å	-	OUTLIER(S) worst is CA-CB-CG: 4.221 σ
A 453	ASP 147.48	-	Favored (63.2%) General / -57.3,-28.7	85% (*m-20*) chi angles: 294.3,332.4	0.143Å	-	-
A 454	TYR 165.21	-	Favored (10.93%) General / -95.9,-36.9	9.9% (*t80*) chi angles: 176.3,37.8	0.066Å	-	-
A 455	ASN 156.34	-	Favored (86.59%) General / -67.1,-39.6	19.9% (*m120*) chi angles: 298.3,141	0.105Å	-	OUTLIER(S) worst is CA-CB-CG: 5.64 σ
A 456	GLU 175.15	-	Favored (98.32%) General / -63.6,-42.2	18.1% (*tp10*) chi angles: 177.9,61.1,57.5	0.055Å	-	-
A 457	THR 165.06	-	Favored (96.2%) General / -61.7,-40.8	90.6% (*m*) chi angles: 300.7	0.139Å	-	OUTLIER(S) worst is CA-CB-OG1: 4.306 σ

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 458		VAL	161.19	-	Favored (48.04%) Isoleucine or valine / -65.7,-29.8	33.9% (*m*) chi angles: 299.3	0.348Å	-	OUTLIER(S) worst is N-CA-CB: 4.43 σ
A 459		HIS	176.5	-	Favored (85.45%) General / -67.4,-40.9	61.4% (*m80*) chi angles: 286.6,96.2	0.163Å	-	-
A 460		LYS	171.96	-	Favored (77.15%) General / -67.6,-34.5	35.2% (*mmtt*) chi angles: 267.6,288.3,173.6,186.5	0.122Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 138.32	Clashscore: 1.18	Outliers: 7 of 620	Poor rotamers: 12 of 557	Outliers: 14 of 591	Outliers: 0 of 628	Outliers: 57 of 628
A 461		LYS	163.13	-	Favored (79.85%) General / -64.8,-35.0	7.5% (*ttpt*) chi angles: 190.6,227.5,64,169.9	0.098Å	-	-
A 462		THR	170.99	-	Favored (66.4%) General / -71.9,-31.4	11.2% (*p*) chi angles: 44.7	0.234Å	-	-
A 463		GLU	170.83	-	Favored (98.73%) General / -62.5,-41.3	45.9% (*mt-10*) chi angles: 284.3,181.8,233.3	0.081Å	-	-
A 464		VAL	159.58	-	Favored (86.24%) Isoleucine or valine / -65.7,-47.4	57.9% (*t*) chi angles: 170.9	0.093Å	-	-
A 465		VAL	179.58	-	Favored (96.71%) Isoleucine or valine / -62.5,-46.3	12.8% (*t*) chi angles: 161.1	0.202Å	-	-
A 466		ILE	193.98	-	Favored (96.8%) Isoleucine or valine / -64.3,-42.9	58.5% (*mt*) chi angles: 298.4,181.4	0.136Å	-	-
A 467		THR	199.53	-	Favored (68.03%) General / -53.2,-48.6	89.2% (*m*) chi angles: 297.8	0.102Å	-	-

A 468	LEU 199.47	-	Favored (97.56%) General / -62.6,-40.6	21.6% (*tp*) chi angles: 189.6,53.3	0.074Å	-	-
A 469	ASP 181.25	-	Favored (98.18%) General / -62.5,-40.9	62.9% (*m-20*) chi angles: 294.1,303.5	0.108Å	-	-
A 470	PHE 191.68	-	Favored (27.07%) General / -84.9,-26.7	19.7% (*m-85*) chi angles: 308.8,307.6	0.152Å	-	-
A 471	CYS 197.22	-	Favored (41.84%) General / -79.5,-33.9	7.6% (*t*) chi angles: 198.6	0.172Å	-	-
A 472	ILE 195.94	-	Favored (72.35%) Isoleucine or valine / -71.3,-39.1	35.3% (*pt*) chi angles: 67,170.1	0.277Å	-	OUTLIER(S) worst is N-CA-CB: 4.332 σ
A 473	ARG 191.69	-	Favored (76.38%) General / -62.1,-34.5	25.2% (*ttm-85*) chi angles: 200.4,153.5,290.5,268.5	0.088Å	-	-
A 474	ASN 202.36	-	Favored (54.26%) General / -52.1,-37.5	31.5% (*t30*) chi angles: 179.2,71	0.079Å	-	-
A 475	ILE 173.76	-	Favored (5.29%) Isoleucine or valine / -98.9,-36.0	2.1% (*mp*) chi angles: 290.2,112.3	0.143Å	-	-
A 476	GLU 178.99	-	Favored (28.45%) General / -83.3,-29.2	35% (*mt-10*) chi angles: 292.6,194.9,44.4	0.148Å	-	-
A 477	LYS 179.16	-	Favored (72.24%) General / -62.1,-31.8	76.1% (*tttt*) chi angles: 170.2,186.6,167.4,173.5	0.107Å	-	-
A 478	THR 179.47	-	Allowed (1.11%) General / -77.7,14.2	2.1% (*m*) chi angles: 322.4	0.124Å	-	-
A 479	VAL 187.6	-	Favored (7.55%) Isoleucine or valine /	23.9% (*m*) chi angles: 302.4	0.187Å	-	-

-105.0,-17.2

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 480		LYS	185.02	-	Favored (12.9%) General / -95.9,-31.9	43.9% (*tptt*) chi angles: 167.8,69.4,189,187.3	0.074Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 138.32	Clashscore: 1.18	Outliers: 7 of 620	Poor rotamers: 12 of 557	Outliers: 14 of 591	Outliers: 0 of 628	Outliers: 57 of 628
A 481		VAL	185.6	-	Favored (44.12%) Isoleucine or valine / -117.9,139.7	3.6% (*m*) chi angles: 313.6	0.055Å	-	OUTLIER(S) worst is C-N-CA: 5.039 σ
A 482		TYR	197.76	-	-	1.3% (*t80*) chi angles: 184.8,10.4	0.05Å	-	OUTLIER(S) worst is CA-CB-CG: 4.705 σ
A 492		ALA	165.5	0.403Å N with A 494 GLU OE2	-	-	0.159Å	-	-
A 493		ALA	177.38	-	Favored (74.69%) General / -62.9,-33.1	-	0.111Å	-	-
A 494		GLU	212.79	0.403Å OE2 with A 492 ALA N	Favored (74.66%) General / -63.2,-33.0	0.2% chi angles: 72.8,312.7,308.8	0.201Å	-	-
A 495		LEU	176.51	-	Favored (76.59%) General / -57.6,-39.3	13.4% (*mt*) chi angles: 295.3,153.2	0.122Å	-	-
A 496		GLY	167.13	-	Favored (35.6%) Glycine / -76.4,-37.6	-	-	-	-
A 497		GLU	191.29	-	Favored (82.18%) General / -59.2,-48.3	38% (*mt-10*) chi angles: 287,188.5,254.9	0.087Å	-	-
A 498		ILE	164.26	-	Favored (90.54%) Isoleucine or valine / -66.0,-41.9	41.1% (*mt*) chi angles: 283.6,164.7	0.164Å	-	-
A		SER	181.93	-	Favored (95.7%)	87.9% (*p*)	0.153Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
499					General / -60.6,-45.0	chi angles: 61.6			
A 500		ASP 182.01	-		Favored (73.01%) General / -70.9,-37.2	15.9% (*m-20*) chi angles: 303.5,358.6	0.103Å	-	-
A 501		ILE 194.67	-		Favored (16.15%) Isoleucine or valine / -76.5,-25.0	75.3% (*mt*) chi angles: 302.1,174.1	0.246Å	-	-
A 502		HIS 192.32	-		Favored (77.95%) General / -63.8,-34.5	41% (*t60*) chi angles: 186.2,48.1	0.116Å	-	OUTLIER(S) worst is CA-CB-CG: 7.723 σ
A 503		THR 181.17	-		Favored (74.35%) General / -69.1,-43.5	12.9% (*p*) chi angles: 76.3	0.255Å	-	OUTLIER(S) worst is N-CA-CB: 4.6 σ
A 504		LYS 168.92	-		Favored (65.97%) General / -70.5,-45.3	25.7% (*mttt*) chi angles: 298.6,144.4,195.7,155.5	0.14Å	-	-
A 505		LEU 177.68	-		Favored (78.51%) General / -66.8,-34.8	57.8% (*mt*) chi angles: 293,184.1	0.134Å	-	-
A 506		LEU 177.58	-		Favored (65.35%) General / -70.6,-29.0	19.8% (*tp*) chi angles: 191.1,53.5	0.076Å	-	-
A 507		ARG 215.96	-		Favored (82.53%) General / -67.4,-37.1	15.6% (*ttp85*) chi angles: 186.4,218.2,54.1,84.1	0.099Å	-	-
A 508		LEU 181.33	-		Favored (90.99%) General / -65.9,-40.0	19.2% (*mt*) chi angles: 289.8,155.4	0.134Å	-	-
A 509		SER 151.81	-		Favored (91.78%) General / -61.9,-39.4	13% (*t*) chi angles: 190.7	0.091Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 138.32	Clashscore: 1.18	Outliers: 7 of 620	Poor rotamers: 12 of 557	Outliers: 14 of 591	Outliers: 0 of 628	Outliers: 57 of 628

A 510	SER 171.19	-	Favored (57.03%) General / -77.1,-32.8	16.6% (*p*) chi angles: 49.3	0.27Å	-	-
A 511	SER 171.4	-	Favored (99.67%) General / -62.9,-42.0	60.3% (*m*) chi angles: 291.8	0.129Å	-	-
A 512	GLN 175.14	-	Favored (89.19%) General / -59.2,-41.7	1.6% (*tm0?*) chi angles: 191.6,275.5,280.7	0.069Å	-	-
A 513	GLY 169.83	-	Favored (73.28%) Glycine / -69.4,-33.9	-	-	-	-
A 514	THR 176.28	-	Favored (80.33%) General / -67.8,-36.3	1.9% (*p*) chi angles: 37.7	0.18Å	-	-
A 515	ILE 182.39	-	Favored (62.65%) Isoleucine or valine / -68.3,-49.9	67.6% (*mt*) chi angles: 291.5,161.5	0.107Å	-	-
A 516	GLU 192.44	-	Allowed (0.71%) General / -46.1,-64.6	7.2% (*tp10*) chi angles: 186.4,75.8,83.6	0.044Å	-	-
A 517	THR 179.77	-	Favored (58.52%) General / -77.4,-16.9	37.2% (*p*) chi angles: 52.9	0.228Å	-	-
A 518	SER 160.88	-	Favored (42.14%) General / -79.3,-26.9	95.2% (*p*) chi angles: 63.6	0.214Å	-	-
A 519	LEU 159.95	-	Favored (98.04%) General / -62.7,-40.7	30.9% (*mt*) chi angles: 284.5,182.3	0.066Å	-	-
A 520	GLN 166.04	-	Favored (67.75%) General / -67.8,-28.6	92.9% (*mt-30*) chi angles: 293.3,183.7,339.3	0.142Å	-	-
A 521	ASP 146.86	-	Favored (72.59%) General / -70.3,-34.3	8.8% (*t70*) chi angles: 199.3,74.1	0.169Å	-	-

# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 522	ILE 143.84	-	Favored (96.79%) Isoleucine or valine / -63.5,-45.8	25% (*mt*) chi angles: 288.8,185.1	0.171Å	-	-
A 523	ASP 150.24	-	Favored (69.65%) General / -55.0,-50.1	38% (*t70*) chi angles: 188.2,59.5	0.063Å	-	-
A 524	SER 144.08	-	Favored (13.12%) General / -51.2,-29.0	12.3% (*t*) chi angles: 191	0.059Å	-	-
A 525	ARG 152.34	-	Favored (25.51%) General / -84.2,-30.6	58.8% (*mtt180*) chi angles: 305.7,158.9,196.1,189.4	0.091Å	-	-
A 526	LEU 147.23	-	Favored (56.25%) General / -82.8,-13.4	18.2% (*mt*) chi angles: 308,164	0.076Å	-	-
A 527	SER 158.35	-	Favored (21.91%) Pre-proline / -62.1,161.8	27.8% (*p*) chi angles: 77.8	0.035Å	-	-
A 528	PRO 161.05	-	Allowed (1.31%) Trans-proline / -70.5,78.0	74.4% (*Cg_exo*) chi angles: 333.7	0.059Å	-	-
A 529	GLY 150.34	-	Allowed (0.76%) Glycine / 153.7,-29.6	-	-	-	-

# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
	Avg: 138.32	Clashscore: 1.18	Outliers: 7 of 620	Poor rotamers: 12 of 557	Outliers: 14 of 591	Outliers: 0 of 628	Outliers: 57 of 628
A 530	GLY 142.91	-	Allowed (1.75%) Glycine / -74.0,48.8	-	-	-	-
A 531	SER 152.98	-	Allowed (0.37%) General / 75.8,-20.2	1.1% (*m*) chi angles: 266.6	0.219Å	-	-
A 532	LEU 142.39	-	Favored (13.56%) General / -109.6,-18.1	1% chi angles: 223.4,80.8	0.134Å	-	-

A 533	ALA 157.05	-	Favored (18.64%) General / -56.3,148.4	-	0.019Å	-	-
A 534	ASP 154.38	-	Allowed (0.33%) General / -76.9,18.8	14% (p-10) chi angles: 68.1,312.6	0.13Å	-	-
A 535	ALA 140.97	-	Favored (70.2%) General / -53.9,-48.3	-	0.086Å	-	-
A 536	TRP 138.65	0.519Å CH2 with A 616 SER HA	Favored (93.86%) General / -62.0,-45.4	26% (p-90) chi angles: 68.4,284.8	0.102Å	-	OUTLIER(S) worst is CE3-CD2-CG: 4.268 σ
A 537	ALA 140.09	-	Favored (84.34%) General / -63.5,-36.6	-	0.07Å	-	-
A 538	HIS 139.86	-	Favored (59.98%) General / -77.9,-12.4	1.8% (t-80) chi angles: 219.7,302.8	0.044Å	-	OUTLIER(S) worst is C-N-CA: 4.289 σ
A 539	GLN 156.83	-	Allowed (0.31%) General / -106.4,-108.0	46.1% (mt-30) chi angles: 295.1,152.7,348.6	0.098Å	-	OUTLIER(S) worst is C-N-CA: 6.157 σ
A 540	GLU 148.14	-	OUTLIER (0%) General / 16.3,-102.3	20.5% (tp10) chi angles: 205.2,67.3,24	0.252Å	-	-
A 541	GLY 122.45	0.423Å O with A 543 HIS CE1	Allowed (0.58%) Glycine / -59.6,-172.6	-	-	-	-
A 542	THR 115.1	-	Favored (26.04%) General / -76.5,164.4	62.2% (p) chi angles: 56.8	0.078Å	-	-
A 543	HIS 143.91	0.423Å CE1 with A 541 GLY O	Favored (27.9%) Pre-proline / -136.9,166.4	6.7% (m80) chi angles: 320.7,81.4	0.088Å	-	-
A 544	PRO 118.47	-	Favored (82.96%) Trans-proline / -60.6,-26.5	75.5% (Cg_exo) chi angles: 328.2	0.049Å	-	-
			Favored				

# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 545	LYS 124.56	-	(67.12%) General / -58.8,-29.8	55.9% (*tttp*) chi angles: 185.8,176.5,159.3,62.6	0.086Å	-	-
A 546	ASP 138.51	-	Favored (48.64%) General / -77.9,-23.9	0.6% chi angles: 318.2,353.4	0.089Å	-	OUTLIER(S) worst is CA-CB-CG: 4.795 σ
A 547	ARG 115.42	-	Favored (9.56%) General / 64.2,36.3	52.5% (*mtp85*) chi angles: 298.1,188.5,60.1,67.6	0.134Å	-	-
A 548	ASN 103.07	-	Favored (61.96%) General / -73.7,-28.9	79.4% (*m-20*) chi angles: 283.6,324.5	0.127Å	-	-
A 549	VAL 85.55	-	Favored (16.82%) Isoleucine or valine / -79.8,-36.1	83.1% (*t*) chi angles: 179	0.121Å	-	-

# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
	Avg: 138.32	Clashscore: 1.18	Outliers: 7 of 620	Poor rotamers: 12 of 557	Outliers: 14 of 591	Outliers: 0 of 628	Outliers: 57 of 628
A 550	GLU 117.45	-	Favored (76.18%) General / -67.1,-33.8	3.1% (*mp0*) chi angles: 312.5,93.5,296.9	0.111Å	-	-
A 551	LYS 146.44	-	Favored (78.54%) General / -64.6,-47.5	65.4% (*mttm*) chi angles: 285.1,173.4,182.2,303.4	0.075Å	-	-
A 552	LEU 86.55	-	Favored (96.29%) General / -63.1,-40.0	58.4% (*mt*) chi angles: 304.2,184.2	0.14Å	-	-
A 553	GLN 120.07	-	Favored (95.16%) General / -64.0,-39.9	55.7% (*tp60*) chi angles: 195.8,66.7,38.4	0.113Å	-	-
A 554	VAL 70.54	-	Favored (22.7%) Isoleucine or valine / -51.7,-52.3	3.3% (*t*) chi angles: 156.2	0.101Å	-	-
A 555	LEU 79.97	-	Favored (79.36%) General / -64.8,-34.9	21.4% (*mt*) chi angles: 298.8,159.1	0.101Å	-	-

A 556	LEU 83.02	-	Favored (65.94%) General / -71.7,-30.7	19.9% (*tp*) chi angles: 193.9,57.5	0.034Å	-	-
A 557	ASN 87.94	-	Favored (60.8%) General / -73.0,-44.5	76.9% (*m-20*) chi angles: 300.7,329	0.069Å	-	-
A 558	CYS 104.39	-	Favored (71.69%) General / -54.1,-44.7	52.9% (*m*) chi angles: 306.7	0.093Å	-	-
A 559	MET 69.61	-	Favored (72.46%) General / -71.0,-39.2	88.9% (*mtp*) chi angles: 293.6,180.3,60.4	0.058Å	-	-
A 560	THR 98.31	-	Favored (88.41%) General / -66.8,-40.7	23.7% (*m*) chi angles: 291.2	0.112Å	-	-
A 561	GLU 97.7	-	Favored (84.32%) General / -59.6,-47.8	50.3% (*tt0*) chi angles: 184.6,185.1,38	0.045Å	-	-
A 562	ILE 75.82	-	Favored (87.79%) Isoleucine or valine / -60.0,-41.9	64.2% (*mt*) chi angles: 286.9,168.6	0.088Å	-	-
A 563	TYR 86.71	-	Favored (77.79%) General / -58.7,-49.4	9.6% (*t80*) chi angles: 162.7,55.6	0.112Å	-	-
A 564	TYR 128.63	-	Favored (69.83%) General / -65.0,-28.9	48.1% (*m-85*) chi angles: 285.5,294.5	0.206Å	-	-
A 565	GLN 95.44	-	Favored (64.11%) General / -63.2,-52.0	3.6% (*tp-100*) chi angles: 196,69.4,283.2	0.195Å	-	OUTLIER(S) worst is N-CA-CB: 4.06 σ
A 566	PHE 86.24	-	Favored (65.97%) General / -66.9,-23.1	5.4% (*m-30*) chi angles: 301.1,359.5	0.161Å	-	OUTLIER(S) worst is CA-CB-CG: 4.807 σ
A 567	LYS 124.28	-	Favored (89.27%) General / -59.5,-46.3	18.8% (*mtpp*) chi angles: 293.3,208.2,79.4,62.3	0.142Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 568		LYS	123.84	-	Favored (85.9%) General / -66.0,-44.0	21.5% (*mtmt*) chi angles: 279.2,169.6,276.6,151.5	0.143Å	-	-
A 569		ASP	103.56	-	Favored (93.99%) General / -60.1,-42.0	7.1% (*m-20*) chi angles: 306.9,359.7	0.113Å	-	-
			Avg: 138.32	Clashscore: 1.18	Outliers: 7 of 620	Poor rotamers: 12 of 557	Outliers: 14 of 591	Outliers: 0 of 628	Outliers: 57 of 628
A 570		LYS	121.63	-	Favored (94.41%) General / -64.6,-39.8	43.1% (*tttp*) chi angles: 179.9,191.5,168.5,78.5	0.088Å	-	-
A 571		ALA	111.53	-	Favored (76.7%) General / -67.6,-34.3	-	0.096Å	-	-
A 572		GLU	145.44	-	Favored (7.51%) General / -64.0,-58.2	1.7% (*tp10*) chi angles: 168.1,25.4,75.5	0.085Å	-	OUTLIER(S) worst is C-N-CA: 4.599 σ
A 573		ARG	167.59	-	OUTLIER (0.02%) General / 96.3,-28.0	42.6% (*mtm180*) chi angles: 307,162.6,301.7,146.3	0.209Å	-	-
A 574		ARG	158.14	-	Favored (20.16%) General / -139.8,126.2	59.7% (*ttt85*) chi angles: 186.1,175.3,185.8,86.5	0.046Å	-	-
A 575		LEU	121.35	-	Favored (15.58%) General / -92.4,159.4	4.3% (*mp*) chi angles: 270.1,41.7	0.065Å	-	-
A 576		ALA	110.19	-	Favored (20.7%) General / -75.3,168.1	-	0.037Å	-	-
A 577		TYR	95.54	-	Favored (94.98%) General / -62.9,-39.6	30.7% (*t80*) chi angles: 177.4,278.9	0.155Å	-	-
A 578		ASN	127.88	-	Favored (73.7%) General /	1.7% (*m-20*) chi angles: 309,10.7	0.18Å	-	OUTLIER(S) worst is CA-CB-CG: 4.135 σ

-65.3,-48.3

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 579		GLU	111.96	-	Favored (71.47%) General / -59.5,-33.6	5.2% (*mp0*) chi angles: 293.3,86.8,310	0.104Å	-	-
A 580		GLU	149.59	-	Favored (89.33%) General / -58.6,-43.1	10% (*tt0*) chi angles: 200.8,206.5,3	0.051Å	-	-
A 581		GLN	126.37	-	Favored (24.74%) General / -86.6,-25.9	3.4% (*mm-40*) chi angles: 335.2,312,339.9	0.255Å	-	-
A 582		ILE	105.54	-	Favored (96.71%) Isoleucine or valine / -64.6,-43.4	18.5% (*mt*) chi angles: 283.8,153.6	0.139Å	-	-
A 583		HIS	108.67	-	Favored (60.91%) General / -50.9,-46.3	23.3% (*t60*) chi angles: 184,101.1	0.027Å	-	-
A 584		LYS	120.48	-	Favored (24.5%) General / -70.9,-51.7	86.7% (*mttt*) chi angles: 295,165.3,187,169.8	0.05Å	-	-
A 585		PHE	142.54	-	Favored (77.88%) General / -56.5,-42.1	14.2% (*m-30*) chi angles: 306.8,323.6	0.092Å	-	-
A 586		ASP	120.74	-	Favored (34.22%) General / -82.7,-23.0	67.2% (*m-20*) chi angles: 299.7,342.8	0.273Å	-	-
A 587		LYS	102.7	-	Favored (90.89%) General / -66.1,-40.5	77.2% (*tttt*) chi angles: 180.5,180.7,162.3,181.2	0.041Å	-	-
A 588		GLN	104.11	-	Favored (76.63%) General / -65.5,-33.7	8.1% (*tt0*) chi angles: 208.1,184.4,116.1	0.059Å	-	-
A 589		LYS	108.05	-	Favored (61.96%) General / -72.7,-27.2	58.6% (*mttt*) chi angles: 298.6,159.8,201.2,166.3	0.125Å	-	-

Avg: Clashscore: Outliers: 7 of   Poor rotamers: 12 of Outliers: Outliers: Outliers: 57

		138.32	1.18	620	557	14 of 591	0 of 628	of 628
A 590	LEU	87.33	0.438Å HD21 with A 415 ALA HA	Favored (73.5%) General / -61.2,-33.5	26.5% (*tp*) chi angles: 191.2,61.5	0.039Å	-	-
A 591	TYR	102.72	-	Favored (11.33%) General / -72.6,-53.6	48.8% (*t80*) chi angles: 166.7,82.9	0.068Å	-	-
A 592	TYR	129.55	-	Favored (92.77%) General / -60.5,-40.9	59.6% (*m-85*) chi angles: 287.9,291	0.154Å	-	-
A 593	HIS	104.1	-	Favored (92.49%) General / -60.6,-45.9	83.9% (*m-70*) chi angles: 298.6,304	0.11Å	-	-
A 594	ALA	79.98	-	Favored (98.4%) General / -62.8,-43.6	-	0.06Å	-	-
A 595	THR	101.51	-	Favored (73.87%) General / -70.6,-39.2	17.7% (*p*) chi angles: 47.3	0.156Å	-	-
A 596	LYS	133.79	-	Favored (77.68%) General / -59.0,-37.8	76.9% (*tttt*) chi angles: 194.4,186.7,184.8,190.6	0.076Å	-	-
A 597	ALA	84.93	-	Favored (67.57%) General / -68.3,-47.4	-	0.07Å	-	-
A 598	MET	96.44	-	Favored (84.91%) General / -67.3,-38.4	68.6% (*mmm*) chi angles: 302.5,308.8,274.7	0.139Å	-	-
A 599	THR	92.32	-	Favored (94.46%) General / -61.7,-40.3	42.6% (*m*) chi angles: 293.3	0.098Å	-	-
A 600	HIS	95.9	-	Favored (96.45%) General / -62.5,-44.4	50.3% (*t60*) chi angles: 197,65.3	0.05Å	-	-
A	PHE	99.41	-	Favored (25.21%)	65.3% (*t80*)	0.023Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
601					General / -59.5,-56.2	chi angles: 176.9,66			
A 602		THR 95.71	-		Favored (61.09%) General / -73.1,-26.1	57.4% (*p*) chi angles: 56.3	0.13Å	-	-
A 603		ASP 114.55	-		Favored (5.94%) General / -106.1,-39.5	4.3% (*m-20*) chi angles: 315.1,339.8	0.141Å	-	OUTLIER(S) worst is CA-CB-CG: 5.126 σ
A 604		GLU 114.38	-		Favored (13.01%) General / -92.7,-36.3	26.5% (*tp10*) chi angles: 171.6,55.6,35.7	0.095Å	-	-
A 605		CYS 113.77	-		Favored (2.05%) General / -88.2,-60.1	56.7% (*m*) chi angles: 306	0.172Å	-	-
A 606		VAL 112.62	-		Favored (38.05%) Isoleucine or valine / -74.6,-47.6	73.8% (*t*) chi angles: 172	0.173Å	-	-
A 607		LYS 144.55	-		Favored (81.38%) General / -57.6,-41.6	29.5% (*mtmm*) chi angles: 275.7,182.6,284,299.6	0.193Å	-	-
A 608		LYS 108.5	-		Favored (75.95%) General / -68.2,-34.2	97.9% (*mttt*) chi angles: 287.1,181.9,176.5,175.1	0.125Å	-	-
A 609		TYR 99.93	-		Favored (80.58%) General / -63.0,-48.0	11.7% (*t80*) chi angles: 157.2,73.6	0.073Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 138.32	Clashscore: 1.18	Outliers: 7 of 620	Poor rotamers: 12 of 557	Outliers: 14 of 591	Outliers: 0 of 628	Outliers: 57 of 628
A 610		GLU 125.32	-		Favored (79.52%) General / -65.3,-34.9	96.7% (*mt-10*) chi angles: 289.6,175,341.6	0.163Å	-	-
A 611		ALA 130.17	-		Favored (62.93%) General / -64.7,-51.4	-	0.05Å	-	-
A		PHE 123.77	-		Favored (77.2%)	14.6% (*t80*)	0.103Å	-	-

612			General / -57.3,-40.2	chi angles: 171.8,100.9			
A 613	LEU 96.02	-	Favored (65.89%) General / -55.6,-51.8	29.4% (*tp*) chi angles: 186.5,70.3	0.037Å	-	-
A 614	ASN 137.1	-	Favored (86.2%) General / -61.1,-47.5	19% (*t-20*) chi angles: 177.4,244.1	0.082Å	-	-
A 615	LYS 149.9	-	Favored (66.3%) General / -67.6,-26.6	81.8% (*mttt*) chi angles: 303.3,191.9,189.9,171.5	0.193Å	-	-
A 616	SER 128.94	0.519Å HA with A 536 TRP CH2	Favored (91.99%) General / -65.8,-41.4	3.8% (*t*) chi angles: 201.7	0.117Å	-	-
A 617	GLU 181.37	-	Favored (94.48%) General / -65.0,-42.4	6.3% (*tt0*) chi angles: 194,213.6,324.8	0.036Å	-	-
A 618	GLU 159.43	-	Favored (86.01%) General / -57.8,-43.7	20.3% (*mm-40*) chi angles: 286.8,294.5,13.3	0.082Å	-	-
A 619	TRP 111.26	-	Favored (92.56%) General / -64.3,-38.9	74% (*t90*) chi angles: 178.4,95.2	0.093Å	-	OUTLIER(S) worst is CE3-CD2-CG: 4.287 σ
A 620	ILE 136.73	-	Favored (97.93%) Isoleucine or valine / -61.4,-45.8	21.8% (*mt*) chi angles: 280.6,159.9	0.125Å	-	-
A 621	ARG 183.85	-	Favored (77.06%) General / -56.6,-48.6	95.6% (*mtt180*) chi angles: 302.1,167.6,186.2,179.5	0.076Å	-	-
A 622	LYS 148.51	-	Favored (92.39%) General / -65.6,-41.8	46% (*mtpt*) chi angles: 297.3,154.2,66.3,182.9	0.076Å	-	-
A 623	MET 138.26	-	Favored (89.71%) General / -66.3,-41.6	11.3% (*tmm?*) chi angles: 179.5,273,306.3	0.103Å	-	-
			Favored				

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 624		LEU	135.56	-	Favored (76.56%) General / -69.0,-35.2	18.7% (*mt*) chi angles: 291.2,192.6	0.181Å	-	-
A 625		HIS	162.77	-	Favored (66.78%) General / -53.5,-49.8	86.4% (*t60*) chi angles: 177.6,71.3	0.058Å	-	-
A 626		LEU	122.61	-	Favored (70.31%) General / -68.0,-30.9	8% (*tt*) chi angles: 192.1,147.5	0.069Å	-	-
A 627		ARG	156.79	-	Favored (51.57%) General / -77.4,-5.9	28% (*ttm-85*) chi angles: 193.8,161.4,274.5,286.3	0.202Å	-	-
A 628		LYS	141.35	-	Favored (10.76%) General / -94.1,-39.1	13.1% (*mptt*) chi angles: 252.8,55,175.3,172.3	0.133Å	-	-
A 629		GLN	163.89	-	Favored (78.77%) General / -61.1,-49.1	5% (*mt-30*) chi angles: 280.2,209.9,237.4	0.167Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 138.32	Clashscore: 1.18	Outliers: 7 of 620	Poor rotamers: 12 of 557	Outliers: 14 of 591	Outliers: 0 of 628	Outliers: 57 of 628
A 630		LEU	144.77	-	Favored (65.77%) General / -70.4,-29.2	31.4% (*tp*) chi angles: 185.2,54.5	0.071Å	-	-
A 631		LEU	143.4	-	Favored (84.61%) General / -60.5,-47.8	53.4% (*tp*) chi angles: 182.2,59.4	0.086Å	-	-
A 632		SER	150.78	-	Favored (7.87%) General / -62.4,-58.4	74.9% (*m*) chi angles: 294.8	0.102Å	-	-
A 633		LEU	148.16	-	Favored (83.56%) General / -58.9,-40.1	81.4% (*mt*) chi angles: 303,176.9	0.126Å	-	-
A 634		THR	160.09	-	Favored (90.87%) General / -61.9,-46.1	87.9% (*m*) chi angles: 301.1	0.068Å	-	-
					Favored				OUTLIER(S)

A 635	ASN 172.86	-	(56.83%) General / -76.9,-19.9	7.5% (*m120*) chi angles: 303.6,161.5	0.151Å	-	worst is CA-CB-CG: 5.61 σ
A 636	GLN 173.74	-	Favored (47.56%) General / -78.6,-22.2	1.6% (*mt-30*) chi angles: 306.4,223.4,249	0.186Å	-	-
A 637	CYS 154.13	-	Favored (75.86%) General / -63.9,-33.5	58.3% (*m*) chi angles: 285.6	0.152Å	-	-
A 638	PHE 162.79	-	Favored (61.97%) General / -73.2,-28.0	10.3% (*m-30*) chi angles: 309.2,326.7	0.228Å	-	-
A 639	ASP 181.64	-	Favored (68.03%) General / -53.9,-49.7	3.4% (*m-20*) chi angles: 309.9,1.5	0.147Å	-	OUTLIER(S) worst is CA-CB-CG: 5.084 σ
A 640	ILE 172.46	-	Favored (11.43%) Isoleucine or valine / -80.3,-23.2	1.7% (*pt*) chi angles: 75.5,200.4	0.257Å	-	-
A 641	GLU 166.31	-	Favored (60.56%) General / -64.3,-52.0	55% (*tt0*) chi angles: 193,174.7,330.8	0.089Å	-	-
A 642	GLU 179.18	-	Favored (62.88%) General / -72.5,-28.5	6.5% (*mm-40*) chi angles: 287.3,285.2,44	0.187Å	-	-
A 643	GLU 178.42	-	Favored (76.42%) General / -57.7,-49.5	42.3% (*mm-40*) chi angles: 276.5,302.7,114.6	0.118Å	-	-
A 644	VAL 152.76	-	Favored (69.86%) Isoleucine or valine / -61.6,-35.9	31% (*m*) chi angles: 294.7	0.23Å	-	-
A 645	SER 160.58	-	Favored (79.13%) General / -56.1,-46.2	52.8% (*m*) chi angles: 300	0.064Å	-	-
A 646	LYS 180.81	-	Favored (68.38%) General / -53.2,-44.9	31.8% (*ttmt*) chi angles: 184,199.3,304.8,173.2	0.027Å	-	-
			Favored				

# Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 647	TYR 176.38	-		(43.75%) General / -79.8,-21.9	65.4% (*m-85*) chi angles: 306.1,283.3	0.17Å	-	-
A 648	GLN 163.27	-		Favored (65.42%) General / -67.1,-49.3	7.9% (*tp-100*) chi angles: 183.1,62.3,208.5	0.062Å	-	OUTLIER(S) worst is CB-CG-CD: 4.897 σ
A 649	GLU 161.46	-		Favored (83.67%) General / -57.7,-42.4	45.4% (*mt-10*) chi angles: 293.6,181.2,78	0.093Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 138.32	Clashscore: 1.18	Outliers: 7 of 620	Poor rotamers: 12 of 557	Outliers: 14 of 591	Outliers: 0 of 628	Outliers: 57 of 628
A 650		TYR 183.65	-		Favored (13.27%) General / -65.8,-56.2	29% (*t80*) chi angles: 182.7,101.6	0.121Å	-	-
A 651		THR 180.77	-		Favored (14.35%) General / -90.4,-36.8	3.1% (*m*) chi angles: 319.8	0.176Å	-	-
A 652		ASN 160.65	-		Favored (29.68%) General / -78.3,-42.7	25.8% (*t-20*) chi angles: 184.7,265.2	0.093Å	-	-
A 653		GLU 174.64	-		Allowed (1.28%) General / -101.8,71.1	29.8% (*mt-10*) chi angles: 306.8,201.1,323.7	0.166Å	-	-
A 654		LEU 133.87	-		Favored (56.09%) General / -116.2,129.0	2.2% (*tp*) chi angles: 169.5,38	0.147Å	-	-
A 655		GLN 137.84	-		Favored (46.91%) General / -72.4,138.0	2.4% (*mm-40*) chi angles: 321,264.8,261.9	0.086Å	-	OUTLIER(S) worst is C-N-CA: 4.143 σ
A 656		GLU 135.94	-		Favored (12.52%) General / -161.2,143.9	13.2% (*tp10*) chi angles: 182.9,40.8,45.3	0.117Å	-	OUTLIER(S) worst is CB-CG-CD: 5.439 σ
A 657		THR 170.56	-		-	82.1% (*m*) chi angles: 297.3	0.115Å	-	-