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All-Atom Contacts	Clashscore, all atoms:	8.45		96th percentile* (N=63, 2.81Å - 9999Å)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	0	0.00%	Goal: <1%
	Ramachandran outliers	0	0.00%	Goal: <0.05%
	Ramachandran favored	596	96.13%	Goal: >98%
	MolProbity score^	1.72		100th percentile* (N=2131, 3.06Å ± 0.25Å)
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	Bad backbone bonds:	0 / 5166	0.00%	Goal: 0%
	Bad backbone angles:	0 / 6976	0.00%	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: 137.21	Clashscore: 8.45	Outliers: 0 of 620	Poor rotamers: 0 of 557	Outliers: 0 of 591	Outliers: 0 of 628	Outliers: 0 of 628
A -1		ALA	123.55	-	-	-	0.019Å	-	-
A 0		MET	172.86	-	Favored (50.7%) General / -69.5,135.9	25.5% (*mmt*) chi angles: 297.8,297.4,182.4	0.002Å	-	-
A 1		GLY	116.09	-	Favored (6.26%) Glycine / -153.0,138.3	-	-	-	-
A 2		GLN	127.24	-	Favored (16.28%) General / -73.9,170.0	12.6% (*mm-40*) chi angles: 295.8,268.5,54.4	0.018Å	-	-
A 3		SER	109.02	-	Favored (11%) General / -155.4,177.8	82.3% (*p*) chi angles: 60.7	0.011Å	-	-
				0.816Å	Favored				

A 4	THR 107.77	HG22 with A 5 SER N	(6.16%) General / -148.5,-178.1	98.3% (*m*) chi angles: 299	0.042Å	-	-
A 5	SER 109.81	0.816Å N with A 4 THR HG22	Favored (98.37%) General / -61.0,-42.4	31.2% (*t*) chi angles: 173.4	0.024Å	-	-
A 6	ASN 116.09	-	Favored (11.89%) General / -115.1,-12.8	5.7% (*m-20*) chi angles: 292.7,24.4	0.036Å	-	-
A 7	HIS 108.38	0.449Å O with A 4 THR N	Favored (42.31%) General / -132.1,158.2	63% (*m80*) chi angles: 302.8,80.2	0.03Å	-	-
A 8	LEU 104.7	0.647Å HD23 with A 29 LYS HG2	Favored (33.04%) General / -150.6,151.7	4.4% (*pp*) chi angles: 59.3,87.2	0.028Å	-	-
A 9	TRP 106.94	-	Favored (39.38%) General / -156.8,160.6	43.8% (*p90*) chi angles: 58,95.7	0.023Å	-	-
A 10	LEU 122.38	-	Favored (23.31%) General / -94.4,147.4	91.4% (*mt*) chi angles: 300.4,177.7	0.025Å	-	-
A 11	LEU 119.97	-	Favored (60.88%) General / -74.5,-14.8	83.2% (*mt*) chi angles: 294.5,180	0.017Å	-	-
A 12	SER 103.15	-	Favored (62.44%) General / -73.7,-29.7	75.6% (*p*) chi angles: 58.3	0.006Å	-	-
A 13	ASP 103.76	0.48Å HB3 with A 25 ARG HB3	Favored (7.82%) General / -80.9,98.3	71.7% (*m-20*) chi angles: 299.8,330.4	0.022Å	-	-
A 14	ILE 114.63	-	Favored (35.71%) Isoleucine or valine / -118.4,141.9	9.9% (*tp*) chi angles: 194.8,59.4	0.064Å	-	-
A 15	LEU 110.97	-	Favored (2.63%) General / -116.9,-48.9	61.2% (*mt*) chi angles: 305.1,183	0.006Å	-	-
A	GLY 116.68	-	Favored (9.3%) Glycine /	-	-	-	-

16   -146.7,141.2

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 17		GLN	144.81	-	Favored (9.26%) General / -119.3,103.2	5.9% (*tp60*) chi angles: 202.8,79.7,336.2	0.012Å	-	-
A 18		GLY	133.21	-	Favored (23.04%) Glycine / -106.3,179.9	-	-	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 137.21	Clashscore: 8.45	Outliers: 0 of 620	Poor rotamers: 0 of 557	Outliers: 0 of 591	Outliers: 0 of 628	Outliers: 0 of 628
A 19		ALA	132.84	-	Favored (12.6%) General / -73.0,-52.9	-	0.023Å	-	-
A 20		THR	151.75	0.509Å O with A 41 ASN N	Favored (21.65%) General / -85.7,-33.2	13.2% (*m*) chi angles: 312.3	0.026Å	-	-
A 21		ALA	123.02	-	Favored (25.66%) General / -140.6,166.1	-	0.032Å	-	-
A 22		ASN	135.96	0.605Å OD1 with A 41 ASN ND2	Favored (52%) General / -130.2,149.2	17.7% (*m120*) chi angles: 298.5,143.6	0.012Å	-	-
A 23		VAL	105.73	-	Favored (60.93%) Isoleucine or valine / -112.8,119.7	89.5% (*t*) chi angles: 175.3	0.05Å	-	-
A 24		PHE	102.18	-	Favored (21.31%) General / -114.0,158.3	67.7% (*m-85*) chi angles: 304.3,88.3	0.041Å	-	-
A 25		ARG	111.61	0.48Å HB3 with A 13 ASP HB3	Favored (19.16%) General / -83.8,111.4	77.8% (*ttt180*) chi angles: 178.1,184.7,180.3,181.6	0.023Å	-	-
A 26		GLY	96.73	-	Favored (15.98%) Glycine / -123.7,170.7	-	-	-	-
A 27		ARG	98.7	0.435Å HG2 with A 34 LEU HD23	Favored (47.01%) General / -131.1,155.4	40.1% (*mtp85*) chi angles: 313.4,187.6,75,103.7	0.03Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 28		HIS	103.33	0.408Å CE1 with A 30 LYS HB2	Favored (37.9%) General / -78.0,133.6	23.4% (*t-80*) chi angles: 189.7,242.1	0.031Å	-	-
A 29		LYS	136.01	0.647Å HG2 with A 8 LEU HD23	Favored (75.3%) General / -61.6,-34.2	61.6% (*mtpt*) chi angles: 294.8,176.4,62.6,178.8	0.036Å	-	-
A 30		LYS	137.81	0.408Å HB2 with A 28 HIS CE1	Allowed (1.04%) General / -84.2,-65.2	74.6% (*mmtt*) chi angles: 304.6,290.9,177.5,181.8	0.009Å	-	-
A 31		THR	110.04	-	Favored (60.12%) General / -73.4,-43.6	58.6% (*p*) chi angles: 65.1	0.02Å	-	-
A 32		GLY	95.32	-	Favored (56.66%) Glycine / 94.7,11.6	-	-	-	-
A 33		ASP	96.01	-	Favored (38.44%) General / -76.0,147.8	62.5% (*m-20*) chi angles: 302.5,331.5	0.001Å	-	-
A 34		LEU	85.55	0.435Å HD23 with A 27 ARG HG2	Favored (36.43%) General / -79.3,132.4	95.5% (*mt*) chi angles: 292.5,174.8	0.018Å	-	-
A 35		PHE	92.11	-	Favored (47.22%) General / -136.9,157.2	93% (*m-85*) chi angles: 291.8,88.4	0.025Å	-	-
A 36		ALA	99.75	0.684Å HB3 with A 86 MET HB2	Favored (34.34%) General / -86.8,126.0	-	0.027Å	-	-
A 37		ILE	101.13	-	Favored (31.57%) Isoleucine or valine / -105.2,110.6	47.5% (*mm*) chi angles: 304.6,300.8	0.01Å	-	-
A 38		LYS	120.65	0.596Å HD3 with A 84 LEU HD12	Favored (10.66%) General / -99.0,99.6	37.9% (*tttp*) chi angles: 203.1,180.7,188.4,67.8	0.015Å	-	-
			Avg: 137.21	Clashscore: 8.45	Outliers: 0 of 620	Poor rotamers: 0 of 557	Outliers: 0 of 591	Outliers: 0 of 628	Outliers: 0 of 628

A 39	VAL 127.96	-	Favored (49.55%) Isoleucine or valine / -100.3,120.3	18.9% (*t*) chi angles: 189.2	0.028Å	-	-
A 40	PHE 140.16	0.422Å HD1 with A 20 THR HG22	Favored (19.98%) General / -77.4,118.6	71.3% (*m-85*) chi angles: 286.3,275.1	0.049Å	-	-
A 41	ASN 159.01	0.605Å ND2 with A 22 ASN OD1	Favored (28.79%) General / -88.1,141.2	6.1% (*m-20*) chi angles: 299.8,14.7	0.035Å	-	-
A 42	ASN 178.62	-	Allowed (0.28%) General / 54.1,75.3	39.5% (*t30*) chi angles: 179.4,23.2	0.044Å	-	-
A 43	ILE 195.75	-	Allowed (1.61%) Isoleucine or valine / -131.3,92.4	11% (*tt*) chi angles: 177.1,176.6	0.133Å	-	-
A 44	SER 214.02	-	Allowed (0.33%) General / -143.7,-51.4	78.9% (*p*) chi angles: 59.5	0.011Å	-	-
A 45	PHE 209.89	-	Favored (62.85%) General / -69.1,-14.2	34.6% (*p90*) chi angles: 52.1,271.7	0.042Å	-	-
A 46	LEU 224.64	-	Allowed (0.41%) General / -102.8,-87.7	73.6% (*mt*) chi angles: 300.4,183.3	0.006Å	-	-
A 47	ARG 231.78	-	Favored (15.65%) Pre-proline / 45.6,57.8	18.1% (*mmt85*) chi angles: 277.2,290.7,173,93.7	0.05Å	-	-
A 48	PRO 236.75	0.515Å HG2 with A 52 GLN HG3	Allowed (1.28%) Trans-proline / -87.6,80.7	91.6% (*Cg_endo*) chi angles: 31	0.057Å	-	-
A 49	VAL 237.54	-	Allowed (1.86%) Isoleucine or valine / -69.4,-1.7	31% (*m*) chi angles: 294.7	0.024Å	-	-
A 50	ASP 246.39	-	Favored (4.06%) General / -92.2,-53.9	30.8% (*m-20*) chi angles: 307.5,328.8	0.033Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 51		VAL	222.27	-	Favored (42.74%) Isoleucine or valine / -73.3,-48.3	59.9% (*t*) chi angles: 181	0.016Å	-	-
A 52		GLN	212.86	0.515Å HG3 with A 48 PRO HG2	Favored (66.05%) General / -66.8,-21.5	80.3% (*mt-30*) chi angles: 281.8,179.3,355.4	0.039Å	-	-
A 53		MET	204.62	-	Allowed (0.85%) General / -59.1,-64.7	45.5% (*ttm*) chi angles: 176.7,186.4,298.6	0.019Å	-	-
A 54		ARG	193.77	-	Favored (76.75%) General / -63.7,-33.9	18.4% (*ptt-85*) chi angles: 57.7,171.2,203.2,271.2	0.004Å	-	-
A 55		GLU	182.79	-	Favored (70.59%) General / -61.6,-50.9	69.3% (*mt-10*) chi angles: 276.6,185.1,351.7	0.015Å	-	-
A 56		PHE	184.21	-	Favored (64.67%) General / -68.6,-25.0	22.6% (*m-30*) chi angles: 297.9,337.9	0.015Å	-	-
A 57		GLU	172.78	-	Favored (63.08%) General / -73.1,-29.7	86.4% (*mt-10*) chi angles: 285.7,165.6,4.2	0.001Å	-	-
A 58		VAL	158.47	-	Favored (40.96%) Isoleucine or valine / -74.7,-46.8	25.5% (*t*) chi angles: 164.4	0.016Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 137.21	Clashscore: 8.45	Outliers: 0 of 620	Poor rotamers: 0 of 557	Outliers: 0 of 591	Outliers: 0 of 628	Outliers: 0 of 628
A 59		LEU	154.8	-	Favored (65.31%) General / -67.6,-20.0	80.7% (*mt*) chi angles: 296.4,181.9	0.008Å	-	-
A 60		LYS	144.64	-	Favored (23.5%) General / -66.3,-54.5	35.7% (*tptt*) chi angles: 158.3,64.5,191.8,175.3	0.009Å	-	-
A 61		LYS	144.43	0.412Å HA with A 61 LYS HD2	Favored (62.17%) General / -71.8,-15.3	17.1% (*tptm*) chi angles: 200.4,55.3,181.9,298.1	0.022Å	-	-

A 62	LEU 133.78	-	Favored (4.87%) General / -66.1,113.9	7.9% (*tt*) chi angles: 193.7,152.9	0.018Å	-	-
A 63	ASN 143.55	-	Favored (44.33%) General / -131.0,131.5	10% (*t30*) chi angles: 175.5,83.3	0.015Å	-	-
A 64	HIS 141.74	-	Favored (27.95%) General / -156.8,153.2	2.1% (*t60*) chi angles: 196.2,22.3	0.009Å	-	-
A 65	LYS 128.17	0.507Å O with A 154 LYS NZ	Favored (67.52%) General / -68.1,-28.6	63.1% (*tttm*) chi angles: 182.1,173.5,175.1,292.9	0.016Å	-	-
A 66	ASN 111.06	-	Favored (14.6%) General / -101.2,21.0	26.9% (*m120*) chi angles: 301.3,130.3	0.02Å	-	-
A 67	ILE 119.81	-	Favored (47.77%) Isoleucine or valine / -136.4,130.7	72.8% (*mt*) chi angles: 296.3,178.3	0.007Å	-	-
A 68	VAL 97.05	-	Favored (10.79%) Isoleucine or valine / -61.2,122.1	90% (*t*) chi angles: 175.3	0.014Å	-	-
A 69	LYS 123.38	-	Favored (40.85%) General / -75.6,133.6	54.6% (*tptt*) chi angles: 185.7,58.1,180.6,178.1	0.019Å	-	-
A 70	LEU 124.33	-	Favored (40%) General / -96.5,123.0	54.9% (*tp*) chi angles: 172.2,62.1	0.026Å	-	-
A 71	PHE 111.78	-	Favored (4.89%) General / -91.8,-52.1	75.2% (*m-85*) chi angles: 293.3,288.8	0.046Å	-	-
A 72	ALA 114.9	-	Favored (40.93%) General / -155.1,162.8	-	0.031Å	-	-
A 73	ILE 137.59	-	Favored (44.82%) Isoleucine or valine / -117.4,114.2	5.2% (*mp*) chi angles: 299.4,91.1	0.016Å	-	-

# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 74	GLU 142.17	0.531Å OE1 with A 4 THR HG21	Favored (12.62%) General / -126.2,169.7	94.4% (mt-10) chi angles: 301,174.8,355.5	0.015Å	-	-
A 75	GLU 175.07	-	Favored (55.38%) General / -112.6,131.9	95.2% (mt-10) chi angles: 298.9,183.3,354.8	0.024Å	-	-
A 76	GLU 138.88	0.404Å OE1 with A 78 THR N	Favored (41.01%) General / -58.2,144.3	6.3% (tm-20) chi angles: 212.5,287.2,329	0.02Å	-	-
A 77	THR 126.34	-	Favored (8.25%) General / -62.1,-58.3	47.5% (p) chi angles: 55.5	0.021Å	-	-
A 78	THR 153.5	0.404Å N with A 76 GLU OE1	Allowed (1.93%) General / -86.4,-60.7	64.9% (p) chi angles: 63	0.024Å	-	-
# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
	Avg: 137.21	Clashscore: 8.45	Outliers: 0 of 620	Poor rotamers: 0 of 557	Outliers: 0 of 591	Outliers: 0 of 628	Outliers: 0 of 628
A 79	THR 141.02	-	Favored (60.77%) General / -71.3,-11.2	81.8% (p) chi angles: 60.9	0.025Å	-	-
A 80	ARG 148.04	-	Favored (13.62%) General / 57.7,26.9	77.4% (mtp180) chi angles: 298.5,179.9,60.2,179.9	0.055Å	-	-
A 81	HIS 141.96	-	Favored (33%) General / -79.4,146.2	1.9% (m-70) chi angles: 284,2.6	0.01Å	-	-
A 82	LYS 162.58	-	Favored (40.27%) General / -75.2,131.2	33.6% (mmtp) chi angles: 296.3,306.6,181.1,64	0.013Å	-	-
A 83	VAL 133.16	-	Favored (72.8%) Isoleucine or valine / -122.5,125.6	49% (t) chi angles: 168.4	0.01Å	-	-
A 84	LEU 122.03	0.596Å HD12 with A 38 LYS HD3	Favored (31.32%) General / -94.8,139.4	48.8% (mt) chi angles: 306.1,184.5	0.017Å	-	-
			Favored (6.43%)				

A 85	ILE 107.84	-	Isoleucine or valine / -104.7,98.1	37.9% (*mm*) chi angles: 308.2,299.3	0.003Å	-	-
A 86	MET 112.48	0.684Å HB2 with A 36 ALA HB3	Favored (12.38%) General / -92.9,166.5	42.9% (*mmm*) chi angles: 317.6,284.7,287.9	0.042Å	-	-
A 87	GLU 107.09	-	Favored (37.47%) General / -79.6,139.3	9.7% (*pt-20*) chi angles: 58.3,166.8,328.4	0.022Å	-	-
A 88	PHE 86.13	-	Favored (34.22%) General / -79.2,129.2	40.3% (*t80*) chi angles: 178.1,57.1	0.037Å	-	-
A 89	CYS 89.59	-	Favored (23.62%) Pre-proline / -112.2,93.9	39.3% (*m*) chi angles: 307.7	0.023Å	-	-
A 90	PRO 69.16	-	Favored (95.96%) Trans-proline / -57.0,-33.7	50.7% (*Cg_exo*) chi angles: 335.3	0.07Å	-	-
A 91	CYS 90.27	-	Favored (58.13%) General / -76.2,-8.9	62.1% (*m*) chi angles: 303.4	0.019Å	-	-
A 92	GLY 87.85	-	Favored (21.43%) Glycine / 85.6,-146.2	-	-	-	-
A 93	SER 101.64	-	Favored (3.25%) General / -114.8,-177.9	85.6% (*p*) chi angles: 61.2	0.012Å	-	-
A 94	LEU 98.24	-	Favored (73.79%) General / -66.1,-32.4	54.2% (*tp*) chi angles: 180,58.2	0.016Å	-	-
A 95	TYR 119.11	-	Favored (80.31%) General / -57.7,-40.8	81% (*t80*) chi angles: 176.5,84.7	0.024Å	-	-
A 96	THR 98.81	-	Favored (89.59%) General / -63.8,-38.0	34.6% (*m*) chi angles: 306.4	0.013Å	-	-
			Favored (82.26%)				

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 97		VAL	93.51	-	Isoleucine or valine / -66.3,-38.6	35.1% (*t*) chi angles: 185.8	0.015Å	-	-
A 98		LEU	99.55	-	Favored (61.62%) General / -72.1,-20.4	91.8% (*mt*) chi angles: 298.6,179	0.009Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 137.21	Clashscore: 8.45	Outliers: 0 of 620	Poor rotamers: 0 of 557	Outliers: 0 of 591	Outliers: 0 of 628	Outliers: 0 of 628
A 99		GLU	114.64	-	Favored (64.51%) General / -68.5,-19.7	17.9% (*mm-40*) chi angles: 283.9,276,16.7	0.01Å	-	-
A 100		GLU	92.11	0.432Å HA with A 101 PRO HD3	Favored (78.72%) Pre-proline / -73.6,134.8	54.4% (*mt-10*) chi angles: 305.4,182.6,204.5	0.002Å	-	-
A 101		PRO	101.21	0.432Å HD3 with A 100 GLU HA	Favored (70.16%) Trans-proline / -63.5,-25.4	47% (*Cg_exo*) chi angles: 337.2	0.065Å	-	-
A 102		SER	121.02	0.617Å O with A 427 ARG NH2	Favored (68.02%) General / -65.7,-27.0	26.6% (*m*) chi angles: 304.4	0.024Å	-	-
A 103		ASN	88.03	0.414Å HB3 with A 107 LEU HD23	Favored (19.03%) General / -110.2,19.3	60.3% (*m-20*) chi angles: 307.9,317.8	0.01Å	-	-
A 104		ALA	94.04	-	Favored (70.5%) General / -65.3,-29.7	-	0.019Å	-	-
A 105		TYR	110.69	-	Favored (14.92%) General / -110.6,22.9	85.3% (*m-85*) chi angles: 293,284	0.026Å	-	-
A 106		GLY	83.68	-	Favored (10.47%) Glycine / 114.2,151.8	-	-	-	-
A 107		LEU	103.72	0.414Å HD23 with A 103 ASN HB3	Favored (90.38%) Pre-proline / -69.7,157.1	82.1% (*mt*) chi angles: 301.2,180.7	0.037Å	-	-
A					Favored (60.94%)	72.2% (*Cg_exo*)			

# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
108	PRO 95.76	-	Trans-proline / -58.6,151.7	chi angles: 332.7	0.075Å	-	-
A 109	GLU 124.77	0.538Å OE1 with A 325 TYR OH	Favored (91.75%) General / -59.0,-44.0	75.1% (*tt0*) chi angles: 188.7,168.3,188.9	0.035Å	-	-
A 110	SER 98.75	-	Favored (88.34%) General / -63.3,-46.1	80.1% (*p*) chi angles: 60	0.002Å	-	-
A 111	GLU 104.59	-	Favored (72.12%) General / -64.6,-31.1	43.3% (*tp10*) chi angles: 187.4,73.2,187.7	0.007Å	-	-
A 112	PHE 102.62	-	Favored (80.22%) General / -68.7,-38.5	75.1% (*t80*) chi angles: 181.9,85.7	0.008Å	-	-
A 113	LEU 107.17	-	Favored (80.16%) General / -64.0,-35.3	96% (*mt*) chi angles: 295.4,176.2	0.01Å	-	-
A 114	ILE 104.73	-	Favored (94.81%) Isoleucine or valine / -64.6,-45.6	60.6% (*mt*) chi angles: 298.4,180.9	0.02Å	-	-
A 115	VAL 101.2	-	Favored (71.31%) Isoleucine or valine / -59.4,-51.5	59.7% (*t*) chi angles: 171	0.006Å	-	-
A 116	LEU 105.38	-	Favored (81.27%) General / -57.9,-48.0	51.6% (*tp*) chi angles: 173.5,59.7	0.003Å	-	-
A 117	ARG 108.47	-	Favored (91.49%) General / -63.9,-44.9	8.5% (*tmm_?*) chi angles: 174.5,250.2,299.3,169.6	0.023Å	-	-
A 118	ASP 107.18	-	Favored (69.87%) General / -70.7,-42.9	93.7% (*m-20*) chi angles: 291.9,337.4	0.036Å	-	-
	Avg: 137.21	Clashscore: 8.45	Outliers: 0 of 620	Poor rotamers: 0 of 557	Outliers: 0 of 591	Outliers: 0 of 628	Outliers: 0 of 628

A 119	VAL 107.7	-	Favored (97.79%) Isoleucine or valine / -61.5,-45.9	37% (*t*) chi angles: 165.5	0.024Å	-	-
A 120	VAL 118.86	-	Favored (98.76%) Isoleucine or valine / -61.5,-45.4	18.7% (*t*) chi angles: 162.5	0.027Å	-	-
A 121	GLY 127.8	-	Favored (96.25%) Glycine / -60.2,-45.3	-	-	-	-
A 122	GLY 118.85	-	Favored (70.47%) Glycine / -69.4,-43.2	-	-	-	-
A 123	MET 206.75	-	Favored (86.41%) General / -64.7,-37.1	27.9% (*ttt*) chi angles: 182.4,179.8,179	0.006Å	-	-
A 124	ASN 131.92	-	Favored (88.32%) General / -66.5,-38.9	22.4% (*t-20*) chi angles: 171.6,264.8	0.007Å	-	-
A 125	HIS 146.65	-	Favored (77.68%) General / -66.2,-34.3	55.1% (*t-80*) chi angles: 188.8,266.5	0.006Å	-	-
A 126	LEU 134.79	-	Favored (68.89%) General / -72.0,-34.5	95.7% (*mt*) chi angles: 297.9,178.4	0.02Å	-	-
A 127	ARG 157.69	0.408Å HH21 with A 128 GLU HG2	Favored (84.77%) General / -67.6,-40.3	13.4% (*ttp180*) chi angles: 184.8,222.2,69,181.5	0.013Å	-	-
A 128	GLU 156.81	0.408Å HG2 with A 127 ARG HH21	Favored (67.19%) General / -64.8,-23.3	98.8% (*mt-10*) chi angles: 293,181.3,351.4	0.021Å	-	-
A 129	ASN 149.59	-	Favored (55.36%) General / -91.4,-4.8	89.4% (*m-20*) chi angles: 295.5,327.4	0.021Å	-	-
A 130	GLY 166.79	-	Favored (45%) Glycine / 90.7,-19.4	-	-	-	-
			Favored				

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 131		ILE	154.06	-	(23.57%) Isoleucine or valine / -71.1,137.6	13.5% (*pt*) chi angles: 54.6,184.7	0.076Å	-	-
A 132		VAL	166.23	-	Favored (30.6%) Isoleucine or valine / -112.2,140.7	44.5% (*t*) chi angles: 183.9	0.027Å	-	-
A 133		HIS	145.81	-	Allowed (0.96%) General / -97.3,-65.5	5.4% (*t-160*) chi angles: 196.3,158.4	0.03Å	-	-
A 134		ARG	161.33	-	Allowed (0.25%) General / 67.5,-13.0	79.8% (*mtt85*) chi angles: 302.4,178,176.7,95.3	0.072Å	-	-
A 135		ASP	161.97	-	Favored (21.15%) General / -110.6,17.0	11.3% (*t70*) chi angles: 196.3,81.5	0.021Å	-	-
A 136		ILE	129.9	-	Favored (6.39%) Isoleucine or valine / -63.2,119.1	1.9% (*mt*) chi angles: 303,211.1	0.088Å	-	-
A 137		LYS	121.36	0.621Å HG2 with A 139 GLY H	Favored (26.52%) Pre-proline / -145.7,145.7	73.1% (*tttt*) chi angles: 168.2,195.1,174.5,183.7	0.065Å	-	-
A 138		PRO	105.38	0.478Å HD3 with A 210 THR HG23	Favored (5.03%) Trans-proline / -46.8,-26.8	6.3% (*Cg_exo*) chi angles: 357.5	0.052Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 137.21	Clashscore: 8.45	Outliers: 0 of 620	Poor rotamers: 0 of 557	Outliers: 0 of 591	Outliers: 0 of 628	Outliers: 0 of 628
A 139		GLY	98.77	0.621Å H with A 137 LYS HG2	Favored (86.74%) Glycine / -67.2,-34.7	-	-	-	-
A 140		ASN	117.42	-	Favored (29.95%) General / -103.7,15.0	3.7% (*p-10*) chi angles: 63.9,270.7	0.061Å	-	-
A 141		ILE	102.16	-	Favored (12.36%) Isoleucine or valine /	60.1% (*mt*) chi angles: 299.9,180.6	0.005Å	-	-

-107.9,101.3

A 142	MET 97.97	-	Favored (27.65%) General / -79.1,159.2	56.2% (*mmm*) chi angles: 311.9,314.6,297.7	0.022Å	-	-
A 143	ARG 91.15	-	Favored (42.82%) General / -129.4,128.3	59.5% (*ttt-85*) chi angles: 167.8,180.6,178.5,260.1	0.012Å	-	-
A 144	VAL 100.14	-	Favored (28.06%) Isoleucine or valine / -125.3,162.4	35.2% (*m*) chi angles: 298.2	0.007Å	-	-
A 145	ILE 80.8	-	Favored (44.11%) Isoleucine or valine / -100.5,116.5	55.2% (*mt*) chi angles: 293.5,181.5	0.003Å	-	-
A 146	GLY 76.86	-	Favored (33.12%) Glycine / -66.9,170.4	-	-	-	-
A 147	GLU 122.92	-	Favored (67.37%) General / -65.2,-24.5	95.5% (*mt-10*) chi angles: 295.8,184.8,351.4	0.007Å	-	-
A 148	ASP 104.68	-	Favored (56.79%) General / -89.8,0.8	6% (*p-10*) chi angles: 70.4,284.7	0.004Å	-	-
A 149	GLY 94.87	-	Favored (25.03%) Glycine / 96.6,-25.7	-	-	-	-
A 150	GLN 121.05	-	Favored (45.84%) General / -72.9,146.9	82% (*mt-30*) chi angles: 281.6,181.6,341.2	0.024Å	-	-
A 151	SER 111.5	-	Favored (50.72%) General / -67.2,149.3	12.6% (*m*) chi angles: 310.6	0.021Å	-	-
A 152	VAL 85.55	-	Favored (53.29%) Isoleucine or valine / -131.9,124.4	93.5% (*t*) chi angles: 178.1	0.017Å	-	-
A			Favored (37.2%)	78.1% (*m-85*)			

# Alt Res High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
153 TYR 105.88	-	General / -100.2,138.5	chi angles: 288.1,265.9	0.055Å	-	-
A 154 LYS 113.27	0.507Å NZ with A 65 LYS O	Favored (43.57%) General / -132.2,157.7	60.1% (*mttm*) chi angles: 302.9,169.5,176,294.6	0.019Å	-	-
A 155 LEU 110.28	-	Favored (27.87%) General / -106.2,148.5	47.9% (*mt*) chi angles: 308.7,180.4	0.02Å	-	-
A 156 THR 121.66	-	Allowed (0.85%) General / -134.4,-56.2	1.1% (*t*) chi angles: 165.4	0.077Å	-	-
A 157 ASP 110.35	-	Favored (14.23%) General / -87.2,102.2	30.4% (*t0*) chi angles: 186.9,33.3	0.025Å	-	-
A 158 PHE 133.88	-	Favored (15.51%) General / -162.2,172.6	31.3% (*p90*) chi angles: 51.1,85.4	0.01Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 137.21	Clashscore: 8.45	Outliers: 0 of 620	Poor rotamers: 0 of 557	Outliers: 0 of 591	Outliers: 0 of 628	Outliers: 0 of 628
A 159		GLY	165.41	-	Favored (82.14%) Glycine / 74.4,12.6	-	-	-	-
A 160		ALA	162.12	-	Favored (54.24%) General / -94.7,4.1	-	0.018Å	-	-
A 161		ALA	185	-	Favored (58.49%) General / -87.4,-2.3	-	0.024Å	-	-
A 162		ARG	197.58	-	Favored (3.13%) General / -68.8,-59.4	13.7% (*mmt85*) chi angles: 272.2,297.1,188.8,90.9	0.034Å	-	-
A 163		GLU	217.36	-	Favored (33.01%) General / -93.1,-11.4	31.7% (*tt0*) chi angles: 204.7,178.3,10.4	0.039Å	-	-
A 164		LEU	179.17	-	-	37.5% (*mt*) chi angles: 286.1,182	0.015Å	-	-
A									

175	GLY 157.17	-	-	-	-	-	-
A 176	THR 168.44	-	Favored (40.52%) General / -75.7,146.1	8.1% (*m*) chi angles: 314.2	0.017Å	-	-
A 177	GLU 168.25	-	Favored (47.78%) General / -52.4,-34.4	13.7% (*pm0*) chi angles: 60.6,281,355.1	0.075Å	-	-
A 178	GLU 160.23	-	Favored (41.95%) General / -83.2,-17.7	43.8% (*mp0*) chi angles: 301.6,90.4,8	0.013Å	-	-
A 179	TYR 139.24	-	Favored (29.51%) General / -107.5,10.1	63.1% (*m-85*) chi angles: 300.1,79.6	0.011Å	-	-
A 180	LEU 159.41	0.401Å O with A 205 TRP NE1	Favored (40.72%) General / -75.4,146.4	19.2% (*mt*) chi angles: 278.8,181.1	0.03Å	-	-
A 181	HIS 173.12	0.448Å O with A 185 TYR N	Favored (51.71%) Pre-proline / -80.6,140.9	58.9% (*t-80*) chi angles: 183.1,270.7	0.044Å	-	-
A 182	PRO 169.81	0.422Å HB3 with A 238 ILE HG22	Favored (5.08%) Trans-proline / -44.2,-53.0	1.7% (*Cg_endo*) chi angles: 5	0.045Å	-	-
A 183	ASP 179.54	-	Favored (57.77%) General / -75.5,-26.1	13.6% (*m-20*) chi angles: 300.6,274.2	0.011Å	-	-
A 184	MET 204.55	-	Favored (45.98%) General / -88.8,-11.0	24.4% (*ttt*) chi angles: 193.5,180.5,177.9	0.018Å	-	-
A 185	TYR 163.48	0.448Å N with A 181 HIS O	Favored (89.59%) General / -62.7,-46.1	20% (*t80*) chi angles: 197.2,278.4	0.01Å	-	-
A 186	GLU 146.41	-	-	88.7% (*tt0*) chi angles: 181.1,180.6,359.1	0.003Å	-	-
A 199	GLY 180.86	-	-	-	-	-	-
A 200	ALA 190.65	-	Favored (56.84%) General /	-	0.019Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 137.21	Clashscore: 8.45	Outliers: 0 of 620	Poor rotamers: 0 of 557	Outliers: 0 of 591	Outliers: 0 of 628	Outliers: 0 of 628
A 201		THR	190.42	-	Favored (83.05%) General / -63.6,-36.2	97.2% (*m*) chi angles: 299.3	0.014Å	-	-
A 202		VAL	180.39	-	Favored (27.74%) Isoleucine or valine / -57.6,-26.6	11.4% (*m*) chi angles: 287.9	0.023Å	-	-
A 203		ASP	179.78	0.493Å O with A 207 ILE HG12	Allowed (0.38%) General / -66.8,-68.4	62.8% (*m-20*) chi angles: 283,328.8	0.039Å	-	-
A 204		LEU	152.64	-	Favored (11.45%) General / -53.4,-24.0	71.1% (*mt*) chi angles: 304.3,180.4	0.022Å	-	-
A 205		TRP	156.49	0.401Å NE1 with A 180 LEU O	Favored (5.45%) General / -61.9,-59.2	58.7% (*t-105*) chi angles: 181.1,268.8	0.011Å	-	-
A 206		SER	131.82	-	Favored (72.31%) General / -61.0,-32.8	57.6% (*m*) chi angles: 299.4	0.003Å	-	-
A 207		ILE	131.04	0.493Å HG12 with A 203 ASP O	Favored (92.59%) Isoleucine or valine / -64.8,-41.6	21.6% (*mm*) chi angles: 313.9,300.9	0.027Å	-	-
A 208		GLY	104.35	-	Favored (86.71%) Glycine / -67.5,-43.4	-	-	-	-
A 209		VAL	119.84	-	Favored (63.33%) Isoleucine or valine / -62.1,-34.4	60.1% (*t*) chi angles: 181.1	0.013Å	-	-
A 210		THR	102.22	0.478Å HG23 with A 138 PRO HD3	Favored (71.12%) General / -68.7,-45.6	86.6% (*m*) chi angles: 301.2	0.013Å	-	-

A 211	PHE 108.98	-	Favored (94.6%) General / -64.8,-40.1	15% (*m-30*) chi angles: 286.9,343.2	0.034Å	-	-
A 212	TYR 135.11	-	Favored (93.91%) General / -64.7,-39.6	52.8% (*t80*) chi angles: 181.2,273.9	0.027Å	-	-
A 213	HIS 104.21	-	Favored (70.52%) General / -65.6,-29.9	12.2% (*t-160*) chi angles: 197.9,180	0.01Å	-	-
A 214	ALA 92.89	-	Favored (34.3%) General / -81.2,-29.8	-	0.021Å	-	-
A 215	ALA 93.98	-	Favored (14.66%) General / -85.7,-42.0	-	0.022Å	-	-
A 216	THR 120.85	0.546Å HG23 with A 264 PRO HG3	Favored (15.93%) General / -89.1,-36.1	63.2% (*m*) chi angles: 303.6	0.017Å	-	-
A 217	GLY 117.96	-	Favored (67.56%) Glycine / 92.2,3.4	-	-	-	-
A 218	SER 108.31	-	Favored (19.46%) General / -141.6,168.6	33.9% (*m*) chi angles: 303.7	0.011Å	-	-
A 219	LEU 102.24	-	Favored (72.4%) Pre-proline / -77.5,145.9	89.8% (*mt*) chi angles: 290.3,172.9	0.016Å	-	-
A 220	PRO 113.16	-	Favored (7.05%) Trans-proline / -58.3,-51.7	59% (*Cg_exo*) chi angles: 334.3	0.066Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 137.21	Clashscore: 8.45	Outliers: 0 of 620	Poor rotamers: 0 of 557	Outliers: 0 of 591	Outliers: 0 of 628	Outliers: 0 of 628
A 221		PHE 136.97		-	Favored (24.6%) General / -110.8,112.6	5.7% (*m-85*) chi angles: 321.2,279.7	0.025Å	-	-
A		ARG 127.09		-	Favored (21.3%)	62.5% (*mtm-85*) chi angles:	0.02Å	-	-

222			Pre-proline / -127.5,117.5	311.2,188.5,309.1,264.9			
A 223	PRO 146.83	-	Favored (24.04%) Trans-proline / -70.0,167.7	37.7% (*Cg_exo*) chi angles: 340.3	0.092Å	-	-
A 224	PHE 166.76	-	Favored (62.68%) General / -68.7,-48.9	84.3% (*t80*) chi angles: 180.5,72.3	0.031Å	-	-
A 225	GLU 199.61	-	Favored (40%) General / -72.1,-49.0	36.1% (*tp10*) chi angles: 187.2,60.4,34.7	0.014Å	-	-
A 226	GLY 176.91	-	Favored (19.08%) Glycine / 125.6,-164.8	-	-	-	-
A 227	PRO 191.98	-	Favored (2.2%) Trans-proline / -75.1,81.5	61.6% (*Cg_endo*) chi angles: 27.5	0.05Å	-	-
A 228	ARG 215.26	0.412Å HB3 with A 229 ARG H	Allowed (0.16%) General / -139.7,-143.5	12.6% (*mmm180*) chi angles: 271.5,301,308.4,169.9	0.004Å	-	-
A 229	ARG 205.6	0.412Å H with A 228 ARG HB3	Favored (58.49%) General / -83.1,-10.8	7.4% (*ptm-85*) chi angles: 56.3,186.2,301.5,269.7	0.007Å	-	-
A 230	ASN 208.64	-	Favored (16.36%) General / -98.1,18.4	16.7% (*m120*) chi angles: 297.2,87.8	0.005Å	-	-
A 231	LYS 179.74	0.569Å HG2 with A 234 MET HB3	Favored (8.5%) General / -83.1,10.3	60.9% (*tttt*) chi angles: 207.1,188.3,183.9,178.2	0.021Å	-	-
A 232	GLU 215.08	-	Favored (77.83%) General / -62.1,-35.1	46.6% (*mt-10*) chi angles: 312.1,166.8,179.2	0.052Å	-	-
A 233	VAL 161.58	0.447Å O with A 237 ILE HG13	Favored (92.18%) Isoleucine or valine / -63.6,-41.3	58.3% (*t*) chi angles: 180.7	0.016Å	-	-
A 234	MET 154.41	0.569Å HB3 with A 231 LYS HG2	Favored (69.37%) General / -53.3,-46.5	21.8% (*tpp*) chi angles: 161.7,82.1,75.8	0.01Å	-	-
A			Favored (78.17%)	49.2% (*t80*)			

# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
235	TYR 169.56	-	General / -63.1,-34.7	chi angles: 190.7,70.2	0.022Å	-	-
A 236	LYS 161.29	-	Favored (78.89%) General / -68.4,-36.3	87% (*tttt*) chi angles: 179.3,183.3,177,180.9	0.004Å	-	-
A 237	ILE 144.5	0.515Å HG12 with A 257 ILE HD13	Favored (88.78%) Isoleucine or valine / -64.1,-47.8	73.7% (*mt*) chi angles: 300.3,176.7	0.035Å	-	-
A 238	ILE 159.73	0.422Å HG22 with A 182 PRO HB3	Favored (84.14%) Isoleucine or valine / -67.1,-39.9	58.7% (*mt*) chi angles: 303.8,178.6	0.034Å	-	-
A 239	THR 157.03	-	Favored (59.9%) General / -77.2,-13.7	37.8% (*p*) chi angles: 53	0.022Å	-	-
A 240	GLY 168.86	-	Favored (50.21%) Glycine / -64.6,-51.6	-	-	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 137.21	Clashscore: 8.45	Outliers: 0 of 620	Poor rotamers: 0 of 557	Outliers: 0 of 591	Outliers: 0 of 628	Outliers: 0 of 628
A 241		LYS	186.37	-	Allowed (1.48%) Pre-proline / 32.8,58.7	22.8% (*pttm*) chi angles: 53.8,173.7,182.2,301.1	0.1Å	-	-
A 242		PRO	150.34	-	Favored (5.75%) Trans-proline / -76.3,120.7	72.3% (*Cg_endo*) chi angles: 29.2	0.046Å	-	-
A 243		SER	163.79	-	Favored (2.37%) General / 51.1,-127.6	95.8% (*p*) chi angles: 64.8	0.045Å	-	-
A 244		GLY	150.26	-	Favored (7.41%) Glycine / -110.5,31.4	-	-	-	-
A 245		ALA	153.84	-	Favored (49.46%) General / -68.8,134.2	-	0.018Å	-	-
					Favored				

A 246	ILE 140.58	-	(9.28%) Isoleucine or valine / -102.6,-5.7	15.2% (*pt*) chi angles: 53.8,182.9	0.029Å	-	-
A 247	SER 132.57	-	Favored (25.08%) General / -157.9,152.7	45% (*p*) chi angles: 54.1	0.025Å	-	-
A 248	GLY 109.63	-	Allowed (1.03%) Glycine / -157.0,121.1	-	-	-	-
A 249	VAL 129.57	-	Favored (40.94%) Isoleucine or valine / -138.1,131.1	78.9% (*t*) chi angles: 172.4	0.022Å	-	-
A 250	GLN 144.59	-	Favored (36.62%) General / -91.6,126.4	1.5% (*pt20*) chi angles: 52.1,169,171.1	0.043Å	-	-
A 251	LYS 134.46	0.427Å HB2 with A 251 LYS HE3	Favored (57.02%) General / -89.3,0.1	37% (*mtmt*) chi angles: 304.7,165.5,300.7,179.5	0.006Å	-	-
A 252	ALA 136.06	-	Favored (39.45%) General / -142.6,160.9	-	0.021Å	-	-
A 253	GLU 144.42	-	Favored (7.06%) General / -63.5,117.7	87.2% (*tt0*) chi angles: 183.5,178.1,6.3	0.017Å	-	-
A 254	ASN 150.84	-	Favored (30.88%) General / 55.4,41.6	16.3% (*t-20*) chi angles: 205.2,335.1	0.049Å	-	-
A 255	GLY 140.87	-	Favored (23.62%) Glycine / -106.0,-177.4	-	-	-	-
A 256	PRO 145.25	-	Favored (44.13%) Trans-proline / -67.2,161.2	51.1% (*Cg_endo*) chi angles: 25.1	0.064Å	-	-
A 257	ILE 144.38	0.515Å HD13 with A 237 ILE HG12	Favored (54.45%) Isoleucine or valine / -103.2,121.5	37.3% (*mt*) chi angles: 306.7,163	0.019Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 258		ASP	122.2	-	Favored (12.19%) General / -78.3,109.2	23.5% (*t0*) chi angles: 197,324.1	0.017Å	-	-
A 259		TRP	149.87	-	Favored (20.37%) General / -96.0,150.5	98.4% (*m95*) chi angles: 294.2,98.7	0.013Å	-	-
A 260		SER	122.34	-	Favored (8.31%) General / -156.9,130.8	40% (*t*) chi angles: 176.6	0.008Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 137.21	Clashscore: 8.45	Outliers: 0 of 620	Poor rotamers: 0 of 557	Outliers: 0 of 591	Outliers: 0 of 628	Outliers: 0 of 628
A 261		GLY	119.69	-	Favored (27.94%) Glycine / -99.0,25.5	-	-	-	-
A 262		ASP	129.18	0.469Å OD1 with A 263 MET N	Favored (10.57%) General / -140.3,174.4	13.1% (*t0*) chi angles: 204,330.8	0.012Å	-	-
A 263		MET	400	0.469Å N with A 262 ASP OD1	Favored (60.25%) Pre-proline / -84.5,152.3	26% (*mmt*) chi angles: 292.8,300.4,176.9	0.012Å	-	-
A 264		PRO	112.68	0.546Å HG3 with A 216 THR HG23	Favored (34.22%) Trans-proline / -66.7,163.1	42.2% (*Cg_endo*) chi angles: 24.1	0.059Å	-	-
A 265		VAL	119.47	0.5Å HB with A 395 GLU HB2	Favored (37.72%) Isoleucine or valine / -71.7,-30.3	12.7% (*t*) chi angles: 191.3	0.015Å	-	-
A 266		SER	118.71	-	Favored (50.36%) General / -74.2,-6.9	81.9% (*p*) chi angles: 60.6	0.004Å	-	-
A 267		CYS	115.76	-	Favored (54.67%) General / -60.8,132.7	46.8% (*t*) chi angles: 185.2	0.007Å	-	-
A 268		SER	137.62	-	Favored (56.1%) General / -84.0,-2.2	45.8% (*m*) chi angles: 302.3	0.009Å	-	-

A 269	LEU 125.86	-	Favored (34.53%) General / -77.3,152.5	85.3% (*mt*) chi angles: 297.5,181.5	0.004Å	-	-
A 270	SER 115.12	-	Favored (37.31%) General / -71.0,158.0	97.5% (*p*) chi angles: 64.7	0.027Å	-	-
A 271	ARG 161.13	-	Favored (91.19%) General / -64.5,-38.5	29.4% (*tpt180*) chi angles: 186.1,55.5,182.4,177.7	0.014Å	-	-
A 272	GLY 116.77	-	Favored (90.83%) Glycine / -61.1,-35.5	-	-	-	-
A 273	LEU 110.92	-	Favored (62.27%) General / -74.8,-37.8	42% (*tp*) chi angles: 182,55.7	0.004Å	-	-
A 274	GLN 119.79	-	Favored (76.31%) General / -63.1,-33.8	79.5% (*mt-30*) chi angles: 298.7,182.4,19.1	0.008Å	-	-
A 275	VAL 124.57	-	Favored (63.76%) Isoleucine or valine / -64.8,-33.5	92.7% (*t*) chi angles: 175.6	0.02Å	-	-
A 276	LEU 128.82	-	Favored (20.04%) General / -85.6,-37.0	76.9% (*mt*) chi angles: 302.5,182.4	0.003Å	-	-
A 277	LEU 115.58	-	Favored (62.15%) General / -74.9,-34.3	44.5% (*tp*) chi angles: 180.3,55.9	0.02Å	-	-
A 278	THR 136.22	-	Favored (80.9%) Pre-proline / -54.3,-51.1	20% (*m*) chi angles: 289.9	0.131Å	-	-
A 279	PRO 124.49	0.605Å O with A 283 ASN ND2	Favored (34.78%) Trans-proline / -67.5,-31.0	38% (*Cg_exo*) chi angles: 340.7	0.072Å	-	-
A 280	VAL 121.92	-	Favored (36.77%) Isoleucine or valine / -59.4,-54.3	97.6% (*t*) chi angles: 176.2	0.001Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 137.21	Clashscore: 8.45	Outliers: 0 of 620	Poor rotamers: 0 of 557	Outliers: 0 of 591	Outliers: 0 of 628	Outliers: 0 of 628
A 281		LEU	126.84	-	Favored (75.17%) General / -67.2,-33.3	65.9% (*mt*) chi angles: 301.6,184.3	0.005Å	-	-
A 282		ALA	135.91	-	Favored (83.36%) General / -66.8,-36.8	-	0.024Å	-	-
A 283		ASN	152.63	0.605Å ND2 with A 279 PRO O	Favored (40.32%) General / -82.5,-18.8	64.6% (*m-80*) chi angles: 292.8,277.3	0.041Å	-	-
A 284		ILE	137.72	-	Favored (10.34%) Isoleucine or valine / -102.1,0.6	25.5% (*pt*) chi angles: 66.3,179.9	0.018Å	-	-
A 285		LEU	156.51	-	Favored (2.06%) General / -118.3,83.7	54.2% (*mt*) chi angles: 289.2,181.4	0.037Å	-	-
A 286		GLU	177.4	-	Favored (7.49%) General / -168.5,155.5	12.8% (*pt-20*) chi angles: 49.1,189.5,337.7	0.018Å	-	-
A 287		ALA	183.86	-	Favored (61.46%) General / -74.4,-29.3	-	0.02Å	-	-
A 288		ASP	191.52	-	Favored (31.99%) General / -76.0,127.0	65.4% (*m-20*) chi angles: 301.7,329.5	0.008Å	-	-
A 289		GLN	191.78	-	Favored (49.09%) General / -79.6,-3.9	81.3% (*mt-30*) chi angles: 297.5,184.4,4.6	0.022Å	-	-
A 290		GLU	194.24	-	Favored (66.01%) General / -61.7,-52.0	28.7% (*mm-40*) chi angles: 318,289.7,334	0.04Å	-	-
A 291		LYS	178.94	-	Favored (19.96%) General / -103.6,-8.4	5.1% (*mptt*) chi angles: 310.7,93.2,183.6,177.5	0.008Å	-	-

# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 292	CYS 174.64	-	Favored (47.43%) General / -72.8,144.8	46.2% (*t*) chi angles: 182.9	0.021Å	-	-
A 293	TRP 151.69	0.402Å CH2 with A 301 GLU HG3	Favored (27.63%) General / -78.1,161.2	34.3% (*m0*) chi angles: 283.8,350.6	0.021Å	-	-
A 294	GLY 144.08	-	Favored (34.91%) Glycine / -96.7,-179.3	-	-	-	-
A 295	PHE 169.93	-	Favored (70.03%) General / -66.3,-29.8	9.3% (*p90*) chi angles: 45.2,75.6	0.065Å	-	-
A 296	ASP 139.81	-	Favored (62.18%) General / -73.2,-43.0	35.7% (*m-20*) chi angles: 281.6,316.4	0.019Å	-	-
A 297	GLN 152.44	-	Favored (88.15%) General / -61.1,-47.0	39.1% (*mm-40*) chi angles: 285.7,280.7,351.9	0.033Å	-	-
A 298	PHE 135.95	-	Favored (75.8%) General / -61.1,-49.8	83.7% (*t80*) chi angles: 173.3,78.5	0.008Å	-	-
A 299	PHE 126.49	-	Favored (93.99%) General / -62.6,-39.5	77% (*t80*) chi angles: 182.9,83.9	0.016Å	-	-
A 300	ALA 122.68	-	Favored (71.05%) General / -62.2,-50.6	-	0.023Å	-	-
# Alt Res	**High B**	**Clash > 0.4Å**	**Ramachandran**	**Rotamer**	**Cβ deviation**	**Bond lengths**	**Bond angles**
	Avg: 137.21	Clashscore: 8.45	Outliers: 0 of 620	Poor rotamers: 0 of 557	Outliers: 0 of 591	Outliers: 0 of 628	Outliers: 0 of 628
A 301	GLU 128.31	0.402Å HG3 with A 293 TRP CH2	Favored (78.5%) General / -68.8,-41.5	67% (*mm-40*) chi angles: 307.6,300.2,327.6	0.014Å	-	-
A 302	THR 129.11	-	Favored (71.73%) General / -67.0,-47.4	21.4% (*p*) chi angles: 48.8	0.027Å	-	-
A			Favored				

303	SER 118.85	-	(77.37%) General / -62.4,-34.8	78.3% (*p*) chi angles: 59.1	0.006Å	-	-
A 304	ASP 123.99	-	Favored (90.25%) General / -58.7,-43.4	11.3% (*t70*) chi angles: 171.7,266.2	0.011Å	-	-
A 305	ILE 120.36	-	Favored (92.78%) Isoleucine or valine / -64.0,-41.5	69.2% (*mt*) chi angles: 300.6,177.9	0.011Å	-	-
A 306	LEU 130.03	-	Favored (68.39%) General / -68.6,-29.8	72.5% (*mt*) chi angles: 300,170.8	0.009Å	-	-
A 307	HIS 129.02	-	Favored (60.12%) General / -74.3,-26.3	4.1% (*m-70*) chi angles: 296.9,348.7	0.017Å	-	-
A 308	ARG 120.98	-	Favored (54.92%) General / -66.0,146.2	94% (*mtt-85*) chi angles: 299.6,175.9,181,272.3	0.005Å	-	-
A 309	MET 147.9	-	Favored (5.51%) General / -94.4,178.7	11.1% (*ptp*) chi angles: 53.7,170.6,50.5	0.013Å	-	-
A 310	VAL 145.82	-	Favored (56.27%) Isoleucine or valine / -110.1,133.2	4.8% (*p*) chi angles: 53.8	0.049Å	-	-
A 311	ILE 130.83	-	Favored (31.02%) Isoleucine or valine / -117.7,110.5	48.2% (*mm*) chi angles: 303.7,298.5	0.009Å	-	-
A 312	HIS 142.25	-	Favored (26.51%) General / -86.8,119.0	49.1% (*m80*) chi angles: 296.4,111.1	0.017Å	-	-
A 313	VAL 130.9	-	Favored (42.28%) Isoleucine or valine / -133.0,120.9	46% (*t*) chi angles: 168	0.011Å	-	-
A 314	PHE 124.34	-	Favored (24.55%) General /	2.5% (*t80*) chi angles: 189.9,23.6	0.012Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
					-105.8,111.8				
A 315		SER	125.77	-	Favored (21.46%) General / -84.4,113.8	42.4% (*t*) chi angles: 177.8	0.014Å	-	-
A 316		LEU	129.77	-	Favored (67.82%) General / -69.1,-29.7	76.3% (*mt*) chi angles: 293,180.6	0.011Å	-	-
A 317		GLN	160.11	-	Favored (87.75%) General / -62.0,-46.8	7.5% (*mm100*) chi angles: 299.8,288.1,158.2	0.021Å	-	-
A 318		GLN	122.88	0.534Å HA with A 389 THR HA	Favored (31.78%) General / -99.9,-3.7	28% (*mp0*) chi angles: 300,92.4,340.9	0.016Å	-	-
A 319		MET	128.96	-	Favored (16.78%) General / 54.7,50.0	18.9% (*ttt*) chi angles: 198.1,182,183.2	0.041Å	-	-
A 320		THR	113.03	-	Favored (45.23%) General / -131.6,133.7	64.7% (*p*) chi angles: 57	0.022Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 137.21	Clashscore: 8.45	Outliers: 0 of 620	Poor rotamers: 0 of 557	Outliers: 0 of 591	Outliers: 0 of 628	Outliers: 0 of 628
A 321		ALA	115.48	-	Favored (24.65%) General / -88.1,148.0	-	0.023Å	-	-
A 322		HIS	108.97	-	Favored (42.07%) General / -138.9,147.2	71.6% (*m-70*) chi angles: 303.1,264.6	0.005Å	-	-
A 323		LYS	145.16	-	Favored (12.9%) General / -119.9,107.2	60.6% (*mttp*) chi angles: 298.5,187.2,184.7,61.8	0.011Å	-	-
A 324		ILE	123.8	-	Favored (49.51%) Isoleucine or valine / -98.2,122.1	5% (*mp*) chi angles: 296.6,89.8	0.041Å	-	-
A 325		TYR	131.03	0.538Å OH with A 109 GLU OE1	Favored (25.11%) General / -90.9,113.0	66.7% (*m-85*) chi angles: 288.8,80.3	0.013Å	-	-

A 326	ILE 139.38	-	Favored (31.16%) Isoleucine or valine / -134.8,146.1	27.2% (*mt*) chi angles: 308.6,182.7	0.043Å	-	-
A 327	HIS 120.11	-	Favored (42.24%) General / -71.7,153.1	91.1% (*m-70*) chi angles: 288.9,276.6	0.003Å	-	-
A 328	SER 160.43	0.486Å HA with A 367 ALA HB3	Favored (63.99%) General / -69.1,-21.8	95.9% (*p*) chi angles: 63.7	0.014Å	-	-
A 329	TYR 144.93	-	Favored (53.38%) General / -92.8,-4.2	43.1% (*p90*) chi angles: 55.4,86.3	0.041Å	-	-
A 330	ASN 131.53	-	Favored (29.57%) General / -74.5,161.7	13.7% (*m-20*) chi angles: 293.5,13.8	0.03Å	-	-
A 331	THR 135.81	-	Favored (4.85%) General / -94.5,-179.3	81.6% (*p*) chi angles: 61	0.004Å	-	-
A 332	ALA 120.91	-	Favored (59.77%) General / -80.5,-9.1	-	0.02Å	-	-
A 333	THR 127.98	-	Favored (25.61%) General / -73.8,-49.4	98% (*m*) chi angles: 299.1	0.003Å	-	-
A 334	ILE 125.31	-	Favored (51.31%) Isoleucine or valine / -65.7,-30.8	17% (*mt*) chi angles: 313.4,180.5	0.018Å	-	-
A 335	PHE 134.83	-	Favored (74.31%) General / -61.4,-50.1	39.8% (*t80*) chi angles: 164.8,72.9	0.006Å	-	-
A 336	HIS 134.31	-	Favored (75.45%) General / -61.5,-34.4	5.3% (*m-70*) chi angles: 291.7,342.4	0.005Å	-	-
A 337	GLU 142.51	0.524Å HG3 with A 341 LYS HE3	Favored (75.55%) General / -67.5,-45.5	31.2% (*tp10*) chi angles: 174.1,59.5,35.5	0.013Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 338		LEU	124.75	0.449Å HD23 with A 341 LYS HD2	Favored (87.68%) General / -66.9,-39.8	83.2% (mt) chi angles: 291.4,177.8	0.019Å	-	-
A 339		VAL	118.56	-	Favored (77.16%) Isoleucine or valine / -61.1,-37.3	53.7% (t) chi angles: 170.3	0.025Å	-	-
A 340		TYR	135.57	-	Favored (88.22%) General / -64.4,-37.6	36.9% (t80) chi angles: 163.8,75.9	0.007Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 137.21	Clashscore: 8.45	Outliers: 0 of 620	Poor rotamers: 0 of 557	Outliers: 0 of 591	Outliers: 0 of 628	Outliers: 0 of 628
A 341		LYS	127.6	0.524Å HE3 with A 337 GLU HG3	Favored (69.85%) General / -65.2,-29.1	99.3% (mttt) chi angles: 293.2,175.8,181.2,177.7	0.024Å	-	-
A 342		GLN	141.9	-	Favored (7.79%) General / -98.0,-41.8	81.1% (mt-30) chi angles: 300.3,181,13.6	0.013Å	-	-
A 343		THR	125.01	-	Favored (27%) General / -98.3,-8.5	78.3% (p) chi angles: 61.6	0.02Å	-	-
A 344		LYS	125.07	-	Favored (25.75%) General / 57.2,42.3	72.4% (mmtt) chi angles: 290.7,303.9,178.4,179.9	0.07Å	-	-
A 345		ILE	127.72	-	Favored (75.25%) Isoleucine or valine / -118.2,128.5	31.6% (mt) chi angles: 308.3,181.6	0.023Å	-	-
A 346		ILE	150.46	-	Favored (16.16%) Isoleucine or valine / -58.7,141.0	19.9% (mt) chi angles: 313.6,177.9	0.011Å	-	-
A 347		SER	128.51	-	Favored (61.02%) General / -53.8,-35.2	34.3% (m) chi angles: 303.7	0.008Å	-	-
A 348		SER	152.34	-	Favored (57.72%) General / -78.7,-16.0	73% (p) chi angles: 58	0.003Å	-	-

A 349	ASN 161.2	-	Favored (40.85%) General / -96.9,-4.0	11.1% (*m120*) chi angles: 289.6,79.8	0.022Å	-	-
A 350	GLN 143.28	-	Favored (24.23%) General / -83.8,118.9	82% (*mt-30*) chi angles: 299.9,173,8.1	0.006Å	-	-
A 351	GLU 142.69	0.509Å OE2 with A 627 ARG NH2	Favored (51.82%) General / -122.0,128.7	28% (*mt-10*) chi angles: 306.9,168.5,250.1	0.015Å	-	-
A 352	LEU 167.03	-	Favored (31.22%) General / -101.8,143.8	56.2% (*mt*) chi angles: 306.7,181.9	0.018Å	-	-
A 353	ILE 138.82	-	Favored (57.53%) Isoleucine or valine / -133.4,133.5	51.4% (*mt*) chi angles: 300,182.8	0.018Å	-	-
A 354	TYR 159.95	-	Favored (16.47%) General / -143.2,126.4	89.7% (*t80*) chi angles: 178.6,81.1	0.02Å	-	-
A 355	GLU 142.42	-	Favored (32.01%) General / 53.7,41.7	83.7% (*mt-10*) chi angles: 281.6,186.1,174.4	0.087Å	-	-
A 356	GLY 142.15	-	Favored (64.77%) Glycine / 92.8,-14.6	-	-	-	-
A 357	ARG 160.11	-	Favored (42.21%) General / -123.5,152.1	94.1% (*mtt-85*) chi angles: 300.9,183.6,178.9,273.8	0.008Å	-	-
A 358	ARG 163.06	0.652Å HB3 with A 449 LEU HD21	Favored (43.68%) General / -71.6,151.6	10.6% (*ptp85*) chi angles: 54.4,174,58.1,91.7	0.021Å	-	-
A 359	LEU 180.56	-	Favored (19.53%) General / -131.6,118.0	22.1% (*tp*) chi angles: 192.6,59.4	0.014Å	-	-
A 360	VAL 166.23	-	Favored (39.61%) Isoleucine or valine / -86.2,123.5	1.7% (*p*) chi angles: 44.6	0.046Å	-	-

# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
	Avg: 137.21	Clashscore: 8.45	Outliers: 0 of 620	Poor rotamers: 0 of 557	Outliers: 0 of 591	Outliers: 0 of 628	Outliers: 0 of 628
A 361	LEU 168.19	-	Favored (50.47%) General / -111.5,123.6	9.8% (*mp*) chi angles: 269.5,59.9	0.007Å	-	-
A 362	GLU 171.82	0.4Å HA with A 363 PRO HD3	Favored (98.08%) Pre-proline / -66.0,142.7	29% (*mp0*) chi angles: 284.7,70.6,28.8	0.004Å	-	-
A 363	PRO 138.91	0.4Å HD3 with A 362 GLU HA	Favored (38.39%) Trans-proline / -57.6,-19.6	56.4% (*Cg_exo*) chi angles: 334.4	0.053Å	-	-
A 364	GLY 148.2	-	Favored (13.85%) Glycine / -116.4,18.0	-	-	-	-
A 365	ARG 183.62	-	Favored (37.01%) General / -77.6,130.6	72.2% (*ttt180*) chi angles: 193,178,185.8,182.3	0.015Å	-	-
A 366	LEU 134.93	-	Favored (38%) General / -71.0,157.6	60.9% (*mt*) chi angles: 299,185.4	0.013Å	-	-
A 367	ALA 132.58	0.486Å HB3 with A 328 SER HA	Favored (60.3%) General / -75.8,-14.4	-	0.034Å	-	-
A 368	GLN 146.47	0.466Å HG2 with A 328 SER HB2	Favored (68.93%) General / -68.0,-29.8	80.2% (*mt-30*) chi angles: 302.9,179.2,353.4	0.026Å	-	-
A 369	HIS 150.64	-	Favored (38.55%) General / -99.6,11.7	15.2% (*m80*) chi angles: 313.7,77.5	0.017Å	-	-
A 370	PHE 152.62	0.429Å CD1 with A 367 ALA HA	Favored (97.02%) Pre-proline / -69.0,151.9	4.9% (*m-85*) chi angles: 271.8,52	0.018Å	-	-
A 371	PRO 152.47	-	Favored (37.25%) Trans-proline / -66.8,162.5	38.6% (*Cg_endo*) chi angles: 23.5	0.054Å	-	-
			Favored	69.8% (*tttt*)			

# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 372	LYS 167.38	-	(25.66%) General / -71.8,124.8	chi angles: 203.8,170.4,187.2,177	0.021Å	-	-
A 373	THR 131.97	-	Favored (50.35%) General / -131.4,143.2	6.8% (*t*) chi angles: 178.2	0.036Å	-	-
A 374	THR 121.2	-	Favored (8.13%) General / -126.9,175.3	44.3% (*p*) chi angles: 66.8	0.042Å	-	-
A 375	GLU 125.59	-	Favored (58.7%) General / -75.2,-21.3	19.4% (*pt-20*) chi angles: 60.5,175.4,168.1	0.025Å	-	-
A 376	GLU 126.27	-	Favored (36.2%) General / -95.8,-7.8	15.7% (*pt-20*) chi angles: 48.2,185.9,175	0.018Å	-	-
A 377	ASN 136.99	-	Favored (20.91%) Pre-proline / -142.5,73.0	26.7% (*t-20*) chi angles: 183.2,258.4	0.013Å	-	-
A 378	PRO 126.05	-	Allowed (0.27%) Trans-proline / -94.1,-171.7	48.5% (*Cg_endo*) chi angles: 35.3	0.097Å	-	-
A 379	ILE 134.89	-	Favored (40.66%) Isoleucine or valine / -99.4,115.6	60.3% (*mt*) chi angles: 299.9,180.6	0.02Å	-	-
A 380	PHE 123.17	-	Favored (41.58%) General / -74.5,147.8	81.7% (*m-85*) chi angles: 290.5,83.6	0.018Å	-	-
# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
	Avg: 137.21	Clashscore: 8.45	Outliers: 0 of 620	Poor rotamers: 0 of 557	Outliers: 0 of 591	Outliers: 0 of 628	Outliers: 0 of 628
A 381	VAL 135.06	-	Favored (61.18%) Isoleucine or valine / -122.8,120.6	22.8% (*t*) chi angles: 163.3	0.033Å	-	-
A 382	VAL 142.33	-	Favored (20.15%) Isoleucine or valine /	11.7% (*t*) chi angles: 191.8	0.029Å	-	-

			-115.8,146.5				
A 383	SER 144.56	-	Favored (46.34%) General / -127.8,153.6	23% (*t*) chi angles: 187	0.014Å	-	-
A 384	ARG 158.39	0.422Å NH2 with A 631 LEU HD22	Favored (53.13%) General / -77.6,-35.3	18.3% (*mmm180*) chi angles: 307.9,295.2,303.2,195	0.028Å	-	-
A 385	GLU 172.99	-	Favored (51.3%) Pre-proline / -80.7,140.7	15.3% (*pt-20*) chi angles: 56.1,178.4,333.2	0.011Å	-	-
A 386	PRO 155.55	-	Favored (26.32%) Trans-proline / -64.6,130.4	41.9% (*Cg_exo*) chi angles: 337.7	0.071Å	-	-
A 387	LEU 152.06	-	Favored (48.29%) General / -133.3,142.0	57.9% (*mt*) chi angles: 285,173.8	0.011Å	-	-
A 388	ASN 123.71	-	Favored (52.4%) General / -69.4,146.0	33.4% (*m120*) chi angles: 301.7,119.2	0.003Å	-	-
A 389	THR 136.55	0.534Å HA with A 318 GLN HA	Favored (25.48%) General / -87.7,115.9	12% (*p*) chi angles: 76.7	0.026Å	-	-
A 390	ILE 132.6	-	Favored (13.52%) Isoleucine or valine / -90.6,-49.5	41.7% (*mm*) chi angles: 307.3,300.2	0.009Å	-	-
A 391	GLY 111.94	-	Favored (46.05%) Glycine / 81.3,-164.8	-	-	-	-
A 392	LEU 111.24	-	Favored (26.67%) General / -76.4,123.9	60.3% (*tp*) chi angles: 178,59.2	0.015Å	-	-
A 393	ILE 119.28	-	Favored (29.42%) Isoleucine or valine / -100.8,111.1	45% (*mm*) chi angles: 297.2,299.3	0.009Å	-	-
A 394	TYR 123.33	-	Favored (12.57%) General /	51.6% (*p90*) chi angles: 58.5,87.9	0.015Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
					-130.6,171.9				
A 395		GLU	120.59	0.5Å HB2 with A 265 VAL HB	Favored (26.61%) General / -97.1,114.9	47.2% (*tp10*) chi angles: 181,69.5,26.6	0.015Å	-	-
A 396		LYS	133.25	-	Favored (8.52%) General / -72.9,112.0	99.4% (*mttt*) chi angles: 294,183.9,179,180.8	0.011Å	-	-
A 397		ILE	106.38	-	Favored (74.73%) Isoleucine or valine / -122.6,126.9	23.9% (*mt*) chi angles: 312.4,168.7	0.015Å	-	-
A 398		SER	129.83	-	Favored (8.65%) General / -95.3,171.6	53.7% (*m*) chi angles: 299.9	0.007Å	-	-
A 399		LEU	103.5	-	Favored (84%) Pre-proline / -75.1,148.2	88.3% (*mt*) chi angles: 301.6,177.4	0.018Å	-	-
A 400		PRO	106.49	-	Favored (10.01%) Trans-proline / -86.2,160.4	33.8% (*Cg_endo*) chi angles: 22	0.051Å	-	-
#	**Alt**	**Res**	**High B**	**Clash > 0.4Å**	**Ramachandran**	**Rotamer**	**Cβ deviation**	**Bond lengths**	**Bond angles**
			Avg: 137.21	Clashscore: 8.45	Outliers: 0 of 620	Poor rotamers: 0 of 557	Outliers: 0 of 591	Outliers: 0 of 628	Outliers: 0 of 628
A 401		LYS	142.69	-	Favored (46.09%) General / -72.2,135.4	98% (*mttt*) chi angles: 297.7,182.3,178.6,180.8	0.013Å	-	-
A 402		VAL	114.58	-	Favored (42.72%) Isoleucine or valine / -100.1,116.1	97% (*t*) chi angles: 176.1	0.004Å	-	-
A 403		HIS	135.43	-	Favored (41.21%) Pre-proline / -85.7,145.3	2.3% (*m-70*) chi angles: 297,359.5	0.008Å	-	-
A 404		PRO	139.14	-	Favored (11.29%) Trans-proline / -74.7,-1.6	73.4% (*Cg_endo*) chi angles: 28.4	0.056Å	-	-
A 405		ARG	170.9	0.428Å HG3 with A 407 ASP H	Favored (54.75%) General /	29.1% (*tpt180*) chi angles: 187.8,53.8,179.1,174.2	0.019Å	-	-

			-64.8,146.5				
A 406	TYR 132.52	0.433Å CZ with A 580 GLU HG3	Favored (42.95%) General / -86.8,4.0	68.3% (*t80*) chi angles: 177.8,66.5	0.04Å	-	-
A 407	ASP 129.99	0.428Å H with A 405 ARG HG3	Allowed (0.27%) General / -49.8,109.3	29.1% (*t0*) chi angles: 197,336.2	0.008Å	-	-
A 408	LEU 112.53	-	Favored (87.03%) General / -60.7,-39.0	80% (*mt*) chi angles: 297.1,182.6	0.01Å	-	-
A 409	ASP 123.12	-	Favored (88.27%) General / -65.7,-43.7	5% (*m-20*) chi angles: 305.2,81	0.029Å	-	-
A 410	GLY 116.48	-	Favored (97.45%) Glycine / -64.8,-41.5	-	-	-	-
A 411	ASP 106.85	-	Favored (71.26%) General / -66.3,-30.8	67.7% (*m-20*) chi angles: 299,345.8	0.013Å	-	-
A 412	ALA 104.2	-	Favored (41.36%) General / -73.3,-47.6	-	0.019Å	-	-
A 413	SER 96.14	-	Favored (95.59%) General / -64.9,-40.7	74.9% (*m*) chi angles: 294.8	0.008Å	-	-
A 414	MET 115.3	-	Favored (83.16%) General / -65.3,-36.1	10.8% (*tmm?*) chi angles: 184.4,272.1,306.8	0.011Å	-	-
A 415	ALA 101.82	-	Favored (70.43%) General / -63.9,-50.0	-	0.019Å	-	-
A 416	LYS 108.76	0.414Å HB2 with A 563 TYR CE1	Favored (97.05%) General / -61.2,-41.5	59% (*tttp*) chi angles: 172.2,175.4,167.7,53.6	0.009Å	-	-
A 417	ALA 100.94	-	Favored (23.78%) General / -63.5,-55.5	-	0.02Å	-	-
			Favored				

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 418		ILE	95.89	-	(54.93%) Isoleucine or valine / -67.3,-31.9	14.7% (*tt*) chi angles: 195.9,174.3	0.089Å	-	-
A 419		THR	97.18	-	Favored (61.47%) General / -75.2,-34.6	23.1% (*m*) chi angles: 309.6	0.01Å	-	-
A 420		GLY	87.98	-	Favored (98.11%) Glycine / -62.8,-39.5	-	-	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 137.21	Clashscore: 8.45	Outliers: 0 of 620	Poor rotamers: 0 of 557	Outliers: 0 of 591	Outliers: 0 of 628	Outliers: 0 of 628
A 421		VAL	100.27	-	Favored (95.9%) Isoleucine or valine / -64.0,-45.7	92.6% (*t*) chi angles: 176.9	0.009Å	-	-
A 422		VAL	90.04	-	Favored (75.33%) Isoleucine or valine / -65.8,-35.5	59% (*t*) chi angles: 180.3	0.033Å	-	-
A 423		CYS	96.83	-	Favored (92.8%) General / -59.4,-44.4	29.6% (*m*) chi angles: 281.1	0.024Å	-	-
A 424		TYR	124.52	-	Favored (99.86%) General / -62.9,-42.6	77.5% (*t80*) chi angles: 183.5,82.7	0.008Å	-	-
A 425		ALA	90.59	-	Favored (93.55%) General / -62.1,-39.8	-	0.018Å	-	-
A 426		CYS	91.5	-	Favored (65.45%) General / -72.3,-31.2	31.2% (*t*) chi angles: 189.8	0.004Å	-	-
A 427		ARG	134.36	0.617Å NH2 with A 102 SER O	Favored (72.79%) General / -68.1,-45.7	41.9% (*ttm105*) chi angles: 183.1,178.4,302.6,104.6	0.013Å	-	-
A 428		ILE	105.88	-	Favored (96.45%) Isoleucine or	43.6% (*mm*) chi angles: 298.1,303.3	0.01Å	-	-

			valine / -63.6,-42.5			
A 429	ALA 98.07	-	Favored (76.76%) General / -60.9,-35.5	-	0.019Å	-	-
A 430	SER 108.34	-	Favored (76.87%) General / -69.2,-36.2	46.4% (*t*) chi angles: 179	0.014Å	-	-
A 431	THR 106.15	-	Favored (75.23%) General / -70.0,-40.2	40.2% (*m*) chi angles: 305.7	0.008Å	-	-
A 432	LEU 111.22	-	Favored (97.59%) General / -61.2,-41.9	93.6% (*mt*) chi angles: 294.1,177.3	0.007Å	-	-
A 433	LEU 106.33	-	Favored (79.75%) General / -66.5,-35.2	54.1% (*tp*) chi angles: 179.4,57.7	0.001Å	-	-
A 434	LEU 108.65	-	Favored (87.47%) General / -64.2,-45.6	60.3% (*tp*) chi angles: 174,63	0.011Å	-	-
A 435	TYR 105.24	-	Favored (87.15%) General / -59.3,-40.8	6.5% (*m-30*) chi angles: 277,9.6	0.016Å	-	-
A 436	GLN 114.12	0.491Å OE1 with A 542 THR N	Favored (67.34%) General / -69.5,-46.2	77.9% (*mt-30*) chi angles: 299.6,184.8,15.6	0.018Å	-	-
A 437	GLU 109.49	0.436Å OE2 with A 440 ARG NH1	Favored (68.62%) General / -67.5,-29.3	68.3% (*mm-40*) chi angles: 286.4,297.6,301.9	0.03Å	-	-
A 438	LEU 116.75	-	Favored (54.01%) General / -77.5,-34.9	27.9% (*mt*) chi angles: 281.2,178.7	0.014Å	-	-
A 439	MET 115.98	-	Favored (84.57%) General / -63.6,-46.7	5.2% (*tpt*) chi angles: 211.2,65.3,177.3	0.026Å	-	-
A 440	ARG 120.91	0.436Å NH1 with A 437 GLU OE2	Favored (84.48%) General / -59.1,-40.2	82.8% (*mtt85*) chi angles: 297.2,181.8,181.3,94.1	0.007Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 137.21	Clashscore: 8.45	Outliers: 0 of 620	Poor rotamers: 0 of 557	Outliers: 0 of 591	Outliers: 0 of 628	Outliers: 0 of 628
A 441		LYS	140.16	-	Favored (64.81%) General / -71.2,-44.8	51.8% (*mtpt*) chi angles: 291.2,181.2,55.7,183.7	0.006Å	-	-
A 442		GLY	123.45	-	Favored (92.38%) Glycine / -61.4,-36.4	-	-	-	-
A 443		ILE	134.01	-	Favored (77.46%) Isoleucine or valine / -70.5,-43.9	51.1% (*mt*) chi angles: 289.8,179.9	0.03Å	-	-
A 444		ARG	137.01	-	Favored (85.3%) General / -62.4,-37.3	33.8% (*ttm105*) chi angles: 187.3,195.1,303.9,104.8	0.009Å	-	-
A 445		TRP	140.95	-	Favored (82.07%) General / -68.1,-41.2	48.3% (*m0*) chi angles: 292.5,358.4	0.026Å	-	-
A 446		LEU	119.7	-	Favored (85.55%) General / -66.5,-43.3	30.2% (*tp*) chi angles: 186.8,55.4	0.022Å	-	-
A 447		ILE	137.95	0.481Å O with A 451 LYS HB2	Favored (43.37%) Isoleucine or valine / -66.8,-28.5	37.6% (*pt*) chi angles: 64.8,175.5	0.055Å	-	-
A 448		GLU	140.34	-	Favored (25.9%) General / -85.8,-26.1	35.3% (*mm-40*) chi angles: 291.7,295.7,283.1	0.004Å	-	-
A 449		LEU	149.67	0.652Å HD21 with A 358 ARG HB3	Favored (36.72%) General / -77.9,-41.4	18.7% (*tp*) chi angles: 195.2,58.7	0.011Å	-	-
A 450		ILE	138.84	-	Favored (35.6%) Isoleucine or valine / -70.5,-28.6	47.9% (*mt*) chi angles: 298.4,183.5	0.036Å	-	-
A		LYS	149.31	0.661Å HG3 with A	Favored (78.11%)	38.4% (*tttt*) chi angles:	0.023Å	-	-

# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
451		526 LEU HD23	General / -63.8,-34.5	214.1,165.7,187.9,176.4			
A 452	ASP 146.14	-	Favored (75.05%) General / -67.9,-33.6	11.9% (*m-20*) chi angles: 282.8,21.2	0.009Å	-	-
A 453	ASP 149.53	-	Favored (78.62%) General / -65.8,-34.6	78.9% (*m-20*) chi angles: 297.8,340.1	0.016Å	-	-
A 454	TYR 157.41	0.426Å CZ with A 523 ASP HB2	Favored (77.21%) General / -69.1,-36.0	80.9% (*t80*) chi angles: 178.5,85.1	0.017Å	-	-
A 455	ASN 154.7	-	Favored (73.62%) General / -66.3,-32.3	25.9% (*m120*) chi angles: 294.9,133.7	0.032Å	-	-
A 456	GLU 161.47	-	Favored (29.69%) General / -84.2,-25.3	12% (*pt-20*) chi angles: 80.8,177.3,38.5	0.025Å	-	-
A 457	THR 168.05	-	Favored (68.56%) General / -72.2,-34.6	46.4% (*m*) chi angles: 305.2	0.011Å	-	-
A 458	VAL 176.95	-	Favored (94.1%) Isoleucine or valine / -61.9,-42.3	49.4% (*t*) chi angles: 168.5	0.012Å	-	-
A 459	HIS 176.1	-	Favored (85.31%) General / -63.2,-46.8	26% (*m170*) chi angles: 286.2,140.1	0.027Å	-	-
A 460	LYS 169.7	-	Favored (72.26%) General / -64.0,-31.2	37.7% (*mmtt*) chi angles: 267.2,298.6,179.9,181.2	0.023Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 137.21	Clashscore: 8.45	Outliers: 0 of 620	Poor rotamers: 0 of 557	Outliers: 0 of 591	Outliers: 0 of 628	Outliers: 0 of 628
A 461		LYS 174.84	-		Favored (78.7%) General / -66.7,-45.5	8% (*ttpt*) chi angles: 182.3,227.7,65.3,177.7	0.016Å	-	-
A					Favored	39.5% (*p*)			

462	THR 172.6	-	(73.27%)	chi angles: 53.4	0.021Å	-	-
A 463	GLU 176.01	-	Favored (89.89%) General / -62.0,-32.7	77.2% (*mt-10*) chi angles: 297.3,178.3,200.4	0.013Å	-	-
A 464	VAL 175.88	-	Favored (58.8%) Isoleucine or valine / -69.1,-33.5	45.4% (*t*) chi angles: 183.6	0.018Å	-	-
A 465	VAL 184.02	-	Favored (81.26%) Isoleucine or valine / -63.9,-49.5	11.8% (*t*) chi angles: 160.8	0.046Å	-	-
A 466	ILE 196.61	-	Favored (92.11%) Isoleucine or valine / -61.6,-41.9	71.6% (*mt*) chi angles: 298.7,178.3	0.005Å	-	-
A 467	THR 186.69	-	Favored (80.29%) General / -60.0,-48.8	75.8% (*m*) chi angles: 297	0.03Å	-	-
A 468	LEU 178.39	-	Favored (2.67%) General / -57.5,-61.2	31.4% (*tp*) chi angles: 179.9,72.1	0.003Å	-	-
A 469	ASP 186.97	-	Favored (29.14%) General / -48.4,-50.9	87.1% (*m-20*) chi angles: 291.7,332.5	0.03Å	-	-
A 470	PHE 209.1	-	Favored (25.71%) General / -75.5,-47.7	1.7% (*t80*) chi angles: 208.4,117.4	0.077Å	-	-
A 471	CYS 191.71	-	Favored (73.47%) General / -54.7,-44.6	38.3% (*t*) chi angles: 174.9	0.042Å	-	-
A 472	ILE 180.4	0.491Å O with A 476 GLU HG3	Favored (68.34%) Isoleucine or valine / -69.6,-35.9	14% (*pt*) chi angles: 70.7,183.2	0.089Å	-	-
A 473	ARG 188.36	-	Favored (98.31%) General / -63.6,-41.8	59.7% (*ttm-85*) chi angles: 176.3,173.1,298.1,275.1	0.018Å	-	-

# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 474	ASN 193.04	-	Favored (95.76%) General / -60.3,-44.1	37% (*t-20*) chi angles: 195.3,327.3	0.05Å	-	-
A 475	ILE 180.07	0.513Å HD13 with A 501 ILE HG21	Favored (22.51%) Isoleucine or valine / -74.5,-28.6	35.4% (*mt*) chi angles: 305.9,161.1	0.106Å	-	-
A 476	GLU 203.43	0.491Å HG3 with A 472 ILE O	Favored (55.61%) General / -77.3,-19.9	57.8% (*mt-10*) chi angles: 297.2,198.4,337.3	0.023Å	-	-
A 477	LYS 182.01	-	Favored (15.64%) General / -91.0,-33.2	5% (*tttt*) chi angles: 129.3,197.9,174.5,185.4	0.009Å	-	-
A 478	THR 174.73	-	Favored (67.8%) General / -62.1,-25.5	7.4% (*m*) chi angles: 314.6	0.025Å	-	-
A 479	VAL 166.36	1.126Å HG12 with A 498 ILE HD13	Favored (9.38%) Isoleucine or valine / -82.4,-22.6	27.3% (*m*) chi angles: 296	0.031Å	-	-
A 480	LYS 171.17	-	Favored (37.25%) General / -80.6,-27.6	53.5% (*tptt*) chi angles: 179.8,56.5,183.8,177.3	0.024Å	-	-
# Alt Res	**High B**	**Clash > 0.4Å**	**Ramachandran**	**Rotamer**	**Cβ deviation**	**Bond lengths**	**Bond angles**
	Avg: 137.21	Clashscore: 8.45	Outliers: 0 of 620	Poor rotamers: 0 of 557	Outliers: 0 of 591	Outliers: 0 of 628	Outliers: 0 of 628
A 481	VAL 172.33	-	Allowed (0.92%) Isoleucine or valine / -118.6,-175.7	35.3% (*m*) chi angles: 298.1	0.006Å	-	-
A 482	TYR 204.22	-	-	55.8% (*t80*) chi angles: 190.3,77.4	0.039Å	-	-
A 492	ALA 152.66	-	-	-	0.02Å	-	-
A 493	ALA 165.19	-	Favored (3.51%) General / -67.4,-59.3	-	0.02Å	-	-
			Favored	46% (*mt-10*)			

A 494	GLU 235.17	-	(84.54%) General / -63.5,-36.7	chi angles: 305.6,157.4,353.9	0.004Å	-	-
A 495	LEU 155.3	-	Favored (99.53%) General / -63.0,-41.2	83% (mt) chi angles: 300.8,174.4	0.004Å	-	-
A 496	GLY 161.62	-	Favored (96.76%) Glycine / -64.1,-43.8	-	-	-	-
A 497	GLU 188.7	0.42Å O with A 501 ILE HG13	Favored (32.34%) General / -60.9,-55.5	82.3% (mt-10) chi angles: 303.6,167.2,348.1	0.029Å	-	-
A 498	ILE 151.91	1.126Å HD13 with A 479 VAL HG12	Favored (27.3%) Isoleucine or valine / -50.7,-48.8	33.9% (mt) chi angles: 286.4,156.6	0.018Å	-	-
A 499	SER 173.4	-	Favored (92.66%) General / -60.2,-45.6	80.2% (p) chi angles: 60.1	0.01Å	-	-
A 500	ASP 164.29	-	Favored (96.66%) General / -61.2,-41.3	84% (m-20) chi angles: 296.4,337.8	0.006Å	-	-
A 501	ILE 178.62	0.513Å HG21 with A 475 ILE HD13	Favored (88.47%) Isoleucine or valine / -66.9,-45.0	56.9% (mt) chi angles: 305.3,166.7	0.004Å	-	-
A 502	HIS 165.09	-	Favored (81.88%) General / -56.8,-45.9	82.4% (t60) chi angles: 182,62	0.006Å	-	-
A 503	THR 170	0.499Å O with A 507 ARG HG2	Favored (68.37%) General / -60.2,-51.7	39.2% (p) chi angles: 53.3	0.013Å	-	-
A 504	LYS 190.62	0.407Å HD3 with A 647 TYR CZ	Favored (72.2%) General / -55.4,-41.2	94.6% (mttt) chi angles: 289.1,171.5,175.8,184.5	0.024Å	-	-
A 505	LEU 167.08	0.457Å HD22 with A 472 ILE HG22	Favored (68.72%) General / -66.3,-28.5	69.7% (mt) chi angles: 298.5,168.7	0.003Å	-	-
			Favored				

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 506		LEU	181.86	-	(33.89%) General / -81.6,-27.9	54.3% (*mt*) chi angles: 288.5,180.7	0.02Å	-	-
A 507		ARG	185.49	0.499Å HG2 with A 503 THR O	Favored (85.99%) General / -62.6,-37.4	39.4% (*mmt180*) chi angles: 303.7,292.3,188.2,181.6	0.038Å	-	-
A 508		LEU	176.49	-	Favored (14.05%) General / -88.1,-40.1	70.1% (*mt*) chi angles: 304.3,181	0.008Å	-	-
A 509		SER	158.65	-	Favored (70.36%) General / -66.2,-30.0	37.2% (*t*) chi angles: 182.2	0.016Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 137.21	Clashscore: 8.45	Outliers: 0 of 620	Poor rotamers: 0 of 557	Outliers: 0 of 591	Outliers: 0 of 628	Outliers: 0 of 628
A 510		SER	163.15	-	Favored (65.29%) General / -68.7,-47.9	85.4% (*p*) chi angles: 61.2	0.01Å	-	-
A 511		SER	159.44	-	Favored (68.84%) General / -66.4,-28.7	90.2% (*p*) chi angles: 62.6	0.003Å	-	-
A 512		GLN	158.69	-	Favored (76.31%) General / -64.2,-33.7	17.8% (*tm0?*) chi angles: 178.8,267.6,324	0.01Å	-	-
A 513		GLY	163.64	-	Favored (58.77%) Glycine / -72.9,-34.6	-	-	-	-
A 514		THR	160.83	-	Favored (71.15%) General / -66.1,-48.4	27.7% (*p*) chi angles: 71.1	0.03Å	-	-
A 515		ILE	163.58	-	Favored (93.07%) Isoleucine or valine / -63.8,-41.6	63.5% (*mt*) chi angles: 300.7,179.4	0.014Å	-	-
A 516		GLU	164.58	0.428Å O with A 520 GLN HG2	Favored (70.14%) General / -53.9,-44.0	23.9% (*tp10*) chi angles: 161.4,65.2,22.9	0.015Å	-	-
A					Favored				

517	THR	156.2	-	(29.74%) General / -82.1,-33.5	61.6% (*p*) chi angles: 56.7	0.029Å	-	-
A 518	SER	145.52	-	Favored (65.06%) General / -68.9,-26.4	89% (*p*) chi angles: 65.4	0.009Å	-	-
A 519	LEU	153.27	-	Favored (66.34%) General / -72.9,-34.0	38.6% (*mt*) chi angles: 284.7,180.3	0.01Å	-	-
A 520	GLN	165.1	0.428Å HG2 with A 516 GLU O	Favored (68.92%) General / -65.5,-28.1	77.2% (*mm-40*) chi angles: 303.7,298.5,332	0.008Å	-	-
A 521	ASP	147.84	-	Favored (72.97%) General / -70.9,-37.5	17.5% (*t70*) chi angles: 174.7,84	0.014Å	-	-
A 522	ILE	143.21	-	Favored (82.97%) Isoleucine or valine / -68.2,-40.6	25.7% (*mt*) chi angles: 293.3,186.9	0.023Å	-	-
A 523	ASP	149.69	0.426Å HB2 with A 454 TYR CZ	Favored (77.84%) General / -64.5,-34.3	17.6% (*t70*) chi angles: 179.6,88.6	0.013Å	-	-
A 524	SER	146.84	0.4Å O with A 527 SER OG	Favored (79.18%) General / -64.7,-34.8	48.3% (*t*) chi angles: 179.5	0.022Å	-	-
A 525	ARG	140.55	0.61Å HD3 with A 626 LEU HD12	Favored (71.67%) General / -71.3,-39.1	90.7% (*mtt180*) chi angles: 290.4,172,163.1,185.9	0.016Å	-	-
A 526	LEU	139.38	0.661Å HD23 with A 451 LYS HG3	Favored (60.16%) General / -73.7,-21.6	4.9% (*mp*) chi angles: 265,45.8	0.004Å	-	-
A 527	SER	146.45	0.4Å OG with A 524 SER O	Favored (96.51%) Pre-proline / -69.2,152.8	94.8% (*p*) chi angles: 63.5	0.022Å	-	-
A 528	PRO	154.24	-	Favored (28.9%) Trans-proline / -55.4,128.1	78.7% (*Cg_exo*) chi angles: 332.1	0.066Å	-	-
A				Favored				

# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
529 GLY	137.5	-	(75.8%) Glycine / 79.8,17.2	-	-	-	-
	Avg: 137.21	Clashscore: 8.45	Outliers: 0 of 620	Poor rotamers: 0 of 557	Outliers: 0 of 591	Outliers: 0 of 628	Outliers: 0 of 628
A 530 GLY	147.78	-	Favored (7.22%) Glycine / -94.4,30.9	-	-	-	-
A 531 SER	145.62	-	Allowed (0.89%) General / 65.7,-2.2	33.4% (*t*) chi angles: 183.6	0.09Å	-	-
A 532 LEU	128.38	0.638Å HD22 with A 626 LEU HD13	Favored (12.46%) General / -116.8,0.3	14.7% (*tp*) chi angles: 196.8,71.4	0.011Å	-	-
A 533 ALA	137.09	-	Favored (26.81%) General / -60.1,151.4	-	0.019Å	-	-
A 534 ASP	136.73	-	Favored (7.19%) General / -90.3,17.4	11.4% (*p30*) chi angles: 47.9,24.1	0.007Å	-	-
A 535 ALA	126.54	-	Favored (75.45%) General / -60.5,-35.2	-	0.022Å	-	-
A 536 TRP	126.35	-	Favored (82.89%) General / -63.7,-36.1	61.1% (*p-90*) chi angles: 66.7,270.7	0.022Å	-	-
A 537 ALA	128.62	-	Favored (58.39%) General / -76.7,-18.7	-	0.019Å	-	-
A 538 HIS	154.16	-	Favored (20.14%) General / -93.5,14.0	1.3% (*t-80*) chi angles: 203.9,342.9	0.037Å	-	-
A 539 GLN	144.58	-	Allowed (1.01%) General / -131.6,-55.0	88% (*mt-30*) chi angles: 292,167.2,346.8	0.026Å	-	-
A 540 GLU	145.57	-	Favored (65.32%) General /	29.6% (*tp10*) chi angles:	0.04Å	-	-

			-62.8,-51.9	200,69.7,16.8		

#	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 541	GLY 117.94	-	Favored (21.52%) Glycine / -75.7,-166.9	-	-	-	-
A 542	THR 119.24	0.491Å N with A 436 GLN OE1	Favored (15.26%) General / -102.3,159.6	24.3% (*p*) chi angles: 50	0.007Å	-	-
A 543	HIS 129.71	-	Favored (62.91%) Pre-proline / -128.9,160.6	37.2% (*m80*) chi angles: 308.3,80.2	0.029Å	-	-
A 544	PRO 112.24	-	Favored (45.44%) Trans-proline / -59.4,-18.4	71.3% (*Cg_exo*) chi angles: 332.5	0.066Å	-	-
A 545	LYS 124.7	-	Favored (71.02%) General / -64.0,-29.9	63.8% (*tttp*) chi angles: 180.8,184.3,177.4,63.1	0.027Å	-	-
A 546	ASP 114.81	-	Favored (65.53%) General / -70.2,-28.7	64.1% (*m-20*) chi angles: 302.1,331.9	0.01Å	-	-
A 547	ARG 119.3	-	Favored (23.97%) General / 58.0,34.2	72.4% (*mtp85*) chi angles: 302.5,181.6,60,88.2	0.04Å	-	-
A 548	ASN 108.37	-	Favored (87.36%) General / -62.3,-37.9	93.1% (*m-20*) chi angles: 290.7,327.9	0.032Å	-	-
A 549	VAL 100.21	-	Favored (83.94%) Isoleucine or valine / -67.3,-39.9	50.5% (*t*) chi angles: 182.4	0.014Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 137.21	Clashscore: 8.45	Outliers: 0 of 620	Poor rotamers: 0 of 557	Outliers: 0 of 591	Outliers: 0 of 628	Outliers: 0 of 628
A 550		GLU 98.99	-	Favored (92.69%) General / -65.0,-39.0	40.2% (*mp0*) chi angles: 289.2,82.8,343.2	0.01Å	-	-
A		LYS 112.24	-	Favored (96.46%)	67.1% (*mttm*) chi angles:	0.008Å	-	-

551			General / -60.6,-42.4	288.1,174.8,177.6,292.5			
A 552	LEU 93.74	-	Favored (73.4%) General / -70.5,-35.8	80.6% (*mt*) chi angles: 296,181.6	0.012Å	-	-
A 553	GLN 117.57	-	Favored (79.3%) General / -67.3,-35.4	56.1% (*tp60*) chi angles: 186.7,61.9,29.7	0.026Å	-	-
A 554	VAL 82.03	-	Favored (80.73%) Isoleucine or valine / -58.3,-49.8	39.9% (*t*) chi angles: 166.4	0.006Å	-	-
A 555	LEU 85.22	-	Favored (71.43%) General / -67.5,-31.4	83.2% (*mt*) chi angles: 300.4,174	0.022Å	-	-
A 556	LEU 95.69	-	Favored (71.75%) General / -70.1,-33.4	23.5% (*tp*) chi angles: 189,53.9	0.006Å	-	-
A 557	ASN 92.44	-	Favored (78.98%) General / -69.0,-40.0	95.1% (*m-20*) chi angles: 292.8,332.2	0.013Å	-	-
A 558	CYS 100.27	-	Favored (98.67%) General / -61.3,-42.4	70.7% (*m*) chi angles: 297.5	0.019Å	-	-
A 559	MET 82.1	-	Favored (75.72%) General / -69.8,-40.6	77.5% (*mtp*) chi angles: 294.4,182.1,56.5	0.005Å	-	-
A 560	THR 90.5	-	Favored (89.77%) General / -64.7,-38.1	47.8% (*m*) chi angles: 305.1	0.013Å	-	-
A 561	GLU 118.91	-	Favored (93.28%) General / -63.0,-45.2	87.4% (*tt0*) chi angles: 183.7,180.1,6.3	0.014Å	-	-
A 562	ILE 85.88	-	Favored (82.65%) Isoleucine or valine / -63.1,-38.7	54.8% (*mt*) chi angles: 292.8,181.5	0.027Å	-	-
A	TYR 89.82	0.527Å CZ with A	Favored (51.62%)	12.4% (*t80*)	0.029Å	-	-

# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
563		567 LYS HD2	General / -59.2,-54.0	chi angles: 158.9,65.2			
A 564	TYR 110.4	-	Favored (67.81%) General / -64.2,-24.8	48.1% (m-85) chi angles: 283.8,290.4	0.033Å	-	-
A 565	GLN 90.36	-	Favored (69.69%) General / -71.3,-41.6	11.4% (tp-100) chi angles: 179.5,52.2,235.7	0.008Å	-	-
A 566	PHE 98.2	-	Favored (68.51%) General / -67.1,-28.8	11.1% (m-30) chi angles: 283.7,2.2	0.023Å	-	-
A 567	LYS 100.52	0.527Å HD2 with A 563 TYR CZ	Favored (92.1%) General / -65.6,-40.0	29.1% (mtpp) chi angles: 292.5,183.5,61.4,61.9	0.055Å	-	-
A 568	LYS 106.18	0.424Å HB2 with A 568 LYS HE3	Favored (63.67%) General / -71.2,-27.6	25.2% (ttmt) chi angles: 205.1,165.8,303.4,176.5	0.02Å	-	-
A 569	ASP 103.98	-	Favored (34.06%) General / -81.4,-28.9	84.5% (m-20) chi angles: 296,336.7	0.008Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 137.21	Clashscore: 8.45	Outliers: 0 of 620	Poor rotamers: 0 of 557	Outliers: 0 of 591	Outliers: 0 of 628	Outliers: 0 of 628
A 570		LYS	112.51	-	Favored (75.97%) General / -68.8,-34.7	86.9% (tttt) chi angles: 178.5,183.2,174.8,180.2	0.006Å	-	-
A 571		ALA	115.45	-	Favored (67.01%) General / -67.8,-27.7	-	0.022Å	-	-
A 572		GLU	139.54	-	Favored (48.94%) General / -83.3,-15.8	32.4% (mm-40) chi angles: 315.9,303,323.1	0.005Å	-	-
A 573		ARG	166.9	-	Allowed (0.1%) General / 66.2,-24.2	39.3% (mtm105) chi angles: 305.4,183,301.2,103	0.105Å	-	-
A 574		ARG	136.84	-	Favored (28.79%) General /	6.8% (ptm105) chi angles: 69.7,165.2,295.3,100.7	0.024Å	-	-

			-153.0,150.0				
A 575	LEU 117.67	0.43Å HD23 with A 579 GLU HB3	Favored (27.34%) General / -121.0,158.7	10.3% (*mp*) chi angles: 271.5,57.2	0.021Å	-	-
A 576	ALA 111.3	-	Favored (13.95%) General / -70.4,169.4	-	0.029Å	-	-
A 577	TYR 106.96	0.427Å O with A 581 GLN HG2	Favored (81.48%) General / -56.8,-46.4	69.7% (*t80*) chi angles: 183.3,266.9	0.019Å	-	-
A 578	ASN 133.92	-	Favored (72.01%) General / -64.1,-49.5	18.2% (*m120*) chi angles: 298.4,90.2	0.03Å	-	-
A 579	GLU 122.17	0.43Å HB3 with A 575 LEU HD23	Favored (70.52%) General / -61.1,-30.8	23.7% (*mp0*) chi angles: 278.6,66.8,18.6	0.004Å	-	-
A 580	GLU 135.02	0.433Å HG3 with A 406 TYR CZ	Favored (91.47%) General / -64.3,-44.5	82.8% (*tt0*) chi angles: 174.9,175.1,359.8	0.008Å	-	-
A 581	GLN 123.02	0.427Å HG2 with A 577 TYR O	Favored (38.92%) General / -80.2,-31.4	26.9% (*mm-40*) chi angles: 320.4,307,337	0.046Å	-	-
A 582	ILE 106.71	-	Favored (86.84%) Isoleucine or valine / -63.7,-39.8	55.8% (*mt*) chi angles: 291.4,180.2	0.018Å	-	-
A 583	HIS 100.07	-	Favored (84.19%) General / -59.1,-40.0	32.4% (*t60*) chi angles: 179.8,98.6	0.033Å	-	-
A 584	LYS 130.87	-	Favored (65.01%) General / -73.1,-40.4	98.7% (*mttt*) chi angles: 297,174.9,183.8,176.1	0.006Å	-	-
A 585	PHE 111.12	-	Favored (77.88%) General / -62.1,-49.0	18.3% (*m-30*) chi angles: 291.2,332	0.017Å	-	-
A 586	ASP 101.81	-	Favored (74.08%) General / -66.5,-32.6	72.4% (*m-20*) chi angles: 299.5,337.9	0.01Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 587		LYS	104.18	-	Favored (85.83%) General / -63.9,-37.0	87.6% (tttt) chi angles: 180.4,181.1,177.5,179.6	0.005Å	-	-
A 588		GLN	126.97	-	Favored (68.21%) General / -72.5,-35.4	64.4% (tt0) chi angles: 184.2,177.4,355.9	0.004Å	-	-
A 589		LYS	104.59	-	Favored (61.67%) General / -71.9,-24.5	96.9% (mttt) chi angles: 297.7,173.4,183.4,176.5	0.002Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 137.21	Clashscore: 8.45	Outliers: 0 of 620	Poor rotamers: 0 of 557	Outliers: 0 of 591	Outliers: 0 of 628	Outliers: 0 of 628
A 590		LEU	92.75	-	Favored (89.29%) General / -64.5,-37.9	27.6% (tp) chi angles: 190.1,66.1	0.039Å	-	-
A 591		TYR	101.43	-	Favored (64.78%) General / -70.0,-46.7	35.6% (t80) chi angles: 164.5,83.8	0.016Å	-	-
A 592		TYR	139.78	-	Favored (90.15%) General / -61.6,-39.1	9.4% (m-30) chi angles: 284.6,330.6	0.031Å	-	-
A 593		HIS	96.33	-	Favored (89.09%) General / -64.4,-45.1	8% (m-70) chi angles: 283.3,330.3	0.01Å	-	-
A 594		ALA	88.51	-	Favored (85%) General / -64.4,-46.1	-	0.029Å	-	-
A 595		THR	93.62	-	Favored (85.87%) General / -64.3,-37.0	58% (p) chi angles: 56.4	0.006Å	-	-
A 596		LYS	123.31	-	Favored (87.8%) General / -65.2,-37.6	35.8% (ttmt) chi angles: 187.7,189.4,306.5,175.5	0.021Å	-	-
A 597		ALA	95.22	-	Favored (55.01%) General / -73.8,-44.6	-	0.019Å	-	-
A 598		MET	117.7	-	Favored (89.41%) General /	94.4% (mmm) chi angles:	0.011Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
					-63.2,-38.0	291.9,300.7,300.8			
A 599		THR	103.5	-	Favored (86.03%) General / -64.9,-45.4	94.3% (m) chi angles: 298.1	0.004Å	-	-
A 600		HIS	95.11	-	Favored (65.51%) General / -67.6,-24.4	82.7% (t60) chi angles: 183.9,74.2	0.007Å	-	-
A 601		PHE	100.01	-	Favored (28.44%) General / -73.3,-49.2	65.3% (t80) chi angles: 171.6,70.6	0.011Å	-	-
A 602		THR	104.18	-	Favored (29.42%) General / -81.5,-36.3	81.6% (p) chi angles: 61	0.017Å	-	-
A 603		ASP	113.52	-	Favored (55.77%) General / -84.1,-12.0	3.7% (m-20) chi angles: 298.6,22.5	0.036Å	-	-
A 604		GLU	116.55	-	Allowed (1.46%) General / -124.2,-59.7	45.4% (tp10) chi angles: 176.1,73.7,12.3	0.016Å	-	-
A 605		CYS	103.65	-	Favored (19.99%) General / -69.0,-53.6	66.1% (m) chi angles: 302.2	0.017Å	-	-
A 606		VAL	110.8	-	Favored (37.64%) Isoleucine or valine / -64.9,-53.8	77.5% (t) chi angles: 174.3	0.03Å	-	-
A 607		LYS	124.69	-	Favored (91.45%) General / -59.0,-44.5	18.5% (mtmm) chi angles: 264,195.4,283.2,292.1	0.054Å	-	-
A 608		LYS	112.13	-	Favored (62.87%) General / -70.5,-24.5	96.3% (mttt) chi angles: 292.3,187.9,176,181.6	0.036Å	-	-
A 609		TYR	107.34	-	Favored (59.09%) General / -72.6,-45.5	10.6% (t80) chi angles: 156.6,75.3	0.01Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg:	Clashscore:	Outliers: 0 of	Poor rotamers: 0 of	Outliers:	Outliers:	Outliers:

		137.21	8.45	620	557	0 of 591	0 of 628	0 of 628
A 610	GLU	106.87	-	Favored (76.1%) General / -64.2,-33.6	98.6% (*mt-10*) chi angles: 297.1,179.5,348.8	0.007Å	-	-
A 611	ALA	121.61	-	Favored (76.98%) General / -69.6,-37.4	-	0.021Å	-	-
A 612	PHE	114.98	-	Favored (75.42%) General / -68.5,-34.2	66.8% (*t80*) chi angles: 183.9,87.6	0.026Å	-	-
A 613	LEU	114.67	-	Favored (63.59%) General / -74.3,-34.8	61.9% (*tp*) chi angles: 177.3,59.6	0.007Å	-	-
A 614	ASN	128.42	-	Favored (81.59%) General / -66.2,-45.2	28% (*t-20*) chi angles: 181,268.6	0.014Å	-	-
A 615	LYS	152.35	-	Favored (59.91%) General / -76.9,-12.1	97.7% (*mttt*) chi angles: 291.6,186.2,176,179.2	0.013Å	-	-
A 616	SER	121.75	-	Favored (74.82%) General / -70.1,-40.4	41.2% (*t*) chi angles: 181.3	0.005Å	-	-
A 617	GLU	138.79	0.403Å O with A 621 ARG HG3	Favored (94.11%) General / -62.7,-39.5	70.5% (*mt-10*) chi angles: 304,190.6,184.2	0.017Å	-	-
A 618	GLU	151.41	-	Favored (38.71%) General / -59.2,-55.1	10.2% (*mm-40*) chi angles: 308.6,278.5,27.5	0.013Å	-	-
A 619	TRP	116.27	-	Favored (71.35%) General / -64.2,-30.3	78.9% (*t90*) chi angles: 188,92.2	0.01Å	-	-
A 620	ILE	131.47	-	Favored (92.95%) Isoleucine or valine / -65.5,-45.3	17.6% (*mt*) chi angles: 282.7,181.5	0.045Å	-	-
A 621	ARG	150.09	0.403Å HG3 with A 617 GLU O	Favored (82.03%) General / -58.8,-48.2	93.9% (*mtt180*) chi angles: 302.4,172.1,192.6,177.7	0.044Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 622		LYS	131.99	-	Favored (71.08%) General / -67.7,-31.2	48.9% (*mtpt*) chi angles: 307.7,168.6,67.8,181	0.013Å	-	-
A 623		MET	128.86	-	Favored (50.94%) General / -73.4,-46.0	12% (*tmm?*) chi angles: 184.5,272,304.2	0.012Å	-	-
A 624		LEU	131.66	-	Favored (76.76%) General / -65.3,-33.8	39.9% (*mt*) chi angles: 287.9,183	0.028Å	-	-
A 625		HIS	137.4	-	Favored (83.97%) General / -65.5,-45.3	69.3% (*t60*) chi angles: 174.8,60.2	0.011Å	-	-
A 626		LEU	124.35	0.638Å HD13 with A 532 LEU HD22	Favored (90.43%) General / -63.6,-38.3	6.1% (*tt*) chi angles: 175.9,141.1	0.02Å	-	-
A 627		ARG	148.5	0.509Å NH2 with A 351 GLU OE2	Favored (72.45%) General / -66.2,-31.5	62.6% (*ttt180*) chi angles: 197,181.7,188,188.3	0.01Å	-	-
A 628		LYS	130.46	-	Favored (66.68%) General / -72.9,-39.1	24.4% (*tptt*) chi angles: 216.1,64.4,175.3,183	0.018Å	-	-
A 629		GLN	135.85	0.476Å OE1 with A 525 ARG NH1	Favored (72.81%) General / -65.0,-48.7	84.5% (*mt-30*) chi angles: 288.4,186.1,346.7	0.014Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 137.21	Clashscore: 8.45	Outliers: 0 of 620	Poor rotamers: 0 of 557	Outliers: 0 of 591	Outliers: 0 of 628	Outliers: 0 of 628
A 630		LEU	137.96	-	Favored (76.75%) General / -61.0,-35.4	58.2% (*tp*) chi angles: 181.8,61.2	0.002Å	-	-
A 631		LEU	134.45	0.422Å HD22 with A 384 ARG NH2	Favored (51.02%) General / -63.2,-53.6	45.4% (*tp*) chi angles: 177.5,69.6	0.019Å	-	-
A 632		SER	146.02	-	Favored (79.72%) General / -60.6,-48.9	62.4% (*m*) chi angles: 298.9	0.006Å	-	-
					Favored				

A 633	LEU 144.87	-	(68.8%) General / -62.8,-26.5	76.9% (*mt*) chi angles: 296.6,182.8	0.021Å	-	-
A 634	THR 147.78	-	Favored (28.38%) General / -77.8,-44.1	51.6% (*m*) chi angles: 304.8	0.003Å	-	-
A 635	ASN 156.16	-	Favored (68.99%) General / -66.3,-28.8	29.7% (*m120*) chi angles: 292.3,126.8	0.037Å	-	-
A 636	GLN 157.51	-	Favored (71.42%) General / -66.4,-30.9	80.6% (*mt-30*) chi angles: 289.4,180.7,20.7	0.016Å	-	-
A 637	CYS 157.11	-	Favored (74.53%) General / -65.8,-32.8	92.1% (*m*) chi angles: 293.5	0.004Å	-	-
A 638	PHE 155.45	-	Favored (58.38%) General / -75.8,-28.5	19.2% (*m-30*) chi angles: 291.3,334.8	0.015Å	-	-
A 639	ASP 175.04	-	Favored (67.05%) General / -72.0,-32.4	75.4% (*m-20*) chi angles: 298.9,333.9	0.003Å	-	-
A 640	ILE 166.46	-	Favored (10.08%) Isoleucine or valine / -94.4,-7.3	27.5% (*pt*) chi angles: 67.1,178.4	0.006Å	-	-
A 641	GLU 155.13	-	Favored (61.2%) General / -75.2,-32.2	72.3% (*tt0*) chi angles: 185.9,185.9,15.6	0.022Å	-	-
A 642	GLU 180.51	-	Favored (39.98%) General / -85.6,-16.2	24.9% (*mm-40*) chi angles: 320.2,296.1,338	0.006Å	-	-
A 643	GLU 176.77	-	Favored (37.12%) General / -80.0,-35.5	7.1% (*mm-40*) chi angles: 288.7,286.6,75.8	0.007Å	-	-
A 644	VAL 168.2	-	Favored (12.97%) Isoleucine or valine / -79.0,-10.9	28.6% (*m*) chi angles: 294.1	0.022Å	-	-
A			Favored (47.03%)	49.5% (*m*)			

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
645		SER	166.19	-	General / -84.7,-15.0	chi angles: 300.4	0.012Å	-	-
A 646		LYS	161.59	-	Favored (28.62%) General / -99.3,-6.1	37.7% (*ttmt*) chi angles: 195.8,178.6,297.9,181.8	0.019Å	-	-
A 647		TYR	169.42	0.407Å CZ with A 504 LYS HD3	Favored (4.93%) General / -112.2,-37.7	20.6% (*m-30*) chi angles: 291.7,338.3	0.038Å	-	-
A 648		GLN	190.41	-	Favored (63.59%) General / -69.7,-20.4	24.2% (*pt20*) chi angles: 72.3,181.9,346.8	0.008Å	-	-
A 649		GLU	164.97	-	Favored (16.61%) General / -107.5,22.0	75% (*mt-10*) chi angles: 299.7,190.6,9.9	0.013Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 137.21	Clashscore: 8.45	Outliers: 0 of 620	Poor rotamers: 0 of 557	Outliers: 0 of 591	Outliers: 0 of 628	Outliers: 0 of 628
A 650		TYR	183.92	-	Allowed (0.66%) General / -99.5,-72.6	45.5% (*t80*) chi angles: 191.5,87.4	0.01Å	-	-
A 651		THR	179.91	-	Favored (46.83%) General / -77.7,-38.6	28.8% (*m*) chi angles: 307.5	0.01Å	-	-
A 652		ASN	167.29	-	Favored (66.79%) General / -60.6,-26.1	22.9% (*t-20*) chi angles: 185.1,280.8	0.005Å	-	-
A 653		GLU	161	-	Favored (3.71%) General / -107.5,34.1	88.2% (*mt-10*) chi angles: 304.5,181.4,350.1	0.018Å	-	-
A 654		LEU	143.13	-	Favored (58.82%) General / -64.5,140.0	47.6% (*tp*) chi angles: 174.6,57.4	0.011Å	-	-
A 655		GLN	132.92	-	Favored (28.93%) General / -91.2,141.3	21.6% (*mm-40*) chi angles: 289.6,282.9,27.4	0.029Å	-	-
A 656		GLU	128.51	-	Favored (7.64%) General /	15.8% (*tp10*) chi angles: 183.5,47.8,55.3	0.009Å	-	-

-166.4,150.6

A 657	THR 134.37	-	-	55.9% (*m*) chi angles: 304.5	0.008Å	-	-
A 701	BX7 143.81	0.403Å S02 with A 38 LYS NZ	-	-	-	-	-

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