Viewing MYO7A_60-686.pdb_54_1H-multi.table

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All-Atom Contacts	Clashscore, all atoms:	1.19		99th percentile* (N=1784, all resolutions
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	5	0.90%	Goal: <1%
	Ramachandran outliers	8	1.28%	Goal: <0.05%
	Ramachandran favored	559	89.44%	Goal: >98%
	MolProbity score^	1.40		97th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	13	2.19%	Goal: 0
	Bad backbone bonds:	0 / 5180	0.00%	Goal: 0%
	Bad backbone angles:	66 / 6990	0.94%	Goal: <0.1%

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

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

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

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.75	Clashscore: 1.19	Outliers: 8 of 625	Poor rotamers: 5 of 555	Outliers: 13 of 594	Outliers: 0 of 627	Outliers: 6 of 627
A 60		HIS	50	-	-	24.8% (*p80*) chi angles: 60.2,71.5	0.046Å	-	OUTLIER(worst is CA-CB-CG 4.798 σ
A 61		PRO	50	-	Favored (5.96%) Trans-proline / -53.6,160.0	54.1% (*Cg_exo*) chi angles: 334.6	0.07Å	-	-

A 62	THR	50	-	Favored (73.66%) General / -67.7,-32.8	1.4% (*p*) chi angles: 36.1	0.137Å	-	-
A 63	SER	50	-	Favored (71.41%) General / -62.0,-31.1	49.5% (*p*) chi angles: 54.4	0.09Å	-	-
A 64	VAL	50	-	Allowed (0.28%) Isoleucine or valine / -80.6,16.9	40.8% (*t*) chi angles: 184.7	0.158Å	-	-
A 65	HIS	50	-	Favored (19.76%) General / -84.8,111.6	63.6% (*m-70*) chi angles: 285.5,305.1	0.082Å	-	-
A 66	GLY	50	-	Favored (32.51%) Glycine / 108.6,0.7	-	-	-	-
A 67	VAL	50	-	Favored (10.86%) Isoleucine or valine / -50.6,134.5	6.2% (*p*) chi angles: 74.8	0.142Å	-	-
A 68	GLU	50	-	Favored (40.07%) General / -80.9,-22.1	2.1% (*mt-10*) chi angles: 299.6,234.4,297.6	0.096Å	-	-
A 69	ASP	50	-	Favored (44.92%) General / -129.3,129.5	36.6% (*t0*) chi angles: 194.8,336.9	0.022Å	-	-
A 70	MET	50	-	Favored (47.91%) General / -83.5,0.1	54% (*mtm*) chi angles: 299.3,202,285.1	0.169Å	-	-
A 71	ILE	50	-	Favored (46.61%) Isoleucine or valine / -59.8,-31.1	20.7% (*pt*) chi angles: 70,179.1	0.161Å	-	-
A 72	ARG	50	-	Favored (3.55%)	75.1% (*mtp85*) chi angles: 298.3,180.6,70.2,84.5	0.092Å	-	-

# Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 73	LEU	50	-	Favored (43.64%) General / -80.3,11.5	57% (*mt*) chi angles: 298.8,186	0.083Å	-	-
A 74	GLY	50	-	Allowed (0.28%) General / -70.8,152.6	-	-	-	-
A 75	ASP	50	-	Favored (44.94%) Glycine / -74.9,-86.2	43.4% (*p30*) chi angles: 57.3,13.1	0.131Å	-	OUTLIER(worst is CA-CB-CG 4.916 σ
A 76	LEU	50	-	Allowed (1.59%) General / -63.3,149.7	57.7% (*tp*) chi angles: 181.9,63.8	0.051Å	-	-
A 77	ASN	50	-	Favored (11.92%) General / -136.2,76.3	17.3% (*p30*) chi angles: 68.1,68.4	0.054Å	-	-
A 78	GLU	50	-	Favored (70.92%) General / -140.9,173.0	61.4% (*mt-10*) chi angles: 290.4,199,2.7	0.092Å	-	-
A 79	ALA	50	-	Favored (58.53%) General / -57.5,-36.0	-	0.09Å	-	-
# Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 55.75	Clashscore: 1.19	Outliers: 8 of 625	Poor rotamers: 5 of 555	Outliers: 13 of 594	Outliers: 0 of 627	Outliers: (of 627
A 80	GLY	50	-	Favored (4.2%) Glycine / -100.0,-36.4	-	-	-	-
A 81	ILE	50	-	Favored (20.82%) Isoleucine or valine / -80.9,-46.5	20.6% (*tt*) chi angles: 186.8,169.7	0.084Å	-	-

A 82	LEU	50	0.404Å HD11 with A 652 CYS SG	Favored (74.56%) General / -63.7,-32.9	34.4% (*tp*) chi angles: 187.9,64.3	0.057Å	-	-
A 83	ARG	50	-	Favored (67.95%) General / -70.9,-31.4	37.5% (*ttm-85*) chi angles: 191.5,179.5,289.3,254.7	0.138Å	-	-
A 84	ASN	50	-	Favored (51.97%) General / -77.5,-36.8	18.3% (*t30*) chi angles: 197.9,67.6	0.145Å	-	-
A 85	LEU	50	-	Favored (96.13%) General / -64.2,-40.5	97.1% (*mt*) chi angles: 294,173.4	0.132Å	-	-
A 86	LEU	50	-	Favored (76.21%) General / -58.7,-49.8	19.6% (*tp*) chi angles: 165.5,57.9	0.085Å	-	-
A 87	ILE	50	-	Favored (89.52%) Isoleucine or valine / -66.9,-43.1	40.4% (*pt*) chi angles: 62.2,176.3	0.267Å	-	-
A 88	ARG	50	-	Favored (78.62%) General / -62.0,-35.5	77.4% (*mtp85*) chi angles: 287.1,176.1,68.3,85.6	0.129Å	-	-
A 89	TYR	50	-	Favored (94.5%) General / -63.2,-39.4	77.4% (*t80*) chi angles: 184.7,74.8	0.087Å	-	-
A 90	ARG	50	-	Favored (91.41%) General / -59.2,-45.4	76.8% (*mtp85*) chi angles: 294.7,173.7,61.1,80.5	0.096Å	-	-
A 91	ASP	50	-	Favored (58.17%) General / -80.5,-14.5	2% (*m-20*) chi angles: 315.3,349.7	0.079Å	-	-
A 92	HIS	50	-	Allowed (0.1%) General /	78.8% (*m-70*) chi angles: 309.2,284.6	0.182Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
							86.3,18.0		
A 93		LEU	50	-	Favored (9.66%) General / -85.4,78.7	44.1% (*mt*) chi angles: 309,175.5	0.05Å	-	-
A 94		ILE	50	-	Favored (16.35%) Isoleucine or valine / -74.4,-15.5	49.5% (*mm*) chi angles: 301,298.8	0.133Å	-	-
A 95		TYR	50	-	Favored (36.93%) General / -108.7,144.0	69.7% (*m-85*) chi angles: 295.5,292.6	0.101Å	-	-
A 96		THR	50	-	Favored (16.94%) General / -151.7,136.2	26.1% (*m*) chi angles: 308.4	0.078Å	-	-
A 97		TYR	50	-	Favored (30.71%) General / -79.0,152.8	30.2% (*m-85*) chi angles: 295.9,309.1	0.044Å	-	-
A 98		THR	50	-	Allowed (1.86%) General / -138.0,52.2	1.4% (*p*) chi angles: 36.1	0.086Å	-	-
A 99		GLY	50	-	Favored (11.62%) Glycine / 92.5,-133.2	-	-	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.75	Clashscore: 1.19	Outliers: 8 of 625	Poor rotamers: 5 of 555	Outliers: 13 of 594	Outliers: 0 of 627	Outliers: 6 of 627
A 100		SER	50	-	Allowed (0.16%) General / -69.1,12.4	49.7% (*m*) chi angles: 300.9	0.045Å	-	-
A 101		ILE	50	-	Favored (8.68%) Isoleucine or valine / -143.8,170.8	50.5% (*mm*) chi angles: 301.7,300.1	0.089Å	-	-

A 102	LEU	50	-	Favored (46.7%) General / -121.6,146.7	37.6% (*tp*) chi angles: 181.9,70.2	0.104Å	-	-
A 103	VAL	50	-	Favored (19.89%) Isoleucine or valine / -111.5,144.2	88.6% (*t*) chi angles: 177.2	0.054Å	-	-
A 104	ALA	50	-	Favored (10.63%) General / -136.0,113.3	-	0.114Å	-	-
A 105	VAL	50	-	Favored (42.37%) Isoleucine or valine / -90.4,128.3	38.9% (*t*) chi angles: 185.3	0.027Å	-	-
A 106	ASN	50	-	Favored (91.94%) Pre-proline / -64.8,126.9	55.1% (*t-20*) chi angles: 191.8,348.8	0.048Å	-	-
A 107	PRO	50	-	Allowed (0.92%) Trans-proline / -91.1,-19.4	41.2% (*Cg_endo*) chi angles: 36.3	0.038Å	-	-
A 108	TYR	99.99	-	Favored (19.45%) General / 50.0,49.9	11% (*t80*) chi angles: 203,70	0.178Å	-	-
A 109	GLN	50	-	Favored (3.3%) General / -171.5,152.7	5.9% (*pt20*) chi angles: 65.9,164.7,124.9	0.059Å	-	-
A 110	LEU	50	-	Favored (48.95%) General / -72.0,144.1	45% (*tp*) chi angles: 185.3,61.1	0.035Å	-	-
A 111	LEU	50	-	Favored (28.81%) General / -136.3,127.9	82.3% (*mt*) chi angles: 301.8,175.6	0.073Å	-	-
A 112	SER	50	-	Favored (4.96%) General / -79.0,68.3	69% (*p*) chi angles: 57.5	0.05Å	-	-

A 113	ILE	50	-	Favored (2.68%) Isoleucine or valine / -129.1,5.7	1.1% (*pt*) chi angles: 85.2,192.4	0.191Å	-	-
A 114	TYR	50	-	Favored (10.1%) General / -120.0,-4.2	25.1% (*m-85*) chi angles: 313.2,298.1	0.043Å	-	-
A 115	SER	50	-	Favored (98.69%) Pre-proline / -66.7,148.6	42.4% (*t*) chi angles: 181.1	0.1Å	-	-
A 116	PRO	50	-	Favored (38.1%) Trans-proline / -55.3,-23.5	21.1% (*Cg_endo*) chi angles: 19.5	0.181Å	-	-
A 117	GLU	50	0.403Å OE2 with A 118 HIS CE1	Favored (74.93%) General / -63.9,-33.1	6.7% (*pm0*) chi angles: 69.1,294.5,341.4	0.146Å	-	-
A 118	HIS	50	0.403Å CE1 with A 117 GLU OE2	Favored (58.84%) General / -74.5,-23.2	56.1% (*m80*) chi angles: 300,72.7	0.093Å	-	-
A 119	ILE	50	-	Favored (15.27%) Isoleucine or valine / -82.0,-37.8	15.9% (*tt*) chi angles: 190.4,160.2	0.113Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.75	Clashscore: 1.19	Outliers: 8 of 625	Poor rotamers: 5 of 555	Outliers: 13 of 594	Outliers: 0 of 627	Outliers: (of 627
A 120	ARG	50	-		Favored (71.6%) General / -71.1,-35.1	76.1% (*mtp85*) chi angles: 293.9,177.9,63.5,78	0.113Å	-	-
A 121	GLN	50	-		Favored (73.13%) General / -63.5,-31.9	37.5% (*tt0*) chi angles: 171.6,177.6,79.3	0.107Å	-	-

A 122	TYR	50	-	Favored (54.55%) General / -93.3,-2.9	2.7% (*m-30*) chi angles: 299.6,10.2	0.048Å	-	-
A 123	THR	50	-	Favored (56.33%) General / -65.2,136.2	37.3% (*p*) chi angles: 52.9	0.022Å	-	-
A 124	ASN	50	-	Favored (2.8%) General / 75.0,-2.6	11% (*t-20*) chi angles: 191.9,235.2	0.048Å	-	OUTLIER(worst is CA-CB-CG 5.674 σ
A 125	LYS	50	-	Favored (31.39%) General / -87.2,138.6	69.6% (*mmtt*) chi angles: 288.6,298.1,179.7,193.4	0.062Å	-	-
A 126	LYS	50	-	Favored (39.48%) General / -74.0,154.2	55% (*mtpt*) chi angles: 302.8,167.9,69.3,176.4	0.037Å	-	-
A 127	ILE	50	-	Favored (34.92%) Isoleucine or valine / -55.9,-33.5	31% (*mm*) chi angles: 310.9,301.9	0.205Å	-	-
A 128	GLY	50	-	Favored (87.29%) Glycine / -82.6,-7.6	-	-	-	-
A 129	GLU	50	-	Favored (54.72%) General / -87.6,-9.3	41.3% (*mt-10*) chi angles: 299.6,186.6,255.4	0.096Å	-	-
A 130	MET	50	-	Favored (3.12%) Pre-proline / -154.1,175.3	19% (*ptm*) chi angles: 60.6,166.2,299.3	0.113Å	-	-
A 131	PRO	50	-	Favored (13.75%) Trans-proline / -83.7,156.2	57.1% (*Cg_endo*) chi angles: 26.2	0.068Å	-	-
A 132	PRO	50	-	Favored (44.09%) Trans-proline / -51.0,135.2	5.2% (*Cg_exo*) chi angles: 322.1	0.088Å	-	-

A 133	HIS	50	-	Allowed (0.47%) General / -178.8,149.9	34.2% (*t-80*) chi angles: 203.3,293	0.106Å	-	OUTLIER(worst is CA-CB-CG 6.246 σ
A 134	ILE	50	-	Favored (6.37%) Isoleucine or valine / -46.5,-44.3	38.1% (*mm*) chi angles: 295.2,296.5	0.132Å	-	OUTLIER(worst is C-N-CA: 4.109 σ
A 135	PHE	50	-	Favored (91.03%) General / -60.2,-40.7	19.4% (*m-30*) chi angles: 294.2,347.9	0.036Å	-	OUTLIER(worst is CA-CB-CG 6.724 σ
A 136	ALA	50	-	Favored (90.38%) General / -64.5,-38.3	-	0.045Å	-	-
A 137	ILE	50	-	Favored (65.46%) Isoleucine or valine / -69.7,-35.4	10.9% (*tp*) chi angles: 195,64	0.117Å	-	-
A 138	ALA	50	-	Favored (79.77%) General / -68.3,-36.8	-	0.075Å	-	-
A 139	ASP	50	-	Favored (76.98%) General / -68.3,-43.7	5.3% (*t70*) chi angles: 203.4,279.5	0.07Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.75	Clashscore: 1.19	Outliers: 8 of 625	Poor rotamers: 5 of 555	Outliers: 13 of 594	Outliers: 0 of 627	Outliers: 6 of 627
A 140	ASN	50	-		Favored (82.95%) General / -59.0,-48.1	6.6% (*t-20*) chi angles: 184.4,221.5	0.076Å	-	OUTLIER(worst is CA-CB-CG 4.687 σ
A 141	CYS	50	-		Favored (87.4%) General / -67.0,-40.0	14.5% (*p*) chi angles: 75.1	0.208Å	-	-

A 142	TYR	50	-	Favored (91.67%) General / -60.3,-40.8	61% (*t80*) chi angles: 176,65.2	0.064Å	-	-
A 143	PHE	99.99	-	Favored (93.59%) General / -64.9,-39.5	41.1% (*t80*) chi angles: 193.9,77.4	0.074Å	-	-
A 144	ASN	50	-	Favored (55.28%) General / -76.2,-25.7	18.5% (*m120*) chi angles: 286.8,132.7	0.128Å	-	-
A 145	MET	50	-	Favored (88.33%) General / -65.7,-43.8	40.8% (*ttp*) chi angles: 185.2,196.2,73.4	0.029Å	-	-
A 146	LYS	50	-	Favored (71.56%) General / -71.2,-35.5	28.3% (*mmmt*) chi angles: 293.9,306.8,300.2,169.6	0.101Å	-	-
A 147	ARG	50	-	Favored (23.77%) General / -88.7,-21.6	52.2% (*mmm-85*) chi angles: 291.7,299.2,300.3,270.6	0.113Å	-	-
A 148	ASN	50	-	Favored (11.61%) General / -116.7,-5.6	1.6% (*m-20*) chi angles: 313.7,357.1	0.077Å	-	-
A 149	SER	50	-	Favored (24.71%) General / 49.7,45.2	0.4% chi angles: 259.7	0.183Å	-	-
A 150	ARG	50	-	Favored (47.08%) General / -135.2,144.8	58.7% (*ttm-85*) chi angles: 181.9,182.2,288.3,274.1	0.106Å	-	-
A 151	ASP	50	-	Favored (57.35%) General / -62.7,143.5	3% (*m-20*) chi angles: 311.6,256.3	0.032Å	-	-
A 152	GLN	50	-	Favored (10.39%) General / -126.5,172.3	33.3% (*mm-40*) chi angles: 315.5,279,297.3	0.058Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 153		CYS	50	-	Favored (27.02%) General / -150.0,146.4	3.7% (*p*) chi angles: 82.8	0.045Å	-	-
A 154		CYS	50	-	Favored (10.18%) General / -114.6,102.6	22.9% (*m*) chi angles: 280.2	0.056Å	-	-
A 155		ILE	50	-	Favored (21.28%) Isoleucine or valine / -101.7,107.3	2.4% (*tp*) chi angles: 168.6,58.3	0.185Å	-	-
A 156		ILE	50	-	Favored (43.18%) Isoleucine or valine / -101.0,115.7	68.3% (*mt*) chi angles: 302.6,176.3	0.126Å	-	-
A 157		SER	50	-	Favored (4.42%) General / -106.4,178.9	21.2% (*t*) chi angles: 188.3	0.061Å	-	-
A 158		GLY	50	-	Favored (11.48%) Glycine / 121.1,161.7	-	-	-	-
A 159		GLU	50	-	Favored (2.95%) General / -73.2,-178.5	12.7% (*pt-20*) chi angles: 61.4,170.2,118.3	0.14Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.75	Clashscore: 1.19	Outliers: 8 of 625	Poor rotamers: 5 of 555	Outliers: 13 of 594	Outliers: 0 of 627	Outliers: 6 of 627
A 160		SER	50	-	Favored (10.57%) General / -73.9,113.0	9.4% (*t*) chi angles: 192.8	0.044Å	-	-
A 161		GLY	50	-	Favored (57.6%) Glycine / 86.5,19.1	-	-	-	-

A 162	ALA	50	-	Favored (59.4%) General / -80.9,-12.5	-	0.092Å	-	-
A 163	GLY	50	-	Favored (24.6%) Glycine / 113.4,2.1	-	-	-	-
A 164	LYS	50	-	Favored (74.43%) General / -56.0,-41.1	35% (*mtmm*) chi angles: 299.6,182.7,303.7,302.3	0.116Å	-	-
A 165	THR	50	-	Favored (43.9%) General / -52.9,-53.8	5.2% (*m*) chi angles: 284.9	0.074Å	-	-
A 166	GLU	50	-	Favored (68.08%) General / -71.8,-41.7	20.2% (*mm-40*) chi angles: 315.9,313.6,313.2	0.099Å	-	-
A 167	SER	50	-	Favored (90.09%) General / -60.1,-40.6	50% (*m*) chi angles: 301.1	0.086Å	-	-
A 168	THR	50	-	Favored (92.42%) General / -60.8,-46.0	76.6% (*m*) chi angles: 297	0.099Å	-	-
A 169	LYS	50	-	Favored (75.7%) General / -61.5,-34.6	50.1% (*mtmt*) chi angles: 291.6,181.3,295.9,197.1	0.128Å	-	-
A 170	LEU	50	-	Favored (76.99%) General / -67.5,-34.4	48.7% (*mt*) chi angles: 296.8,164.3	0.109Å	-	-
A 171	ILE	99.99	-	Favored (86.98%) Isoleucine or valine / -66.9,-41.0	33.3% (*mt*) chi angles: 296.3,185.9	0.119Å	-	-
A 172	LEU	50	-	Favored (84.96%) General /	92.4% (*mt*) chi angles: 297.9,173	0.087Å	-	-

# Alt	Res		High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
					-58.0,-46.6				
A 173	GLN	50	-		Favored (79.11%) General / -56.1,-46.1	26.5% (*tt0*) chi angles: 186,205.1,1.7	0.03Å	-	-
A 174	PHE	50	-		Favored (68.55%) General / -63.2,-50.9	52.8% (*t80*) chi angles: 190.9,78.2	0.083Å	-	-
A 175	LEU	50	-		Favored (79.6%) General / -67.3,-35.5	45.1% (*mt*) chi angles: 302.8,168.3	0.129Å	-	-
A 176	ALA	50	-		Favored (72.91%) General / -59.8,-34.4	-	0.066Å	-	-
A 177	ALA	50	-		Favored (20.16%) General / -84.9,-37.9	-	0.036Å	-	-
A 178	ILE	50	-		Favored (6.03%) Isoleucine or valine / -86.2,-28.9	17.1% (*tt*) chi angles: 194.1,172.4	0.151Å	-	-
A 179	SER	50	-		Favored (14.44%) General / -109.9,-13.5	23% (*t*) chi angles: 187.6	0.091Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.75	Clashscore: 1.19	Outliers: 8 of 625	Poor rotamers: 5 of 555	Outliers: 13 of 594	Outliers: 0 of 627	Outliers: 6 of 627
A 180	GLY	50	-		Favored (27.65%) Glycine / -61.8,161.7	-	-	-	-
A 181	GLN	99.99	-		Favored (13.2%) General / -117.4,8.9	8.3% (*pt20*) chi angles: 55.6,167.5,29.9	0.099Å	-	-

A 182	HIS	99.99	-	OUTLIER (0.03%) General / 80.1,46.7	12.1% (*t-160*) chi angles: 183.3,217.1	0.186Å	-	-
A 183	SER	99.99	-	Favored (6.06%) General / -84.4,-176.0	1.4% (*m*) chi angles: 322.7	0.133Å	-	OUTLIER(worst is C-N-CA: 9.813 σ
A 184	TRP	50	-	Allowed (0.5%) General / 57.8,-109.9	93% (*m95*) chi angles: 286.7,97.1	0.429Å	-	OUTLIER(worst is CE3-CD2-C 4.793 σ
A 185	ILE	50	-	Allowed (0.18%) Isoleucine or valine / -35.1,-50.0	8.9% (*tp*) chi angles: 184,65.9	0.117Å	-	-
A 186	GLU	50	-	Favored (90.84%) General / -64.3,-38.4	5.3% (*mp0*) chi angles: 305,94.4,45.6	0.172Å	-	-
A 187	GLN	50	-	Favored (86.76%) General / -57.9,-44.2	4.6% (*tp-100*) chi angles: 181.2,69.8,281.5	0.084Å	-	-
A 188	GLN	50	-	Favored (80.53%) General / -61.5,-36.4	97.9% (*mt-30*) chi angles: 295,178.4,322.8	0.106Å	-	-
A 189	VAL	50	-	Favored (46.58%) Isoleucine or valine / -68.9,-30.4	4.4% (*m*) chi angles: 311.8	0.29Å	-	-
A 190	LEU	50	-	Favored (53.09%) General / -73.5,-45.5	5.8% (*mp*) chi angles: 274.6,44.8	0.069Å	-	-
A 191	GLU	50	-	Favored (57.9%) General / -77.6,-8.5	4.5% (*mm-40*) chi angles: 279.1,285.4,64.8	0.136Å	-	-
A 192	ALA	50	-	Favored (76.09%)	-	0.067Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 193		THR	50	-	Favored (7.18%) General / -60.9,-35.2	40.2% (*p*) chi angles: 67.8	0.351Å	-	-
A 194		PRO	50	-	Favored (31.22%) Pre-proline / -68.1,-35.3	92.5% (*Cg_exo*) chi angles: 329.1	0.074Å	-	-
A 195		ILE	50	-	Favored (83.14%) Trans-proline / -64.2,-39.3	15.1% (*tt*) chi angles: 186.4,159.4	0.151Å	-	-
A 196		LEU	50	-	Favored (75.62%) Isoleucine or valine / -68.5,-44.4	71.4% (*mt*) chi angles: 291.8,180.6	0.055Å	-	-
A 197		GLU	50	-	Favored (49.38%) General / -56.8,-40.2	68.4% (*mt-10*) chi angles: 294.2,187.9,22.5	0.132Å	-	-
A 198		ALA	50	-	Favored (10.06%) General / -93.0,-6.0	-	0.065Å	-	-
A 199		PHE	50	-	Favored (30.78%) General / -90.2,-44.0	71.8% (*m-85*) chi angles: 292,79.9	0.119Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.75	Clashscore: 1.19	Outliers: 8 of 625	Poor rotamers: 5 of 555	Outliers: 13 of 594	Outliers: 0 of 627	Outliers: 6 of 627
A 200		GLY	50	-	Favored (12.62%) General / -84.4,-21.4 Glycine / -120.2,3.8	-	-	-	-
A 201		ASN	50	0.473Å OD1 with A 211 SER HA	Favored (33.73%) General / -124.0,157.8	97% (*m-20*) chi angles: 291.2,343.2	0.066Å	-	OUTLIER(worst is CA-CB-CG 7.96 σ

A 202	ALA	50	-	Favored (33.24%) General / -154.9,166.5	-	0.105Å	-	-
A 203	LYS	50	-	Favored (15.47%) General / -79.3,111.3	66% (*tttt*) chi angles: 178.9,199,179.9,193.8	0.036Å	-	-
A 204	THR	50	-	Favored (11.05%) General / -97.7,167.3	74.5% (*p*) chi angles: 58.1	0.084Å	-	-
A 205	ILE	50	-	Favored (28.86%) Isoleucine or valine / -56.8,-28.8	89.6% (*mt*) chi angles: 295.4,166.2	0.209Å	-	-
A 206	ARG	50	-	Favored (35.29%) General / -89.6,-14.2	85.7% (*mtt-85*) chi angles: 288.5,174.6,171.1,281.1	0.139Å	-	-
A 207	ASN	50	-	Allowed (0.21%) General / -176.2,127.6	66.3% (*t30*) chi angles: 191.7,30.6	0.093Å	-	-
A 208	ASP	50	-	Favored (2.38%) General / -42.4,-58.0	13.2% (*t0*) chi angles: 172,30.4	0.046Å	-	-
A 209	ASN	50	-	Allowed (1.14%) General / -97.7,53.8	46.5% (*t30*) chi angles: 203.3,37.2	0.131Å	-	-
A 210	SER	50	-	Favored (37.41%) General / -78.6,136.1	21.8% (*t*) chi angles: 188.1	0.064Å	-	-
A 211	SER	50	0.473Å HA with A 201 ASN OD1	Favored (34.6%) General / -84.1,134.1	47.3% (*m*) chi angles: 289.4	0.073Å	-	-
A 212	ARG	50	-	Favored (10.99%) General /	17.1% (*mmm180*) chi angles: 321.3,308.7,307.8,155.2	0.147Å	-	-

# Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
				-119.8,1.2				
A 213	PHE	50	-	Favored (39.52%) General / -122.7,153.4	5% (*p90*) chi angles: 80.7,292.3	0.083Å	-	-
A 214	GLY	50	-	Favored (23.48%) Glycine / -95.3,162.0	-	-	-	-
A 215	LYS	50	-	Favored (18.56%) General / -157.9,145.6	17.1% (*pttm*) chi angles: 63.1,184.2,186.6,268	0.056Å	-	-
A 216	TYR	50	-	Favored (23.18%) General / -126.1,117.5	79.5% (*t80*) chi angles: 177,85.5	0.102Å	-	-
A 217	ILE	50	-	Favored (59.32%) Isoleucine or valine / -117.2,134.9	23.9% (*pt*) chi angles: 56.7,180.8	0.123Å	-	-
A 218	ASP	50	-	Favored (28.29%) General / -103.4,114.2	16.2% (*m-20*) chi angles: 286.6,284.3	0.043Å	-	-
A 219	ILE	50	-	Favored (37.08%) Isoleucine or valine / -81.9,129.7	46.6% (*mm*) chi angles: 301.2,303.8	0.163Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.75	Clashscore: 1.19	Outliers: 8 of 625	Poor rotamers: 5 of 555	Outliers: 13 of 594	Outliers: 0 of 627	Outliers: 6 of 627
A 220		HIS	50	-	Favored (46.48%) General / -100.4,130.1	56.4% (*m170*) chi angles: 292.6,176.5	0.067Å	-	-
A 221		PHE	50	-	Favored (26.71%) General / -118.0,157.5	53.9% (*m-85*) chi angles: 307.3,92	0.094Å	-	-

A 222	ASN	50	-	Favored (5.04%) General / -100.7,177.3	24.9% (*p30*) chi angles: 60.6,55.9	0.124Å	-	-
A 223	LYS	50	-	Favored (72.61%) General / -62.4,-31.9	31% (*mmmt*) chi angles: 293.5,301.8,301.2,181.5	0.19Å	-	-
A 224	ARG	50	-	Favored (83.48%) General / -66.0,-44.9	60.1% (*ttm-85*) chi angles: 179.5,174.8,291.5,280.5	0.128Å	-	-
A 225	GLY	50	-	Favored (3.68%) Glycine / 137.5,-14.6	-	-	-	-
A 226	ALA	50	-	Favored (20.76%) General / -71.4,166.9	-	0.022Å	-	-
A 227	ILE	50	-	Favored (4.35%) Isoleucine or valine / -77.1,162.1	30.5% (*mt*) chi angles: 311.3,169.5	0.209Å	-	-
A 228	GLU	50	-	Allowed (1.35%) General / -139.9,-5.0	2% (*pt-20*) chi angles: 44.6,157.1,83.2	0.084Å	-	-
A 229	GLY	50	-	Favored (26.73%) Glycine / 155.3,-156.1	-	-	-	-
A 230	ALA	50	-	Favored (18.95%) General / -163.1,155.9	-	0.147Å	-	-
A 231	LYS	50	-	Favored (24.67%) General / -134.3,123.7	27% (*tptp*) chi angles: 176.4,69.9,185.1,65.6	0.088Å	-	-
A 232	ILE	50	-	Favored (47.09%) Isoleucine or	43% (*pt*) chi angles: 64.8,171.2	0.107Å	-	OUTLIER(worst is C-N-CA: 4.382 σ

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
					valine / -98.6,130.7				
A 233		GLU	50	-	Favored (10.37%) General / -104.2,100.6	22.8% (*tt0*) chi angles: 187.8,204.9,9.2	0.084Å	-	-
A 234		GLN	99.99	-	Favored (33.09%) General / -90.8,136.4	7.3% (*pm0*) chi angles: 85.3,291.5,10.8	0.046Å	-	-
A 235		TYR	50	-	Favored (7.59%) General / -101.2,171.5	24.6% (*m-85*) chi angles: 309,304.3	0.034Å	-	-
A 236		LEU	50	-	Allowed (1.73%) General / -43.9,141.1	85.2% (*mt*) chi angles: 298.6,171.9	0.036Å	-	-
A 237		LEU	50	-	Favored (26.18%) General / -101.7,147.7	17% (*tp*) chi angles: 177.8,77.6	0.137Å	-	-
A 238		GLU	50	-	Favored (3.93%) General / -77.4,80.4	38.6% (*tt0*) chi angles: 187.8,190.6,40.6	0.07Å	-	-
A 239		LYS	50	-	Favored (74.15%) General / -62.8,-32.9	38% (*mtmt*) chi angles: 312,186.7,303.6,175	0.115Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.75	Clashscore: 1.19	Outliers: 8 of 625	Poor rotamers: 5 of 555	Outliers: 13 of 594	Outliers: 0 of 627	Outliers: 6 of 627
A 240		SER	50	-	Favored (69.84%) General / -58.1,-34.1	23.3% (*p*) chi angles: 50.9	0.078Å	-	-
A 241		ARG	50	-	Favored (63.89%) General / -57.3,-29.4	52.5% (*ttm-85*) chi angles: 180.7,163.7,300.6,279.9	0.156Å	-	-

A 242	VAL	50	-	Favored (93.32%) Isoleucine or valine / -63.2,-41.6	17.9% (*t*) chi angles: 189.4	0.089Å	-	-
A 243	CYS	50	-	Favored (22.02%) General / -91.2,-20.4	18% (*p*) chi angles: 71.4	0.17Å	-	-
A 244	ARG	50	-	Favored (15.19%) General / -155.6,138.4	62% (*ttm-85*) chi angles: 185,178.6,294.7,270.6	0.096Å	-	-
A 245	GLN	50	-	Favored (5.8%) General / -117.1,175.0	6.3% (*mp0*) chi angles: 303.3,89.4,65.7	0.052Å	-	-
A 246	ALA	50	-	Favored (15.39%) General / -107.4,160.8	-	0.046Å	-	-
A 247	LEU	50	-	Favored (40.5%) General / -54.0,131.6	8% (*tt*) chi angles: 189.3,144.4	0.049Å	-	OUTLIER(worst is C-N-CA: 4.586 σ
A 248	ASP	50	-	OUTLIER (0.03%) General / 89.5,-33.7	36.1% (*t70*) chi angles: 181.5,69	0.175Å	-	-
A 249	GLU	50	-	Favored (37.39%) General / -75.9,151.2	34% (*mt-10*) chi angles: 303.6,200.2,318.7	0.037Å	-	-
A 250	ARG	50	-	Favored (13.88%) General / -102.1,161.2	28.9% (*mtm180*) chi angles: 293.3,212.5,299.4,180.3	0.059Å	-	-
A 251	ASN	50	-	Allowed (1.31%) General / -69.7,-177.8	12.5% (*t-20*) chi angles: 206.1,330.3	0.098Å	-	-
A 252	TYR	50	-	Favored (26.89%) General / -54.4,142.4	79.2% (*m-85*) chi angles: 288.8,278.6	0.026Å	-	-

# Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 253	HIS	50	-	Favored (69.01%) General / -55.2,-38.9	40% (*m-70*) chi angles: 306.9,313.1	0.166Å	-	OUTLIER(worst is CA-CB-CG 5.212 σ
A 254	VAL	50	-	Favored (2.07%) Isoleucine or valine / -44.7,-41.1	1.9% (*m*) chi angles: 278.8	0.218Å	-	-
A 255	PHE	50	-	Favored (95.74%) General / -64.1,-40.2	64% (*m-85*) chi angles: 300.7,294.1	0.092Å	-	-
A 256	TYR	50	-	Favored (67.11%) General / -72.0,-41.8	50.8% (*m-85*) chi angles: 308.9,277.7	0.131Å	-	-
A 257	CYS	50	-	Favored (72.94%) General / -58.7,-35.6	41.4% (*m*) chi angles: 307.4	0.099Å	-	-
A 258	MET	50	-	Favored (55.27%) General / -76.0,-25.1	48.1% (*tpp*) chi angles: 196,59.3,71	0.042Å	-	-
A 259	LEU	50	-	Favored (16.21%) General / -96.2,-24.5	53.1% (*mt*) chi angles: 305.5,172.6	0.087Å	-	-

# Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 55.75	Clashscore: 1.19	Outliers: 8 of 625	Poor rotamers: 5 of 555	Outliers: 13 of 594	Outliers: 0 of 627	Outliers: 6 of 627
A 260	GLU	50	-	Favored (13.41%) General / -95.1,-31.7	16.1% (*tp10*) chi angles: 172.8,44,36.7	0.093Å	-	-
A 261	GLY	50	-	Favored (18.39%) Glycine / -115.3,14.5	-	-	-	-

A 262	MET	50	-	Favored (25.04%) General / -87.1,148.9	55.6% (*ttm*) chi angles: 186.5,172.9,291.3	0.053Å	-	-
A 263	SER	50	-	Favored (47.66%) General / -70.9,148.6	4.7% (*t*) chi angles: 200.2	0.062Å	-	OUTLIER(worst is C-N-CA: 5.282 σ
A 264	GLU	50	-	OUTLIER (0.01%) General / -27.3,-78.5	2.4% (*pt-20*) chi angles: 47.7,215.6,66.9	0.118Å	-	-
A 265	ASP	99.99	-	Favored (48.74%) General / -86.2,2.0	33.7% (*m-20*) chi angles: 276.7,7.8	0.232Å	-	-
A 266	GLN	50	-	Favored (75.99%) General / -70.0,-38.2	53.1% (*tt0*) chi angles: 189.6,186.4,346.5	0.165Å	-	-
A 267	LYS	50	-	Favored (78.48%) General / -68.6,-36.4	41.6% (*mtpt*) chi angles: 301.8,193.9,72.7,170.4	0.174Å	-	-
A 268	LYS	50	-	Favored (93.58%) General / -64.3,-39.3	27.4% (*tptp*) chi angles: 186.7,65,182.4,59.5	0.051Å	-	-
A 269	LYS	50	-	Favored (68.66%) General / -71.7,-33.4	8.9% (*tptp*) chi angles: 179.6,63.7,217.7,59.9	0.077Å	-	-
A 270	LEU	50	-	Favored (29.73%) General / -98.3,-7.1	46.5% (*mt*) chi angles: 309.1,179.4	0.147Å	-	-
A 271	GLY	50	-	Favored (44.63%) Glycine / 76.2,35.1	-	-	-	-
A 272	LEU	50	-	Favored (49.06%) General / -103.6,124.6	85% (*mt*) chi angles: 301.5,176.2	0.037Å	-	-

# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 273	GLY 50	-	Favored (2.82%) Glycine / -83.5,-136.2	-	-	-	-
A 274	GLN 50	-	Allowed (1.53%) General / -107.3,-169.4	18.6% (*pt20*) chi angles: 67.7,185.9,57.2	0.149Å	-	-
A 275	ALA 50	-	Favored (30.96%) General / -84.1,-22.9	-	0.124Å	-	-
A 276	SER 50	-	Favored (94.08%) General / -63.2,-39.2	5.3% (*p*) chi angles: 43.2	0.064Å	-	OUTLIER(worst is C-N-CA: 4.929 σ
A 277	ASP 50	-	Allowed (0.18%) General / -66.3,9.0	0.3% chi angles: 322.5,348.4	0.078Å	-	OUTLIER(worst is CA-CB-CG 5.439 σ
A 278	TYR 50	0.431Å CD1 with A 326 LEU HB3	Favored (31.02%) General / -136.6,129.5	59.3% (*m-85*) chi angles: 290.8,294.8	0.064Å	-	-
A 279	ASN 50	-	Favored (70.39%) General / -58.8,-33.5	87.1% (*m-20*) chi angles: 296.3,331.6	0.079Å	-	-
# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
	Avg: 55.75	Clashscore: 1.19	Outliers: 8 of 625	Poor rotamers: 5 of 555	Outliers: 13 of 594	Outliers: 0 of 627	Outliers: (of 627
A 280	TYR 50	-	Favored (56.66%) General / -77.2,-7.9	22.4% (*m-30*) chi angles: 295.8,332.5	0.074Å	-	-
A 281	LEU 50	-	Favored (6.23%) General / -120.7,-22.6	23.8% (*mt*) chi angles: 313.4,175.6	0.12Å	-	-
A 282	ALA 50	-	Favored (27.02%)	-	0.039Å	-	-

A 283	MET	50	-	General / -83.3,-31.1 Favored (64.32%) General / -57.2,-30.2	14.9% (*ptp*) chi angles: 81.1,173.1,75.8	0.21Å	-	-
A 284	GLY	50	-	Favored (78.37%) Glycine / -82.8,-13.3	-	-	-	-
A 285	ASN	50	-	Allowed (0.05%) General / 84.9,-35.4	20.6% (*t-20*) chi angles: 185.5,251.2	0.156Å	-	-
A 286	CYS	50	-	Favored (25.45%) General / -102.0,112.7	53.6% (*t*) chi angles: 180.4	0.037Å	-	-
A 287	ILE	50	-	Favored (7.6%) Isoleucine or valine / -95.6,-15.5	59.8% (*mt*) chi angles: 306.2,173	0.214Å	-	-
A 288	THR	50	-	Allowed (0.89%) General / -118.0,-162.7	30.4% (*p*) chi angles: 51.3	0.113Å	-	-
A 289	CYS	50	-	Favored (2.82%) General / -171.4,150.1	1.7% (*p*) chi angles: 40.2	0.062Å	-	-
A 290	GLU	50	-	Favored (45.06%) General / -59.1,130.0	22.3% (*pt-20*) chi angles: 68.9,170.6,21.2	0.088Å	-	-
A 291	GLY	50	-	Favored (76.45%) Glycine / 72.5,11.3	-	-	-	-
A 292	ARG	50	-	Favored (51.15%) General / -121.4,127.4	60.2% (*ttm-85*) chi angles: 188.5,179.1,302.5,282.9	0.09Å	-	-
A 293	VAL	50	-	Favored (7.91%)	61.3% (*t*) chi angles: 180.1	0.049Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
					Isoleucine or valine / -109.9,99.1				
A 294		ASP	50	-	Favored (24.19%) General / -55.8,-22.5	16% (*m-20*) chi angles: 302.2,276.9	0.238Å	-	-
A 295		SER	50	-	Favored (71.81%) General / -68.1,-46.1	23.7% (*p*) chi angles: 51	0.104Å	-	-
A 296		GLN	50	-	Favored (90.29%) General / -59.7,-41.2	95.9% (*mt-30*) chi angles: 293.8,180.6,341.3	0.073Å	-	-
A 297		GLU	50	0.451Å O with A 301 ILE HG23	Favored (85.59%) General / -59.1,-47.4	12.5% (*mm-40*) chi angles: 297.4,294.5,268.4	0.113Å	-	-
A 298		TYR	50	-	Favored (82.97%) General / -58.3,-40.8	28.4% (*t80*) chi angles: 188.9,56	0.06Å	-	-
A 299		ALA	50	-	Favored (98.3%) General / -63.3,-40.8	-	0.07Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.75	Clashscore: 1.19	Outliers: 8 of 625	Poor rotamers: 5 of 555	Outliers: 13 of 594	Outliers: 0 of 627	Outliers: 6 of 627
A 300		ASN	50	-	Favored (98.82%) General / -61.9,-43.5	25.4% (*t-20*) chi angles: 180.2,252.3	0.056Å	-	-
A 301		ILE	50	0.451Å HG23 with A 297 GLU O	Favored (96.14%) Isoleucine or valine / -63.5,-46.1	4.4% (*tp*) chi angles: 174.3,71	0.095Å	-	-
A 302		ARG	50	-	Favored (79.72%) General /	36.8% (*mtm180*) chi angles: 291.7,202.2,281.4,192.7	0.205Å	-	-

				-68.0,-36.3			
A 303	SER	50	-	Favored (95.46%) General / -61.1,-45.3	74.4% (*m*) chi angles: 295	0.067Å	-	-
A 304	ALA	50	-	Favored (94.78%) General / -60.0,-44.0	-	0.069Å	-	-
A 305	MET	50	-	Favored (85.52%) General / -57.7,-44.1	62.1% (*mtt*) chi angles: 286.8,175,179	0.077Å	-	-
A 306	LYS	50	-	Favored (84.64%) General / -66.7,-37.4	29.2% (*mtpp*) chi angles: 294.6,175.8,64.8,57.6	0.12Å	-	-
A 307	VAL	50	-	Favored (13.69%) Isoleucine or valine / -78.0,-21.6	23.3% (*m*) chi angles: 302.5	0.187Å	-	-
A 308	LEU	50	-	Favored (54.3%) General / -81.3,-15.8	72.2% (*mt*) chi angles: 298.9,169.6	0.098Å	-	-
A 309	MET	50	-	OUTLIER (0.03%) General / 89.7,23.6	39.7% (*tpp*) chi angles: 199.8,58.7,67.7	0.181Å	-	-
A 310	PHE	50	-	Favored (29.42%) General / -72.8,126.2	78.2% (*m-85*) chi angles: 290,282.4	0.087Å	-	-
A 311	THR	50	-	Favored (25.9%) General / -68.8,162.7	81% (*p*) chi angles: 61.2	0.096Å	-	-
A 312	ASP	50	-	Favored (98.24%) General / -62.6,-40.9	23.6% (*t0*) chi angles: 196.7,34.8	0.107Å	-	-
A 313	THR	50	-	Favored (69.5%)	5.1% (*p*) chi angles: 41.7	0.142Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 314		GLU	50	-	Favored (85.59%) General / -53.5,-45.0	72.9% (*mt-10*) chi angles: 291.3,179.7,316.2	0.095Å	-	-
A 315		ASN	50	-	Favored (95.64%) General / -66.1,-37.4	6.2% (*m120*) chi angles: 311,149.7	0.118Å	-	OUTLIER(worst is CA-CB-CG 5.543 σ
A 316		TRP	50	-	Favored (77.07%) General / -61.1,-40.9	19.2% (*m0*) chi angles: 304.8,3.8	0.12Å	-	OUTLIER(worst is CE3-CD2-C(4.446 σ
A 317		GLU	99.99	-	Favored (80.5%) General / -67.7,-44.6	42.8% (*mt-10*) chi angles: 284.3,198.2,325.9	0.214Å	-	-
A 318		ILE	50	-	Favored (81.97%) Isoleucine or valine / -66.7,-35.6	14.9% (*mt*) chi angles: 309.6,155.3	0.229Å	-	-
A 319		SER	50	-	Favored (81.54%) General / -65.8,-38.3	49.4% (*m*) chi angles: 300.8	0.099Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.75	Clashscore: 1.19	Outliers: 8 of 625	Poor rotamers: 5 of 555	Outliers: 13 of 594	Outliers: 0 of 627	Outliers: 6 of 627
A 320		LYS	50	-	Favored (74.53%) General / -64.7,-35.6	97.3% (*mttt*) chi angles: 297.2,180.1,185.9,180.7	0.117Å	-	-
A 321		LEU	50	-	Favored (72.41%) General / -55.1,-44.2	8.5% (*mp*) chi angles: 279.5,73.9	0.124Å	-	-
A 322		LEU	50	-	Favored (92.53%) General / -65.1,-48.8	84.6% (*mt*) chi angles: 297.5,170.7	0.119Å	-	-

A 323	ALA	50	-	Favored (93.56%) General / -65.4,-41.7	-	0.019Å	-	-
A 324	ALA	50	-	Favored (67.87%) General / -72.0,-33.3	-	0.134Å	-	-
A 325	ILE	50	-	Favored (72.59%) Isoleucine or valine / -65.0,-34.7	50.1% (*mt*) chi angles: 305.1,179.9	0.236Å	-	-
A 326	LEU	50	0.431Å HB3 with A 278 TYR CD1	Favored (93.04%) General / -65.6,-41.1	81.7% (*mt*) chi angles: 303.2,177.3	0.079Å	-	-
A 327	HIS	50	-	Favored (85.52%) General / -64.6,-36.8	70.9% (*m-70*) chi angles: 302.2,307.7	0.16Å	-	-
A 328	LEU	50	-	Favored (91.22%) General / -63.7,-38.5	83.3% (*mt*) chi angles: 293.2,167.7	0.108Å	-	-
A 329	GLY	50	-	Favored (73.72%) Glycine / -67.7,-22.7	-	-	-	-
A 330	ASN	50	-	Favored (8.77%) General / -92.2,18.0	37.2% (*m-20*) chi angles: 295.6,2.5	0.059Å	-	-
A 331	LEU	50	-	Favored (30.23%) General / -78.0,126.0	48.7% (*mt*) chi angles: 289.3,162.6	0.062Å	-	-
A 332	GLN	50	-	Favored (51.26%) General / -116.0,138.4	36.1% (*mt-30*) chi angles: 299.4,177.1,241	0.081Å	-	-
A 333	TYR	50	-	Favored (12.31%) General /	72.5% (*m-85*) chi angles: 298,291.8	0.047Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
					-125.2,109.0				
A 334		GLU	50	-	Favored (11.91%) General / -92.7,167.4	17.7% (*mp0*) chi angles: 309.9,77.6,33.4	0.055Å	-	-
A 335		ALA	50	-	Favored (28.46%) General / -83.5,146.3	-	0.039Å	-	-
A 336		ARG	99.99	-	Favored (2.6%) General / -82.2,-169.8	69.2% (*mtt-85*) chi angles: 292.9,198.2,171.7,261.9	0.052Å	-	-
A 337		THR	50	-	Favored (26.75%) General / -49.2,-38.5	25.5% (*p*) chi angles: 50.4	0.052Å	-	-
A 338		PHE	99.99	-	Favored (16.72%) General / -90.8,104.1	63.9% (*m-85*) chi angles: 303.6,291.4	0.034Å	-	-
A 339		GLU	99.99	-	Favored (17.54%) General / -97.7,-20.6	86.5% (*tt0*) chi angles: 186.2,173.6,4.8	0.065Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.75	Clashscore: 1.19	Outliers: 8 of 625	Poor rotamers: 5 of 555	Outliers: 13 of 594	Outliers: 0 of 627	Outliers: 6 of 627
A 340		ASN	99.99	-	Favored (7.84%) General / -101.9,-38.3	10.5% (*p30*) chi angles: 44.2,44.5	0.103Å	-	-
A 341		LEU	99.99	-	Favored (6.82%) General / -88.5,83.8	8.2% (*tt*) chi angles: 191.5,157.2	0.09Å	-	-
A 342		ASP	99.99	-	Allowed (0.16%) General / 58.7,-103.0	61.4% (*m-20*) chi angles: 297.7,301	0.307Å	-	OUTLIER(worst is C-N-CA: 7.221 σ
A 343		ALA	50	-	Favored (41.21%)	-	0.101Å	-	-

A 344	CYS	50	-	General / -129.7,127.8 Favored (7.47%) General / -100.4,171.9	15.3% (*p*) chi angles: 73.9	0.082Å	-	-
A 345	GLU	50	-	Favored (5.66%) General / -141.2,-178.6	13.1% (*pt-20*) chi angles: 51.8,185.4,41.1	0.086Å	-	-
A 346	VAL	50	-	Allowed (0.33%) Isoleucine or valine / -139.9,79.8	3.4% (*p*) chi angles: 52	0.115Å	-	-
A 347	LEU	50	-	Favored (82.06%) General / -62.6,-47.8	48.9% (*mt*) chi angles: 292.3,162.5	0.066Å	-	-
A 348	PHE	99.99	-	Favored (5.38%) General / -92.0,77.8	89.9% (*m-85*) chi angles: 296.7,284.5	0.155Å	-	OUTLIER(worst is CA-CB-CG 5.806 σ
A 349	SER	50	-	OUTLIER (0.02%) Pre-proline / -71.4,5.9	7.2% (*m*) chi angles: 280.8	0.146Å	-	OUTLIER(worst is CA-C-N: 4.923 σ
A 350	PRO	99.99	-	Favored (92.22%) Trans-proline / -60.9,-32.2	28.7% (*Cg_exo*) chi angles: 325	0.075Å	-	-
A 351	SER	50	-	Favored (73.84%) General / -70.6,-38.1	22.9% (*p*) chi angles: 50.8	0.118Å	-	-
A 352	LEU	50	-	Favored (75.7%) General / -59.9,-50.0	14.7% (*tp*) chi angles: 188.7,78.3	0.034Å	-	-
A 353	ALA	50	-	Favored (91.39%) General / -65.7,-42.3	-	0.079Å	-	-

A 354	THR	50	-	Favored (84.04%) General / -67.0,-37.4	23.4% (*p*) chi angles: 49.7	0.203Å	-	-
A 355	ALA	50	-	Favored (78.93%) General / -66.6,-45.5	-	0.079Å	-	-
A 356	ALA	50	-	Favored (52.35%) General / -77.7,-34.9	-	0.086Å	-	-
A 357	SER	50	-	Favored (88.19%) General / -58.7,-42.3	28.8% (*t*) chi angles: 185.2	0.041Å	-	-
A 358	LEU	50	-	Favored (24.12%) General / -87.0,-25.8	11% (*tp*) chi angles: 200.3,48.1	0.087Å	-	-
A 359	LEU	99.99	-	Favored (58.88%) General / -79.8,-7.8	81% (*mt*) chi angles: 294.1,167.8	0.136Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.75	Clashscore: 1.19	Outliers: 8 of 625	Poor rotamers: 5 of 555	Outliers: 13 of 594	Outliers: 0 of 627	Outliers: 6 of 627
A 360		GLU	50	-	Allowed (1.62%) General / 69.1,40.1	54.1% (*mm-40*) chi angles: 299.3,280.6,356.8	0.138Å	-	OUTLIER(worst is CB-CG-CD 4.121 σ
A 361		VAL	50	0.496Å HB with A 580 LEU HD21	Allowed (0.17%) Isoleucine or valine / -120.0,-157.4	33.7% (*m*) chi angles: 299.4	0.186Å	-	-
A 362		ASN	50	-	Favored (39.21%) Pre-proline / -112.5,121.3	21% (*t-20*) chi angles: 183.8,287.4	0.116Å	-	-

A 363	PRO	50	-	Favored (3.73%) Trans-proline / -71.5,-39.4	8.5% (*Cg_endo*) chi angles: 10.4	0.241Å	-	-
A 364	PRO	50	-	Favored (71.61%) Trans-proline / -60.2,-39.1	5.9% (*Cg_exo*) chi angles: 322.2	0.056Å	-	-
A 365	ASP	50	-	Favored (99.63%) General / -61.7,-43.0	57.1% (*t0*) chi angles: 176.7,358	0.113Å	-	OUTLIER(worst is CA-CB-CG 5.552 σ
A 366	LEU	50	-	Favored (78.95%) General / -57.5,-40.5	33.1% (*tp*) chi angles: 186.4,56.3	0.14Å	-	-
A 367	MET	50	-	Favored (45.47%) General / -59.1,-54.6	66.8% (*ttp*) chi angles: 178.8,176.9,70.1	0.041Å	-	-
A 368	SER	50	-	Favored (99.12%) General / -63.2,-41.3	58.9% (*m*) chi angles: 299.3	0.089Å	-	-
A 369	CYS	50	-	Favored (59.96%) General / -75.5,-17.8	23.6% (*p*) chi angles: 56.3	0.167Å	-	-
A 370	LEU	50	-	Favored (17.6%) General / -82.9,-42.5	55.3% (*mt*) chi angles: 295.3,164.5	0.107Å	-	-
A 371	THR	50	-	Favored (7.42%) General / -106.0,-34.9	57.7% (*p*) chi angles: 65.2	0.069Å	-	-
A 372	SER	50	-	Allowed (1.64%) General / -134.8,62.5	15.7% (*m*) chi angles: 308.2	0.087Å	-	-
A 373	ARG	99.99	0.465Å HD3 with A 574 HIS HB3	Favored (26.42%) General / -102.0,147.6	46.4% (*ttp85*) chi angles: 186.3,193.6,63.1,101	0.141Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 374		THR	50	-	Favored (31.23%) General / -76.8,158.0	31.7% (*p*) chi angles: 69.4	0.129Å	-	-
A 375		LEU	50	-	Favored (13.17%) General / -157.9,138.8	60.6% (*tp*) chi angles: 174.2,62	0.107Å	-	-
A 376		ILE	50	-	Favored (28.54%) Isoleucine or valine / -69.1,126.1	42.7% (*mm*) chi angles: 297.4,296.2	0.123Å	-	-
A 377		THR	50	-	Favored (4.51%) General / -113.3,93.7	74.3% (*m*) chi angles: 303.1	0.077Å	-	-
A 378		ARG	50	-	OUTLIER (0.04%) General / 74.7,-78.6	43.9% (*ttm-85*) chi angles: 173.7,195.9,294.9,272.3	0.192Å	-	-
A 379		GLY	50	-	Allowed (1.21%) Glycine / -148.7,14.7	-	-	-	OUTLIER(worst is C-N-CA: 4.538 σ

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.75	Clashscore: 1.19	Outliers: 8 of 625	Poor rotamers: 5 of 555	Outliers: 13 of 594	Outliers: 0 of 627	Outliers: 6 of 627
A 380		GLU	99.99	-	Favored (34.57%) General / -107.8,144.8	19.4% (*tt0*) chi angles: 170.5,198.7,54.8	0.178Å	-	-
A 381		THR	99.99	-	Allowed (1.96%) General / -103.8,82.0	59.2% (*m*) chi angles: 304.1	0.064Å	-	-
A 382		VAL	50	-	Favored (16.44%) Isoleucine or valine / -85.5,140.1	96.6% (*t*) chi angles: 176.1	0.034Å	-	-

A 383	SER	50	-	Favored (12.24%) General / -89.6,99.2	42.5% (*t*) chi angles: 177.8	0.031Å	-	-
A 384	THR	50	-	Favored (18.98%) Pre-proline / -71.8,113.3	64.7% (*p*) chi angles: 62.2	0.063Å	-	-
A 385	PRO	50	-	Favored (43.71%) Trans-proline / -74.8,154.4	47.1% (*Cg_endo*) chi angles: 35.4	0.07Å	-	-
A 386	LEU	50	-	Favored (52.23%) General / -129.0,139.0	83.7% (*mt*) chi angles: 301.2,175.4	0.102Å	-	-
A 387	SER	50	-	Favored (18.87%) General / -67.8,164.7	78.5% (*p*) chi angles: 70.2	0.067Å	-	-
A 388	ARG	50	-	Favored (44.67%) General / -49.7,-42.2	32.1% (*ptt-85*) chi angles: 58.4,187.1,176.8,267.4	0.166Å	-	-
A 389	GLU	50	-	Favored (73.46%) General / -70.5,-40.5	45.8% (*tt0*) chi angles: 191.7,173.6,321.4	0.042Å	-	-
A 390	GLN	50	-	Favored (82.92%) General / -64.7,-36.0	52.2% (*mt-30*) chi angles: 301.5,167.8,280	0.08Å	-	-
A 391	ALA	50	-	Favored (87.51%) General / -66.6,-38.7	-	0.059Å	-	-
A 392	LEU	99.99	-	Favored (93.1%) General / -61.9,-45.6	35.6% (*mt*) chi angles: 291.7,160	0.149Å	-	-
A 393	ASP	50	-	Favored (44.9%) General / -78.8,-24.2	21.7% (*t70*) chi angles: 197.8,52.9	0.317Å	-	OUTLIER(worst is CB-CA-N: 5.005 σ

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 394		VAL	50	-	Favored (97.63%) Isoleucine or valine / -63.9,-43.0	13.6% (*p*) chi angles: 62.9	0.284Å	-	OUTLIER(worst is CB-CA-N: 4.918 σ
A 395		ARG	50	-	Favored (74.37%) General / -57.6,-50.1	5.1% (*tmm_?*) chi angles: 183.7,284.5,307.8,293.8	0.104Å	-	-
A 396		ASP	50	-	Favored (90.87%) General / -58.8,-44.1	10.4% (*m-20*) chi angles: 294.1,16.4	0.132Å	-	-
A 397		ALA	50	-	Favored (96.77%) General / -63.8,-40.5	-	0.107Å	-	-
A 398		PHE	50	0.553Å O with A 402 ILE HG23	Favored (78.1%) General / -62.3,-48.8	19.5% (*t80*) chi angles: 179.3,46.4	0.112Å	-	-
A 399		VAL	50	-	Favored (82.18%) Isoleucine or valine / -59.7,-40.4	24.2% (*t*) chi angles: 163.6	0.132Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.75	Clashscore: 1.19	Outliers: 8 of 625	Poor rotamers: 5 of 555	Outliers: 13 of 594	Outliers: 0 of 627	Outliers: 6 of 627
A 400		LYS	50	-	Favored (81.28%) General / -61.9,-36.4	39.6% (*mtmt*) chi angles: 288.5,173.3,290.5,204.5	0.137Å	-	-
A 401		GLY	50	-	Favored (24.61%) Glycine / -82.6,-33.6	-	-	-	-
A 402		ILE	50	0.553Å HG23 with A 398 PHE O	Favored (83.76%) Isoleucine or valine / -62.6,-49.4	6.9% (*tp*) chi angles: 179.4,65.6	0.071Å	-	-

A 403	TYR	50	-	Favored (60.8%) General / -74.3,-41.7	34.2% (*t80*) chi angles: 195.4,85.9	0.047Å	-	-
A 404	GLY	50	-	Favored (94.42%) Glycine / -66.1,-39.0	-	-	-	-
A 405	ARG	50	-	Favored (36.19%) General / -80.9,-27.6	94.2% (*mtt180*) chi angles: 303.6,179.4,183,193.6	0.112Å	-	-
A 406	LEU	50	-	Favored (70.77%) General / -55.3,-40.1	36.7% (*tp*) chi angles: 173.7,55.4	0.043Å	-	-
A 407	PHE	50	-	Favored (82.39%) General / -66.7,-36.4	15.2% (*t80*) chi angles: 202.1,81	0.166Å	-	-
A 408	VAL	50	-	Favored (97.79%) Isoleucine or valine / -63.6,-42.9	1.6% (*p*) chi angles: 84.1	0.261Å	-	-
A 409	TRP	50	-	Favored (62.31%) General / -74.6,-39.4	12% (*t90*) chi angles: 181.7,107.9	0.113Å	-	OUTLIER(worst is CE3-CD2-C(4.551 σ
A 410	ILE	50	-	Favored (66.78%) Isoleucine or valine / -56.9,-39.7	78.2% (*mt*) chi angles: 299,165.3	0.24Å	-	OUTLIER(worst is CB-CA-N: 4.057 σ
A 411	VAL	50	-	Favored (83.51%) Isoleucine or valine / -68.4,-44.5	33.8% (*t*) chi angles: 165.2	0.16Å	-	-
A 412	ASP	50	-	Favored (59.25%) General / -74.8,-25.8	7.7% (*t70*) chi angles: 206.9,49	0.235Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 413		LYS 50	-		Favored (73.95%) General / -61.9,-33.3	17% (mmmt) chi angles: 289.1,268.3,292.8,192.8	0.074Å	-	-
A 414		ILE 50	-		Favored (13.86%) Isoleucine or valine / -78.5,-15.0	2.3% (mt) chi angles: 323.4,190.7	0.24Å	-	-
A 415		ASN 50	-		Allowed (0.11%) General / -89.5,-94.4	82.8% (m-20) chi angles: 294.2,310.3	0.12Å	-	-
A 416		ALA 99.99	-		Favored (3.33%) General / 55.0,20.7	-	0.069Å	-	-
A 417		ALA 99.99	-		Favored (43.88%) General / -99.8,2.3	-	0.083Å	-	-
A 418		ILE 99.99	-		Favored (9.71%) Isoleucine or valine / -104.9,-5.9	4.2% (mt) chi angles: 311.9,196.4	0.161Å	-	-
A 419		TYR 99.99	-		Favored (8.71%) General / -95.3,-42.1	85.7% (t80) chi angles: 179.9,82.6	0.028Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.75	Clashscore: 1.19	Outliers: 8 of 625	Poor rotamers: 5 of 555	Outliers: 13 of 594	Outliers: 0 of 627	Outliers: 6 of 627
A 420		LYS 99.99	-		Favored (62.84%) Pre-proline / -63.8,-41.2	90.6% (mttt) chi angles: 303.8,170.4,184.1,176.2	0.173Å	-	-
A 421		PRO 99.99	-		Favored (17.66%) Trans-proline / -69.0,-34.1	54.6% (Cg_exo) chi angles: 334.5	0.196Å	-	-

A 422	PRO	99.99	-	Favored (14.77%) Trans-proline / -75.5,-21.6	82.6% (*Cg_exo*) chi angles: 331.9	0.091Å	-	-
A 423	SER	99.99	-	Favored (57.96%) General / -80.3,-6.5	60.6% (*m*) chi angles: 299.1	0.063Å	-	-
A 424	GLN	99.99	-	Allowed (1.5%) General / -145.1,14.8	72.9% (*mt-30*) chi angles: 303,183.5,296.8	0.043Å	-	OUTLIER(worst is C-N-CA: 4.075 σ
A 425	ASP	50	-	Allowed (0.83%) General / 41.0,39.4	5.8% (*m-20*) chi angles: 295.4,21.2	0.113Å	-	-
A 426	VAL	50	-	Allowed (1.48%) Isoleucine or valine / -89.2,77.8	21.6% (*t*) chi angles: 188	0.191Å	-	-
A 427	LYS	50	-	Favored (5.97%) General / -44.7,127.0	94.9% (*mttt*) chi angles: 290.2,188.4,179.1,184	0.048Å	-	-
A 428	ASN	50	-	Favored (58.81%) General / -54.2,-33.6	42.1% (*m-20*) chi angles: 303.2,347.3	0.141Å	-	-
A 429	SER	50	-	Allowed (0.52%) General / -84.6,31.7	93.5% (*p*) chi angles: 66.9	0.076Å	-	-
A 430	ARG	50	-	Favored (42.28%) General / -96.8,-3.3	97.9% (*mtt180*) chi angles: 294,172,167.9,173.5	0.046Å	-	OUTLIER(worst is C-N-CA: 4.851 σ
A 431	ARG	50	-	Allowed (0.23%) General / -130.1,-140.6	8.5% (*mtm-85*) chi angles: 323,200.5,284.9,240.4	0.152Å	-	OUTLIER(worst is C-N-CA: 6.3
A 432	SER	50	-	Favored (2.52%) General / -115.0,-174.6	75.3% (*p*) chi angles: 58.3	0.034Å	-	-

# Alt Res			High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 433	ILE	50	-		Favored (64.74%) Isoleucine or valine / -130.1,133.2	11.4% (*mt*) chi angles: 317.4,171.2	0.185Å	-	-
A 434	GLY	50	-		Favored (15.85%) Glycine / -106.4,144.5	-	-	-	-
A 435	LEU	99.99	-		Favored (43.28%) General / -125.9,125.7	7.4% (*mt*) chi angles: 322.5,179.5	0.07Å	-	-
A 436	LEU	50	-		Favored (26.33%) General / -101.3,113.3	27.9% (*tp*) chi angles: 190,66.1	0.037Å	-	-
A 437	ASP	50	-		Favored (3.09%) General / -95.2,68.3	14.4% (*t0*) chi angles: 171.6,27.9	0.098Å	-	OUTLIER(worst is CA-CB-CG 6.491 σ
A 438	ILE	50	0.569Å HG22 with A 439 PHE H		Allowed (0.46%) Isoleucine or valine / -73.3,178.9	5.1% (*pt*) chi angles: 75.8,155	0.228Å	-	-
A 439	PHE	50	0.569Å H with A 438 ILE HG22		Favored (25.37%) General / -81.9,155.2	3.2% (*m-85*) chi angles: 274.9,39.9	0.046Å	-	OUTLIER(worst is CA-CB-CG 6.813 σ

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.75	Clashscore: 1.19	Outliers: 8 of 625	Poor rotamers: 5 of 555	Outliers: 13 of 594	Outliers: 0 of 627	Outliers: (of 627
A 440	GLY	50	-		Favored (11.28%) Glycine / -90.9,132.4	-	-	-	-
A 441	PHE	50	-		Favored (23.29%) General / -50.1,131.8	55.3% (*t80*) chi angles: 188.6,86.9	0.076Å	-	-

A 442	GLU	50	-	Favored (31.06%) General / -145.6,145.7	9.1% (*pt-20*) chi angles: 45.4,188.5,37.8	0.097Å	-	-
A 443	ASN	50	-	Favored (4.53%) General / -145.6,108.5	11.9% (*t-20*) chi angles: 174.2,296.1	0.068Å	-	-
A 444	PHE	50	-	Favored (3.47%) General / -107.2,-177.8	17% (*m-85*) chi angles: 314,303.2	0.053Å	-	-
A 445	ALA	50	-	Favored (93.07%) General / -63.5,-38.9	-	0.098Å	-	-
A 446	VAL	50	-	Favored (19.47%) Isoleucine or valine / -114.3,145.9	86.9% (*t*) chi angles: 177.7	0.085Å	-	-
A 447	ASN	50	-	Favored (4.18%) General / -137.7,100.3	68% (*m-80*) chi angles: 299.2,288.8	0.062Å	-	-
A 448	SER	50	-	Favored (2.57%) General / -88.2,-169.5	7.7% (*t*) chi angles: 195.9	0.19Å	-	-
A 449	PHE	50	-	Favored (75.08%) General / -57.3,-39.0	7.1% (*t80*) chi angles: 172.9,36.2	0.032Å	-	OUTLIER(worst is CA-CB-CG 5.096 σ
A 450	GLU	50	-	Favored (84.28%) General / -57.6,-46.4	6.7% (*mp0*) chi angles: 308.7,86,316.5	0.08Å	-	-
A 451	GLN	50	-	Favored (88.6%) General / -64.3,-37.8	7.4% (*mp0*) chi angles: 281.8,60.6,71.7	0.114Å	-	-
A 452	LEU	50	-	Favored (88.46%) General /	62.8% (*tp*) chi angles: 178.1,64.8	0.067Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
					-59.5,-46.6				
A 453		CYS	50	-	Favored (98.71%) General / -63.4,-42.8	91.2% (*m*) chi angles: 295.1	0.108Å	-	-
A 454		ILE	50	-	Favored (79.77%) Isoleucine or valine / -67.9,-38.3	8% (*mt*) chi angles: 310,148.5	0.227Å	-	-
A 455		ASN	50	-	Favored (58.24%) General / -76.0,-29.3	87% (*m-20*) chi angles: 295.9,317	0.129Å	-	-
A 456		PHE	99.99	-	Favored (84.55%) General / -65.3,-36.6	4.2% (*m-30*) chi angles: 276.3,319.3	0.132Å	-	-
A 457		ALA	50	-	Favored (97.06%) General / -62.4,-40.6	-	0.092Å	-	-
A 458		ASN	50	-	Favored (92.25%) General / -65.8,-40.6	3.8% (*m-80*) chi angles: 284.5,247.5	0.127Å	-	OUTLIER(worst is CA-CB-CG 4.456 σ
A 459		GLU	50	-	Favored (97.04%) General / -62.6,-44.1	8.9% (*tp10*) chi angles: 202.2,68.6,61.4	0.036Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.75	Clashscore: 1.19	Outliers: 8 of 625	Poor rotamers: 5 of 555	Outliers: 13 of 594	Outliers: 0 of 627	Outliers: 6 of 627
A 460		HIS	99.99	-	Favored (73.46%) General / -66.4,-32.2	92.4% (*m-70*) chi angles: 290.3,287.4	0.14Å	-	-
A 461		LEU	50	-	Favored (68.34%) General / -72.5,-37.6	23.6% (*tp*) chi angles: 190,70.1	0.198Å	-	-

A 462	GLN	50	-	Favored (74.02%) General / -64.6,-32.4	58.9% (*tp60*) chi angles: 182.4,58.7,32.7	0.187Å	-	-
A 463	GLN	50	-	Favored (90.82%) General / -62.4,-38.7	63.4% (*tp60*) chi angles: 189.6,69.8,62.4	0.082Å	-	-
A 464	PHE	50	-	Favored (80%) General / -68.6,-37.5	44.5% (*t80*) chi angles: 189.6,64.9	0.085Å	-	-
A 465	PHE	50	-	Favored (35.54%) General / -66.6,-53.3	88.6% (*t80*) chi angles: 181.5,76.8	0.07Å	-	-
A 466	VAL	50	-	Favored (58.31%) Isoleucine or valine / -60.4,-34.6	3.5% (*p*) chi angles: 79.4	0.15Å	-	-
A 467	ARG	50	-	Favored (80.15%) General / -67.5,-43.7	63.4% (*ttm-85*) chi angles: 186.7,175.5,298.9,277.2	0.102Å	-	-
A 468	HIS	50	-	Favored (44.35%) General / -79.9,-21.1	57.7% (*t-80*) chi angles: 197.6,286	0.218Å	-	-
A 469	VAL	50	-	Favored (8.88%) Isoleucine or valine / -108.1,-16.0	1.5% (*p*) chi angles: 84.4	0.292Å	-	-
A 470	PHE	50	-	Allowed (1.52%) General / -132.7,-29.3	4.6% (*m-85*) chi angles: 324.4,289.3	0.144Å	-	-
A 471	LYS	50	-	Favored (3.35%) General / -79.0,-58.2	54% (*tttm*) chi angles: 192.7,186.9,179.1,299.1	0.148Å	-	-
A 472	LEU	50	-	Favored (64.83%) General / -73.6,-34.0	52.4% (*mt*) chi angles: 302.1,169	0.147Å	-	-

# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 473	GLU 50	-	Favored (96.1%) General / -64.5,-40.7	29.9% (*mm-40*) chi angles: 306,279.5,316.1	0.127Å	-	-
A 474	GLN 50	-	Favored (50.75%) General / -77.8,-29.5	36.8% (*mt-30*) chi angles: 294.6,187.1,106.4	0.185Å	-	-
A 475	GLU 50	-	Favored (59.49%) General / -77.3,-15.3	88% (*mt-10*) chi angles: 290.2,169.1,333.4	0.166Å	-	-
A 476	GLU 50	-	Favored (55.68%) General / -70.8,-48.1	50.1% (*mt-10*) chi angles: 286.6,195.4,22.5	0.068Å	-	-
A 477	TYR 50	-	Favored (91.86%) General / -59.3,-42.6	10.4% (*m-30*) chi angles: 307.7,332.1	0.101Å	-	-
A 478	ASP 50	-	Favored (57.99%) General / -79.2,-15.5	42.1% (*m-20*) chi angles: 302.4,348.2	0.096Å	-	-
A 479	LEU 50	-	Favored (13.3%) General / -93.7,-34.3	50.8% (*tp*) chi angles: 184.3,62.1	0.059Å	-	-
# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
	Avg: 55.75	Clashscore: 1.19	Outliers: 8 of 625	Poor rotamers: 5 of 555	Outliers: 13 of 594	Outliers: 0 of 627	Outliers: 6 of 627
A 480	GLU 50	-	Favored (39.07%) General / -81.0,-22.8	5.2% (*mm-40*) chi angles: 301,270.4,57.2	0.073Å	-	-
A 481	SER 50	-	Allowed (0.1%) General / 78.9,40.8	19.1% (*t*) chi angles: 188.9	0.164Å	-	-
A 482	ILE 50	-	Allowed (0.12%)	86.8% (*mt*) chi angles: 298.3,174.8	0.127Å	-	-

				Isoleucine or valine / -74.7,16.8			
A 483	ASP	50	-	Allowed (1.51%) General / 60.2,62.9	20.8% (*t0*) chi angles: 178.9,34	0.131Å	-	-
A 484	TRP	50	-	Favored (39.39%) General / -122.7,122.7	63.5% (*t-105*) chi angles: 178,265.7	0.047Å	-	OUTLIER(worst is CE3-CD2-C 4.075 σ
A 485	LEU	50	-	Favored (7.34%) General / -83.7,90.6	5.4% (*tt*) chi angles: 191.5,138.7	0.04Å	-	-
A 486	HIS	99.99	-	Favored (5.12%) General / -55.4,119.1	2.5% (*p80*) chi angles: 49.1,52.4	0.081Å	-	OUTLIER(worst is CA-CB-CG 4.606 σ
A 487	ILE	99.99	-	Favored (17.69%) Isoleucine or valine / -93.0,139.7	72.9% (*mt*) chi angles: 295.8,178.1	0.139Å	-	-
A 488	GLU	99.99	-	Favored (23.37%) General / -77.3,166.3	5.6% (*pm0*) chi angles: 83.9,302.6,353	0.062Å	-	OUTLIER(worst is CB-CG-CD 5.054 σ
A 489	PHE	99.99	-	Favored (2.51%) General / -173.9,155.1	47.1% (*p90*) chi angles: 57.6,93.9	0.043Å	-	-
A 490	THR	99.99	-	Favored (8.78%) General / -130.8,106.9	11.1% (*t*) chi angles: 184.6	0.129Å	-	OUTLIER(worst is C-N-CA: 7.759 σ
A 491	ASP	50	-	Allowed (0.13%) General / 77.0,-178.2	30.7% (*t0*) chi angles: 200,16.1	0.253Å	-	-
A 492	ASN	50	-	Favored (4.15%) General / -133.4,13.3	7% (*m120*) chi angles: 312.4,141.9	0.038Å	-	OUTLIER(worst is CA-CB-CG 6.557 σ

# Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 493	GLN 50	-	Favored (72.23%) General / -60.0,-33.6	7.4% (tp60) chi angles: 189.8,58.5,101	0.168Å	-	-
A 494	ASP 50	-	Favored (18.49%) General / -67.7,-54.6	28.4% (t0) chi angles: 180.8,29.7	0.085Å	-	-
A 495	ALA 50	-	Favored (31.98%) General / -52.9,-30.1	-	0.094Å	-	-
A 496	LEU 50	-	Favored (50.12%) General / -76.3,-40.9	43% (mt) chi angles: 297.4,188.5	0.098Å	-	-
A 497	ASP 99.99	-	Favored (15.3%) General / 50.6,52.2	5.1% (m-20) chi angles: 265.9,330.8	0.155Å	-	OUTLIER(worst is CA-CB-CG 4.565 σ
A 498	MET 99.99	-	Favored (24.18%) General / -87.7,-23.4	94.8% (mmm) chi angles: 295.6,291.8,284.7	0.219Å	-	-
A 499	ILE 99.99	-	Favored (16.56%) Isoleucine or valine / -74.6,-17.6	46% (mm) chi angles: 301,296.5	0.124Å	-	-

# Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 55.75	Clashscore: 1.19	Outliers: 8 of 625	Poor rotamers: 5 of 555	Outliers: 13 of 594	Outliers: 0 of 627	Outliers: 6 of 627
A 500	ALA 99.99	-	Allowed (0.33%) General / -78.4,39.6	-	0.081Å	-	-
A 501	ASN 50	-	Favored (58.36%) General / -78.1,-16.0	34.3% (m120) chi angles: 294,111.1	0.1Å	-	-

A 502	LYS	50	-	Allowed (1.55%) Pre-proline / -159.1,104.3	24.5% (*tptp*) chi angles: 172.7,63,189.9,63.9	0.046Å	-	-
A 503	PRO	50	-	Favored (19.17%) Cis-proline / -88.8,142.9	11.3% (*Cg_endo*) chi angles: 40	0.075Å	-	-
A 504	MET	99.99	-	Favored (6.91%) General / -52.3,121.4	23.7% (*mmt*) chi angles: 296.5,304.9,175.7	0.049Å	-	OUTLIER(worst is C-N-CA: 4.276 σ
A 505	ASN	50	-	Allowed (1.29%) General / -54.7,162.2	41.4% (*t-20*) chi angles: 193.6,327.9	0.143Å	-	OUTLIER(worst is CA-CB-CG 5.816 σ
A 506	ILE	50	-	Favored (23.11%) Isoleucine or valine / -51.8,-38.7	47.2% (*pt*) chi angles: 63.8,172.5	0.143Å	-	-
A 507	ILE	50	-	Favored (12.47%) Isoleucine or valine / -71.0,-9.2	15.1% (*pt*) chi angles: 74.8,170.8	0.197Å	-	-
A 508	SER	50	-	Favored (6.55%) General / -106.8,-36.9	9.1% (*t*) chi angles: 193.1	0.081Å	-	-
A 509	LEU	50	-	Favored (83.2%) General / -62.0,-37.0	62.6% (*mt*) chi angles: 300.6,169.5	0.104Å	-	-
A 510	ILE	50	-	Favored (54.23%) Isoleucine or valine / -60.4,-33.5	20.6% (*pt*) chi angles: 70,179	0.205Å	-	-
A 511	ASP	50	-	Favored (62.88%) General / -74.6,-37.1	70.1% (*m-20*) chi angles: 300.2,335.3	0.109Å	-	-
A 512	GLU	50	-	Favored (59.21%)	2.4% (*tt0*) chi angles: 191.3,224.6,319.5	0.036Å	-	-

# Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 513	GLU	50	-	General / -58.8,-53.4 Favored (73.99%) General / -69.9,-34.8	15.8% (*tp10*) chi angles: 206.7,70.8,9.3	0.057Å	-	-
A 514	SER	50	-	Favored (72.13%) General / -60.8,-32.8	30.4% (*m*) chi angles: 286.5	0.187Å	-	-
A 515	LYS	50	-	Favored (62.23%) General / -74.8,-37.9	34.8% (*ttpt*) chi angles: 192.8,166,60,181.7	0.129Å	-	-
A 516	PHE	50	-	Favored (61.87%) Pre-proline / -55.7,125.7	8.8% (*t80*) chi angles: 186.8,36.7	0.037Å	-	-
A 517	PRO	50	-	Favored (33.71%) Trans-proline / -70.4,-14.0	68.9% (*Cg_exo*) chi angles: 327.8	0.086Å	-	-
A 518	LYS	50	-	Favored (17.42%) General / -114.0,10.0	32.1% (*mmmt*) chi angles: 295.7,294.7,297.7,186.6	0.077Å	-	-
A 519	GLY	50	-	Favored (25.02%) Glycine / -73.5,138.4	-	-	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.75	Clashscore: 1.19	Outliers: 8 of 625	Poor rotamers: 5 of 555	Outliers: 13 of 594	Outliers: 0 of 627	Outliers: 6 of 627
A 520		THR	50	-	Favored (4.21%) General / -117.0,178.8	75.9% (*p*) chi angles: 58.7	0.039Å	-	-
A 521		ASP	50	-	Favored (58.15%) General / -75.0,-22.9	69% (*m-20*) chi angles: 287.8,320.9	0.155Å	-	-

A 522	THR	50	-	Favored (72.85%) General / -70.8,-39.7	21.1% (*p*) chi angles: 48.7	0.181Å	-	-
A 523	THR	50	-	Favored (80.77%) General / -68.5,-40.4	67.5% (*p*) chi angles: 59.4	0.189Å	-	-
A 524	MET	50	-	Favored (7.09%) General / -47.2,-56.2	53.2% (*tpp*) chi angles: 178.4,74.7,75.5	0.041Å	-	-
A 525	LEU	50	-	Favored (95.52%) General / -60.5,-44.8	2.3% (*tt*) chi angles: 184.3,130	0.1Å	-	-
A 526	HIS	50	-	Favored (80.93%) General / -61.2,-36.8	19.5% (*t-160*) chi angles: 189.3,184.9	0.12Å	-	-
A 527	LYS	50	-	Favored (81.22%) General / -59.0,-39.3	10.2% (*tppt?*) chi angles: 176.8,74,68.4,148.9	0.037Å	-	-
A 528	LEU	50	-	Favored (52.93%) General / -77.7,-34.2	26.5% (*mt*) chi angles: 311.1,185	0.13Å	-	-
A 529	ASN	99.99	-	Favored (2.45%) General / -137.6,35.8	45.8% (*p30*) chi angles: 60.8,22.7	0.161Å	-	-
A 530	SER	99.99	-	Allowed (0.17%) General / -57.8,104.1	0.9% chi angles: 211.6	0.046Å	-	OUTLIER(worst is C-N-CA: 4.718 σ
A 531	GLN	99.99	-	Allowed (0.06%) General / 27.1,68.4	12.2% (*pt20*) chi angles: 54.4,179,114.7	0.164Å	-	-
A 532	HIS	99.99	-	Favored (31.05%) General / -147.7,148.5	27.6% (*p80*) chi angles: 71.8,80.8	0.065Å	-	OUTLIER(worst is C-N-CA: 6.641 σ

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 533		LYS	50	-	Allowed (0.52%) General / 72.0,43.6	28.2% (*mmmt*) chi angles: 309.7,288.6,291.8,187	0.229Å	-	-
A 534		LEU	50	-	Allowed (0.1%) General / -145.7,-103.6	59.1% (*mt*) chi angles: 284.8,172.4	0.171Å	-	-
A 535		ASN	50	-	Favored (3.32%) General / -46.5,142.1	21.7% (*t-20*) chi angles: 180.5,282	0.055Å	-	-
A 536		ALA	50	-	Favored (18.9%) General / -86.6,-36.3	-	0.066Å	-	-
A 537		ASN	50	-	Favored (34.44%) General / -84.6,-18.8	5.7% (*m120*) chi angles: 296.9,171.7	0.168Å	-	OUTLIER(worst is CA-CB-CG 5.695 σ
A 538		TYR	50	-	Favored (27.97%) General / -80.0,123.6	8.5% (*t80*) chi angles: 189.4,291.3	0.033Å	-	-
A 539		ILE	50	-	Favored (26.99%) Pre-proline / -121.7,124.8	45% (*mm*) chi angles: 297.3,300.4	0.084Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.75	Clashscore: 1.19	Outliers: 8 of 625	Poor rotamers: 5 of 555	Outliers: 13 of 594	Outliers: 0 of 627	Outliers: 6 of 627
A 540		PRO	50	-	Favored (2.79%) Trans-proline / -85.6,125.0	7.3% (*Cg_exo*) chi angles: 351.4	0.089Å	-	-
A 541		PRO	50	-	Favored (3.79%) Trans-proline / -82.5,-178.1	51.5% (*Cg_endo*) chi angles: 35.1	0.063Å	-	-
A 542		LYS	50	-	Favored (11.63%)	51.6% (*mtmt*) chi angles:	0.076Å	-	-

			General / -117.4,-1.9	303.7,185.9,294.6,176.4			
A 543	ASN 50	-	Favored (19.08%) General / -95.2,-20.6	17.2% (*t-20*) chi angles: 179.8,241.3	0.06Å	-	-
A 544	ASN 99.99	-	Favored (57.62%) General / -62.6,135.9	9.8% (*p-10*) chi angles: 50.7,324.8	0.058Å	-	-
A 545	HIS 99.99	-	Favored (52.78%) General / -79.1,-18.7	34.1% (*p80*) chi angles: 63,85.2	0.144Å	-	OUTLIER(worst is CA-CB-CG 4.662 σ
A 546	GLU 99.99	-	OUTLIER (0.01%) General / 176.1,-35.7	47.6% (*tt0*) chi angles: 170.1,193.8,349.3	0.168Å	-	OUTLIER(worst is CA-CB-CG 4.142 σ
A 547	THR 50	-	Favored (13.27%) General / -104.7,-22.1	73.2% (*p*) chi angles: 58	0.093Å	-	-
A 548	GLN 50	-	Favored (17.21%) General / -103.5,157.2	79.7% (*mt-30*) chi angles: 292,182,31.7	0.068Å	-	-
A 549	PHE 50	-	Favored (3.3%) General / -139.3,-172.2	35.8% (*p90*) chi angles: 64.4,100.3	0.067Å	-	-
A 550	GLY 50	-	Favored (34.78%) Glycine / -160.3,165.1	-	-	-	-
A 551	ILE 99.99	-	Favored (22.91%) Isoleucine or valine / -139.3,150.5	80.9% (*mt*) chi angles: 295.1,176.2	0.092Å	-	-
A 552	ASN 50	-	Favored (16.3%) General / -90.6,103.6	27.6% (*t-20*) chi angles: 202.8,8.2	0.025Å	-	-
A 553	HIS 50	-	Favored (13.37%)	79% (*m-70*) chi angles: 284.9,287.6	0.089Å	-	OUTLIER(worst is CA-CB-CG

# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			General / -91.5,165.4				4.381 σ
A 554	PHE 50	-	Favored (16.79%) General / -46.8,-42.4	8.4% (*p90*) chi angles: 77.7,110	0.142Å	-	-
A 555	ALA 50	-	Favored (56.56%) General / -93.8,1.1	-	0.115Å	-	-
A 556	GLY 50	-	Favored (7.34%) Glycine / 138.3,157.2	-	-	-	-
A 557	ILE 50	-	Favored (17.79%) Isoleucine or valine / -61.4,141.2	45.5% (*pt*) chi angles: 64.3,172.6	0.088Å	-	-
A 558	VAL 50	-	Favored (48.25%) Isoleucine or valine / -135.8,129.6	28% (*t*) chi angles: 186.4	0.052Å	-	-
A 559	TYR 50	-	Favored (34.9%) General / -92.7,134.6	2.8% (*m-30*) chi angles: 288,29.8	0.062Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.75	Clashscore: 1.19	Outliers: 8 of 625	Poor rotamers: 5 of 555	Outliers: 13 of 594	Outliers: 0 of 627	Outliers: 6 of 627
A 560		TYR	50	-	Favored (47.32%) General / -115.5,142.0	97.8% (*m-85*) chi angles: 294.5,276.7	0.038Å	-	-
A 561		GLU	50	-	Favored (32.8%) General / -105.7,116.9	6.8% (*tp10*) chi angles: 176.2,41.1,81.5	0.113Å	-	-
A 562		THR	50	-	Favored (59.91%) General /	5.6% (*m*) chi angles: 316.3	0.134Å	-	-

				-77.8,-11.7			
A 563	GLN	50	-	Favored (6.01%) General / -54.4,120.0	26% (*tt0*) chi angles: 184.5,180.6,106.1	0.036Å	-	-
A 564	GLY	50	-	Favored (70.13%) Glycine / 90.9,3.8	-	-	-	-
A 565	PHE	50	-	Favored (99.2%) General / -63.1,-41.0	3.4% (*m-30*) chi angles: 275.9,33.6	0.156Å	-	-
A 566	LEU	50	-	Favored (77.66%) General / -58.5,-49.4	29.4% (*mt*) chi angles: 280.5,176.2	0.168Å	-	-
A 567	GLU	50	-	Favored (31.47%) General / -84.0,-21.8	29.9% (*mm-40*) chi angles: 294.9,321.8,304.8	0.197Å	-	-
A 568	LYS	50	-	Favored (63.79%) General / -71.2,-27.8	97.9% (*mttt*) chi angles: 294,180,176.1,186.4	0.117Å	-	-
A 569	ASN	50	-	Favored (18.29%) General / -89.0,-31.1	64% (*t30*) chi angles: 193.3,43.4	0.099Å	-	-
A 570	ARG	50	-	Favored (64.08%) General / -73.4,-31.8	97.5% (*mtt180*) chi angles: 294.8,164.3,176.6,168.5	0.117Å	-	-
A 571	ASP	50	-	Favored (16.11%) General / 52.2,51.5	32.9% (*t0*) chi angles: 198.8,18.8	0.161Å	-	-
A 572	THR	50	-	Favored (49.21%) General / -68.8,134.0	0.9% chi angles: 32.7	0.066Å	-	-
A 573	LEU	50	-	Favored (50.26%) General / -127.3,147.1	27.7% (*tp*) chi angles: 188.7,56.2	0.032Å	-	-

# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 574	HIS 99.99	0.465Å HB3 with A 373 ARG HD3	Favored (29%) General / -89.5,118.3	6.8% (*m170*) chi angles: 273.6,210.3	0.048Å	-	-
A 575	GLY 50	-	Favored (59.15%) Glycine / -54.0,-49.4	-	-	-	-
A 576	ASP 50	-	Favored (70.12%) General / -59.4,-32.3	0.4% chi angles: 316.2,16.9	0.148Å	-	OUTLIER(worst is CA-CB-CG 4.453 σ
A 577	ILE 50	-	Favored (84.66%) Isoleucine or valine / -62.2,-39.6	5.2% (*tp*) chi angles: 186.7,79.7	0.065Å	-	-
A 578	ILE 50	-	Favored (76.25%) Isoleucine or valine / -65.3,-35.8	21.5% (*tt*) chi angles: 187.2,167.4	0.129Å	-	-
A 579	GLN 50	-	Favored (65.54%) General / -71.8,-43.4	35.3% (*mt-30*) chi angles: 293.4,167.5,239.8	0.098Å	-	-
# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
	Avg: 55.75	Clashscore: 1.19	Outliers: 8 of 625	Poor rotamers: 5 of 555	Outliers: 13 of 594	Outliers: 0 of 627	Outliers: 6 of 627
A 580	LEU 50	0.496Å HD21 with A 361 VAL HB	Favored (37.25%) General / -54.9,-54.8	5.2% (*tt*) chi angles: 186,171.4	0.05Å	-	-
A 581	VAL 50	-	Favored (17.82%) Isoleucine or valine / -72.3,-15.4	9.8% (*p*) chi angles: 72.2	0.25Å	-	-
A 582	HIS 50	-	Favored (77.91%) General / -59.4,-37.4	45.9% (*m170*) chi angles: 290,152.5	0.098Å	-	-

A 583	SER	50	-	Favored (35.49%) General / -82.3,1.7	24% (*m*) chi angles: 304.8	0.041Å	-	-
A 584	SER	50	-	Favored (12.5%) General / -56.2,151.5	22.8% (*t*) chi angles: 186.7	0.046Å	-	-
A 585	ARG	50	-	Favored (39.74%) General / -91.2,-10.9	35.5% (*ptt-85*) chi angles: 58.1,187.7,186.4,274.6	0.185Å	-	OUTLIER(worst is CD-NE-CZ 4.031 σ
A 586	ASN	99.99	0.417Å HB3 with A 589 ILE HG22	Favored (47.12%) General / -73.0,140.1	20.9% (*t-20*) chi angles: 181.5,296	0.088Å	-	OUTLIER(worst is CA-CB-CG 7.756 σ
A 587	LYS	50	-	Favored (47.2%) General / -69.5,-50.2	28.3% (*mmmt*) chi angles: 291.4,284.4,293.1,190	0.061Å	-	-
A 588	PHE	99.99	-	Favored (77.16%) General / -64.2,-48.1	79.3% (*t80*) chi angles: 178.1,70.1	0.042Å	-	-
A 589	ILE	99.99	0.472Å HA with A 592 ILE HG12	Favored (49.43%) Isoleucine or valine / -68.0,-30.8	8.1% (*mt*) chi angles: 315.6,157	0.376Å	-	OUTLIER(worst is CB-CA-N: 5.172 σ
A 590	LYS	50	-	Favored (87.59%) General / -65.2,-44.6	34.4% (*ttpt*) chi angles: 197.5,167.8,67.7,174.2	0.145Å	-	-
A 591	GLN	50	-	Favored (83.59%) General / -63.1,-47.3	56.4% (*tt0*) chi angles: 185.3,186.7,350.6	0.137Å	-	-
A 592	ILE	50	0.472Å HG12 with A 589 ILE HA	Favored (9.49%) Isoleucine or valine / -64.2,-11.2	11.3% (*pt*) chi angles: 68.6,156.9	0.161Å	-	-
A 593	PHE	50	-	Favored (11.77%)	49% (*m-85*) chi angles: 281.7,277	0.185Å	-	OUTLIER(worst is CA-CB-CG

# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			General / -115.6,-11.1				4.325 σ
A 594	GLN 99.99	-	Favored (16.45%) General / -159.0,144.7	7.9% (pt20) chi angles: 50.9,166.7,102.1	0.069Å	-	-
A 595	ALA 99.99	-	Allowed (0.77%) General / 72.8,38.1	-	0.135Å	-	-
A 596	ASP 99.99	-	Favored (3.05%) General / -157.1,-169.7	4.8% (t0) chi angles: 207.4,312.9	0.087Å	-	OUTLIER(worst is CA-CB-CG 4.178 σ
A 597	VAL 99.99	-	OUTLIER (0.07%) Isoleucine or valine / -84.3,47.2	9.8% (p) chi angles: 72.2	0.223Å	-	-
A 598	ALA 50	-	Favored (34.82%) General / -86.0,-17.6	-	0.021Å	-	-
A 599	MET 50	-	Favored (4.82%) General / -68.0,173.1	15% (ptm) chi angles: 66.6,197.6,274.7	0.047Å	-	-
# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
	Avg: 55.75	Clashscore: 1.19	Outliers: 8 of 625	Poor rotamers: 5 of 555	Outliers: 13 of 594	Outliers: 0 of 627	Outliers: 6 of 627
A 600	GLY 50	-	Favored (15.16%) Glycine / -118.1,157.5	-	-	-	-
A 601	ALA 50	-	Favored (2.39%) General / -73.0,-177.4	-	0.112Å	-	-
A 602	GLU 50	-	Favored (29.89%) General / -142.7,137.3	13.2% (tp10) chi angles: 187.5,66.3,341.6	0.118Å	-	-

A 603	THR	50	-	Allowed (1.74%) General / -120.7,81.3	17.6% (*p*) chi angles: 47.2	0.139Å	-	-
A 604	ARG	50	-	Allowed (0.08%) General / 85.7,-54.6	31% (*ttm-85*) chi angles: 179,181.7,284.6,251.4	0.241Å	-	-
A 605	LYS	50	-	Allowed (0.05%) General / -164.5,16.5	14.2% (*tptp*) chi angles: 188.1,60.2,210.7,70.7	0.129Å	-	-
A 606	ARG	50	-	Favored (25.61%) General / -145.0,136.9	41.3% (*mmm-85*) chi angles: 293,298.4,296.3,259.9	0.165Å	-	-
A 607	SER	50	-	Favored (7.87%) Pre-proline / -54.4,154.9	14.9% (*m*) chi angles: 308.9	0.032Å	-	-
A 608	PRO	50	-	Favored (11.53%) Trans-proline / -73.6,127.3	21.7% (*Cg_endo*) chi angles: 38.4	0.03Å	-	-
A 609	THR	50	-	Allowed (1.16%) General / -53.8,161.3	34.9% (*p*) chi angles: 52.3	0.029Å	-	-
A 610	LEU	50	-	Favored (86.99%) General / -63.1,-37.4	6.5% (*tt*) chi angles: 197.2,154	0.085Å	-	-
A 611	SER	50	-	Favored (85.21%) General / -57.6,-44.0	44.2% (*t*) chi angles: 178.4	0.033Å	-	-
A 612	SER	50	-	Favored (99.62%) General / -62.2,-42.8	24.4% (*t*) chi angles: 186.1	0.094Å	-	-
A 613	GLN	50	-	Favored (93.18%) General / -65.4,-40.1	61.2% (*mt-30*) chi angles: 292.3,170.8,71.5	0.062Å	-	-

# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 614 PHE 50		-	Favored (90.46%) General / -66.3,-41.0	93.4% (*t80*) chi angles: 177,77.7	0.081Å	-	-
A 615 LYS 50		-	Favored (95.02%) General / -60.0,-43.6	29.1% (*mtmm*) chi angles: 286.8,184.2,280.8,279.9	0.134Å	-	-
A 616 ARG 50		-	Favored (79.61%) General / -68.7,-37.5	93.3% (*mtm-85*) chi angles: 295.6,190.1,301.6,281.1	0.18Å	-	-
A 617 SER 50		-	Favored (86.73%) General / -64.8,-45.3	58.4% (*m*) chi angles: 290.9	0.062Å	-	-
A 618 LEU 50		-	Favored (80.9%) General / -65.1,-46.5	45.8% (*tp*) chi angles: 177.1,69.4	0.051Å	-	-
A 619 GLU 50		-	Favored (70.24%) General / -70.8,-33.0	14.9% (*pt-20*) chi angles: 74.4,187.7,123.4	0.14Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.75	Clashscore: 1.19	Outliers: 8 of 625	Poor rotamers: 5 of 555	Outliers: 13 of 594	Outliers: 0 of 627	Outliers: 6 of 627
A 620		LEU 50		-	Favored (81.73%) General / -60.3,-48.4	46.8% (*tp*) chi angles: 182.2,57	0.043Å	-	-
A 621		LEU 50		-	Favored (72.65%) General / -58.0,-50.7	34.9% (*tp*) chi angles: 171.3,56.7	0.059Å	-	-
A 622		MET 50		-	Favored (79.39%) General / -62.0,-35.7	53.8% (*mmm*) chi angles: 302.2,321.7,295.6	0.14Å	-	-
A 623		ARG 50		-	Favored (99.28%)	62.3% (*ttm-85*) chi angles:	0.064Å	-	-

				General / -62.9,-41.2	189.8,176.7,298,276.6			
A 624	THR	50	-	Favored (90.27%) General / -66.0,-39.2	24% (*m*) chi angles: 309.2	0.077Å	-	-
A 625	LEU	50	-	Favored (61%) General / -74.1,-14.7	75% (*mt*) chi angles: 303.3,181.1	0.126Å	-	-
A 626	GLY	50	-	Favored (65.73%) Glycine / -81.7,-19.5	-	-	-	-
A 627	ALA	50	-	Favored (13.84%) General / -91.5,-36.2	-	0.026Å	-	-
A 628	CYS	50	-	Favored (17.17%) General / -92.1,156.8	25.6% (*p*) chi angles: 57.8	0.035Å	-	-
A 629	GLN	50	-	Favored (43.69%) Pre-proline / -83.0,113.1	47.4% (*tt0*) chi angles: 189.5,162.3,7.4	0.071Å	-	-
A 630	PRO	50	-	Allowed (0.97%) Trans-proline / -95.0,139.1	12% (*Cg_endo*) chi angles: 39.9	0.061Å	-	-
A 631	PHE	50	-	Favored (33.85%) General / -122.3,120.4	84.3% (*m-85*) chi angles: 300.1,265.9	0.106Å	-	-
A 632	PHE	50	-	Favored (44%) General / -101.4,134.8	2.4% (*m-85*) chi angles: 309.5,246	0.105Å	-	-
A 633	VAL	50	-	Favored (69.53%) Isoleucine or valine / -116.8,131.4	96.6% (*t*) chi angles: 176.7	0.1Å	-	-
A 634	ARG	50	-	Favored (7.98%) General / -113.5,99.7	34.8% (*mmm-85*) chi angles: 317.1,303.5,296.2,269.8	0.04Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 635		CYS	50	-	Favored (31.73%) General / -84.0,125.1	66.2% (*m*) chi angles: 302.2	0.042Å	-	-
A 636		ILE	50	-	Favored (51.89%) Isoleucine or valine / -119.3,137.8	2% (*mm*) chi angles: 329.4,289.8	0.127Å	-	-
A 637		LYS	99.99	-	Favored (96.53%) Pre-proline / -68.2,144.2	19.7% (*mtpp*) chi angles: 286.7,172.6,76.4,95	0.096Å	-	-
A 638		PRO	50	-	Favored (2.07%) Trans-proline / -89.0,-17.2	21.2% (*Cg_endo*) chi angles: 38.4	0.019Å	-	-
A 639		ASN	50	-	Favored (19.19%) General / -165.6,163.9	9.2% (*p30*) chi angles: 56.5,82.5	0.048Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.75	Clashscore: 1.19	Outliers: 8 of 625	Poor rotamers: 5 of 555	Outliers: 13 of 594	Outliers: 0 of 627	Outliers: 6 of 627
A 640		GLU	50	-	Favored (76.49%) General / -69.5,-41.2	7.5% (*mm-40*) chi angles: 286,292.6,31.7	0.088Å	-	OUTLIER(worst is C-N-CA: 4.652 σ
A 641		PHE	50	-	Favored (7.4%) General / -68.4,-1.9	99.6% (*m-85*) chi angles: 297.6,96.6	0.071Å	-	-
A 642		LYS	50	-	Favored (9.16%) General / 61.0,45.8	24.7% (*mtpp*) chi angles: 297.1,167.8,55.9,56.6	0.075Å	-	-
A 643		LYS	50	-	Favored (46.35%) Pre-proline / -116.6,150.9	29.7% (*mtpp*) chi angles: 298.3,186.2,72.8,63.3	0.053Å	-	-
A 644		PRO	50	-	Favored (8.73%)	9.9% (*Cg_endo*) chi angles: 40.3	0.086Å	-	-

				Trans-proline / -87.0,161.6				
A 645	MET	50	-	Favored (18.74%) General / 56.0,31.8	15.1% (*ptp*) chi angles: 77.7,183.7,83.4	0.202Å	-	-
A 646	LEU	50	-	Favored (16.45%) General / -136.5,119.5	48% (*tp*) chi angles: 184.4,64.1	0.15Å	-	-
A 647	PHE	50	-	Allowed (1.9%) General / -132.5,80.5	63.3% (*t80*) chi angles: 187.6,82.8	0.079Å	-	-
A 648	ASP	50	-	Allowed (1.22%) General / -61.5,109.6	9.6% (*m-20*) chi angles: 307.7,352.2	0.071Å	-	-
A 649	ARG	50	-	Favored (9.54%) General / -47.8,-35.0	50.2% (*mmm-85*) chi angles: 296.2,294,303.6,292.4	0.09Å	-	-
A 650	HIS	50	-	Favored (34.83%) General / -82.2,-24.8	19.6% (*t-160*) chi angles: 192.9,190.8	0.069Å	-	OUTLIER(worst is CA-CB-CG 4.082 σ
A 651	LEU	50	-	Favored (7.22%) General / -95.5,-45.1	2.8% (*tt*) chi angles: 169,139.4	0.051Å	-	-
A 652	CYS	50	0.404Å SG with A 82 LEU HD11	Favored (80.83%) General / -64.6,-35.4	1.7% (*p*) chi angles: 39.6	0.214Å	-	-
A 653	VAL	50	-	Favored (68.34%) Isoleucine or valine / -64.5,-34.2	6.1% (*p*) chi angles: 74.9	0.23Å	-	-
A 654	ARG	50	-	Favored (35.69%) General / -55.6,-55.1	65.2% (*mtp85*) chi angles: 281.5,182,68.2,77.4	0.101Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 655		GLN	50	-	Favored (72.5%) General / -59.4,-34.5	39.5% (*mt-30*) chi angles: 291.5,165.2,93	0.064Å	-	-
A 656		LEU	50	-	Favored (70.92%) General / -71.6,-38.9	46.7% (*mt*) chi angles: 302.3,168.2	0.155Å	-	-
A 657		ARG	50	-	Favored (73.85%) General / -68.2,-45.2	82.7% (*mtm-85*) chi angles: 286.9,185.2,294.1,257.3	0.111Å	-	-
A 658		TYR	99.99	-	Favored (59.58%) General / -76.4,-17.0	18.1% (*m-30*) chi angles: 305.9,316.7	0.126Å	-	-
A 659		SER	50	-	Favored (45.62%) General / -79.6,-21.0	23.9% (*m*) chi angles: 285.3	0.062Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.75	Clashscore: 1.19	Outliers: 8 of 625	Poor rotamers: 5 of 555	Outliers: 13 of 594	Outliers: 0 of 627	Outliers: 6 of 627
A 660		GLY	50	-	Favored (32.94%) Glycine / 79.0,34.8	-	-	-	-
A 661		MET	50	-	Favored (74.54%) General / -69.0,-43.6	53.8% (*tpp*) chi angles: 193.3,66.3,72.4	0.094Å	-	-
A 662		MET	50	-	Favored (68.98%) General / -72.3,-37.6	41.4% (*mtt*) chi angles: 297.9,186.8,203.7	0.109Å	-	OUTLIER(worst is C-N-CA: 4.852 σ
A 663		GLU	50	-	Favored (96.54%) General / -62.4,-40.5	26.2% (*mp0*) chi angles: 307.3,80.5,341.7	0.087Å	-	OUTLIER(worst is CB-CG-CD 5.609 σ
A 664		THR	50	-	Favored (69.14%)	52.5% (*m*) chi angles: 295.6	0.035Å	-	-

A 665	ILE	50	-	General / -53.4,-44.8 Favored (14.53%) Isoleucine or valine / -77.3,-23.4	1.3% (*mt*) chi angles: 331.2,184.4	0.289Å	-	-
A 666	ARG	50	-	Favored (90.19%) General / -66.2,-40.4	63.7% (*mtt180*) chi angles: 293.9,174.4,180.4,120.9	0.151Å	-	-
A 667	ILE	50	-	Favored (41.2%) Isoleucine or valine / -67.1,-28.0	32.2% (*mm*) chi angles: 299.8,292.2	0.245Å	-	-
A 668	ARG	50	-	Favored (10.03%) General / -93.5,18.3	13.5% (*ttt180*) chi angles: 204.2,176.4,169,126.4	0.128Å	-	-
A 669	ARG	50	-	Favored (4.7%) General / -122.5,-25.6	53.5% (*mtp85*) chi angles: 297.1,160.5,71.9,99.9	0.104Å	-	-
A 670	ALA	50	-	Favored (7.48%) General / -122.7,-15.4	-	0.018Å	-	-
A 671	GLY	50	-	Favored (16.46%) Glycine / -109.2,172.7	-	-	-	-
A 672	TYR	50	-	Favored (4.29%) Pre-proline / -111.2,84.0	67.5% (*m-85*) chi angles: 303.8,85.8	0.062Å	-	-
A 673	PRO	50	-	Allowed (0.31%) Trans-proline / -73.1,32.8	3% (*Cg_exo*) chi angles: 354.8	0.055Å	-	-
A 674	ILE	50	-	Allowed (0.11%) Isoleucine or valine / -176.1,135.1	49.2% (*pt*) chi angles: 60.6,172.3	0.067Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 675		ARG 99.99	-		Favored (40.67%) General / -136.7,159.8	24.1% (*ptt-85*) chi angles: 55.1,179.2,194.6,289.7	0.059Å	-	-
A 676		TYR 99.99	-		Favored (4.64%) General / 53.8,24.8	25.9% (*p90*) chi angles: 68.2,79.9	0.196Å	-	-
A 677		SER 99.99	-		Favored (21.26%) General / -86.1,154.6	33.4% (*t*) chi angles: 183.6	0.025Å	-	-
A 678		PHE 99.99	-		Allowed (1.15%) General / -92.3,32.8	51% (*p90*) chi angles: 58.1,90	0.058Å	-	-
A 679		VAL 99.99	-		Favored (49.21%) Isoleucine or valine / -98.2,128.9	14.8% (*p*) chi angles: 63.9	0.121Å	-	OUTLIER(worst is C-N-CA: 4.241 σ
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.75	Clashscore: 1.19	Outliers: 8 of 625	Poor rotamers: 5 of 555	Outliers: 13 of 594	Outliers: 0 of 627	Outliers: 6 of 627
A 680		GLU 99.99	-		Favored (6.46%) General / -107.5,-36.5	1.1% (*pm0*) chi angles: 79.5,298.8,41.8	0.047Å	-	OUTLIER(worst is CB-CG-CD 5.464 σ
A 681		PHE 99.99	-		Allowed (0.16%) General / -68.5,11.7	14.3% (*p90*) chi angles: 66.4,74.5	0.13Å	-	-
A 682		VAL 99.99	-		Favored (41.58%) Isoleucine or valine / -134.5,160.2	5.9% (*p*) chi angles: 75.1	0.108Å	-	-
A 683		GLU 99.99	-		Favored (56.49%) General / -59.6,133.9	6.7% (*pm0*) chi angles: 50.3,275.1,47.7	0.052Å	-	-

A 684	ARG 50	-	Favored (7.28%) General / -156.6,128.4	26.2% (*ptt-85*) chi angles: 56.2,194.9,180,292	0.08Å	-	-
A 685	TYR 99.99	-	Allowed (0.3%) General / -92.6,-151.8	3% (*m-85*) chi angles: 281.3,39.6	0.225Å	-	OUTLIER(worst is C-CA-CB: 4.439 σ
A 686	ARG 99.99	-	-	60.5% (*mtp85*) chi angles: 285.9,181.5,57.3,70.2	0.055Å	-	-
z 687	MG 10.71	-	-	-	-	-	-

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