Viewing TIMP3_mb_24-199H-multi.table

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All-Atom Contacts	Clashscore, all atoms:	65.39		1st percentile* (N=1784, all resolutions)		
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.					
Protein Geometry	Poor rotamers	2	1.28%	Goal: <1%		
	Ramachandran outliers	2	1.15%	Goal: <0.05%		
	Ramachandran favored	161	92.53%	Goal: >98%		
	MolProbity score^	2.83		30th percentile* (N=27675, 0Å - 99Å)		
	Cβ deviations >0.25Å	0	0.00%	Goal: 0		
	Bad backbone bonds:	0 / 1478	0.00%	Goal: 0%		
	Bad backbone angles:	26 / 1985	1.31%	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: 90.85	Clashscore: 65.39	Outliers: 2 of 174	Poor rotamers: 2 of 156	Outliers: 0 of 161	Outliers: 0 of 176	Outliers: 24 of 176
24		CYS	87.04	0.561Å SG with 117 LEU HD12	-	24.6% (p) chi angles: 56.8	0.037Å	-	-
25		THR	24.62	0.44Å HG22 with 26 CYS N	Favored (50.42%) General / -127.8,147.7	94.5% (m) chi angles: 300	0.086Å	-	-
26		CYS	33.67	0.44Å N with 25 THR HG22	Favored (50.07%) General / -136.7,155.3	56.9% (m) chi angles: 305.9	0.105Å	-	-
27		SER	72.21	0.584Å HB3 with 28 PRO HD2	Favored (60.88%) Pre-proline / -84.4,152.4	75.5% (m) chi angles: 294.4	0.097Å	-	-
28		PRO	105.42	0.584Å HD2 with 27 SER HB3	Favored (78.91%) Trans-proline / -64.2,142.1	61.3% (Cg_endo) chi angles: 27.4	0.049Å	-	-

29	SER	74.32	-	Favored (34.42%) General / -138.2,134.3	47.9% (*t*) chi angles: 179.8	0.127Å	-	-
30	HIS	58.63	0.656Å CG with 31 PRO HD2	Favored (99.04%) Pre-proline / -66.5,146.4	55% (*t-80*) chi angles: 181.9,280.6	0.078Å	-	OUTLIER(S) worst is CD2-NE2-CE1: 4.427 σ
31	PRO	156.31	0.656Å HD2 with 30 HIS CG	Favored (97.9%) Trans-proline / -57.8,-34.2	15.5% (*Cg_endo*) chi angles: 16.6	0.166Å	-	-
32	GLN	55.77	0.509Å HE22 with 184 CYS HB3	Favored (87.17%) General / -66.8,-41.7	42.1% (*tt0*) chi angles: 174.5,181.7,309.3	0.139Å	-	-
33	ASP	43.92	0.812Å OD2 with 147 ILE HB	Favored (95.59%) General / -63.5,-39.9	70.4% (*m-20*) chi angles: 280.5,358.4	0.136Å	-	-
34	ALA	33.59	-	Favored (97.26%) General / -64.0,-41.8	-	0.095Å	-	-
35	PHE	114.34	-	Favored (75.19%) General / -60.0,-50.1	56.8% (*t80*) chi angles: 176.7,271.8	0.071Å	-	-
36	CYS	53.31	-	Favored (84.27%) General / -67.3,-38.0	73.6% (*m*) chi angles: 288.7	0.105Å	-	-
37	ASN	41.77	-	Favored (80.82%) General / -68.3,-37.8	97.3% (*m-20*) chi angles: 292.4,340.9	0.074Å	-	OUTLIER(S) worst is CA-CB-CG: 4.559 σ
38	SER	81.74	0.529Å OG with 105 THR HB	Favored (51.32%) General / -68.8,147.7	59.1% (*m*) chi angles: 299.3	0.087Å	-	-
39	ASP	52.85	1.178Å HB3 with 108 VAL HG13	Favored (69.73%) General / -70.7,-43.1	97.4% (*m-20*) chi angles: 289.3,347.5	0.046Å	-	OUTLIER(S) worst is CA-CB-CG: 4.685 σ
40	ILE	73.04	0.996Å HG13 with 108 VAL HG12	Favored (37.51%) Isoleucine or valine / -135.6,143.1	61.5% (*mt*) chi angles: 296.8,159.8	0.216Å	-	-
				Favored				

41	VAL	59.51	0.782Å HG22 with 105 THR HG22	(57.07%) Isoleucine or valine / -132.8,128.5	94.3% (*t*) chi angles: 178.2	0.106Å	-	-
42	ILE	65.65	1.095Å HD13 with 79 VAL HG11	Favored (15.23%) Isoleucine or valine / -144.3,160.6	46.8% (*pt*) chi angles: 61.1,170	0.109Å	-	-
43	ARG	90.42	-	Favored (51.03%) General / -103.7,128.5	77.7% (*ttt180*) chi angles: 176.5,182.6,179.6,178.9	0.132Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 90.85	Clashscore: 65.39	Outliers: 2 of 174	Poor rotamers: 2 of 156	Outliers: 0 of 161	Outliers: 0 of 176	Outliers: 24 of 176
44		ALA	60.08	-	Favored (37.58%) General / -157.6,164.1	-	0.092Å	-	-
45		LYS	77.06	-	Favored (50.18%) General / -127.4,149.2	59.3% (*pttt*) chi angles: 63.3,168.6,180,179.4	0.107Å	-	-
46		VAL	60.58	0.483Å HG21 with 95 LEU CD1	Favored (47.29%) Isoleucine or valine / -96.7,121.5	75.3% (*t*) chi angles: 174.1	0.083Å	-	-
47		VAL	58.57	-	Favored (27.35%) Isoleucine or valine / -77.2,-47.2	88.2% (*t*) chi angles: 175.2	0.061Å	-	-
48		GLY	32.55	-	Favored (32.62%) Glycine / -156.3,164.8	-	-	-	-
49		LYS	74.98	0.893Å HD2 with 60 LEU HD23	Favored (50.72%) General / -129.5,142.7	38.3% (*ttpt*) chi angles: 180.1,167.8,64.7,185.2	0.093Å	-	-
50		LYS	140.42	0.754Å O with 61 VAL HG12	Favored (18.96%) General / -154.2,140.9	8.1% (*tmtt?*) chi angles: 206.1,294.3,181.2,173.3	0.121Å	-	-
51		LEU	87.36	0.545Å N with 51 LEU HD22	Favored (32.95%) General /	2% (*mm?*) chi angles: 293.8,295	0.097Å	-	-

				-83.2,139.7				
52	VAL	94.01	-	Favored (42.98%) Isoleucine or valine / -131.9,159.6	27.6% (*m*) chi angles: 295.7	0.09Å	-	-
53	LYS	93.27	-	Favored (19.83%) General / -98.4,107.4	33.6% (*tttp*) chi angles: 195.9,165.6,190.9,79.5	0.092Å	-	-
54	GLU	74.44	0.714Å HG3 with 59 THR HG23	Favored (74.18%) General / -70.5,-38.5	62.9% (*mm-40*) chi angles: 290.1,282.3,344.6	0.103Å	-	-
55	GLY	69.23	-	Allowed (0.78%) Glycine / 173.5,-120.1	-	-	-	-
56	PRO	169.32	-	Favored (61.92%) Trans-proline / -64.7,-24.9	85.2% (*Cg_exo*) chi angles: 331.1	0.114Å	-	-
57	PHE	100.79	-	Favored (38.17%) General / -123.2,154.9	35.3% (*m-85*) chi angles: 278.1,83.4	0.116Å	-	OUTLIER(S) worst is CA-CB-CG: 6.761 σ
58	GLY	32.24	-	Favored (18.62%) Glycine / -101.6,151.7	-	-	-	-
59	THR	106.56	0.714Å HG23 with 54 GLU HG3	Favored (45.08%) General / -132.4,157.2	72.5% (*p*) chi angles: 61.8	0.091Å	-	-
60	LEU	94.77	0.893Å HD23 with 49 LYS HD2	Favored (35.41%) General / -81.8,136.5	8.1% (*mp*) chi angles: 285.1,58.9	0.111Å	-	-
61	VAL	101.03	0.754Å HG12 with 50 LYS O	Favored (60.52%) Isoleucine or valine / -111.6,119.7	7.2% (*p*) chi angles: 58.1	0.049Å	-	-
62	TYR	74.78	-	Favored (46.24%) General / -100.1,125.7	84.3% (*m-85*) chi angles: 292.1,283.5	0.165Å	-	-
63	THR	48.57	0.787Å HG1 with 81 TYR HE1	Favored (34.17%) General / -82.7,138.2	90.1% (*m*) chi angles: 302.6	0.117Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 90.85	Clashscore: 65.39	Outliers: 2 of 174	Poor rotamers: 2 of 156	Outliers: 0 of 161	Outliers: 0 of 176	Outliers: 24 of 176
64		ILE	69.94	0.655Å HD11 with 79 VAL HG13	Favored (34.05%) Isoleucine or valine / -135.9,163.7	28.3% (*pt*) chi angles: 63.9,163.1	0.138Å	-	-
65		LYS	143.03	-	Favored (26.86%) General / -111.2,114.0	0.7% chi angles: 191.5,293.9,180.7,70.6	0.107Å	-	-
66		GLN	74.08	0.654Å OE1 with 79 VAL HG12	Favored (16.91%) General / -79.3,112.8	34.1% (*tt0*) chi angles: 180,185.2,288.1	0.1Å	-	-
67		MET	58.46	-	Favored (62.82%) General / -71.7,-45.1	90.1% (*mtp*) chi angles: 294.9,185.5,70.3	0.067Å	-	-
68		LYS	56.72	-	Favored (17.04%) General / -160.4,149.3	82% (*tttt*) chi angles: 180.2,166.8,178.7,180.2	0.084Å	-	-
69		MET	64.5	0.805Å HE1 with 78 HIS HB2	Favored (29.25%) General / -114.8,116.8	33.3% (*ttm*) chi angles: 182.5,196.6,304.4	0.145Å	-	-
70		TYR	90.58	0.447Å CD1 with 135 LEU HB3	Favored (49.63%) General / -77.5,-38.3	96.4% (*m-85*) chi angles: 293.9,278.2	0.07Å	-	OUTLIER(S) worst is CA-CB-CG: 5.116 σ
71		ARG	127.32	-	Favored (25.9%) General / -163.1,163.5	12.8% (*ptm180*) chi angles: 60.2,168.2,294.3,139.4	0.112Å	-	-
72		GLY	41.79	-	Favored (20.68%) Glycine / 128.0,-166.2	-	-	-	-
73		PHE	122.39	0.857Å HB2 with 78 HIS NE2	Favored (4.9%) General / -51.9,149.5	39.8% (*m-85*) chi angles: 279.9,279.8	0.121Å	-	OUTLIER(S) worst is CA-CB-CG: 5.035 σ
74		THR	55.6	-	Favored (79.78%) General / -63.6,-35.2	86.4% (*m*) chi angles: 301.7	0.063Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
75		LYS	132.35	0.687Å O with 78 HIS HB2	Allowed (1.22%) General / -49.0,115.3	59.7% (*mttm*) chi angles: 292.5,167.7,174.2,290.7	0.07Å	-	-
76		MET	116.79	0.838Å HB2 with 77 PRO HD3	Favored (49.64%) Pre-proline / -66.6,-43.1	89.6% (*mmm*) chi angles: 296.5,292.8,279.9	0.061Å	-	-
77		PRO	219.45	0.838Å HD3 with 76 MET HB2	Favored (43.12%) Trans-proline / -68.6,-17.5	79.2% (*Cg_exo*) chi angles: 332.1	0.079Å	-	-
78		HIS	205.08	0.857Å NE2 with 73 PHE HB2	OUTLIER (0%) General / 15.3,-105.1	52.9% (*t-80*) chi angles: 198.2,289.8	0.215Å	-	OUTLIER(S) worst is CA-CB-CG: 4.647 σ
79		VAL	159.04	1.095Å HG11 with 42 ILE HD13	Favored (2.68%) Isoleucine or valine / -72.9,105.8	6.8% (*p*) chi angles: 55.7	0.055Å	-	-
80		GLN	124.01	-	Favored (18.26%) General / -84.5,-39.9	29.3% (*mm100*) chi angles: 302.1,299,117.4	0.087Å	-	-
81		TYR	64	0.896Å HD2 with 112 LYS HE2	Favored (50.93%) General / -134.2,149.2	86.8% (*m-85*) chi angles: 290.2,276.7	0.129Å	-	-
82		ILE	51.53	0.6Å HD13 with 104 LEU HD22	Favored (67.98%) Isoleucine or valine / -121.6,133.5	96% (*mt*) chi angles: 296,168.6	0.099Å	-	-
83		HIS	54.31	0.41Å CE1 with 61 VAL HG23	Favored (39.07%) General / -115.6,148.9	95.1% (*m-70*) chi angles: 294.8,275.1	0.092Å	-	OUTLIER(S) worst is CD2-NE2-CE1: 4.445 σ
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 90.85	Clashscore: 65.39	Outliers: 2 of 174	Poor rotamers: 2 of 156	Outliers: 0 of 161	Outliers: 0 of 176	Outliers: 24 of 176
84		THR	79.05	1.019Å HG21 with 93 LEU H	Favored (40.32%) General / -156.0,162.5	56% (*m*) chi angles: 304.5	0.118Å	-	-
85		GLU	113.79	0.926Å HG2 with 90 LEU CB	Favored (42.73%) General /	2.8% (*tp10*) chi angles: 194.2,82.4,322.9	0.087Å	-	-

				-70.4,153.7				
86	ALA	41.46	0.876Å HA with 60 LEU CD1	Favored (90.55%) General / -62.8,-38.4	-	0.078Å	-	-
87	SER	90.42	0.725Å OG with 90 LEU HD23	Favored (37.37%) General / -126.6,158.0	75% (*p*) chi angles: 70.6	0.117Å	-	-
88	GLU	77.54	-	Favored (69.88%) General / -66.5,-29.7	26% (*mm-40*) chi angles: 289.4,268.7,346	0.101Å	-	-
89	SER	83.47	-	Favored (75.85%) General / -57.6,-39.0	47.9% (*t*) chi angles: 179.4	0.116Å	-	OUTLIER(S) worst is C-N-CA: 4.844 σ
90	LEU	142.13	0.926Å CB with 85 GLU HG2	Favored (48.89%) General / -77.7,-5.0	2.7% (*mm?*) chi angles: 289.1,293.6	0.094Å	-	-
91	CYS	86.44	0.693Å HA with 117 LEU CD1	Allowed (0.56%) General / 78.6,25.1	38.6% (*m*) chi angles: 307.8	0.193Å	-	-
92	GLY	30.42	0.525Å O with 117 LEU HD21	Favored (53.41%) Glycine / -69.9,156.3	-	-	-	-
93	LEU	149.52	1.162Å HD23 with 117 LEU HD23	Favored (34.36%) General / -112.7,148.6	72.2% (*mt*) chi angles: 291,179.7	0.128Å	-	-
94	LYS	66.98	-	Favored (56.92%) General / -116.9,131.6	78.3% (*tttt*) chi angles: 191.9,164.6,180.1,180.4	0.081Å	-	-
95	LEU	55.69	0.483Å CD1 with 46 VAL HG21	Favored (48.83%) General / -116.2,140.9	80.6% (*mt*) chi angles: 293.5,180	0.101Å	-	-
96	GLU	123.61	0.777Å CG with 99 LYS HD2	Favored (41.23%) General / -76.3,142.5	8% (*tp10*) chi angles: 180.3,84.9,50.9	0.127Å	-	-
97	VAL	79.91	-	Favored (44.76%) Isoleucine or valine / -99.7,132.7	83.3% (*t*) chi angles: 174.8	0.072Å	-	OUTLIER(S) worst is C-N-CA: 7.149 σ

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
98		ASN 139.94		-	Favored (2.79%) General / 69.3,0.2	11.5% (*t-20*) chi angles: 192.3,244.3	0.072Å	-	OUTLIER(S) worst is CA-CB-CG: 5.452 σ
99		LYS 139.34		0.777Å HD2 with 96 GLU CG	Allowed (0.29%) General / -102.5,-97.4	60.4% (*mttm*) chi angles: 294.2,166.9,175.4,290.8	0.163Å	-	-
100		TYR 153		0.543Å CD2 with 123 ARG HD3	Favored (42.74%) General / -54.6,137.8	86.6% (*m-85*) chi angles: 290,87.3	0.115Å	-	-
101		GLN 53.55		-	Favored (35.15%) General / -98.8,139.0	75.4% (*mt-30*) chi angles: 302.4,179.9,25.5	0.123Å	-	-
102		TYR 63.45		-	Favored (51.74%) General / -130.8,150.9	95.8% (*m-85*) chi angles: 297.4,86.9	0.183Å	-	-
103		LEU 70.38		1.161Å HD23 with 120 PHE HE2	Favored (34.55%) General / -88.7,124.9	63% (*tp*) chi angles: 179.9,61.6	0.132Å	-	-

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			Avg: 90.85	Clashscore: 65.39	Outliers: 2 of 174	Poor rotamers: 2 of 156	Outliers: 0 of 161	Outliers: 0 of 176	Outliers: 24 of 176
104		LEU 136.9		0.6Å HD22 with 82 ILE HD13	Favored (35.15%) General / -130.7,125.9	42.5% (*tp*) chi angles: 185,66	0.097Å	-	-
105		THR 107.37		0.782Å HG22 with 41 VAL HG22	Favored (50.28%) General / -116.6,139.6	69.1% (*p*) chi angles: 62	0.073Å	-	-
106		GLY 28.54		-	Favored (36.65%) Glycine / -174.7,-169.4	-	-	-	-
107		ARG 124.72		0.711Å HB2 with 114 TYR CE2	Favored (25.95%) General / -87.1,146.8	70% (*mtt180*) chi angles: 283.8,195.6,170.3,200.4	0.142Å	-	-
108		VAL 160.6		1.178Å HG13 with 39 ASP HB3	Favored (4.66%) Isoleucine or valine / -82.8,149.3	27.5% (*m*) chi angles: 295.8	0.235Å	-	-

109	TYR 288.52	0.666Å HB3 with 112 LYS HB2	Allowed (1.1%) General / -145.1,-160.2	19.3% (*t80*) chi angles: 199.6,71.6	0.103Å	-	OUTLIER(S) worst is CA-CB-CG: 5.154 σ
110	ASP 170.04	-	Favored (8.47%) General / -89.4,90.8	54.5% (*t0*) chi angles: 188.8,7.6	0.116Å	-	OUTLIER(S) worst is CA-CB-CG: 4.741 σ
111	GLY 47.12	-	Favored (65.56%) Glycine / 72.7,5.9	-	-	-	-
112	LYS 124.47	0.896Å HE2 with 81 TYR HD2	Favored (44.88%) General / -124.2,150.7	34.5% (*mmtp*) chi angles: 298.4,299.3,179.6,67.8	0.132Å	-	-
113	MET 95.7	0.531Å CG with 82 ILE HG12	Favored (48.71%) General / -138.6,154.3	28% (*ptm*) chi angles: 62,181.8,286.5	0.073Å	-	-
114	TYR 174.78	0.711Å CE2 with 107 ARG HB2	Favored (53.01%) General / -124.4,134.9	4.6% (*p90*) chi angles: 38.7,271.2	0.152Å	-	-
115	THR 109.46	0.831Å CG2 with 93 LEU HD12	Favored (41.83%) General / -126.5,155.7	14.4% (*t*) chi angles: 189.6	0.082Å	-	-
116	GLY 30.15	-	Favored (22.17%) Glycine / -134.8,172.0	-	-	-	-
117	LEU 72.44	1.162Å HD23 with 93 LEU HD23	Favored (72.26%) General / -61.2,-32.5	96% (*mt*) chi angles: 295.5,175.7	0.119Å	-	-
118	CYS 60.2	-	Favored (65.51%) General / -67.6,-24.3	73.9% (*m*) chi angles: 298.4	0.079Å	-	-
119	ASN 108.88	0.528Å HD21 with 104 LEU HD12	Favored (7.56%) General / -67.2,170.1	6.7% (*p-10*) chi angles: 80.9,318.6	0.193Å	-	-
120	PHE 81.44	1.161Å HE2 with 103 LEU HD23	Favored (17.88%) General / -90.1,105.5	81.3% (*t80*) chi angles: 177.4,70.7	0.045Å	-	-
121	VAL 113.62	0.547Å O with 121	Favored (19.44%) Isoleucine or	7.3% (*p*)	0.047Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		VAL		HG13	valine / -135.1,116.0	chi angles: 57.9			
122		GLU	84.28	0.414Å OE2 with 120 PHE HZ	Favored (43.87%) General / -146.0,157.4	14.1% (*pt-20*) chi angles: 61.3,173.2,317	0.115Å	-	OUTLIER(S) worst is CB-CG-CD: 4.046 σ
123		ARG	119.98	0.543Å HD3 with 100 TYR CD2	Favored (57.38%) General / -62.6,143.3	43.2% (*ttp180*) chi angles: 180.1,178.5,59.8,228.7	0.067Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 90.85	Clashscore: 65.39	Outliers: 2 of 174	Poor rotamers: 2 of 156	Outliers: 0 of 161	Outliers: 0 of 176	Outliers: 24 of 176
124		TRP	73.59	-	Favored (98.6%) General / -62.3,-41.5	68.7% (*t-105*) chi angles: 177.1,262.6	0.094Å	-	-
125		ASP	92.66	-	Favored (70.81%) General / -64.5,-29.8	37.8% (*t0*) chi angles: 197.4,8.2	0.084Å	-	OUTLIER(S) worst is CA-CB-CG: 6.115 σ
126		GLN	63	0.462Å HG2 with 123 ARG HH21	Favored (69.76%) General / -67.7,-30.3	30.8% (*mt-30*) chi angles: 295.9,185,226	0.069Å	-	-
127		LEU	58.74	0.422Å HD11 with 103 LEU HD22	Favored (33.52%) General / -59.3,148.1	87.2% (*mt*) chi angles: 299.1,180.2	0.117Å	-	-
128		THR	31.01	0.586Å HG22 with 129 LEU N	Favored (28.08%) General / -77.3,161.4	88.1% (*m*) chi angles: 302	0.073Å	-	-
129		LEU	96.58	0.76Å H with 129 LEU HD12	Favored (95.24%) General / -60.0,-43.5	3.2% (*mp*) chi angles: 300.8,66.9	0.115Å	-	-
130		SER	39.87	-	Favored (84.01%) General / -65.7,-36.6	79.2% (*p*) chi angles: 59.6	0.058Å	-	-
131		GLN	49.96	-	Favored (93.52%) General / -62.7,-45.3	98.1% (*mt-30*) chi angles: 294.7,180,322.5	0.056Å	-	-
					Favored (78.57%)	51.5% (*mtp180*)			

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
132		ARG	92.2	-	General / -62.5,-48.7	chi angles: 291.5,173,56.3,226.2	0.097Å	-	-
133		LYS	78.98	0.574Å HD3 with 129 LEU O	Favored (78.71%) General / -64.2,-34.7	14.2% (mptt) chi angles: 281.3,68.1,175.9,179.4	0.087Å	-	-
134		GLY	45.26	-	Favored (70.44%) Glycine / -62.2,-28.3	-	-	-	-
135		LEU	68.72	0.447Å HB3 with 70 TYR CD1	Favored (74.48%) General / -60.9,-34.4	80.6% (mt) chi angles: 293.8,180.2	0.072Å	-	-
136		ASN	90.91	-	Allowed (0.07%) General / -65.4,-77.1	82% (m-20) chi angles: 292.1,310.6	0.063Å	-	OUTLIER(S) worst is CA-CB-CG: 5.376 σ
137		TYR	120.25	0.937Å CE2 with 141 LEU HD21	Favored (5.91%) General / -99.2,-45.4	32.2% (t80) chi angles: 196.4,79.6	0.046Å	-	-
138		ARG	171.25	-	Favored (82.48%) General / -62.4,-47.8	66.4% (mtp180) chi angles: 281.9,189.7,66.3,199.1	0.133Å	-	-
139		TYR	84.64	0.448Å CD1 with 32 GLN HB2	Favored (84.32%) General / -63.3,-36.6	48.2% (m-85) chi angles: 285.6,294.7	0.128Å	-	-
140		HIS	77.69	-	Favored (66.63%) General / -56.4,-34.2	59.3% (t-80) chi angles: 183.2,276.9	0.073Å	-	OUTLIER(S) worst is CD2-NE2-CE1: 4.427 σ
141		LEU	74.98	0.937Å HD21 with 137 TYR CE2	Favored (73.65%) General / -61.2,-33.5	85.2% (mt) chi angles: 295.4,180.1	0.1Å	-	OUTLIER(S) worst is C-N-CA: 4.696 σ
142		GLY	92.26	-	Favored (83.4%) Glycine / -78.6,-13.2	-	-	-	-
143		CYS	83.31	-	Favored (62.81%) General / -59.9,-22.8	89.8% (m) chi angles: 291.8	0.133Å	-	-

Avg: Clashscore: Outliers: 2 of   Poor rotamers: 2 of   Outliers: Outliers: Outliers: 24

		90.85	65.39	174	156	0 of 161	0 of 176	of 176
144	ASN	64.15	-	Favored (61.29%) General / -72.7,-25.5	88.1% (*m-20*) chi angles: 296.5,321.1	0.104Å	-	OUTLIER(S) worst is CA-CB-CG: 4.412 σ
145	CYS	62.39	0.696Å O with 146 LYS HE2	Favored (17.89%) General / -83.9,166.5	48.4% (*m*) chi angles: 307	0.108Å	-	-
146	LYS	118.21	0.696Å HE2 with 145 CYS O	Favored (55.37%) General / -120.5,133.7	11.3% (*mmpt?*) chi angles: 300.4,296.9,92.6,166.6	0.152Å	-	-
147	ILE	52.19	0.812Å HB with 33 ASP OD2	Favored (50.9%) Isoleucine or valine / -104.4,118.0	96.9% (*mt*) chi angles: 295.1,170.6	0.056Å	-	-
148	LYS	136.5	-	Favored (53.87%) General / -109.0,132.7	14.8% (*tppt?*) chi angles: 192,69.2,66.8,182.2	0.102Å	-	-
149	SER	33.26	-	Favored (34.96%) General / -79.5,143.3	66.9% (*m*) chi angles: 296.4	0.082Å	-	-
150	CYS	59	-	Favored (8.36%) General / -103.1,98.4	17.7% (*t*) chi angles: 170.8	0.104Å	-	-
151	TYR	151.36	0.778Å HD1 with 152 TYR HD1	Favored (80.94%) General / -62.3,-48.2	36.2% (*p90*) chi angles: 52.2,88.7	0.074Å	-	-
152	TYR	106.76	0.778Å HD1 with 151 TYR HD1	Favored (27.69%) General / -148.9,146.0	85% (*m-85*) chi angles: 291.7,83.3	0.104Å	-	-
153	LEU	148.26	0.868Å CD1 with 154 PRO HA	Favored (90.48%) Pre-proline / -64.6,152.1	46% (*tp*) chi angles: 182.7,67.7	0.101Å	-	-
154	PRO	251.89	0.868Å HA with 153 LEU CD1	Allowed (1.71%) Cis-proline / -70.0,-38.3	61.3% (*Cg_exo*) chi angles: 334.2	0.234Å	-	-
155	CYS	114.23	-	OUTLIER (0%) General / 53.0,155.4	29.5% (*p*) chi angles: 62.4	0.168Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
156		PHE	62.6	0.4Å C with 156 PHE CD1	Favored (24.06%) General / -153.4,169.1	53.1% (*p90*) chi angles: 60.2,88	0.092Å	-	OUTLIER(S) worst is CA-CB-CG: 6.694 σ
157		VAL	119.76	0.678Å HG13 with 164 LEU HG	Favored (51.56%) Isoleucine or valine / -118.5,137.7	28.1% (*m*) chi angles: 295.4	0.143Å	-	-
158		THR	120.05	0.615Å HG22 with 162 GLU OE2	Favored (38.62%) General / -76.0,-44.5	14.5% (*t*) chi angles: 187	0.059Å	-	-
159		SER	98.45	0.589Å OG with 162 GLU HG3	Favored (19.98%) General / -112.0,158.1	81.4% (*p*) chi angles: 60.5	0.081Å	-	-
160		LYS	87.8	0.528Å HB2 with 191 TYR HD1	Favored (81.83%) General / -64.5,-35.7	53.6% (*pttt*) chi angles: 55.2,168.7,178.7,180.7	0.072Å	-	-
161		ASN	109.24	-	Allowed (1.1%) General / -91.0,42.3	38.5% (*p-10*) chi angles: 61.1,341.1	0.086Å	-	OUTLIER(S) worst is CA-CB-CG: 4.627 σ
162		GLU	94.39	0.615Å OE2 with 158 THR HG22	Favored (51%) General / -124.4,142.8	47.7% (*mt-10*) chi angles: 285.2,183.7,43.4	0.171Å	-	-
163		CYS	93.79	0.722Å SG with 147 ILE HG12	Favored (46.98%) General / -115.7,142.2	1% chi angles: 35.2	0.055Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 90.85	Clashscore: 65.39	Outliers: 2 of 174	Poor rotamers: 2 of 156	Outliers: 0 of 161	Outliers: 0 of 176	Outliers: 24 of 176
164		LEU	159.07	0.678Å HG with 157 VAL HG13	Favored (42.08%) General / -97.3,125.8	31.9% (*mt*) chi angles: 283.3,180.3	0.148Å	-	-
165		TRP	88.16	-	Favored (17.13%) General / -88.0,104.9	10.7% (*t90*) chi angles: 187,12.3	0.088Å	-	-
166		THR	146.47	0.634Å O with 169 LEU HG	Favored (46.84%) General / -79.5,-20.6	72.4% (*p*) chi angles: 63.7	0.07Å	-	-

167	ASP 63.4	-	Favored (63.75%) General / -51.9,-44.6	97.1% (*m-20*) chi angles: 286.4,344.7	0.093Å	-	-
168	MET 113.01	0.544Å HE1 with 151 TYR HA	Favored (96.22%) General / -62.9,-44.4	27.8% (*ptm*) chi angles: 64.2,186.2,290.8	0.05Å	-	-
169	LEU 115.51	0.768Å HD12 with 170 SER N	Favored (91.85%) General / -65.9,-41.2	3.2% (*pp*) chi angles: 70.9,76.6	0.056Å	-	-
170	SER 102.96	0.768Å N with 169 LEU HD12	Allowed (0.73%) General / -76.0,-66.9	48.5% (*t*) chi angles: 179.5	0.071Å	-	-
171	ASN 108.78	-	Favored (56.89%) General / -77.0,-31.9	8.3% (*m120*) chi angles: 296.5,164.8	0.075Å	-	OUTLIER(S) worst is CA-CB-CG: 4.345 σ
172	PHE 244.03	-	Favored (12.32%) General / 65.1,28.9	0.7% chi angles: 250.8,276.5	0.162Å	-	OUTLIER(S) worst is CA-CB-CG: 7.581 σ
173	GLY 58.61	-	Favored (6.91%) Glycine / -137.6,134.3	-	-	-	-
174	TYR 76.33	0.548Å HB2 with 175 PRO HD3	Favored (6.75%) Pre-proline / -70.1,-36.9	95.6% (*m-85*) chi angles: 299.8,277.8	0.073Å	-	-
175	PRO 122.45	0.548Å HD3 with 174 TYR HB2	Allowed (0.54%) Trans-proline / -84.2,29.7	12.9% (*Cg_endo*) chi angles: 15.7	0.158Å	-	-
176	GLY 48.47	-	Allowed (1.66%) Glycine / -69.1,-158.8	-	-	-	-
177	TYR 52.75	0.85Å HE2 with 182 TYR HE1	Favored (90.25%) General / -62.2,-46.1	47.1% (*t80*) chi angles: 191.5,84.9	0.064Å	-	-
178	GLN 48.21	-	Favored (90.31%) General / -65.9,-39.1	98.5% (*mt-30*) chi angles: 292.1,180.2,337.2	0.071Å	-	-

Favored

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
179		SER	79.57	0.481Å HA with 30 HIS NE2	(95.64%) General / -62.4,-44.8	47.7% (*t*) chi angles: 179.9	0.089Å	-	-
180		LYS	75.92	-	Favored (13.63%) General / -71.9,-53.3	93.9% (*mttt*) chi angles: 286.7,172.4,173.2,180	0.104Å	-	-
181		HIS	111.5	-	Favored (22.16%) General / -89.2,-24.4	85.8% (*m-70*) chi angles: 286.2,276.5	0.175Å	-	OUTLIER(S) worst is CD2-NE2-CE1: 4.409 σ
182		TYR	139.21	0.85Å HE1 with 177 TYR HE2	Favored (30.51%) General / -115.3,153.7	39.6% (*m-85*) chi angles: 281.2,77.7	0.118Å	-	-
183		ALA	48.48	-	Favored (49.69%) General / -127.8,150.8	-	0.1Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 90.85	Clashscore: 65.39	Outliers: 2 of 174	Poor rotamers: 2 of 156	Outliers: 0 of 161	Outliers: 0 of 176	Outliers: 24 of 176
184		CYS	86.29	0.509Å HB3 with 32 GLN HE22	Favored (18.67%) General / -101.4,107.4	34.8% (*t*) chi angles: 189	0.194Å	-	-
185		ILE	63.28	-	Favored (32.61%) Isoleucine or valine / -115.7,141.5	70.6% (*mt*) chi angles: 300.7,165.1	0.058Å	-	-
186		ARG	108.61	-	Favored (35.83%) General / -89.6,131.0	21.4% (*ttp180*) chi angles: 191,195.8,92.3,177.5	0.105Å	-	-
187		GLN	99.28	-	Favored (9.66%) General / -101.1,168.3	21.9% (*mm100*) chi angles: 301.5,303.7,141.5	0.087Å	-	-
188		LYS	49.14	-	Favored (54.47%) General / -64.4,134.4	91.7% (*mttt*) chi angles: 287.8,167.1,177.9,176.7	0.06Å	-	-
189		GLY	28.93	-	Favored (8.43%) Glycine / 121.5,-19.9	-	-	-	-
					Favored				

190	GLY	31.66	-	(70.77%) Glycine / 91.6,1.8	-	-	-	-	-
191	TYR	104.98	0.528Å HD1 with 160 LYS HB2	Favored (24.7%) General / -93.5,145.2	83.1% (*t80*) chi angles: 183,79.7	0.079Å	-	-	-
192	CYS	93.22	0.48Å SG with 184 CYS SG	Favored (35.55%) General / -118.9,152.8	3.9% (*t*) chi angles: 205.1	0.052Å	-	-	-
193	SER	81.29	0.439Å HG with 191 TYR HE2	Favored (43.04%) General / -152.9,160.5	68.5% (*m*) chi angles: 298	0.104Å	-	-	-
194	TRP	72.7	0.414Å CE3 with 182 TYR HB3	Favored (35.79%) General / -81.3,137.8	99.8% (*m95*) chi angles: 292.5,103.5	0.117Å	-	-	-
195	TYR	58.89	-	Favored (46.22%) General / -133.8,139.3	93.3% (*m-85*) chi angles: 293.1,279.8	0.092Å	-	-	-
196	ARG	181.87	-	Favored (58.17%) General / -77.7,-16.8	5.9% (*ptm-85*) chi angles: 64.3,178,317.5,282.5	0.208Å	-	-	-
197	GLY	39.02	-	Favored (5.19%) Glycine / 105.3,123.3	-	-	-	-	-
198	TRP	57.26	-	Favored (35.54%) General / -79.1,130.5	66.8% (*t90*) chi angles: 171.1,89.7	0.103Å	-	-	-
199	ALA	21.42	-	-	-	0.117Å	-	-	-

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