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All-Atom	Clashscore, all atoms: 108.54			0 th percentile* (N=1784, all resolutions)		
Contacts	Clashscore is the number	r of serious steric over		·laps (> 0.4 Å) per 1000 atoms.		
	Poor rotamers	3	2.78%	Goal: <1%		
	Ramachandran outliers 3 2.		2.46%	Goal: <0.05%		
II I	Ramachandran favored	110 90.16%		Goal: >98%		
Protein Geometry	MolProbity score [^]	3.38		11 th percentile* (N=27675, 0Å - 99Å)		
	Cβ deviations >0.25Å	1	0.86%	Goal: 0		
	Bad backbone bonds:	0 / 1008	0.00%	Goal: 0%		
	Bad backbone angles:	17 / 1367	1.24%	Goal: <0.1%		

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

[^] 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 F	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg:	Clashscore:	Outliers: 3 of	Poor rotamers: 3 of	Outliers:	Outliers:	Outliers: 17
			121.40	108.54	122	108	1 of 116	0 of 124	of 124
48	C	GLY	19.77	0.449Å HA3 with 141 VAL HG11	-	-	-	-	-
49	A	SP	40.91	-	Favored (43.47%) General / -69.5,153.5	85.9% (<i>m-20</i>) chi angles: 288.6,333.4	0.095Å	-	-
50	V	'AL	40.19	0.609Å HG23 with 169 ARG HH11	Favored (28.7%) Isoleucine or valine / -93.0,135.1	91% (<i>t</i>) chi angles: 175.4	0.098Å	-	-
51	L	EU	89.53	0.837Å HB3 with 108 ILE HD11	Favored (56.22%) General / -113.8,131.5	1.9% (<i>mm</i> ?) chi angles: 294.3,294.6	0.092Å	-	-

^{* 100&}lt;sup>th</sup> 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.

52	GLU 66.24 -	Favored (39.97%) General / -116.6,120.8	76.4% (tt0) chi angles: 179.2,189.9,357	0.162Å	-	-
53	0.928Å VAL 115.58 CG1 with 60 HIS HB3	Favored (31.14%) Pre-proline / -113.0,124.7	14.4% (p) chi angles: 64.4	0.073Å	-	-
54	0.534Å PRO 97.7 HD2 with 107 SER O	Favored (9.96%) Trans-proline / -74.8,126.2	7.5% (<i>Cg_endo</i>) chi angles: 9.8	0.181Å	-	-
55	0.61Å ARG 94.79 HB2 with 58 LEU O	Favored (10.62%) General / -116.7,168.0	12% (<i>mmt-85</i>) chi angles: 294,255.5,178.2,260	0.144Å	-	-
56	0.562Å THR 125.76 O with 56 THR HG23	Favored (2.21%) General / -68.5,105.5	9.1% (<i>t</i>) chi angles: 180.1	0.076Å	-	-
57	0.786Å HIS 102.68 C with 58 LEU HD12	Favored (22.09%) General / 58.5,32.4	32.4% (<i>t-80</i>) chi angles: 196.2,262.9	0.122Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.427 σ
58	0.786Å LEU 109.81 HD12 with 57 HIS C	Favored (21.73%) General / -148.5,137.6	6.9% (<i>mp</i>) chi angles: 289.8,66	0.15Å	-	-
59	0.455Å THR 133.72 O with 59 THR HG23	Favored (49.83%) General / -108.0,135.2	11% (<i>t</i>) chi angles: 184.6	0.086Å	-	-
60	0.928Å HIS 72.48 HB3 with 53 VAL CG1	Favored (55.5%) General / -115.5,134.0	73% (<i>t60</i>) chi angles: 187.6,77.4	0.064Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.329 σ
61	0.612Å TYR 127.89 CE1 with 162 GLU HG2	Favored (40.89%) General / -116.6,148.5	39.7% (<i>m-85</i>) chi angles: 281.4,77.4	0.112Å	-	-
62	GLY 40.23 -	Favored (28.8%) Glycine / -148.4,171.4	-	-	-	-
63	0.675Å ILE 59.43 O with 70 VAL HB	Favored (58.49%) Isoleucine or valine /	18.7% (tt) chi angles: 193,165.1	0.052Å	-	-

64	TYR	91.16	0.834Å HA with 70 VAL HG12	-129.5,136.8 Favored (20.55%) General / -82.4,114.0	69.9% (<i>t80</i>) chi angles: 186.6,79.4	0.063Å	-	-
65	LEU	181.96	0.676Å HD21 with 146 GLU OE2	Favored (29.59%) General / -84.0,-25.8	54.6% (<i>tp</i>) chi angles: 180.4,66.1	0.095Å	-	-
66	GLY	43.05	0.602Å HA2 with 64 TYR CE2	Favored (17.44%) Glycine / 112.1,165.8	-	-	-	-
67	ASP	62.4	-	Favored (20.4%) General / 60.0,31.0	25.7% (<i>t0</i>) chi angles: 190.8,43.7	0.07Å	-	-
# .	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C β deviation	Bond lengths	Bond angles
		Avg: 121.40	Clashscore: 108.54	Outliers: 3 of 122	Poor rotamers: 3 of 108		Outliers:	Outliers: 17 of 124
68	ASN	105.13	0.761Å OD1 with 99 LEU HD23	Favored (10.35%) General / 66.6,23.4	54.4% (<i>t30</i>) chi angles: 195.1,49.8	0.045Å	-	OUTLIER(S) worst is CA- CB-CG: 4.195 σ
69	ARG	70.79	0.642Å HG2 with 97 LEU HD23	Favored (40.62%) General / -119.5,150.2	95.4% (<i>mtt-85</i>) chi angles: 297.8,178.8,180.1,274.4	0.16Å	-	-
70	VAL	103.07	1.115Å HG22 with 98 ILE HB	Favored (22.24%) Isoleucine or valine / -129.7,168.7	13% (<i>m</i>) chi angles: 306.9	0.197Å	-	-
71	ALA	56.32	-	Favored (50.92%) General / -112.3,137.1	-	0.104Å	-	-
72	HIS	105.13	0.573Å CD2 with 98 ILE HD11	Favored (6.2%) General / -156.9,-176.8	0.7% chi angles: 63,172.1	0.121Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.43 σ
73	MET	100.8	0.601Å HE1 with 161 CYS CA	Favored (25.36%) General / -94.0,144.6	55.9% (<i>mtm</i>) chi angles: 297.8,185.1,304.9	0.136Å	-	-
			0.717Å	Favored	2.3% (ttt)			

74	MET 162.56	HB3 with 92 VAL CG1	(8.58%) Pre-proline / -115.4,168.3	chi angles: 222.6,178.6,178.1	0.139Å	-	-
75	PRO 169.97	0.689Å CD with 74 MET HG2	Allowed (0.1%) Trans-proline / -33.7,118.1	47.9% (<i>Cg_exo</i>) chi angles: 337.1	0.233Å	-	OUTLIER(S) worst is C-N- CA: 5.886 σ
76	ASP 306.78	1.065Å HB3 with 91 VAL HG12	Allowed (0.12%) General / -174.9,110.0	14.9% (<i>t0</i>) chi angles: 167.5,10.4	0.19Å	-	-
77	ILE 145.25	0.751Å CG2 with 80 ALA HB3	Favored (74.63%) Isoleucine or valine / -123.6,128.6	15.9% (tt) chi angles: 180,165.9	0.08Å	-	-
78	LEU 139.88	0.544Å C with 78 LEU HD13	Favored (69.81%) General / -67.6,-47.4	3.2% (<i>tm</i> ?) chi angles: 181.7,288.5	0.049Å	-	-
79	LEU 138.96	0.661Å O with 79 LEU HD23	Favored (79.25%) General / -68.0,-43.3	3.4% (tt) chi angles: 194,179.9	0.056Å	-	-
80	ALA 216.28	0.751Å HB3 with 77 ILE CG2	Favored (30.74%) General / -59.5,149.1	-	0.116Å	-	-
81	LEU 209.12	-	Favored (4.51%) General / -102.4,178.7	58.3% (<i>mt</i>) chi angles: 295.8,185.3	0.14Å	-	-
82	THR 185.98	-	Favored (8.47%) General / -67.1,116.9	99% (<i>m</i>) chi angles: 298.4	0.087Å	-	-
83	ASP 215.57	-	Allowed (0.27%) General / -122.4,-124.5	40.4% (<i>p30</i>) chi angles: 54.6,6.2	0.037Å	-	-
84	ASP 231.79	-	Favored (24.31%) General / -66.7,161.0	20% (<i>p-10</i>) chi angles: 65.4,325.5	0.106Å	-	OUTLIER(S) worst is CA- CB-CG: 4.122 σ
85	MET 286.26	0.89Å HA with 85 MET HE3	Favored (19.45%) General / -67.4,164.0	3.2% (<i>tpt</i>) chi angles: 186.4,73.3,282.5	0.092Å	-	-
		0.571Å	Favored				

86	GLY	65.7	N with 85 MET HG3	(26.81%) Glycine / 108.9,-21.8	-	-	-	-
87	ARG	191.23	-	Favored (40.07%) General / -93.8,129.7	80.1% (<i>mmt-85</i>) chi angles: 290.5,303.4,176,272.1	0.076Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C β deviation	Bond lengths	Bond angles
		Avg: 121.40	Clashscore: 108.54	Outliers: 3 of 122	Poor rotamers: 3 of 108		Outliers: 0 of 124	Outliers: 17 of 124
88	THR	152.15	0.551Å HG23 with 90 LYS H	Favored (4.23%) General / -145.9,-173.7	10.6% (<i>t</i>) chi angles: 192.4	0.066Å	-	-
89	GLN	104.76	-	Favored (79.01%) General / -68.8,-37.3	8.7% (<i>tt0</i>) chi angles: 186.2,179.7,184.7	0.057Å	-	-
90	LYS	93.54	1.062Å HD3 with 156 LEU HG	Favored (17.66%) General / -115.5,162.1	88.8% (<i>mttt</i>) chi angles: 280.6,174.2,172.1,179.8	0.184Å	-	-
91	VAL	144.05	1.065Å HG12 with 76 ASP HB3	Favored (3.48%) Isoleucine or valine / -104.5,165.4	14.5% (<i>m</i>) chi angles: 306.3	0.265Å	-	-
92	VAL	109.11	0.717Å CG1 with 74 MET HB3	Favored (51.14%) Isoleucine or valine / -123.0,139.0	12.3% (p) chi angles: 62.3	0.091Å	-	-
93	SER	100.09	-	Favored (37.2%) General / -78.7,135.7	48.3% (t) chi angles: 179.6	0.076Å	-	-
94	ASN	89.7	0.46Å HB2 with 74 MET SD	Favored (49.29%) General / -138.1,154.2	47% (<i>t30</i>) chi angles: 195.2,14.7	0.113Å	-	OUTLIER(S) worst is CA- CB-CG: 4.44 σ
95	LYS	199.01	0.905Å CG with 149 LEU HD12	Favored (55.81%) General / -113.0,131.3	1.2% (mmmm) chi angles: 269.9,283.5,310.7,312.1	0.185Å	-	-
96	ARG	120.86	0.585Å HG2 with 97	Favored (10.4%) General /	77.2% (<i>ttt180</i>) chi angles:	0.086Å	-	-

		LEU N	-160.8,177.4	188.2,179,182.3,186.1			
97	LEU 114.45	0.642Å HD23 with 69 ARG HG2	Favored (3.53%) General / -79.6,61.3	76.5% (<i>mt</i>) chi angles: 292.1,179.9	0.168Å	-	-
98	ILE 102.18	1.115Å HB with 70 VAL HG22	Favored (49.17%) Isoleucine or valine / -62.4,-30.5	76.3% (<i>mt</i>) chi angles: 292,163.2	0.125Å	-	-
99	LEU 118.92	0.761 Å HD23 with 68 ASN OD1	Allowed (0.94%) General / -60.6,-64.5	27.5% (<i>tp</i>) chi angles: 190.5,60.2	0.075Å	-	-
100	GLY 45.65	-	Favored (11.45%) Glycine / -74.1,-50.0	-	-	-	-
101	VAL 48.1	0.524Å HG11 with 96 ARG CZ	Favored (47.64%) Isoleucine or valine / -68.4,-51.4	92.1% (<i>t</i>) chi angles: 178	0.052Å	-	-
102	ILE 111.72	1.01Å HG12 with 98 ILE HA	Favored (89.63%) Isoleucine or valine / -65.8,-41.1	31.1% (<i>mm</i>) chi angles: 292.3,298.7	0.115Å	-	-
103	VAL 69.6	0.558Å HG12 with 106 ALA O	Favored (91.53%) Isoleucine or valine / -65.9,-45.3	70.8% (t) chi angles: 179.4	0.082Å	-	-
104	LYS 147.47	0.74Å HG2 with 105 VAL H	Allowed (0.71%) General / 58.1,-141.9	30.1% (<i>ttmt</i>) chi angles: 196.4,163,288.2,180.4	0.056Å	-	-
105	VAL 48.5	0.74Å H with 104 LYS HG2	Favored (73.48%) Isoleucine or valine / -62.7,-36.0	91.7% (t) chi angles: 175.5	0.053Å	-	-
106	ALA 47.63	0.558Å O with 103 VAL HG12	Favored (33.7%) General / -65.2,155.9	-	0.08Å	-	-
107	SER 34.83	0.534Å O with 54 PRO HD2	Favored (15.43%) General / -88.6,164.2	72.3% (<i>m</i>) chi angles: 293.6	0.108Å	-	-
# Al	t Res High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles

	Avg: 121.40	Clashscore: 108.54	Outliers: 3 of 122	Poor rotamers: 3 of 108		Outliers: 0 of 124	Outliers: 17 of 124
108	ILE 149.89	0.842Å HD13 with 109 ARG N	Favored (28.12%) Isoleucine or valine / -138.3,145.6	0% chi angles: 193.3,289.6	0.07Å	-	-
109	ARG 71.55	0.842Å N with 108 ILE HD13	Favored (51.93%) General / -135.2,152.8	31.3% (<i>ptt-85</i>) chi angles: 63.2,185.8,194.6,266.6	0.101Å	-	-
110	VAL 110.2	0.401Å O with 110 VAL HG23	Favored (29.22%) Isoleucine or valine / -80.0,133.7	13% (<i>m</i>) chi angles: 288.6	0.115Å	-	-
111	ASP 70.98	-	Favored (2.04%) General / -139.9,85.7	45.7% (<i>t0</i>) chi angles: 193.1,344.2	0.097Å	-	-
112	THR 83.35	0.733Å HG21 with 115 ASP OD2	Favored (6.37%) General / -90.6,86.4	62.2% (<i>m</i>) chi angles: 303.7	0.084Å	-	-
113	VAL 63.91	-	Favored (77.4%) Isoleucine or valine / -58.6,-50.9	97.8% (<i>t</i>) chi angles: 176.3	0.057Å	-	-
114	GLU 108.53	0.971Å HB2 with 170 TYR CZ	Favored (59.87%) General / -73.7,-23.8	78.5% (<i>mm-40</i>) chi angles: 290.5,301.9,320.1	0.116Å	-	-
115	ASP 58.89	0.733Å OD2 with 112 THR HG21	Favored (70.31%) General / -56.1,-38.2	86.8% (<i>m-20</i>) chi angles: 284.2,352.7	0.076Å	-	OUTLIER(S) worst is CA- CB-CG: 5.794 σ
116	PHE 51.85	0.407Å CG with 117 ALA N	Favored (96.77%) General / -63.1,-40.1	31.8% (<i>p90</i>) chi angles: 73.3,87.4	0.09Å	-	-
117	ALA 39.75	0.407Å N with 116 PHE CG	Favored (72.31%) General / -60.7,-50.7	-	0.106Å	-	-
118	TYR 96.87	0.658Å O with 115 ASP HA	Favored (39.96%) General / -156.5,160.9	1.7% (<i>t80</i>) chi angles: 214.9,282.3	0.083Å	-	OUTLIER(S) worst is CA- CB-CG: 5.344 σ

119	GLY 43.94	0.528Å HA2 with 134 LYS HG3	Favored (29.41%) Glycine / 103.3,-24.7	-	-	-	-
120	ALA 207	-	Favored (40.77%) General / -74.3,149.3	-	0.109Å	-	-
121	ASN 172.2	-	Favored (51.1%) General / -107.7,134.1	90.2% (<i>m-20</i>) chi angles: 293.5,345.3	0.072Å	-	OUTLIER(S) worst is CA- CB-CG: 5.269
122	ILE 130.78	0.483Å O with 122 ILE HG23	Favored (68.73%) Isoleucine or valine / -111.6,127.5	10.2% (<i>tp</i>) chi angles: 188.7,68.1	0.064Å	-	-
123	LEU 105.23	0.536Å O with 123 LEU HD13	Favored (89.47%) General / -63.0,-46.1	3.1% (<i>tm</i> ?) chi angles: 187.9,290.6	0.058Å	-	-
124	VAL 97.35	0.451Å HG23 with 126 HIS ND1	Favored (4.02%) Isoleucine or valine / -97.0,152.1	22% (<i>m</i>) chi angles: 293	0.079Å	-	-
125	ASN 150.15	-	Favored (9.28%) General / -74.2,111.4	52.1% (<i>m-80</i>) chi angles: 294.3,273.3	0.091Å	-	OUTLIER(S) worst is CA- CB-CG: 4.781 σ
126	HIS 200.48	0.451Å ND1 with 124 VAL HG23	Allowed (0.26%) General / -134.3,-98.1	1.9% (<i>m80</i>) chi angles: 261.3,96	0.134Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.491 σ
127	LEU 275.59	1.119Å HD11 with 129 GLU HG3	Favored (2.52%) General / -58.7,114.5	58.3% (<i>tp</i>) chi angles: 182,63.5	0.106Å	-	-
# Al	t Res High B	Clash > 0.4Å	Ramachandran	Rotamer	C β deviation	Bond lengths	Bond angles
	Avg: 121.40	Clashscore: 108.54	Outliers: 3 of 122	Poor rotamers: 3 of 108	Outliers: 1 of 116		Outliers: 17 of 124
128	ASP 178.19	-	Allowed (1.41%) General / -139.8,65.9	67.5% (<i>t0</i>) chi angles: 184.2,353.7	0.146Å	-	OUTLIER(S) worst is CA- CB-CG: 4.402
		1.119Å	Favored	99.2% (mt-10)			

129	GLU 91.62	HG3 with 127 LEU HD11	(45.94%) General / -60.8,-54.4	chi angles: 291,174.4,353.8	0.107Å	-	-
130	SER 195.77	0.496Å HB3 with 129 GLU O	OUTLIER (0.01%) General / 160.3,178.5	91.5% (<i>p</i>) chi angles: 62.8	0.136Å	-	-
131	LEU 240.75	0.438Å HB2 with 130 SER O	Allowed (0.06%) General / 69.0,147.0	79.4% (<i>mt</i>) chi angles: 301.6,181.7	0.071Å	-	-
132	GLN 252.3	0.44Å O with 133 LYS HE3	Favored (37.6%) General / -103.3,118.8	9.4% (tt0) chi angles: 184.6,179.8,197.5	0.101Å	-	-
133	LYS 320.84	0.596Å O with 134 LYS HB2	Favored (13.53%) General / -145.9,172.3	0% chi angles: 199.6,65.9,30.4,66.4	0.112Å	-	-
134	LYS 153.7	0.596Å HB2 with 133 LYS O	OUTLIER (0.03%) General / 166.0,157.2	78.7% (tttt) chi angles: 191.3,164.6,179.5,177.9	0.11Å	-	-
135	ALA 44.8	-	Favored (37.17%) General / -75.9,152.5	-	0.088Å	-	-
136	LEU 131.58	0.791Å HD11 with 140 GLU OE1	Favored (29.85%) General / -76.7,159.9	38.6% (<i>tp</i>) chi angles: 182.2,69.9	0.117Å	-	-
137	LEU 47.71	0.465Å N with 136 LEU HG	Favored (52.97%) General / -60.3,143.4	69.4% (<i>mt</i>) chi angles: 290.9,180.1	0.128Å	-	-
138	ASN 98.48	0.737Å O with 141 VAL HG12	Favored (74.47%) General / -63.4,-32.9	96% (<i>m-20</i>) chi angles: 289.7,333.1	0.054Å	-	OUTLIER(S) worst is CA- CB-CG: 5.84 σ
139	GLU 78.09	0.456Å HA with 139 GLU OE1	Favored (97.45%) General / -61.2,-44.3	4.8% (<i>mm-40</i>) chi angles: 310.9,298.1,31.9	0.123Å	-	-
140	GLU 48.07	0.791Å OE1 with 136 LEU HD11	Favored (75.45%) General / -69.4,-35.0	90% (<i>mt-10</i>) chi angles: 291.5,187.8,4.9	0.092Å	-	-
			Favored				

141	VAL 95.19	0.737Å HG12 with 138 ASN O	(97.69%) Isoleucine or valine / -64.0,-44.1	8.8% (p) chi angles: 68.4	0.071Å	-	-
142	ALA 36.19	0.518Å N with 141 VAL HG13	Favored (94.75%) General / -65.1,-41.9	-	0.081Å	-	-
143	ARG 92.96	0.477Å O with 147 LYS HG3	Favored (91.72%) General / -60.8,-46.1	47.2% (ttt85) chi angles: 183.8,194.5,186.1,94.2	0.117Å	-	-
144	ARG 144.09	0.538Å NH2 with 136 LEU HD22	Favored (88.39%) General / -66.3,-42.4	10.1% (ttm180) chi angles: 200.4,179,313.5,202	0.076Å	-	-
145	ALA 38.34	-	Favored (94.9%) General / -62.6,-45.0	-	0.081Å	-	-
146	GLU 67.61	0.676Å OE2 with 65 LEU HD21	Favored (77.38%) General / -67.0,-34.3	46.4% (<i>mt-10</i>) chi angles: 286.2,182.1,284.6	0.113Å	-	-
147		0.477Å	Favored	57% (mtpt)			
177	LYS 65.08	HG3 with 143 ARG O	(88.67%) General / -61.5,-38.8	chi angles: 295.3,165.5,76,177.5	0.07Å	-	-
	t Res High B		General /	chi angles:	0.07Å Cβ deviation	Bond lengths	- Bond angles
		ARG O Clash >	General / -61.5,-38.8 Ramachandran	chi angles: 295.3,165.5,76,177.5	Cβ deviation Outliers:	lengths	
	t Res High B Avg:	ARG O Clash > 0.4Å Clashscore:	General / -61.5,-38.8 Ramachandran Outliers: 3 of	chi angles: 295.3,165.5,76,177.5 Rotamer Poor rotamers: 3 of	Cβ deviation Outliers:	lengths Outliers:	Outliers: 17
# Al	t Res High B Avg: 121.40	ARG O Clash > 0.4Å Clashscore: 108.54	General / -61.5,-38.8 Ramachandran Outliers: 3 of 122 Favored (70.08%) General /	chi angles: 295.3,165.5,76,177.5 Rotamer Poor rotamers: 3 of 108 62.9% (<i>mt</i>)	C β deviation Outliers: 1 of 116	lengths Outliers:	Outliers: 17
# Al	Avg: 121.40	ARG O Clash > 0.4Å Clashscore: 108.54 - 0.905Å HD12 with 95	General / -61.5,-38.8 Ramachandran Outliers: 3 of 122 Favored (70.08%) General / -64.9,-29.1 Favored (13.75%) General /	chi angles: 295.3,165.5,76,177.5 Rotamer Poor rotamers: 3 of 108 62.9% (<i>mt</i>) chi angles: 293.9,183.7 3.1% (<i>tt</i>)	Cβ deviation Outliers: 1 of 116 0.065Å	lengths Outliers:	Outliers: 17

152	THR 311	0.866Å HG23 with 155 SER H	Favored (9.01%) Pre-proline / -166.5,166.5	11.5% (<i>t</i>) chi angles: 184.9	0.073Å	-	-
153	PRO 236.03	-	Favored (51.99%) Trans-proline / -66.0,-25.4	88.6% (<i>Cg_exo</i>) chi angles: 330.1	0.149Å	-	-
154	TYR 48.95	0.567Å N with 152 THR HG23	Favored (83.48%) General / -64.5,-46.3	60% (<i>m</i> -85) chi angles: 291.1,77.7	0.097Å	-	-
155	SER 151.91	0.866Å H with 152 THR HG23	Favored (71.1%) General / -67.1,-31.0	47.5% (<i>t</i>) chi angles: 180	0.1Å	-	-
156	LEU 156.92	1.062Å HG with 90 LYS HD3	Favored (34.3%) General / -66.2,128.0	44.8% (<i>tp</i>) chi angles: 183.7,67	0.121Å	-	-
15 <i>7</i>	LEU 152.31	0.701Å HD12 with 156 LEU C	Favored (28.05%) General / -152.0,167.6	7.4% (<i>mp</i>) chi angles: 287.2,73.6	0.178Å	-	-
158	TRP 230.38	0.416Å O with 159 ASN HB3	Favored (2.8%) General / -73.3,-59.2	7% (<i>t</i> 90) chi angles: 190.1,0.4	0.043Å	-	-
159	ASN 387.79	0.416Å HB3 with 158 TRP O	OUTLIER (0%) General / 159.6,-153.9	47.8% (<i>p-10</i>) chi angles: 61.6,347.2	0.086Å	-	-
160	ASN 289.26	0.455Å HB3 with 163 HIS ND1	Allowed (0.17%) General / 46.5,73.8	82.4% (<i>m-20</i>) chi angles: 288.6,317.2	0.062Å	-	-
161	CYS 154.33	0.601Å CA with 73 MET HE1	Favored (67.19%) General / -62.5,-23.9	7.4% (<i>t</i>) chi angles: 198.9	0.059Å	-	-
162	GLU 117.13	0.612Å HG2 with 61 TYR CE1	Favored (89.85%) General / -60.3,-46.4	35.5% (<i>mt-10</i>) chi angles: 297,162.7,309	0.107Å	-	-
163	HIS 62.73	0.455Å ND1 with 160 ASN HB3	Favored (86.98%) General / -65.6,-37.5	36% (<i>m80</i>) chi angles: 286.7,111.9	0.108Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.42 σ
			Favored				

164	PHE	69.17	-	(80.14%) General / -60.4,-48.8	91.3% (<i>t80</i>) chi angles: 178.5,79.6	0.06Å	-	-
165	VAL	53.03	0.523Å HG22 with 162 GLU O	Favored (77.85%) Isoleucine or valine / -66.6,-36.7	29.5% (<i>m</i>) chi angles: 295.1	0.071Å	-	-
166	THR	37.87	0.731Å HG23 with 170 TYR CD2	Favored (99.73%) General / -62.7,-42.6	87.9% (<i>m</i>) chi angles: 301.1	0.073Å	-	-
167	TYR	41.1	-	Favored (98.87%) General / -63.4,-41.8	85.6% (<i>t80</i>) chi angles: 180.4,82.1	0.11Å	-	-
44 A I	l4 D	ii:-k p	Clash >	Danis alas das	Dataman	Сβ	Bond	David andles
# Al	it kes	High B	0.4Å	Ramachandran	Rotamer	deviation	lengths	Bond angles
# AI	it kes	Avg: 121.40	0.4Å Clashscore: 108.54	Outliers: 3 of 122	Poor rotamers: 3 of 108	Outliers:	U	O
# Al		Avg:	Clashscore:	Outliers: 3 of	Poor rotamers: 3 of	Outliers:	Outliers:	Outliers: 17
	CYS	Avg: 121.40 50.61	Clashscore:	Outliers: 3 of 122 Favored (72.04%) General /	Poor rotamers: 3 of 108 73% (<i>m</i>)	Outliers: 1 of 116	Outliers:	Outliers: 17
168	CYS ARG	Avg: 121.40 50.61	Clashscore: 108.54 - 0.681Å HD3 with 170	Outliers: 3 of 122 Favored (72.04%) General / -63.2,-50.0 Favored (33.61%) General /	Poor rotamers: 3 of 108 73% (m) chi angles: 297 8.8% (ptm105) chi angles:	Outliers: 1 of 116 0.075Å	Outliers:	Outliers: 17

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