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All-Atom Contacts	Clashscore, all atoms:	27.08		18th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	3	2.10%	Goal: <1%
	Ramachandran outliers	9	5.73%	Goal: <0.05%
	Ramachandran favored	121	77.07%	Goal: >98%
	MolProbity score^	2.94		25th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	1	0.68%	Goal: 0
	Bad backbone bonds:	19 / 1319	1.44%	Goal: 0%
	Bad backbone angles:	12 / 1789	0.67%	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: 51.57	Clashscore: 27.08	Outliers: 9 of 157	Poor rotamers: 3 of 143	Outliers: 1 of 148	Outliers: 9 of 159	Outliers: 8 of 159
A 7		LEU	50	-	-	15% (*mt*) chi angles: 304.4,195.9	0.081Å	-	-
A 8		ASN	50	-	Favored (93.76%) General / -59.6,-43.5	51.1% (*t30*) chi angles: 182.5,53.2	0.021Å	-	-
A 9		VAL	50	-	Favored (16.52%) Isoleucine or valine / -74.7,-18.2	13.1% (*p*) chi angles: 62.7	0.142Å	-	-
A 10		GLU	99.99	-	Favored (61.59%) General / -72.3,-13.8	90% (*mt-10*) chi angles: 296.5,186.6,338.4	0.037Å	-	-
					Favored				

A 11	GLY	50	-	(3.22%) Glycine / 112.8,-38.5	-	-	-	-	-
A 12	VAL	50	-	Favored (3.09%) Isoleucine or valine / -73.5,165.5	67.3% (*t*) chi angles: 179.6	0.081Å	-	-	-
A 13	LYS	50	-	Favored (9.57%) General / -143.6,117.9	28% (*tptp*) chi angles: 186,69,179.1,62.5	0.152Å	-	-	-
A 14	LYS	50	-	Favored (14.37%) General / -106.4,161.7	6.8% (*ptmt*) chi angles: 82.8,145.9,293.3,180.5	0.112Å	-	-	-
A 15	THR	50	-	Favored (12.63%) General / -152.1,131.1	70.5% (*p*) chi angles: 59.1	0.039Å	-	-	-
A 16	ILE	50	-	Favored (23.25%) Isoleucine or valine / -96.1,137.8	45.6% (*pt*) chi angles: 58.3,173	0.028Å	-	-	-
A 17	LEU	50	0.486Å HD11 with A 86 GLU OE1	Allowed (0.83%) General / -80.9,-66.8	95.9% (*mt*) chi angles: 296.4,174.4	0.047Å	-	-	-
A 18	HIS	50	0.462Å HB2 with A 84 VAL HG12	Favored (20.01%) General / -122.4,113.9	38.4% (*m170*) chi angles: 302.7,158.1	0.062Å	OUTLIER(S) worst is CD2-- NE2: 4.316 σ	-
A 19	GLY	50	-	Favored (30.05%) Glycine / -62.0,122.9	-	-	-	-	-
A 20	GLY	50	-	Allowed (0.25%) Glycine / -72.9,-136.5	-	-	-	-	-
A 21	THR	50	-	Favored (41.73%) General / -140.2,148.5	69.9% (*p*) chi angles: 64.1	0.052Å	-	-	-
A 22	GLY	50	-	Favored (31.14%) Glycine /	-	-	-	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
					90.4,-165.3				
A 23		GLU	50	-	Favored (26.84%) General / -95.0,143.0	46% (*mt-10*) chi angles: 298.7,181.7,272.8	0.038Å	-	-
A 24		LEU	50	-	Favored (17.4%) Pre-proline / -79.2,111.0	1.9% (*tm?*) chi angles: 194.4,295.8	0.087Å	-	-
A 25		PRO	50	-	Allowed (0.31%) Trans-proline / -69.9,-169.0	90% (*Cg_endo*) chi angles: 31.9	0.097Å	-	-
A 26		ASN	50	-	Favored (3.03%) General / -61.1,-60.9	64.9% (*m-80*) chi angles: 291.6,277.7	0.061Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 51.57	Clashscore: 27.08	Outliers: 9 of 157	Poor rotamers: 3 of 143	Outliers: 1 of 148	Outliers: 9 of 159	Outliers: 8 of 159
A 27		PHE	50	-	Favored (3.68%) General / 59.9,55.9	70.8% (*m-85*) chi angles: 287.1,279.5	0.076Å	-	-
A 28		ILE	50	-	Allowed (0.74%) Isoleucine or valine / -118.8,-173.7	48.6% (*pt*) chi angles: 61.3,173.1	0.087Å	-	-
A 29		THR	50	-	Allowed (0.11%) General / -63.5,96.0	72.8% (*p*) chi angles: 59.9	0.078Å	-	-
A 30		GLY	50	-	Allowed (1.05%) Glycine / 114.2,39.4	-	-	-	-
A 31		SER	50	-	Favored (56%) General / -112.5,127.2	47.4% (*t*) chi angles: 180.1	0.015Å	-	-
A 32		ARG	50	-	Favored (11.53%) General / -89.6,98.0	21.8% (*tpp85*) chi angles: 182.2,63.4,67.7,82.8	0.015Å	-	-
A					Favored (47.96%)	7% (*p*)			

33	VAL	50	-	Isoleucine or valine / -100.6,118.9	chi angles: 55.9	0.146Å	-	-
A 34	ILE	50	0.68Å HD11 with A 155 GLN HB2	Favored (67.91%) Isoleucine or valine / -111.0,127.7	23.7% (*pt*) chi angles: 71.4,173	0.114Å	-	-
A 35	PHE	50	0.518Å CE1 with A 76 LEU HD22	Favored (18.6%) General / -165.4,166.2	36.4% (*p90*) chi angles: 54.7,275.3	0.047Å	-	-
A 36	HIS	50	0.434Å HB2 with A 152 GLU HB3	Favored (14.38%) General / -92.0,162.4	78.3% (*m-70*) chi angles: 284.1,273.1	0.02Å	OUTLIER(S) worst is CD2-- NE2: 4.298 σ	OUTLIER(S) worst is CB- CG-CD2: 4.278 σ
A 37	PHE	50	0.528Å CD1 with A 59 MET HG2	Favored (33.81%) General / -145.4,148.9	49.5% (*p90*) chi angles: 64.1,274.9	0.01Å	-	-
A 38	ARG	50	0.698Å HB3 with A 150 VAL HG13	Allowed (1.66%) General / -153.8,93.5	6.7% (*tmm_?*) chi angles: 198.1,269.7,291.9,283.2	0.16Å	-	-
A 39	THR	50	-	Favored (28.78%) General / -89.0,118.6	45.7% (*p*) chi angles: 55.2	0.034Å	-	-
A 40	MET	50	0.608Å HG3 with A 148 VAL CG2	Favored (48.7%) General / -134.8,156.5	18.5% (*ptp*) chi angles: 59.6,168.7,79.6	0.152Å	-	OUTLIER(S) worst is CB- CG-SD: 5.056 σ
A 41	LYS	99.99	0.915Å HE2 with A 145 GLN HB3	Favored (58.22%) General / -64.2,143.0	24.4% (*tptp*) chi angles: 188.3,57,187,57.7	0.061Å	-	-
A 42	CYS	50	-	Allowed (0.18%) General / -72.0,-73.7	37.9% (*t*) chi angles: 187.9	0.094Å	-	-
A 43	ASP	50	-	Favored (3.59%) General / -131.8,-6.7	11.6% (*t70*) chi angles: 196,81.4	0.078Å	-	-
A 44	GLU	50	0.559Å HB3 with A 41 LYS HE3	Favored (38.99%) General / -67.0,-52.7	10.2% (*tm-20*) chi angles: 177.9,288.1,325.8	0.114Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 45		GLU	50	0.522Å HB2 with A 44 GLU OE1	Allowed (1.87%) General / -127.5,-39.0	0.8% chi angles: 211.8,300,287	0.047Å	-	-
A 46		ARG	50	0.57Å HG2 with A 46 ARG O	Allowed (0.14%) General / 85.0,17.9	36.9% (*ttm-85*) chi angles: 174.2,198.3,289.2,283.7	0.08Å	-	-
			Avg: 51.57	Clashscore: 27.08	Outliers: 9 of 157	Poor rotamers: 3 of 143	Outliers: 1 of 148	Outliers: 9 of 159	Outliers: 8 of 159
A 47		THR	50	-	Favored (33.04%) General / -82.0,141.7	14.9% (*t*) chi angles: 188.6	0.095Å	-	-
A 48		VAL	50	-	Favored (28.93%) Isoleucine or valine / -90.0,115.1	7.3% (*p*) chi angles: 57.7	0.136Å	-	-
A 49		ILE	50	-	Favored (15.99%) Isoleucine or valine / -81.7,-38.4	50.6% (*pt*) chi angles: 62,172.2	0.112Å	-	-
A 50		ASP	50	-	Favored (35.11%) General / -144.9,149.4	1.5% (*t70*) chi angles: 216.1,299.4	0.071Å	-	-
A 51		ASP	50	-	Favored (3.16%) General / -159.5,120.3	1.7% (*p30*) chi angles: 49.9,81.8	0.037Å	-	-
A 52		SER	50	-	Favored (4.45%) General / -108.5,-42.9	95.6% (*p*) chi angles: 66.3	0.056Å	-	-
A 53		ARG	50	-	Favored (62.13%) General / -63.2,-17.1	0% chi angles: 40.7,61.7,62.6,82	0.192Å	-	-
A 54		GLN	50	-	Favored (88.76%) General / -61.7,-38.7	38.2% (*tt0*) chi angles: 187.3,178,296.6	0.025Å	-	-
A		VAL	50		Favored (5.41%)	13.4% (*p*)	0.135Å		

A 55	VAL	50	-	(5.41%) Isoleucine or valine / -96.9,-21.3	12.4% (*p*) chi angles: 62.3	0.125Å	-	-
A 56	GLY	50	-	Favored (10.12%) Glycine / 84.2,38.5	-	-	-	-
A 57	GLN	50	-	Favored (48.33%) Pre-proline / -120.8,97.6	19.2% (*mm100*) chi angles: 298.4,292.7,100.3	0.013Å	-	-
A 58	PRO	50	-	Favored (40.14%) Trans-proline / -73.0,145.7	88.7% (*Cg_endo*) chi angles: 31.9	0.05Å	-	-
A 59	MET	50	0.591Å HE1 with A 61 ILE HG12	Favored (6.23%) General / -90.8,177.7	3.2% (*ppp?*) chi angles: 53.2,64.7,72.2	0.088Å	-	OUTLIER(S) worst is CG-SD-CE: 6.957 σ
A 60	HIS	50	0.469Å O with A 61 ILE HD13	Favored (35.17%) General / -137.4,133.7	51.5% (*m170*) chi angles: 299.8,160.9	0.035Å	OUTLIER(S) worst is CD2--NE2: 4.995 σ	-
A 61	ILE	50	0.591Å HG12 with A 59 MET HE1	Favored (32.2%) Isoleucine or valine / -115.5,141.6	7.5% (*mm*) chi angles: 298.3,321.4	0.094Å	-	-
A 62	ILE	50	0.411Å N with A 62 ILE HD12	Favored (60.36%) Isoleucine or valine / -105.5,124.2	3.1% (*mp*) chi angles: 296.5,72.1	0.054Å	-	-
A 63	ILE	50	-	Allowed (1.68%) Isoleucine or valine / -73.6,102.0	41% (*mm*) chi angles: 305.2,296.6	0.046Å	-	-
A 64	GLY	50	-	Favored (48.24%) Glycine / 54.6,52.0	-	-	-	-
A 65	ASN	50	-	Allowed (0.19%) General / -148.8,-55.1	21.8% (*t-20*) chi angles: 189.6,296.4	0.039Å	-	-
A 66	MET	50		Favored (4.46%)	25.3% (*ttt*) chi angles:	0.03Å		

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
66		MET	50	-	(4.46%) General / -102.0,-47.8	chi angles: 179.9,184.5,177.3	0.03A	-	-
			Avg: 51.57	Clashscore: 27.08	Outliers: 9 of 157	Poor rotamers: 3 of 143	Outliers: 1 of 148	Outliers: 9 of 159	Outliers: 8 of 159
A 67		PHE	50	0.509Å CE1 with A 61 ILE HD12	Favored (50%) General / -70.5,146.8	1.8% (*t80*) chi angles: 216.7,85.8	0.061Å	-	-
A 68		LYS	50	1.019Å HB2 with A 100 LEU HD12	Favored (17.64%) General / -94.8,-23.1	2.1% (*mppt?*) chi angles: 291.8,60.7,66.6,170.7	0.1Å	-	-
A 69		LEU	50	0.684Å HB2 with A 100 LEU HD13	Favored (15.25%) General / -105.7,105.3	2.3% (*tm?*) chi angles: 189,271.3	0.094Å	-	-
A 70		GLU	50	-	Favored (60.88%) General / -72.8,-24.3	12.2% (*pt-20*) chi angles: 66.7,176.7,56.3	0.131Å	-	-
A 71		VAL	50	0.61Å O with A 75 LEU HG	Favored (62.29%) Isoleucine or valine / -65.5,-33.2	11.4% (*p*) chi angles: 66.6	0.235Å	-	-
A 72		TRP	50	0.59Å CE3 with A 61 ILE HD11	Favored (70.87%) General / -59.8,-32.6	25.5% (*m0*) chi angles: 278.5,13.4	0.045Å	-	-
A 73		GLU	50	0.482Å O with A 77 THR HG23	Favored (67.29%) General / -69.4,-46.3	55.9% (*mt-10*) chi angles: 299.8,176.8,36.3	0.035Å	-	-
A 74		ILE	50	0.61Å HD11 with A 71 VAL HG23	Favored (62.96%) Isoleucine or valine / -68.4,-33.9	48.3% (*pt*) chi angles: 62.6,173.5	0.107Å	-	-
A 75		LEU	50	0.801Å HD21 with A 89 CYS SG	Favored (82.07%) General / -56.9,-46.5	96.1% (*mt*) chi angles: 295.7,174.9	0.059Å	-	-
A 76		LEU	99.99	0.518Å HD22 with A 35 PHE CE1	Favored (40.23%) General / -88.7,-13.2	3.4% (*mp*) chi angles: 276.8,91.9	0.108Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 77		THR	50	0.482Å HG23 with A 73 GLU O	Favored (55.68%) General / -54.9,-29.2	43.2% (*p*) chi angles: 54.7	0.047Å	-	-
A 78		SER	50	-	Favored (59.28%) General / -84.2,-7.7	32.3% (*t*) chi angles: 184.3	0.03Å	-	-
A 79		MET	50	0.5Å HE3 with A 153 LEU HB2	Favored (34.85%) General / -102.3,141.6	5.2% (*mmm*) chi angles: 290.7,253,292	0.04Å	-	-
A 80		ARG	50	0.457Å O with A 153 LEU HD22	Favored (8%) General / -118.2,171.6	39.3% (*ptt180*) chi angles: 60.6,178.1,177.6,178.1	0.004Å	-	-
A 81		VAL	50	0.66Å HA with A 153 LEU CD2	OUTLIER (0.04%) Isoleucine or valine / -52.3,101.9	14.3% (*p*) chi angles: 63.2	0.25Å	-	-
A 82		HIS	50	0.52Å HB3 with A 81 VAL O	OUTLIER (0.01%) General / 93.1,26.4	9.8% (*t-160*) chi angles: 172.4,223.4	0.139Å	OUTLIER(S) worst is CD2-- NE2: 4.595 σ	OUTLIER(S) worst is CA-CB-CG: 4.498 σ
A 83		GLU	50	-	Favored (37.16%) General / -104.9,141.1	29.9% (*tt0*) chi angles: 191.4,171.2,281.2	0.054Å	-	-
A 84		VAL	50	0.462Å HG12 with A 18 HIS HB2	Favored (68.7%) Isoleucine or valine / -122.0,123.3	12.3% (*p*) chi angles: 62.2	0.109Å	-	-
A 85		ALA	50	-	Favored (35.38%) General / -140.0,138.2	-	0.029Å	-	-
A 86		GLU	50	0.486Å OE1 with A 17 LEU HD11	Favored (54.31%) General / -124.8,137.4	11.1% (*pt-20*) chi angles: 56.2,181.6,59.3	0.028Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 51.57	Clashscore: 27.08	Outliers: 9 of 157	Poor rotamers: 3 of 143	Outliers: 1 of 148	Outliers: 9 of 159	Outliers: 8 of 159
A 87		PHE	50	0.415Å CE2 with A 75 LEU CD2	Allowed (1.16%) General /	46.2% (*p90*) chi angles: 55.8,267.5	0.063Å	-	-

87		75 LEU CD2		General / -177.2,155.7	chi angles: 35.6,267.5		
A 88	TRP	50	-	Favored (24.71%) General / -84.6,151.1	39.2% (*p90*) chi angles: 64.8,85.8	0.01Å	-	-
A 89	CYS	50	0.801Å SG with A 75 LEU HD21	Favored (51.64%) General / -127.8,141.2	79.3% (*m*) chi angles: 296.1	0.08Å	-	-
A 90	ASP	50	-	Favored (48.95%) General / -69.1,149.2	15% (*t70*) chi angles: 193.4,84	0.062Å	-	-
A 91	THR	50	-	Favored (61.73%) General / -56.5,-29.2	69.1% (*p*) chi angles: 57.5	0.047Å	-	-
A 92	ILE	50	-	Favored (22.52%) Isoleucine or valine / -55.6,-28.0	48% (*mm*) chi angles: 299.6,299.4	0.082Å	-	-
A 93	HIS	50	-	Favored (11.02%) General / -95.6,-37.1	87.4% (*m-70*) chi angles: 305.4,280.4	0.013Å	OUTLIER(S) worst is CG--ND1: 4.626 σ	OUTLIER(S) worst is CB-CG-CD2: 4.358 σ
A 94	THR	50	-	Favored (4.73%) General / -95.4,24.9	72.6% (*m*) chi angles: 296.8	0.107Å	-	OUTLIER(S) worst is CA-CB-CG2: 4.594 σ
A 95	GLY	50	-	Favored (97.07%) Glycine / -64.4,-39.6	-	-	-	-
A 96	VAL	50	0.509Å HG13 with A 69 LEU HD23	Favored (9.25%) Isoleucine or valine / -103.5,9.1	14.9% (*p*) chi angles: 63.5	0.119Å	-	-
A 97	TYR	50	0.453Å N with A 98 PRO HD2	Favored (94.12%) Pre-proline / -59.3,-42.7	35.8% (*t80*) chi angles: 176.7,55.8	0.055Å	-	-
A 98	PRO	50	0.453Å HD2 with A 97 TYR N	Favored (41.39%) Trans-proline / -68.9,-16.6	98.5% (*Cg_endo*) chi angles: 30.5	0.112Å	-	-
				Favored				

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 99		ILE	50	-	Favored (16.19%) Isoleucine or valine / -87.1,-44.5	50.9% (*mm*) chi angles: 302,300.4	0.052Å	-	-
A 100		LEU	50	1.019Å HD12 with A 68 LYS HB2	Favored (65.05%) General / -70.4,-28.4	6.8% (*tt*) chi angles: 179.8,140.7	0.094Å	-	-
A 101		SER	50	-	Favored (38.69%) General / -53.0,-31.1	24.4% (*t*) chi angles: 186.1	0.039Å	-	-
A 102		ARG	50	-	Allowed (0.8%) General / -81.1,20.5	77.6% (*mtt85*) chi angles: 291.3,188.4,180.7,79	0.011Å	-	-
A 103		SER	50	-	Allowed (0.3%) General / -145.7,-35.5	79.7% (*p*) chi angles: 59.8	0.121Å	-	-
A 104		LEU	50	0.803Å HD23 with A 100 LEU HD23	Favored (67.51%) General / -64.2,-24.0	3.6% (*pp*) chi angles: 71.9,85.8	0.158Å	-	-
A 105		ARG	50	-	Favored (6.35%) General / -83.0,-52.8	17.4% (*tpt180*) chi angles: 161.7,65.5,183.2,189.9	0.053Å	-	-
A 106		GLN	99.99	-	Allowed (1.36%) General / -79.2,-63.7	71.9% (*mt-30*) chi angles: 295.5,181.1,62.9	0.062Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 51.57	Clashscore: 27.08	Outliers: 9 of 157	Poor rotamers: 3 of 143	Outliers: 1 of 148	Outliers: 9 of 159	Outliers: 8 of 159
A 107		MET	50	0.43Å SD with A 113 PRO HD3	Favored (64.05%) General / -57.3,-29.5	36.6% (*mmp*) chi angles: 294.2,296.2,96.5	0.027Å	-	-
A 108		ALA	50	-	Allowed (1.2%) General / -62.3,-3.1	-	0.023Å	-	-
A 109		GLN	50	-	Favored (67.07%) General / 55.6,177.6,22.7	12.4% (*pt20*) chi angles:	0.029Å		

~~109~~	~~GLN~~	~~50~~	-	General / -53.4,-42.5	~~55.0,177.0,22.7~~	~~0.029Å~~	-	-
A 110	GLY	50	0.584Å O with A 116 TRP HB2	OUTLIER (0.03%) Glycine / 166.6,73.5	-	-	-	-
A 111	LYS	50	-	OUTLIER (0.01%) General / 58.2,109.0	31.2% (*mmmt*) chi angles: 298.2,289.5,288.1,185.6	0.071Å	-	-
A 112	ASP	50	-	OUTLIER (0.08%) Pre-proline / 58.9,152.3	1.2% (*m-20*) chi angles: 273.7,84.7	0.103Å	-	-
A 113	PRO	50	0.43Å HD3 with A 107 MET SD	OUTLIER (0.01%) Trans-proline / -59.3,-79.0	57.8% (*Cg_endo*) chi angles: 26.4	0.085Å	-	-
A 114	THR	50	0.852Å HA with A 117 HIS CE1	Favored (72.77%) General / -63.5,-31.6	77% (*p*) chi angles: 58.4	0.207Å	OUTLIER(S) worst is C--N: 5.288 σ	-
A 115	GLU	50	-	Favored (6.3%) General / -55.4,-58.8	10.2% (*tp10*) chi angles: 191,62.9,77.8	0.064Å	-	-
A 116	TRP	50	0.584Å HB2 with A 110 GLY O	Favored (2.62%) General / -123.8,86.7	79.6% (*m95*) chi angles: 300.4,86.3	0.052Å	-	-
A 117	HIS	50	0.852Å CE1 with A 114 THR HA	Favored (4.33%) General / -93.6,78.4	61.5% (*m170*) chi angles: 296.1,161.5	0.065Å	OUTLIER(S) worst is CD2--NE2: 22.445 σ	OUTLIER(S) worst is ND1-CE1-NE2: 6.533 σ
A 118	VAL	50	0.402Å HG22 with A 120 THR HG23	Allowed (0.48%) Isoleucine or valine / -173.5,147.8	12.2% (*p*) chi angles: 62.2	0.086Å	-	-
A 119	HIS	50	-	Favored (2.71%) General / -101.1,84.8	95.7% (*m-70*) chi angles: 292.6,276.7	0.017Å	OUTLIER(S) worst is CG--ND1: 4.472 σ	OUTLIER(S) worst is CB-CG-CD2: 4.105 σ
A 120	THR	50	0.402Å HG23 with A 118 VAL HG22	Allowed (1.71%) General / -131.7,76.5	45.7% (*p*) chi angles: 55.2	0.049Å	-	-
A	CYS	50		OUTLIER (0.04%)	46.3% (*t*)	0.022Å		

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 121		CYS	50	-	(0.04%) General / -162.6,-61.2	40.3% (t) chi angles: 185.1	0.022Å	-	-
A 122		GLY	50	-	Allowed (0.18%) Glycine / -171.2,54.8	-	-	-	-
A 123		LEU	50	-	Favored (3.28%) General / -148.1,101.4	9% (tt) chi angles: 189.2,156.3	0.056Å	-	-
A 124		ALA	50	-	Favored (21.07%) General / -149.0,137.5	-	0.05Å	-	-
A 125		ASN	50	-	Allowed (0.15%) General / 63.2,84.1	35.8% (m120) chi angles: 296,112.4	0.054Å	-	-
A 126		MET	50	-	Allowed (0.61%) General / -166.6,104.8	15.2% (tpt) chi angles: 188.2,62.8,178.8	0.026Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 51.57	Clashscore: 27.08	Outliers: 9 of 157	Poor rotamers: 3 of 143	Outliers: 1 of 148	Outliers: 9 of 159	Outliers: 8 of 159
A 127		PHE	50	-	Favored (9.23%) General / -96.1,97.0	80.6% (t80) chi angles: 182.3,83	0.043Å	-	-
A 128		ALA	50	-	Favored (16.2%) General / -154.7,138.5	-	0.034Å	-	-
A 129		TYR	50	-	Favored (25.87%) General / -92.6,113.6	97.9% (m-85) chi angles: 295.5,272.7	0.029Å	-	-
A 130		HIS	50	-	Allowed (0.17%) General / -68.0,-72.6	23.6% (t-160) chi angles: 184.8,197.7	0.13Å	OUTLIER(S) worst is CG--ND1: 4.662 σ	-
A 131		THR	50	-	Allowed (0.06%) General / 69.3,100.9	24.2% (p) chi angles: 72	0.141Å	-	-

Favored

A 132	LEU	50	-	Favored (45.69%) General / -74.1,141.9	52% (*mt*) chi angles: 300.5,167.4	0.026Å	-	-
A 133	GLY	50	-	OUTLIER (0.09%) Glycine / 144.6,88.1	-	-	-	-
A 134	TYR	50	-	Favored (17.37%) General / -89.2,159.7	98.8% (*m-85*) chi angles: 296.7,274.1	0.031Å	-	-
A 135	GLU	50	-	Favored (6.87%) General / -117.3,-25.9	11.8% (*pt-20*) chi angles: 62.3,176.7,60.4	0.065Å	-	-
A 136	ASP	50	0.426Å O with A 139 GLU HG2	Favored (30.67%) General / -69.4,-52.0	18.7% (*m-20*) chi angles: 296.3,278.2	0.052Å	-	-
A 137	LEU	50	-	Favored (29.72%) General / -88.5,-17.7	2% (*pp*) chi angles: 54.2,100.1	0.158Å	-	-
A 138	ASP	50	-	Favored (61.46%) General / -73.2,-15.3	11.9% (*t70*) chi angles: 195.8,82.9	0.035Å	-	-
A 139	GLU	50	0.426Å HG2 with A 136 ASP O	Favored (66.43%) General / -58.1,-30.7	17.9% (*pt-20*) chi angles: 71.7,187.4,36.7	0.031Å	-	-
A 140	LEU	50	-	Favored (86.24%) General / -67.1,-38.8	75.1% (*mt*) chi angles: 304.5,177.6	0.045Å	-	-
A 141	GLN	50	-	Favored (69.96%) General / -59.2,-32.5	24.8% (*mm-40*) chi angles: 298.4,285.8,269.7	0.014Å	-	-
A 142	LYS	50	-	Favored (16.94%) General / -89.4,-33.3	30.6% (*mtpp*) chi angles: 290,182.6,65.9,66.9	0.014Å	-	-
A 143	GLU	50	0.431Å HG3 with A 143 GLU O	Favored (2.81%) Pre-proline / -155.5,91.4	10.6% (*pt-20*) chi angles: 58,174.4,73.7	0.077Å	-	-

# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 144 PRO 50		-	Favored (49.39%) Trans-proline / -68.6,141.2	72.5% (*Cg_endo*) chi angles: 29.2	0.068Å	-	-
A 145 GLN 50		0.915Å HB3 with A 41 LYS HE2	Favored (23.48%) Pre-proline / -142.7,142.7	23.3% (*mt-30*) chi angles: 296.9,155.5,104.7	0.155Å	-	-
A 146 PRO 50		-	Favored (5.05%) Trans-proline / -74.5,117.7	88.4% (*Cg_endo*) chi angles: 31.2	0.054Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 51.57	Clashscore: 27.08	Outliers: 9 of 157	Poor rotamers: 3 of 143	Outliers: 1 of 148	Outliers: 9 of 159	Outliers: 8 of 159
A 147		LEU	50	-	Favored (16.6%) General / -100.8,157.6	48.7% (*mt*) chi angles: 301.7,168	0.065Å	-	-
A 148		VAL	50	0.608Å CG2 with A 40 MET HG3	Favored (48.61%) Isoleucine or valine / -96.4,123.4	11.2% (*m*) chi angles: 307.7	0.107Å	-	-
A 149		PHE	50	-	Favored (7.61%) General / -110.8,98.5	65.9% (*m-85*) chi angles: 293.3,78.6	0.06Å	-	-
A 150		VAL	50	0.698Å HG13 with A 38 ARG HB3	Favored (10.08%) Isoleucine or valine / -90.3,99.8	6% (*p*) chi angles: 55	0.212Å	-	-
A 151		ILE	50	0.482Å HD12 with A 76 LEU HG	Favored (8.23%) Isoleucine or valine / -94.8,145.3	44.5% (*pt*) chi angles: 59.4,173.9	0.073Å	-	-
A 152		GLU	50	0.434Å HB3 with A 36 HIS HB2	Favored (4.37%) General / -130.8,97.5	26.2% (*tt0*) chi angles: 165.5,169.9,63.1	0.069Å	-	-
A 153		LEU	50	0.66Å CD2 with A 81 VAL HA	Favored (51.27%) General / -70.6,139.0	7.3% (*tt*) chi angles: 192.1,161	0.075Å	-	-
A LEU			50	0.585Å	Allowed (1.87%)	0.1%	0.15Å	-	-

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A 154			O with A 81 VAL HG23	General / -122.1,-55.6	chi angles: 26.1,152.9		
A 155	GLN	50	0.68Å HB2 with A 34 ILE HD11	Favored (41.65%) General / -141.3,159.7	19.7% (*mp0*) chi angles: 303.2,75.3,7.5	0.094Å	-	-
A 156	VAL	50	-	Allowed (0.82%) Isoleucine or valine / -159.6,129.8	2.7% (*p*) chi angles: 50.3	0.109Å	-	-
A 157	ASP	50	-	Favored (39.59%) General / -123.0,153.6	73.3% (*m-20*) chi angles: 299.4,336.1	0.041Å	-	-
A 158	ALA	50	-	Favored (30.77%) Pre-proline / -101.1,159.0	-	0.094Å	-	-
A 159	PRO	50	0.438Å O with A 160 SER HB2	Allowed (0.28%) Trans-proline / -61.8,103.4	68.7% (*Cg_endo*) chi angles: 28	0.055Å	-	-
A 160	SER	50	0.438Å HB2 with A 159 PRO O	OUTLIER (0.01%) General / 147.5,-46.6	34.5% (*t*) chi angles: 183.1	0.112Å	-	-
A 161	ASP	50	-	Favored (10.76%) General / -91.6,-41.5	36.5% (*t0*) chi angles: 190.2,325.1	0.047Å	-	-
A 162	TYR	50	-	Favored (48.33%) General / -72.6,142.2	1.8% (*p90*) chi angles: 93.3,275	0.087Å	-	-
A 163	GLN	50	-	Favored (15.49%) General / -159.7,145.1	4.4% (*pp0?*) chi angles: 68,87.3,51.7	0.031Å	-	-
A 164	ARG	50	-	Favored (26.25%) General / -92.5,143.5	31.7% (*ptt-85*) chi angles: 60.8,176.1,179.2,278	0.024Å	-	-
A 165	GLU	99.99	-	-	52.6% (*mt-10*) chi angles: 298.8,181.3,293.5	0.033Å	-	-

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http://molprobity.biochem.duke.edu/viewtable.php?MolProbSID=6tg769…69b75cr8hl50shh7q53s1cc1jkg4/raw_data/aipl1_sm_7–165H–multi.table   Page 15 of 16