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All-Atom Contacts	Clashscore, all atoms:	1.52		99 th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	5	4.35%	Goal: <1%
	Ramachandran outliers	6	4.58%	Goal: <0.05%
	Ramachandran favored	113	86.26%	Goal: >98%
	MolProbity score^	2.01		75 th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	4	3.28%	Goal: 0
	Bad backbone bonds:	0 / 1043	0.00%	Goal: 0%
	Bad backbone angles:	12 / 1412	0.85%	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	C β deviation	Bond lengths	Bond angles
			Avg: 54.96	Clashscore: 1.52	Outliers: 6 of 131	Poor rotamers: 5 of 115	Outliers: 4 of 122	Outliers: 0 of 133	Outliers: 11 of 133
A 4	SER	50	-	-	-	5.2% (<i>p</i>) chi angles: 43.1	0.139Å	-	-
A 5	HIS	50	-	-	Favored (38.6%) General / -105.3,140.3	45.3% (<i>p</i> -80) chi angles: 63.9,270.3	0.098Å	-	OUTLIER(S) worst is CA-CB-CG: 4.154 Å
A 6	SER	50	-	-	Favored (38.69%) General / -73.6,129.8	70.3% (<i>p</i>) chi angles: 57.6	0.08Å	-	-
A 7	GLY	50	-	-	Favored (13.96%) Glycine / -113.8,171.7	-	-	-	-
					Favored				

A 8	VAL	50	-	(36.37%) Isoleucine or valine / -127.9,144.8	82.3% (<i>t</i>) chi angles: 174.7	0.076Å	-	-
A 9	ASN	50	0.434Å HB2 with C2019 DGU OP2	Favored (4.9%) General / -102.0,177.4	26.9% (<i>p30</i>) chi angles: 55.2,39.6	0.102Å	-	OUTLIER(S) worst is CA- CB-CG: 4.479 σ
A 10	GLN	50	-	Favored (61.62%) General / -72.5,-18.7	32.2% (<i>mt-30</i>) chi angles: 282.5,178,111.5	0.08Å	-	-
A 11	LEU	50	-	Favored (51.78%) General / -80.5,-17.4	4.6% (<i>mp</i>) chi angles: 302.1,93.7	0.106Å	-	-
A 12	GLY	50	-	Favored (54.44%) Glycine / 98.5,8.7	-	-	-	-
A 13	GLY	50	-	Favored (47.28%) Glycine / -87.9,180.0	-	-	-	-
A 14	VAL	50	-	Favored (26.65%) Isoleucine or valine / -122.7,147.9	10.4% (<i>m</i>) chi angles: 287.5	0.033Å	-	-
A 15	PHE	50	-	Favored (4.33%) General / -146.7,-173.9	15.4% (<i>p90</i>) chi angles: 74.7,286	0.058Å	-	-
A 16	VAL	50	-	Favored (43.67%) Isoleucine or valine / -133.5,141.7	55.9% (<i>t</i>) chi angles: 169.5	0.079Å	-	-
A 17	ASN	50	-	Favored (33.86%) General / -78.0,150.8	37% (<i>t30</i>) chi angles: 201,51.9	0.033Å	-	-
A 18	GLY	50	-	Favored (62.21%) Glycine / 56.8,32.8	-	-	-	-
A 19	TRP	50	-	Favored (7.22%) Pre-proline / -161.2,139.6	66.1% (<i>t-105</i>) chi angles: 186.9,263.8	0.071Å	-	OUTLIER(S) worst is CE3- CD2-CG: 4.183 σ

A 20	PRO	50	-	Favored (56.66%) Trans-proline / -69.4,144.7	2.7% (<i>Cg_exo</i>) chi angles: 354.4	0.046Å	-	-	
A 21	LEU	50	-	Favored (34.61%) Pre-proline / -51.5,129.2	16.9% (<i>tp</i>) chi angles: 194.6,70.9	0.054Å	-	-	
A 22	PRO	50	-	Favored (55.59%) Trans-proline / -54.4,145.7	5.9% (<i>Cg_exo</i>) chi angles: 322.2	0.035Å	-	-	
A 23	ASP	50	-	Allowed (1.08%) General / -48.7,-23.6	45.9% (<i>m-20</i>) chi angles: 303,344.4	0.131Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.96	Clashscore: 1.52	Outliers: 6 of 131	Poor rotamers: 5 of 115	Outliers: 4 of 122	Outliers: 0 of 133	Outliers: 11 of 133
A 24	SER	50	-	Favored (76.27%) General / -55.3,-45.9	65.7% (<i>p</i>) chi angles: 57	0.084Å	-	-	
A 25	THR	50	-	Favored (21.02%) General / -87.8,-29.3	2% (<i>m</i>) chi angles: 322.5	0.116Å	-	-	
A 26	ARG	50	-	Favored (76.54%) General / -65.1,-33.7	10.4% (<i>mtp85</i>) chi angles: 311.4,182.4,103.7,87.3	0.141Å	-	-	
A 27	GLN	50	-	Favored (85.51%) General / -60.8,-38.5	1% chi angles: 169.5,69.7,114	0.064Å	-	-	
A 28	LYS	50	-	Favored (74.26%) General / -70.3,-36.4	25.5% (<i>mmmt</i>) chi angles: 308.6,315.8,301.9,180.1	0.173Å	-	-	
A 29	ILE	50	-	Favored (96.87%) Isoleucine or valine / -63.2,-42.5	62.4% (<i>mt</i>) chi angles: 303.9,177.3	0.206Å	-	-	
				Favored (68.86%)	1.00% (<i>m</i>)				

A 30	VAL	50	-	Isoleucine or valine / -69.0,-35.4	1.0% (μ) chi angles: 83.5	0.246Å	-	-
A 31	GLU	50	-	Favored (95.14%) General / -60.3,-42.2	29.2% (<i>mt-10</i>) chi angles: 275.3,178.5,49.2	0.086Å	-	-
A 32	LEU	50	-	Favored (2.6%) General / -86.0,-58.5	28.2% (<i>mt</i>) chi angles: 305.6,189.7	0.14Å	-	-
A 33	ALA	50	-	Favored (99.08%) General / -63.3,-41.8	-	0.102Å	-	-
A 34	HIS	50	-	Favored (38.79%) General / -71.8,-6.1	2.2% (<i>t-80</i>) chi angles: 212.4,314	0.058Å	-	-
A 35	SER	50	-	Favored (20.01%) General / -102.8,-9.4	58.1% (<i>m</i>) chi angles: 291.1	0.059Å	-	-
A 36	GLY	50	-	Allowed (0.61%) Glycine / 131.8,28.4	-	-	-	-
A 37	ALA	50	-	Favored (47.83%) General / -124.6,148.5	-	0.05Å	-	-
A 38	ARG	50	-	Favored (19.67%) Pre-proline / -82.4,169.0	72.7% (<i>mtm180</i>) chi angles: 299,180.3,300,155	0.07Å	-	-
A 39	PRO	50	-	Favored (12.11%) Trans-proline / -53.3,-51.0	3.1% (<i>Cg_exo</i>) chi angles: 321.8	0.043Å	-	-
A 40	CYS	50	-	Favored (73.02%) General / -66.0,-31.9	1.2% (<i>p</i>) chi angles: 87.9	0.213Å	-	-
A 41	ASP	50	-	Favored (90.13%) General / -66.1,-39.8	31.8% (<i>m-20</i>) chi angles: 308.4,321.7	0.167Å	-	-
A 42	ILE	50	-	Favored (10.75%)	5.9% (<i>nt</i>)	0.000Å	-	-

A 42	ILE	50	-	Isoleucine or valine / -81.3,-29.2	chi angles: 64.5,148.7	0.326Å	-	-
A 43	SER	50	-	Favored (91.19%) General / -64.8,-44.0	78.6% (<i>p</i>) chi angles: 59.3	0.102Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
Avg: 54.96				Clashscore: 1.52	Outliers: 6 of 131	Poor rotamers: 5 of 115	Outliers: 4 of 122	Outliers: 0 of 133
A 44	ARG	50	-	Favored (61.21%) General / -73.4,-18.0	33.7% (<i>ttp-105</i>) chi angles: 197.7,179.9,66.9,249.5	0.059Å	-	-
A 45	ILE	50	-	Favored (9.12%) Isoleucine or valine / -110.6,-16.4	18.3% (<i>mt</i>) chi angles: 305.1,188.2	0.265Å	-	-
A 46	LEU	50	-	Favored (20.23%) General / -99.5,-12.3	74.2% (<i>mt</i>) chi angles: 297.6,168.7	0.129Å	-	-
A 47	GLN	50	-	Allowed (0.78%) General / 71.0,41.9	35.4% (<i>mt-30</i>) chi angles: 305.7,181.4,252.6	0.154Å	-	-
A 48	VAL	50	-	Favored (23.8%) Isoleucine or valine / -120.6,153.7	55.4% (<i>t</i>) chi angles: 169.7	0.129Å	-	-
A 49	SER	50	-	Favored (20.02%) General / -64.3,159.8	83.9% (<i>p</i>) chi angles: 68.7	0.048Å	-	-
A 50	ASN	50	-	Favored (87.94%) General / -66.2,-43.0	22.3% (<i>m-20</i>) chi angles: 316,306.2	0.104Å	-	-
A 51	GLY	50	0.418Å HA3 with C2019 DGU O6	Favored (55.87%) Glycine / -75.8,-31.5	-	-	-	-
A 52	CYS	50	-	Favored (99.74%) General / -62.0,-43.0	39.9% (<i>t</i>) chi angles: 175.4	0.06Å	-	-

A 53	VAL	50	-	Allowed (1.42%) Isoleucine or valine / -45.9,-55.5	2.3% (<i>t</i>) chi angles: 150.7	0.171Å	-	-
A 54	SER	50	-	Favored (48.53%) General / -85.3,-13.8	70.8% (<i>m</i>) chi angles: 297.6	0.214Å	-	-
A 55	LYS	50	-	Favored (59.11%) General / -73.2,-9.8	49.1% (<i>mtmt</i>) chi angles: 286.7,187.1,282.6,196.6	0.2Å	-	-
A 56	ILE	50	-	Favored (2.84%) Isoleucine or valine / -90.1,-59.5	3.4% (<i>mp</i>) chi angles: 291.7,77.2	0.151Å	-	-
A 57	LEU	50	-	Favored (75.61%) General / -56.1,-41.6	81.8% (<i>mt</i>) chi angles: 299,182	0.218Å	-	-
A 58	GLY	50	-	Favored (93.34%) Glycine / -60.6,-37.4	-	-	-	-
A 59	ARG	50	-	Favored (55.15%) General / -78.9,-17.7	75.2% (<i>mtm180</i>) chi angles: 295.3,183.3,278.5,184.2	0.141Å	-	-
A 60	TYR	50	-	Favored (61.35%) General / -75.2,-35.8	77.3% (<i>t80</i>) chi angles: 185,76.5	0.135Å	-	-
A 61	TYR	50	-	Favored (73.55%) General / -61.1,-33.6	19.2% (<i>m-30</i>) chi angles: 300.3,338.7	0.128Å	-	-
A 62	GLU	50	-	Allowed (0.1%) General / -89.8,-97.2	7.9% (<i>tm-20</i>) chi angles: 192.7,286.3,309.8	0.217Å	-	OUTLIER(S) worst is C-CA- CB: 4.243 σ
A 63	THR	50	-	Favored (75.38%) General / -65.1,-33.2	1.3% (<i>m</i>) chi angles: 275.7	0.114Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
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		Avg: 54.96	Clashscore: 1.52	Outliers: 6 of 131	Poor rotamers: 5 of 115	Outliers: 4 of 122	Outliers: 0 of 133	Outliers: 11 of 133
A 64	GLY	50	-	Favored (7.77%) Glycine / 106.2,22.6	-	-	-	-
A 65	SER	50	-	Favored (35.41%) General / -77.4,129.2	23.3% (t) chi angles: 187.4	0.056Å	-	-
A 66	ILE	50	-	Favored (7.01%) Isoleucine or valine / -87.2,-22.2	46.7% (pt) chi angles: 62.4,168.6	0.204Å	-	-
A 67	ARG	50	-	Favored (97.01%) Pre-proline / -69.4,150.8	12.7% (mmm180) chi angles: 270.4,294.4,304.6,174.8	0.096Å	-	-
A 68	PRO	50	-	Allowed (0.35%) Trans-proline / -85.9,-167.0	0.3% chi angles: 43.7	0.119Å	-	-
A 69	ARG	50	-	OUTLIER (0.03%) General / -74.7,-150.1	82.9% (mtm180) chi angles: 295,179.6,279.9,175.5	0.166Å	-	-
A 70	ALA	50	-	Favored (52.38%) General / -128.3,138.4	-	0.095Å	-	-
A 71	ILE	50	-	Favored (3.47%) Isoleucine or valine / -85.8,154.2	44% (mt) chi angles: 293.1,155.7	0.117Å	-	-
A 72	GLY	50	0.506Å HA2 with C2013 DAD H2	Favored (45.48%) Glycine / 80.7,172.4	-	-	-	-
A 73	GLY	50	-	Favored (3.1%) Glycine / 96.0,115.9	-	-	-	-
A 74	SER	50	-	Allowed (0.13%) General / -81.5,-155.3	13.1% (p) chi angles: 82.4	0.243Å	-	-
				Favored				

A 75	LYS	50	-	Favored (37.88%) Pre-proline / -140.6,164.2	29.7% (<i>mmtm</i>) chi angles: 308.2,298.9,162.1,307.2	0.039Å	-	-
A 76	PRO	50	-	OUTLIER (0.08%) Trans-proline / -55.8,100.5	0.1% chi angles: 318.1	0.063Å	-	-
A 77	ARG	50	-	Favored (21.9%) General / -86.2,-31.1	84.4% (<i>mtm180</i>) chi angles: 283.5,174.4,283.4,175.3	0.18Å	-	-
A 78	VAL	50	-	Allowed (1.03%) Isoleucine or valine / -125.5,-31.9	7.5% (<i>m</i>) chi angles: 309.2	0.182Å	-	-
A 79	ALA	50	-	Allowed (0.83%) General / -78.7,48.7	-	0.037Å	-	-
A 80	THR	50	-	Favored (3.12%) Pre-proline / -55.2,160.8	65.1% (<i>p</i>) chi angles: 63	0.075Å	-	-
A 81	PRO	50	-	Favored (27.23%) Trans-proline / -47.3,-39.6	0.1% chi angles: 317.9	0.093Å	-	-
A 82	GLU	50	-	Favored (42.33%) General / -79.5,-32.5	44.6% (<i>tt0</i>) chi angles: 185.2,155.4,354.2	0.237Å	-	-
A 83	VAL	50	-	Favored (85.12%) Isoleucine or valine / -59.0,-42.0	23.6% (<i>t</i>) chi angles: 163.4	0.11Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.96	Clashscore: 1.52	Outliers: 6 of 131	Poor rotamers: 5 of 115	Outliers: 4 of 122	Outliers: 0 of 133	Outliers: 11 of 133
A 84	VAL	50	-	Favored (95.61%) Isoleucine or valine / -60.5,-46.3	82.6% (t) chi angles: 174.7	0.069Å	-	-	
A 85	SEP	50	-	Favored (76.95%)	53.9% (m)	0.002Å	-	-	

A 85	SER	50	-	General / -59.8,-36.5	chi angles: 299.9	0.002Å	-	-
A 86	LYS	50	-	Favored (59.71%) General / -73.1,-44.9	70% (<i>mmtt</i>) chi angles: 285,292.8,176.6,186.7	0.086Å	-	-
A 87	ILE	50	-	Favored (66.85%) Isoleucine or valine / -67.1,-34.0	10.7% (<i>mt</i>) chi angles: 298.5,144.4	0.245Å	-	-
A 88	ALA	50	-	Favored (83.21%) General / -58.1,-47.4	-	0.071Å	-	-
A 89	GLN	50	-	Favored (74.1%) General / -55.2,-48.3	29.4% (<i>tt0</i>) chi angles: 188.6,197.1,312.7	0.06Å	-	-
A 90	TYR	50	-	Favored (52.24%) General / -71.9,-47.5	3.9% (<i>m-30</i>) chi angles: 316.2,324.1	0.123Å	-	-
A 91	LYS	50	0.411Å NZ with C2004 DTY OP1	Favored (60.71%) General / -74.8,-16.2	67.2% (<i>mmtt</i>) chi angles: 290.8,282.3,182.3,171.3	0.102Å	-	-
A 92	ARG	50	-	Favored (14%) General / -108.8,-17.2	30.3% (<i>mtp180</i>) chi angles: 302.2,156.4,74.5,161.4	0.167Å	-	-
A 93	GLU	50	-	Favored (12.64%) General / -93.5,-36.0	8.7% (<i>pt-20</i>) chi angles: 88.5,182.4,345.3	0.146Å	-	-
A 94	CYS	50	-	Favored (26.65%) Pre-proline / -139.1,79.4	37.1% (<i>t</i>) chi angles: 188.1	0.048Å	-	-
A 95	PRO	50	-	Favored (7.69%) Trans-proline / -46.1,-30.6	11.7% (<i>Cg_exo</i>) chi angles: 323.1	0.108Å	-	-
A 96	SER	50	-	Favored (9.48%) General / -85.7,78.9	88.7% (<i>p</i>) chi angles: 65.4	0.059Å	-	-
A 97	ILE	50	-	Favored (20.07%) Isoleucine or	19.8% (<i>mt</i>) chi angles: 286.0,105.2	0.08Å	-	-

A 98	PHE	50	-	Favored (9.87%) General / -91.4,170.6	50.1% (<i>m-85</i>) chi angles: 306.9,293.5	0.051Å	-	-	
A 99	ALA	50	-	Favored (87.95%) General / -60.6,-39.4	-	0.089Å	-	-	
A 100	TRP	50	-	Favored (77.06%) General / -69.0,-35.7	63.5% (<i>p-90</i>) chi angles: 53.8,271.6	0.179Å	-	-	
A 101	GLU	50	-	Favored (80.91%) General / -61.1,-36.9	46.8% (<i>mt-10</i>) chi angles: 292.4,188.4,279.4	0.106Å	-	-	
A 102	ILE	50	-	Favored (40.53%) Isoleucine or valine / -71.1,-30.4	48.6% (<i>mt</i>) chi angles: 304.1,181.5	0.319Å	-	-	
A 103	ARG	50	-	Favored (90.36%) General / -61.1,-39.5	31.1% (<i>ttt180</i>) chi angles: 202.3,169.7,184.6,150.8	0.145Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.96	Clashscore: 1.52	Outliers: 6 of 131	Poor rotamers: 5 of 115	Outliers: 4 of 122	Outliers: 0 of 133	Outliers: 11 of 133
A 104	ASP	50	-	Favored (53.63%) General / -80.6,-16.6	25.6% (<i>m-20</i>) chi angles: 284,13.3	0.154Å	-	-	
A 105	ARG	50	-	Favored (98.4%) General / -61.4,-42.2	9.2% (<i>mmt180</i>) chi angles: 273.8,281.6,206.6,138.4	0.108Å	-	-	
A 106	LEU	50	-	Favored (82.12%) General / -61.2,-37.2	4% (<i>mm?</i>) chi angles: 281.5,305.2	0.099Å	-	-	
A 107	LEU	50	-	Favored (45.49%) General / -78.5,-25.4	71.9% (<i>mt</i>) chi angles: 302.6,173.4	0.08Å	-	-	

A 108	SER	50	-	Favored (12.2%) General / -98.4,-31.1	80.9% (<i>p</i>) chi angles: 60.4	0.164Å	-	-
A 109	GLU	50	-	Favored (53.1%) General / -77.2,-26.9	21.5% (<i>mt-10</i>) chi angles: 284.3,205.3,26.2	0.115Å	-	-
A 110	GLY	50	-	Favored (8.5%) Glycine / 89.7,34.4	-	-	-	-
A 111	VAL	50	-	Favored (18.66%) Isoleucine or valine / -82.7,-43.1	97.1% (<i>t</i>) chi angles: 176.2	0.08Å	-	-
A 112	CYS	50	-	Favored (11.22%) General / -98.8,166.6	82.7% (<i>m</i>) chi angles: 300	0.025Å	-	-
A 113	THR	50	0.409Å HB with A 115 ASP OD1	Allowed (0.16%) General / -98.7,-112.3	45.5% (<i>m</i>) chi angles: 305.3	0.239Å	-	OUTLIER(S) worst is C-CA- CB: 4.311 σ
A 114	ASN	50	-	Allowed (1.51%) General / -142.4,31.3	8.6% (<i>m120</i>) chi angles: 291.8,164.1	0.046Å	-	OUTLIER(S) worst is CA- CB-CG: 9.261 σ
A 115	ASP	50	0.409Å OD1 with A 113 THR HB	OUTLIER (0.04%) General / -166.1,20.8	1.5% (<i>p30</i>) chi angles: 37.4,16.2	0.054Å	-	OUTLIER(S) worst is CA- CB-CG: 4.797 σ
A 116	ASN	50	-	OUTLIER (0.01%) General / -173.1,34.8	12.7% (<i>p30</i>) chi angles: 46.6,23.5	0.031Å	-	-
A 117	ILE	50	-	Favored (56.14%) Pre-proline / -96.6,122.8	7.6% (<i>tp</i>) chi angles: 184.7,71.8	0.075Å	-	-
A 118	PRO	50	-	Favored (92.51%) Trans-proline / -61.4,148.6	53.6% (<i>Cg_exo</i>) chi angles: 326.8	0.102Å	-	-
A 119	SER	50	-	Favored (4.98%) General / -96.7,179.4	45% (<i>m</i>) chi angles: 302.4	0.155Å	-	-
				Favored				

A 120	VAL	50	-	(19.92%) Isoleucine or valine / -73.9,-52.6 Favored	51.7% (t) chi angles: 182.3	0.124Å	-	-	
A 121	SER	50	-	(93.4%) General / -64.0,-39.1 Favored	8.5% (t) chi angles: 194.2	0.091Å	-	-	
A 122	SER	50	-	(97.82%) General / -61.0,-42.2 Favored	70% (m) chi angles: 297.3	0.072Å	-	-	
A 123	ILE	50	-	(81.65%) Isoleucine or valine / -64.2,-38.1	28.3% (mt) chi angles: 298.8,186.8	0.255Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
Avg: 54.96			Clashscore: 1.52	Outliers: 6 of 131	Poor rotamers: 5 of 115	Outliers: 4 of 122	Outliers: 0 of 133	Outliers: 11 of 133	
A 124	ASN	50	-	(61.2%) General / -74.7,-29.5 Favored	7% (m-20) chi angles: 287.1,25.3	0.137Å	-	-	
A 125	ARG	50	-	(95.22%) General / -59.9,-43.0 Favored	42.7% (ttp85) chi angles: 181.6,163.3,52.3,65.7	0.093Å	-	-	
A 126	VAL	50	-	(98.66%) Isoleucine or valine / -63.5,-44.3 Favored (74%)	97.8% (t) chi angles: 176.3	0.078Å	-	-	
A 127	LEU	50	-	General / -57.9,-37.4 Favored	98.5% (mt) chi angles: 297.8,177.1	0.161Å	-	-	
A 128	ARG	50	-	(58.94%) General / -75.2,-26.2 Favored	84.5% (mtm-85) chi angles: 296.8,196.8,295,289.4	0.222Å	-	-	
A 129	ASN	50	-	(85.66%) General / -66.2,-37.5 Favored	93.2% (m-20) chi angles: 293.7,333.6	0.107Å	-	-	
A 130	LEU	50	-	(61.22%) General / -72.2,-18.2 Favored	35% (mt) chi angles: 299.6,163.5	0.111Å	-	-	

A 131	ALA	50	-	Favored (68.34%) General / -63.6,-25.7	-	0.109Å	-	-	
A 132	SER	50	-	OUTLIER (0.01%) General / -76.2,-130.1	9.8% (<i>p</i>) chi angles: 84	0.235Å	-	OUTLIER(S) worst is C-CA- CB: 4.143 σ	
A 133	GLU	50	-	Allowed (0.2%) General / 58.9,-104.3	0.8% chi angles: 188.6,233.8,273.5	0.222Å	-	OUTLIER(S) worst is C-N- CA: 6.768 σ	
A 134	LYS	50	-	OUTLIER (0%) General / -50.3,12.8	0.6% chi angles: 60,232.9,170.8,283.6	0.059Å	-	OUTLIER(S) worst is N-CA- C: 4.063 σ	
A 135	GLN	50	-	Favored (12.93%) General / -117.3,7.8	18.5% (<i>mt-30</i>) chi angles: 288.5,158,113.4	0.085Å	-	-	
A 136	GLN	99.99	-	-	4.9% (<i>tp-100</i>) chi angles: 176.4,47.2,205.3	0.08Å	-	OUTLIER(S) worst is CB- CG-CD: 4.217 σ	
B1001	DAD	100.5	-	-	-	-	-	-	
B1002	DAD	102.72	-	-	-	-	-	-	
B1003	DGU	95.24	-	-	-	-	-	-	
B1004	DCY	83.06	-	-	-	-	-	-	
B1005	DAD	74.41	-	-	-	-	-	-	
B1006	DTY	64.72	-	-	-	-	-	-	
B1007	DTY	55.15	-	-	-	-	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg:	Clashscore:	Outliers: 6 of	Poor rotamers: 5 of	Outliers:	Outliers:	Outliers: 11
			54.96	1.52	131	115	4 of 122	0 of 133	of 133
B1008	DTY	63.52	-	-	-	-	-	-	-
B1009	DTY	50.43	-	-	-	-	-	-	-
B1010	DCY	60.49	-	-	-	-	-	-	-
B1011	DAD	62.65	-	-	-	-	-	-	-
B1012	DCY	60.46	-	-	-	-	-	-	-
B1013	DGU	62.87	-	-	-	-	-	-	-
B1014	DCY	66.18	-	-	-	-	-	-	-
B1015	DAD	53.92	-	-	-	-	-	-	-
B1016	DTY	60.67	-	-	-	-	-	-	-

B1017	DGU	53.38	-	-	-	-	-	-	
B1018	DAD	45.88	-	-	-	-	-	-	
B1019	DGU	45.01	-	-	-	-	-	-	
B1020	DTY	47.07	-	-	-	-	-	-	
B1021	DGU	57.3	-	-	-	-	-	-	
B1022	DCY	69.79	-	-	-	-	-	-	
B1023	DAD	85.8	-	-	-	-	-	-	
B1024	DCY	89.37	-	-	-	-	-	-	
B1025	DAD	84.51	-	-	-	-	-	-	
B1026	DGU	87.98	-	-	-	-	-	-	
C2001	DTY	75.67	-	-	-	-	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.96	Clashscore: 1.52	Outliers: 6 of 131	Poor rotamers: 5 of 115	Outliers: 4 of 122	Outliers: 0 of 133	Outliers: 11 of 133
C2002	DTY	77.07	-	-	-	-	-	-	-
C2003	DCY	78.78	-	-	-	-	-	-	-
C2004	DTY	48.81	0.411Å OP1 with A 91 LYS NZ	-	-	-	-	-	-
C2005	DGU	57.01	-	-	-	-	-	-	-
C2006	DTY	69.23	-	-	-	-	-	-	-
C2007	DGU	76.12	-	-	-	-	-	-	-
C2008	DCY	80.78	-	-	-	-	-	-	-
C2009	DAD	74.88	-	-	-	-	-	-	-
C2010	DCY	75.39	-	-	-	-	-	-	-
C2011	DTY	73.29	-	-	-	-	-	-	-
C2012	DCY	61.25	-	-	-	-	-	-	-
C2013	DAD	63.28	0.506Å H2 with A 72 GLY HA2	-	-	-	-	-	-
C2014	DTY	61.51	-	-	-	-	-	-	-
C2015	DGU	43.87	-	-	-	-	-	-	-
C2016	DCY	43.32	-	-	-	-	-	-	-
C2017	DGU	43.75	-	-	-	-	-	-	-
C2018	DTY	44.55	-	-	-	-	-	-	-
C2019	DGU	51.15	0.434Å OP2 with A 9 ASN HB2	-	-	-	-	-	-
C2020	DAD	67.99	-	-	-	-	-	-	-
C2021	DAD	76.69	-	-	-	-	-	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg:	Clashscore:	Outliers: 6 of	Poor rotamers: 5 of	Outliers:	Outliers:	Outliers: 11
			54.96	1.52	131	115	4 of 122	0 of 133	of 133
C2022	DAD		70.65	-	-	-	-	-	-
C2023	DAD		68.53	-	-	-	-	-	-
C2024	DTY		68.92	-	-	-	-	-	-
C2025	DGU		68.54	-	-	-	-	-	-
C2026	DCY		62.68	-	-	-	-	-	-

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