



# Viewing abca4\_sm\_928-1154\_FFX1H-multi.table

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All-Atom Contacts	Clashscore, all atoms:	0.29	99 <sup>th</sup> percentile* (N=1784, all resolutions)	
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	0	0.00%	Goal: <1%
	Ramachandran outliers	3	1.33%	Goal: <0.05%
	Ramachandran favored	203	90.22%	Goal: >98%
	MolProbity score <sup>^</sup>	1.15		99 <sup>th</sup> percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	3	1.46%	Goal: 0
	Bad backbone bonds:	0 / 1778	0.00%	Goal: 0%
	Bad backbone angles:	10 / 2403	0.42%	Goal: <0.1%

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

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

<sup>^</sup> 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: 53.74	Clashscore: 0.29	Outliers: 3 of 225	Poor rotamers: 0 of 190	Outliers: 3 of 205	Outliers: 0 of 227	Outliers: 10 of 227
A 928	GLY	50	-	-	-	-	-	-
A 929	VAL	50	-	Favored (30.23%) Isoleucine or valine / -124.7,146.5	55.6% (t) chi angles: 182	0.101Å	-	-
A 930	CYS	50	-	Favored (4.18%) General / -144.9,106.0	31.7% (p) chi angles: 64.9	0.084Å	-	-
A 931	VAL	50	-	Favored (30.94%) Isoleucine or valine / -70.0,126.8	80.2% (t) chi angles: 174.5	0.086Å	-	-

A 932	LYS	50	-	Favored (4.23%) General / -142.7,103.6	19.7% ( <i>tptp</i> ) chi angles: 192.7,75,196.6,72.9	0.073Å	-	-
A 933	ASN	50	-	Allowed (0.48%) General / 78.1,29.2	2.1% ( <i>m-20</i> ) chi angles: 323.8,321.3	0.086Å	-	-
A 934	LEU	50	-	Favored (12.29%) General / -78.0,109.7	45.5% ( <i>tp</i> ) chi angles: 177.7,55.5	0.033Å	-	-
A 935	VAL	50	0.42Å HA with A 946 VAL O	Favored (45.11%) Isoleucine or valine / -113.3,137.8	8.4% ( <i>p</i> ) chi angles: 68.6	0.138Å	-	-
A 936	LYS	50	-	Favored (19.02%) General / -143.8,129.2	52.1% ( <i>tptt</i> ) chi angles: 182.6,68.7,187.6,181.2	0.039Å	-	-
A 937	ILE	50	-	Favored (3.04%) Isoleucine or valine / -105.1,167.1	23.2% ( <i>pt</i> ) chi angles: 70,177.3	0.062Å	-	-
A 938	PHE	99.99	-	Favored (12.47%) General / -89.5,99.5	50% ( <i>m-85</i> ) chi angles: 306.2,294.8	0.045Å	-	-
A 939	GLU	99.99	-	Favored (63.26%) Pre-proline / -56.7,-38.0	56.3% ( <i>mp0</i> ) chi angles: 296,83.8,353.5	0.157Å	-	-
A 940	PRO	99.99	-	Favored (27.38%) Trans-proline / -69.8,-10.0	32.3% ( <i>Cg_endo</i> ) chi angles: 21.8	0.113Å	-	-
A 941	CYS	99.99	-	Favored (7.31%) General / -125.3,-4.6	17.6% ( <i>p</i> ) chi angles: 71.7	0.152Å	-	-
A 942	GLY	50	-	Favored (97.74%) Glycine / 64.6,40.7	-	-	-	-
A 943	ARG	50	-	Favored (32.82%)	40.7% ( <i>mmt-85</i> ) chi angles:	0.032Å	-	-

				Pre-proline / -129.7,138.3	308.4,299.8,170.4,246.1			
A 944	PRO	50	-	Favored (11.27%) Trans-proline / -83.8,145.0	16.7% ( <i>Cg_endo</i> ) chi angles: 39.1	0.055Å	-	-
A 945	ALA	50	-	Favored (2.82%) General / -128.7,-25.6	-	0.015Å	-	-
A 946	VAL	50	0.42Å O with A 935 VAL HA	Favored (7.43%) Isoleucine or valine / -140.0,115.2	24.7% ( <i>t</i> ) chi angles: 186.9	0.098Å	-	-
A 947	ASP	50	-	Favored (3.31%) General / -119.9,90.4	40.8% ( <i>m-20</i> ) chi angles: 294.1,3.8	0.093Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 53.74	Clashscore: 0.29	Outliers: 3 of 225	Poor rotamers: 0 of 190	Outliers: 3 of 205	Outliers: 0 of 227	Outliers: 10 of 227
A 948	ARG	50	-	Favored (13.65%) General / 57.3,49.2	41% ( <i>mmt180</i> ) chi angles: 292.9,297.6,185.5,186.5	0.193Å	-	-
A 949	LEU	99.99	-	Favored (44%) General / -69.4,153.2	20.9% ( <i>mt</i> ) chi angles: 298,193.6	0.062Å	-	-
A 950	ASN	50	-	Favored (5.38%) General / -148.1,112.8	11.7% ( <i>m-80</i> ) chi angles: 283.1,259.4	0.131Å	-	-
A 951	ILE	50	-	Allowed (1.56%) Isoleucine or valine / -163.1,139.2	9.9% ( <i>tp</i> ) chi angles: 186.4,65.3	0.074Å	-	-
A 952	THR	50	-	Favored (23.35%) General / -99.7,149.4	17.9% ( <i>p</i> ) chi angles: 47.4	0.027Å	-	-
A 953	PHE	50	-	Favored (41.47%) General / -129.8,157.7	17.3% ( <i>m-85</i> ) chi angles: 314.5,302.1	0.053Å	-	-
				Favored				

A 954	TYR	50	-	(49.19%) General / -136.5,151.2	77.1% ( <i>m-85</i> ) chi angles: 304.6,278.8	0.077Å	-	-
A 955	GLU	50	-	Favored (55.41%) General / -62.0,144.2	21.5% ( <i>mp0</i> ) chi angles: 289.2,62.8,38.2	0.057Å	-	-
A 956	ASN	50	-	Allowed (0.22%) General / 82.3,-55.2	14.7% ( <i>t-20</i> ) chi angles: 194.8,286.8	0.166Å	-	-
A 957	GLN	50	-	Favored (4.2%) General / -59.2,116.9	88.7% ( <i>mt-30</i> ) chi angles: 292.8,176.5,1.6	0.082Å	-	-
A 958	ILE	50	-	Favored (15.25%) Isoleucine or valine / -71.1,118.1	29% ( <i>mt</i> ) chi angles: 296.3,153	0.045Å	-	-
A 959	THR	50	-	Favored (50.19%) General / -107.8,124.5	41.4% ( <i>m</i> ) chi angles: 305.6	0.046Å	-	-
A 960	ALA	50	-	Favored (26.13%) General / -102.4,113.1	-	0.01Å	-	-
A 961	PHE	99.99	-	Favored (7.51%) General / -81.2,81.0	71.6% ( <i>t80</i> ) chi angles: 186,80.2	0.093Å	-	-
A 962	LEU	50	-	Favored (47.44%) General / -72.7,139.7	52.4% ( <i>mt</i> ) chi angles: 299.5,186.7	0.068Å	-	-
A 963	GLY	50	-	Allowed (0.89%) Glycine / -178.3,123.8	-	-	-	-
A 964	HIS	50	-	Favored (14.25%) General / -68.4,167.7	19.9% ( <i>m170</i> ) chi angles: 306.3,145.6	0.085Å	-	-
A 965	ASN	50	-	Favored (3.97%) General / -43.4,125.7	1.8% ( <i>m-20</i> ) chi angles: 301,34	0.118Å	-	-
				Favored				

A 966	GLY	50	-	(56.92%) Glycine / 99.8,-2.2	-	-	-	-
A 967	ALA	50	-	Favored (59.76%) General / -78.0,-13.8	-	0.13Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C $\beta$ deviation	Bond lengths	Bond angles
		Avg: 53.74	Clashscore: 0.29	Outliers: 3 of 225	Poor rotamers: 0 of 190	Outliers: 3 of 205	Outliers: 0 of 227	Outliers: 10 of 227
A 968	GLY	50	-	Favored (55.27%) Glycine / 90.7,16.2	-	-	-	-
A 969	LYS	50	-	Favored (85.73%) General / -57.6,-44.8	31% ( <i>mtmm</i> ) chi angles: 308.6,190.1,306.1,300.8	0.143Å	-	-
A 970	THR	50	-	Favored (84.81%) General / -58.5,-41.1	16.5% ( <i>m</i> ) chi angles: 311.5	0.078Å	-	-
A 971	THR	50	-	Favored (88.63%) General / -58.9,-46.2	5.6% ( <i>m</i> ) chi angles: 316.3	0.092Å	-	-
A 972	THR	50	-	Favored (72.95%) General / -56.1,-49.8	4.3% ( <i>m</i> ) chi angles: 317.8	0.133Å	-	-
A 973	LEU	50	-	Favored (62.72%) General / -72.4,-28.1	11.2% ( <i>mp</i> ) chi angles: 273.1,62.1	0.184Å	-	-
A 974	SER	50	-	Favored (83.89%) General / -62.0,-37.2	69.3% ( <i>m</i> ) chi angles: 293.1	0.105Å	-	-
A 975	ILE	50	-	Favored (77.14%) Isoleucine or valine / -69.3,-46.4	17.5% ( <i>mt</i> ) chi angles: 300.8,149.7	0.08Å	-	-
A 976	LEU	50	-	Favored (65.85%) General /	48% ( <i>mt</i> ) chi angles: 304.9,185.6	0.162Å	-	-

A 977	THR	99.99	-	-56.8,-32.6 Favored (57.08%) General / -90.0,0.5	5.8% ( <i>t</i> ) chi angles: 196.4	0.22Å	-	-
A 978	GLY	50	-	Favored (57.99%) Glycine / 74.2,32.8	-	-	-	-
A 979	LEU	50	-	Favored (13.37%) General / -112.1,-14.7	54.9% ( <i>tp</i> ) chi angles: 177.6,57.2	0.041Å	-	-
A 980	LEU	50	-	Favored (3.09%) Pre-proline / -151.1,112.7	54.4% ( <i>tp</i> ) chi angles: 183.5,62.9	0.115Å	-	-
A 981	PRO	50	-	Favored (23.79%) Trans-proline / -78.4,148.5	69.7% ( <i>Cg_endo</i> ) chi angles: 28.1	0.029Å	-	-
A 982	PRO	50	-	Favored (40.34%) Trans-proline / -55.9,151.6	82.3% ( <i>Cg_exo</i> ) chi angles: 331.9	0.121Å	-	-
A 983	THR	50	-	Favored (67.69%) General / -70.5,-30.9	21.9% ( <i>m</i> ) chi angles: 309.9	0.13Å	-	-
A 984	SER	50	-	Allowed (0.17%) General / -175.7,119.5	12.6% ( <i>t</i> ) chi angles: 166.3	0.041Å	-	-
A 985	GLY	50	-	Favored (21.64%) Glycine / 162.6,166.6	-	-	-	-
A 986	THR	50	-	Favored (44.98%) General / -122.5,148.6	1.3% ( <i>m</i> ) chi angles: 275.7	0.152Å	-	-
A 987	VAL	50	-	Allowed (0.32%) Isoleucine or valine / -149.2,100.8	48.2% ( <i>t</i> ) chi angles: 182.8	0.046Å	-	-

#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
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				Avg: 53.74	Clashscore: 0.29	Outliers: 3 of 225	Poor rotamers: 0 of 190	Outliers: 3 of 205	Outliers: 0 of 227	Outliers: 10 of 227
A 988	LEU	50	-	Favored (27.84%) General / -80.1,123.4	10.3% ( <i>mp</i> ) chi angles: 271.5,57.4	0.067Å	-	-		
A 989	VAL	50	-	Favored (10.82%) Isoleucine or valine / -116.8,100.7	45.9% ( <i>t</i> ) chi angles: 183.5	0.031Å	-	-		
A 990	GLY	50	-	Favored (75.15%) Glycine / 69.5,25.8	-	-	-	-		
A 991	GLY	50	-	Favored (78.52%) Glycine / 89.3,1.4	-	-	-	-		
A 992	ARG	50	-	Favored (41.69%) General / -106.0,120.4	13.5% ( <i>mmt85</i> ) chi angles: 297.5,302.9,192.6,110.9	0.083Å	-	-		
A 993	ASP	50	-	Favored (35.31%) General / -76.0,128.6	23.1% ( <i>t0</i> ) chi angles: 201.4,352.9	0.059Å	-	-		
A 994	ILE	50	-	Allowed (0.45%) Isoleucine or valine / -50.8,-63.0	43.4% ( <i>mt</i> ) chi angles: 287.9,180	0.16Å	-	-		
A 995	GLU	50	-	Favored (83.21%) General / -64.8,-36.1	48.1% ( <i>mm-40</i> ) chi angles: 305.6,312.3,316	0.133Å	-	-		
A 996	THR	50	-	Favored (59.89%) General / -77.7,-11.6	11% ( <i>p</i> ) chi angles: 44.6	0.08Å	-	-		
A 997	SER	50	-	Allowed (0.74%) General / -149.2,35.2	36.1% ( <i>t</i> ) chi angles: 175.8	0.076Å	-	-		
A 998	LEU	50	-	Allowed (0.31%) General / -35.0,-63.8	40.3% ( <i>mt</i> ) chi angles: 283.8,164.3	0.123Å	-	-		

A 999	ASP	50	-	Favored (59.25%) General / -80.3,-13.3	6.2% ( <i>m-20</i> ) chi angles: 309.3,89.9	0.196Å	-	OUTLIER(S) worst is CA- CB-CG: 4.199 σ
A1000	ALA	50	-	Favored (73.67%) General / -64.5,-32.1	-	0.12Å	-	-
A1001	VAL	50	-	Favored (15.41%) Isoleucine or valine / -80.8,-51.6	88.2% ( <i>t</i> ) chi angles: 177.8	0.083Å	-	-
A1002	ARG	50	-	Favored (83.65%) General / -64.5,-36.3	33.2% ( <i>mtm180</i> ) chi angles: 297.9,189.7,292.8,212.4	0.21Å	-	-
A1003	GLN	50	-	Favored (60.27%) General / -75.1,-12.3	38.9% ( <i>mt-30</i> ) chi angles: 297.1,172.7,249.3	0.092Å	-	-
A1004	SER	50	-	Favored (40.43%) General / -102.3,7.8	50.9% ( <i>m</i> ) chi angles: 301.4	0.052Å	-	-
A1005	LEU	50	-	Favored (49.4%) General / -126.6,149.5	52.8% ( <i>tp</i> ) chi angles: 172.2,64	0.156Å	-	-
A1006	GLY	50	-	Favored (17.76%) Glycine / -125.8,151.5	-	-	-	-
A1007	MET	99.99	-	Favored (51.65%) General / -133.6,151.1	25.1% ( <i>ptm</i> ) chi angles: 60.2,173.6,280.3	0.033Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 53.74	Clashscore: 0.29	Outliers: 3 of 225	Poor rotamers: 0 of 190	Outliers: 3 of 205	Outliers: 0 of 227	Outliers: 10 of 227
A1008	CYS	50	-	Favored (4.56%) Pre-proline / -145.2,99.5	46.5% ( <i>t</i> ) chi angles: 178.9	0.07Å	-	-
A1009	PRO	50	-	Favored (15.76%)	88.4% ( <i>Cg_endo</i> )	0.018Å	-	-



				Trans-proline / -80.6,170.4	chi angles: 31.2			
A1010	GLN	50	-	Allowed (0.44%) General / -54.6,109.0	59.6% ( <i>tt0</i> ) chi angles: 185.7,170.3,29.8	0.032Å	-	-
A1011	HIS	50	-	Favored (2.05%) General / 72.5,29.5	57.2% ( <i>m80</i> ) chi angles: 284.7,74.1	0.226Å	-	-
A1012	ASN	50	-	Favored (26.31%) General / -52.4,138.8	16.8% ( <i>t30</i> ) chi angles: 170.9,40.1	0.09Å	-	-
A1013	ILE	50	-	Allowed (1.1%) Isoleucine or valine / -154.4,167.0	27.2% ( <i>pt</i> ) chi angles: 52.9,169.7	0.061Å	-	-
A1014	LEU	50	-	Favored (16.2%) General / -105.7,159.2	9.4% ( <i>mp</i> ) chi angles: 278.8,71.4	0.029Å	-	-
A1015	PHE	50	-	Favored (33.17%) General / -64.7,155.6	37.3% ( <i>t80</i> ) chi angles: 186.6,58.4	0.032Å	-	-
A1016	HIS	50	-	Favored (14.31%) General / -108.1,-16.3	19.9% ( <i>m-70</i> ) chi angles: 272,271.3	0.092Å	-	-
A1017	HIS	50	-	Allowed (0.79%) General / -116.6,71.5	39.5% ( <i>t60</i> ) chi angles: 195.2,80.2	0.081Å	-	OUTLIER(S) worst is C-N- CA: 5.561 σ
A1018	LEU	50	-	Allowed (0.16%) General / -178.5,137.9	57.5% ( <i>tp</i> ) chi angles: 182.6,63.2	0.049Å	-	-
A1019	THR	50	-	Favored (41.05%) General / -72.0,154.6	41.6% ( <i>p</i> ) chi angles: 54.4	0.152Å	-	-
A1020	VAL	50	-	Favored (77.49%) Isoleucine or valine / -68.8,-37.5	71.1% ( <i>t</i> ) chi angles: 179.4	0.085Å	-	-

A1021	ALA	50	-	Favored (15.5%) General / -88.5,-37.7	-	0.098Å	-	-
A1022	GLU	50	-	Favored (76.54%) General / -55.4,-45.0	2.8% ( <i>tm-20</i> ) chi angles: 160.8,289.4,318.4	0.063Å	-	-
A1023	HIS	50	-	Favored (11.96%) General / -71.8,-0.7	25.1% ( <i>t-80</i> ) chi angles: 204.4,277.1	0.202Å	-	-
A1024	MET	50	-	Favored (22.18%) General / -84.9,-35.3	24.9% ( <i>mmp</i> ) chi angles: 308.4,293,88	0.112Å	-	-
A1025	LEU	50	-	Favored (91.4%) General / -65.5,-42.9	48.1% ( <i>tp</i> ) chi angles: 172.9,59.1	0.063Å	-	-
A1026	PHE	50	-	Favored (70.97%) General / -56.0,-50.4	2.1% ( <i>t80</i> ) chi angles: 189.5,119.8	0.036Å	-	OUTLIER(S) worst is CA- CB-CG: 4.175 σ
A1027	TYR	50	-	Favored (74.11%) General / -69.2,-33.9	41.7% ( <i>t80</i> ) chi angles: 193.7,76.9	0.162Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 53.74	Clashscore: 0.29	Outliers: 3 of 225	Poor rotamers: 0 of 190	Outliers: 3 of 205	Outliers: 0 of 227	Outliers: 10 of 227
A1028	ALA	50	-	Favored (83.58%) General / -59.4,-39.5	-	0.095Å	-	-
A1029	GLN	50	-	Favored (72.3%) General / -67.2,-31.7	70.3% ( <i>mm-40</i> ) chi angles: 293.5,295.1,340.5	0.127Å	-	-
A1030	LEU	50	-	Favored (76.15%) General / -66.6,-33.7	6.7% ( <i>mp</i> ) chi angles: 272.4,47.1	0.126Å	-	-
A1031	LYS	50	-	OUTLIER (0.02%) General /	5.1% ( <i>ttpm?</i> ) chi angles: 193.6,172.6,90.5,288.1	0.178Å	-	-

A1032	GLY	50	-	-80.2,-113.5 Favored (5.74%) Glycine / -82.3,-146.1	-	-	-	-
A1033	LYS	50	-	Allowed (0.55%) General / -146.2,-7.4	32.2% ( <i>mmtm</i> ) chi angles: 306.5,291.7,160.3,289.5	0.087Å	-	-
A1034	SER	50	-	Favored (11.76%) General / -103.5,164.3	3.6% ( <i>t</i> ) chi angles: 202	0.089Å	-	-
A1035	GLN	50	-	Favored (68.47%) General / -72.5,-36.6	23.9% ( <i>pt20</i> ) chi angles: 65.6,186.9,351.8	0.091Å	-	-
A1036	GLU	50	-	Favored (63.43%) General / -74.4,-34.9	5.9% ( <i>mp0</i> ) chi angles: 322.7,74.7,8.8	0.129Å	-	-
A1037	GLU	50	-	Favored (93.48%) General / -59.6,-42.9	37.3% ( <i>tt0</i> ) chi angles: 185.7,197.8,331.5	0.02Å	-	-
A1038	ALA	50	-	Favored (92.03%) General / -63.2,-38.7	-	0.088Å	-	-
A1039	GLN	50	-	Favored (99.18%) General / -63.2,-42.1	4.8% ( <i>tp60</i> ) chi angles: 175.8,66.3,106.7	0.057Å	-	-
A1040	LEU	50	-	Favored (90.73%) General / -62.3,-46.0	57.4% ( <i>tp</i> ) chi angles: 179.3,58.9	0.05Å	-	-
A1041	GLU	50	-	Favored (45.08%) General / -57.1,-54.6	3.5% ( <i>mt-10</i> ) chi angles: 279.9,227.6,1	0.069Å	-	-
A1042	MET	50	-	Favored (14.84%) General / -52.5,-56.5	51.8% ( <i>ttp</i> ) chi angles: 181.5,164.4,75.9	0.123Å	-	-
A1043	GLU	50	-	Favored (32.62%) General /	72.2% ( <i>mm-40</i> ) chi angles: 290.5,306.1,307	0.224Å	-	-

A1044	ALA	50	-	-83.0,-25.1 Favored (97.21%) General / -62.7,-44.1	-	0.084Å	-	-
A1045	MET	50	-	Favored (54.65%) General / -94.0,-1.4	4.8% ( <i>ptt?</i> ) chi angles: 50.8,165,154.7	0.298Å	-	-
A1046	LEU	50	-	Favored (62.01%) General / -71.1,-46.4	8.2% ( <i>tt</i> ) chi angles: 187.4,143.5	0.073Å	-	-
A1047	GLU	50	-	Favored (88.23%) General / -60.1,-40.1	12.8% ( <i>tm-20</i> ) chi angles: 192.7,288.6,324.7	0.115Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 53.74	Clashscore: 0.29	Outliers: 3 of 225	Poor rotamers: 0 of 190	Outliers: 3 of 205	Outliers: 0 of 227	Outliers: 10 of 227
A1048	ASP	50	-	Favored (45.95%) General / -49.8,-50.1	13.9% ( <i>t70</i> ) chi angles: 176.6,89.8	0.051Å	-	-
A1049	THR	50	-	Favored (51.05%) General / -72.2,-47.4	33.6% ( <i>p</i> ) chi angles: 68.9	0.18Å	-	-
A1050	GLY	50	-	Favored (85.52%) Glycine / 85.9,-4.7	-	-	-	-
A1051	LEU	50	-	Favored (73.42%) General / -66.5,-32.2	85% ( <i>mt</i> ) chi angles: 292.2,167.8	0.126Å	-	-
A1052	HIS	50	-	Allowed (0.14%) General / 57.7,-101.9	75% ( <i>m80</i> ) chi angles: 289.3,79.9	0.267Å	-	-
A1053	HIS	50	-	Favored (65.34%) General / -70.3,-28.6	81.6% ( <i>t60</i> ) chi angles: 184.7,62.2	0.291Å	-	OUTLIER(S) worst is CA-CB-CG: 4.174 σ
				Allowed (0.47%)	27.3% ( <i>mmmt</i> )			

A1054	LYS	50	-	General / -76.4,16.5	chi angles: 287.2,304.7,305.4,174	0.152Å	-	-
A1055	ARG	50	-	Favored (13.45%) General / -118.9,16.4	16% ( <i>tpt85</i> ) chi angles: 201.4,73.1,167.2,72.4	0.07Å	-	-
A1056	ASN	50	-	Favored (4.09%) General / -133.2,21.8	5.1% ( <i>m120</i> ) chi angles: 314.8,142.6	0.109Å	-	OUTLIER(S) worst is CA- CB-CG: 8.548 σ
A1057	GLU	50	-	Favored (4.03%) General / -106.4,-179.8	5.8% ( <i>mm-40</i> ) chi angles: 299.5,287.4,243.2	0.13Å	-	-
A1058	GLU	50	-	Favored (44.96%) General / -71.9,132.9	4.6% ( <i>tp10</i> ) chi angles: 169,58,298.3	0.027Å	-	-
A1059	ALA	50	-	Favored (2.45%) General / -80.0,13.0	-	0.035Å	-	-
A1060	GLN	50	-	Favored (32.75%) General / -83.0,-24.5	10.8% ( <i>pt20</i> ) chi angles: 73.8,199.1,3.7	0.206Å	-	-
A1061	ASP	50	-	Favored (25.35%) General / -96.1,-12.1	16.2% ( <i>p-10</i> ) chi angles: 71.5,153.2	0.146Å	-	-
A1062	LEU	50	-	Favored (8.62%) General / -56.2,121.1	8.8% ( <i>mp</i> ) chi angles: 268.2,66.2	0.078Å	-	-
A1063	SER	50	-	Allowed (1.39%) General / -62.1,172.5	10% ( <i>p</i> ) chi angles: 83.9	0.125Å	-	-
A1064	GLY	50	-	Favored (60.29%) Glycine / -60.2,-23.9	-	-	-	-
A1065	GLY	50	-	Favored (6.01%) Glycine / -97.7,-33.0	-	-	-	-
				Favored				

A1066	MET	50	-	(88.93%) General / -58.5,-43.7	61.6% ( <i>mtt</i> ) chi angles: 291.5,169.7,188	0.089Å	-	-
A1067	GLN	50	-	Favored (85.44%) General / -60.1,-39.2	22% ( <i>pt20</i> ) chi angles: 69.4,186.9,354.8	0.131Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 53.74	Clashscore: 0.29	Outliers: 3 of 225	Poor rotamers: 0 of 190	Outliers: 3 of 205	Outliers: 0 of 227	Outliers: 10 of 227
A1068	ARG	50	-	Favored (66.99%) General / -70.6,-30.3	21.2% ( <i>mmm180</i> ) chi angles: 279.6,297.3,303,159	0.187Å	-	-
A1069	LYS	50	-	Favored (87.49%) General / -65.0,-44.9	20.7% ( <i>mtmt</i> ) chi angles: 301.1,215.9,294,161.1	0.121Å	-	-
A1070	LEU	50	-	Favored (76.75%) General / -61.7,-35.0	7.3% ( <i>tp</i> ) chi angles: 188.1,40.3	0.087Å	-	-
A1071	SER	50	-	Favored (75.87%) General / -57.4,-39.4	15.8% ( <i>m</i> ) chi angles: 308.1	0.089Å	-	-
A1072	VAL	50	-	Favored (14.85%) Isoleucine or valine / -82.7,-38.3	34.1% ( <i>m</i> ) chi angles: 299.1	0.24Å	-	-
A1073	ALA	50	-	Favored (78.25%) General / -60.9,-36.0	-	0.086Å	-	-
A1074	ILE	50	-	Favored (41.02%) Isoleucine or valine / -57.5,-32.1	37.4% ( <i>pt</i> ) chi angles: 66.5,170.7	0.194Å	-	-
A1075	ALA	50	-	Favored (59.59%) General / -81.8,-7.3	-	0.056Å	-	-
				Favored (13.33%)	5.3% ( <i>m-85</i> )			

A1076	PHE	50	-	General / -106.2,-20.7	chi angles: 285.1,55.1	0.065Å	-	-
A1077	VAL	50	-	Favored (16.29%) Isoleucine or valine / -74.5,-15.6	27.3% ( <i>m</i> ) chi angles: 293.9	0.201Å	-	-
A1078	GLY	50	-	Favored (81.81%) Glycine / -85.3,5.8	-	-	-	-
A1079	ASP	50	-	Favored (25.35%) General / 50.9,47.1	35.7% ( <i>t0</i> ) chi angles: 192.6,29	0.184Å	-	-
A1080	ALA	50	-	Favored (19.75%) General / -49.8,129.3	-	0.056Å	-	-
A1081	LYS	50	-	Favored (56.96%) General / -79.3,-16.1	12.2% ( <i>mmtm</i> ) chi angles: 293.8,279.4,141.8,284	0.097Å	-	-
A1082	VAL	50	-	Favored (28.44%) Isoleucine or valine / -137.8,145.8	5% ( <i>p</i> ) chi angles: 54	0.111Å	-	-
A1083	VAL	50	-	Favored (7.23%) Isoleucine or valine / -144.9,125.2	3.3% ( <i>p</i> ) chi angles: 79.8	0.145Å	-	-
A1084	ILE	50	-	Favored (54.77%) Isoleucine or valine / -106.2,118.9	68.1% ( <i>mt</i> ) chi angles: 287.8,166.4	0.095Å	-	-
A1085	LEU	50	-	Favored (5.39%) General / -127.2,98.7	9.3% ( <i>mt</i> ) chi angles: 321.2,172.2	0.038Å	-	-
A1086	ASP	50	-	Favored (30.95%) General / -85.8,123.2	37.5% ( <i>t70</i> ) chi angles: 188.3,61.2	0.022Å	-	-
				Favored	18% ( <i>mm-40</i> )			

A1087	GLU	50	-	(5.38%) Pre-proline / 46.9,48.2	chi angles: 275.4,285.9,4.6	0.122Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
Avg: 53.74				Clashscore: 0.29	Outliers: 3 of 225	Poor rotamers: 0 of 190	Outliers: 3 of 205	Outliers: 0 of 227
A1088	PRO	50	-	Favored (19.08%) Trans-proline / -74.1,-20.4	12% ( <i>Cg_endo</i> ) chi angles: 39.8	0.077Å	-	-
A1089	THR	50	-	Favored (18.44%) General / -113.2,17.7	24.8% ( <i>p</i> ) chi angles: 50.2	0.066Å	-	-
A1090	SER	50	-	Favored (35.78%) General / -77.1,149.7	60.5% ( <i>p</i> ) chi angles: 72.5	0.02Å	-	-
A1091	GLY	50	-	Favored (5.5%) Glycine / 46.7,59.4	-	-	-	-
A1092	VAL	50	-	Favored (3.69%) Isoleucine or valine / -148.5,167.9	3.4% ( <i>p</i> ) chi angles: 79.6	0.12Å	-	-
A1093	ASP	50	-	Favored (20.37%) Pre-proline / -68.5,167.1	6.3% ( <i>p-10</i> ) chi angles: 68.3,281.8	0.063Å	-	-
A1094	PRO	50	-	Favored (14.91%) Trans-proline / -79.3,-10.4	86.4% ( <i>Cg_endo</i> ) chi angles: 31.3	0.084Å	-	-
A1095	TYR	50	-	Favored (6.63%) General / -99.9,-42.9	77.3% ( <i>t80</i> ) chi angles: 172.2,75.3	0.065Å	-	-
A1096	SER	50	-	Favored (74.68%) General / -59.2,-36.0	50.3% ( <i>m</i> ) chi angles: 300.3	0.117Å	-	-
A1097	ARG	50	-	Favored (71.03%) General / -55.1,-40.9	29.9% ( <i>ptt180</i> ) chi angles: 55.4,169.7,187,169.3	0.157Å	-	-



A1098	ARG	50	-	Favored (74.39%) General / -64.4,-48.7	8.3% ( <i>tpt180</i> ) chi angles: 167.1,59.6,195.4,247	0.141Å	-	OUTLIER(S) worst is CD- NE-CZ: 5.002 σ
A1099	SER	50	-	Favored (68.05%) General / -57.4,-33.7	42% ( <i>t</i> ) chi angles: 181.2	0.168Å	-	-
A1100	ILE	99.99	-	Favored (97.66%) Isoleucine or valine / -62.6,-45.9	67.5% ( <i>mt</i> ) chi angles: 287.8,166.2	0.154Å	-	-
A1101	TRP	99.99	-	Favored (97.08%) General / -62.1,-44.2	6.9% ( <i>m0</i> ) chi angles: 313.9,323.3	0.162Å	-	-
A1102	ASP	50	-	Favored (84.97%) General / -59.2,-40.2	18.2% ( <i>m-20</i> ) chi angles: 302.4,278.9	0.114Å	-	-
A1103	LEU	50	-	Favored (94.94%) General / -64.2,-39.9	25.4% ( <i>mt</i> ) chi angles: 293.2,158.2	0.083Å	-	-
A1104	LEU	50	-	Favored (82.5%) General / -59.3,-48.2	62.8% ( <i>mt</i> ) chi angles: 304.8,182.9	0.121Å	-	-
A1105	LEU	50	-	Favored (87.59%) General / -61.3,-38.7	7.4% ( <i>mp</i> ) chi angles: 275.1,76.5	0.147Å	-	-
A1106	LYS	50	-	Favored (81.28%) General / -68.0,-42.2	33.5% ( <i>ttpt</i> ) chi angles: 195,181.2,74.4,188.1	0.031Å	-	-
A1107	TYR	99.99	-	Favored (3.53%) General / -93.9,25.7	23.9% ( <i>m-30</i> ) chi angles: 301.4,315.4	0.052Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 53.74	Clashscore: 0.29	Outliers: 3 of 225	Poor rotamers: 0 of 190	Outliers: 3 of 205	Outliers: 0 of 227	Outliers: 10 of 227

A1108	ARG	99.99	-	Favored (62.38%)	81% ( <i>mtm180</i> ) chi angles:	0.087Å	-	OUTLIER(S) worst is C-N-
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				General / -73.3,-28.9	284,182.9,287.2,183.7		CA: 4.105 $\sigma$
A1109	SER	99.99	-	OUTLIER (0%) General / -7.2,-84.4	75.7% ( <i>p</i> ) chi angles: 58.3	0.17Å	-
A1110	GLY	99.99	-	Allowed (0.57%) Glycine / -126.5,64.7	-	-	-
A1111	ARG	50	-	Favored (6.85%) General / -147.2,116.2	36% ( <i>ttm-85</i> ) chi angles: 197.6,177.6,312.1,261.7	0.096Å	-
A1112	THR	50	-	Favored (6.75%) General / -80.9,83.0	53.1% ( <i>m</i> ) chi angles: 304.7	0.031Å	-
A1113	ILE	50	-	Favored (9.2%) Isoleucine or valine / -77.9,107.0	63.2% ( <i>mt</i> ) chi angles: 300.7,179.5	0.062Å	-
A1114	ILE	50	-	Favored (24.27%) Isoleucine or valine / -122.5,109.5	16.4% ( <i>pt</i> ) chi angles: 48.4,173.5	0.115Å	-
A1115	MET	50	-	Favored (6.02%) General / -111.9,174.1	7.7% ( <i>ptp</i> ) chi angles: 80.1,169,95.5	0.042Å	-
A1116	SER	50	-	Favored (50.58%) General / -126.1,144.9	4% ( <i>p</i> ) chi angles: 89.4	0.036Å	-
A1117	THR	50	-	Favored (13.12%) General / -154.7,134.8	18.2% ( <i>m</i> ) chi angles: 289.1	0.088Å	-
A1118	HIS	50	-	Favored (36.91%) General / -80.6,-30.9	45.5% ( <i>p-80</i> ) chi angles: 71.6,283.9	0.142Å	-
A1119	HIS	99.99	-	Favored (21.11%) General / -58.5,151.1	95.1% ( <i>m-70</i> ) chi angles: 292.5,275.6	0.082Å	-
				Allowed (1.09%)	34.9% ( <i>mtt</i> )		OUTLIER(S)

A1120	MET	50	-	General / -137.6,-23.1	chi angles: 279.1,170.4,165.4	0.151Å	-	worst is C-N- CA: 4.685 $\sigma$
A1121	ASP	50	-	OUTLIER (0.01%) General / -42.9,-15.8	10.4% ( <i>p</i> -10) chi angles: 52,306.7	0.057Å	-	-
A1122	GLU	50	-	Favored (8.68%) General / -121.7,-11.1	96.3% ( <i>mt</i> -10) chi angles: 300.5,179.2,352.6	0.06Å	-	-
A1123	ALA	50	-	Favored (82.53%) General / -59.4,-39.1	-	0.15Å	-	-
A1124	ASP	50	-	Favored (74.36%) General / -66.7,-32.8	1.2% ( <i>m</i> -20) chi angles: 308.1,59.9	0.101Å	-	-
A1125	LEU	50	-	Favored (52.56%) General / -95.9,4.7	8.2% ( <i>mp</i> ) chi angles: 285,71.7	0.059Å	-	-
A1126	LEU	50	-	Favored (17.9%) General / -92.4,-26.7	20.8% ( <i>tp</i> ) chi angles: 192.7,68.3	0.035Å	-	-
A1127	GLY	50	-	Favored (44.11%) Glycine / 173.0,-179.9	-	-	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C $\beta$ deviation	Bond lengths	Bond angles
		Avg: 53.74	Clashscore: 0.29	Outliers: 3 of 225	Poor rotamers: 0 of 190	Outliers: 3 of 205	Outliers: 0 of 227	Outliers: 10 of 227
A1128	ASP	50	-	Favored (22.82%) General / -84.7,-34.8	17.9% ( <i>m</i> -20) chi angles: 307.3,284	0.048Å	-	-
A1129	ARG	50	-	Favored (41.77%) General / -127.5,156.7	45.4% ( <i>mtp</i> 180) chi angles: 285,180.3,62,233.9	0.067Å	-	-
A1130	ILE	50	-	Favored (37.52%) Isoleucine or valine / -131.0,163.2	43.5% ( <i>pt</i> ) chi angles: 63.9,173.9	0.116Å	-	-

A1131	ALA	50	-	Favored (4.87%) General / -152.1,115.9	-	0.07Å	-	-
A1132	ILE	50	-	Favored (45.88%) Isoleucine or valine / -93.4,126.2	46.4% ( <i>pt</i> ) chi angles: 58.8,172.9	0.122Å	-	-
A1133	ILE	50	-	Favored (31.05%) Isoleucine or valine / -119.7,143.5	1.5% ( <i>tt</i> ) chi angles: 194.6,198.6	0.094Å	-	-
A1134	ALA	50	-	Favored (11.8%) General / -146.4,124.1	-	0.082Å	-	-
A1135	GLN	50	-	Favored (4.81%) General / 43.4,55.4	19.5% ( <i>mm100</i> ) chi angles: 302.7,313,108.8	0.138Å	-	-
A1136	GLY	50	-	Favored (68.28%) Glycine / 84.1,-8.1	-	-	-	-
A1137	ARG	50	-	Favored (50.75%) General / -116.8,139.3	38% ( <i>mtt85</i> ) chi angles: 287.9,149.3,184.5,64.2	0.095Å	-	-
A1138	LEU	99.99	-	Favored (25.23%) General / -88.1,146.8	20.5% ( <i>mt</i> ) chi angles: 280.1,160.2	0.074Å	-	-
A1139	TYR	50	-	Favored (2.74%) General / -118.2,-43.2	5.8% ( <i>t80</i> ) chi angles: 178.6,30.5	0.085Å	-	-
A1140	CYS	50	-	Favored (28.37%) General / -147.8,166.2	22.2% ( <i>m</i> ) chi angles: 311.6	0.08Å	-	-
A1141	SER	50	-	Favored (34.09%) General / -158.9,158.8	33.7% ( <i>t</i> ) chi angles: 183.4	0.037Å	-	-

A1142	GLY	50	-	Favored (31.1%) Glycine / 161.9,-159.1	-	-	-	-
A1143	THR	50	-	Favored (11.85%) Pre-proline / -76.1,171.5	66.5% ( <i>p</i> ) chi angles: 59.5	0.051Å	-	-
A1144	PRO	50	-	Favored (34.68%) Trans-proline / -65.8,-35.8	27.5% ( <i>Cg_endo</i> ) chi angles: 20.5	0.127Å	-	-
A1145	LEU	50	-	Favored (93.73%) General / -65.4,-40.7	2% ( <i>tt</i> ) chi angles: 189.4,130.1	0.086Å	-	-
A1146	PHE	50	-	Favored (91.48%) General / -62.6,-38.8	17% ( <i>m-30</i> ) chi angles: 299.7,344.7	0.177Å	-	-
A1147	LEU	50	-	Favored (68.92%) General / -70.3,-31.5	11.5% ( <i>mt</i> ) chi angles: 301.3,199.3	0.215Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
Avg: 53.74				Clashscore: 0.29	Outliers: 3 of 225	Poor rotamers: 0 of 190	Outliers: 3 of 205	Outliers: 0 of 227
A1148	LYS	50	-	Favored (88.66%) General / -65.4,-38.0	87.6% ( <i>mttt</i> ) chi angles: 297.8,182.6,164.5,185.8	0.119Å	-	-
A1149	ASN	50	-	Favored (82.27%) General / -65.7,-36.0	7.3% ( <i>m120</i> ) chi angles: 314,134.3	0.106Å	-	OUTLIER(S) worst is CA- CB-CG: 4.725 σ
A1150	CYS	50	-	Favored (56.3%) General / -77.5,-19.2	34.4% ( <i>t</i> ) chi angles: 189.2	0.095Å	-	-
A1151	PHE	50	-	Favored (9.48%) General / -122.8,3.9	86.7% ( <i>m-85</i> ) chi angles: 289.9,269.8	0.109Å	-	OUTLIER(S) worst is CA- CB-CG: 4.82 σ
A1152	GLY	50	-	Favored (75.82%) Glycine /	-	-	-	-

A1153	THR	50	-	71.4,25.2 Favored (4.64%) General / -99.3,179.3	69.1% ( <i>p</i> ) chi angles: 62	0.109Å	-	-
A1154	GLY	99.99	-	-	-	-	-	-

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