Viewing abca4_sm_1938-2163-FFX1H-multi.table

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All-Atom Contacts	Clashscore, all atoms:	0.58		99th 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	1.34%	Goal: <0.05%
	Ramachandran favored	200	89.29%	Goal: >98%
	MolProbity score^	1.26		99th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	4	1.97%	Goal: 0
	Bad backbone bonds:	0 / 1735	0.00%	Goal: 0%
	Bad backbone angles:	11 / 2349	0.47%	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: 54.20	Clashscore: 0.58	Outliers: 3 of 224	Poor rotamers: 0 of 186	Outliers: 4 of 203	Outliers: 0 of 226	Outliers: 11 of 226
A1938		LEU	50	-	-	4.9% (*mp*) chi angles: 278.1,43	0.067Å	-	-
A1939		ARG	50	-	Favored (48.6%) General / -119.3,141.8	47.3% (*ttp180*) chi angles: 192.5,179,69.9,214.8	0.107Å	-	OUTLIER(S) worst is CD-NE-CZ: 4.007 σ
A1940		LEU	50	-	Favored (4.61%) General / -156.3,121.0	9.2% (*tt*) chi angles: 190,154	0.128Å	-	-
A1941		HIS	50	-	Favored (3.43%) General / -154.8,112.4	5.1% (*t-80*) chi angles: 157.7,262.7	0.1Å	-	OUTLIER(S) worst is C-N-CA: 5.338 σ

A1942	GLU	50	-	Allowed (0.56%) General / 79.2,22.9	51.8% (*mm-40*) chi angles: 306.8,308.6,337.9	0.144Å	-	OUTLIER(S) worst is CB-CG-CD: 4.46 σ
A1943	LEU	50	-	Favored (33.27%) General / -68.2,127.5	8% (*tp*) chi angles: 210.5,68.8	0.042Å	-	-
A1944	THR	50	-	Favored (38.95%) General / -125.5,156.4	32.9% (*p*) chi angles: 51.8	0.039Å	-	-
A1945	LYS	50	-	Favored (13.74%) General / -149.7,130.0	59.3% (*tptt*) chi angles: 180.8,62.4,176.7,178.5	0.073Å	-	-
A1946	ILE	50	-	Favored (5.48%) Isoleucine or valine / -101.3,151.4	47.9% (*pt*) chi angles: 60.5,173	0.094Å	-	-
A1947	TYR	99.99	-	Favored (28.01%) Pre-proline / -118.5,125.1	65.7% (*t80*) chi angles: 185.4,86.1	0.067Å	-	-
A1948	PRO	99.99	-	Favored (23.04%) Trans-proline / -80.3,158.7	9.9% (*Cg_endo*) chi angles: 40.3	0.071Å	-	-
A1949	GLY	99.99	-	Allowed (1.02%) Glycine / 95.8,-69.2	-	-	-	-
A1950	THR	99.99	-	Favored (73.66%) General / -61.5,-33.3	69.9% (*p*) chi angles: 57.6	0.122Å	-	-
A1951	SER	50	-	Favored (7.88%) General / 63.5,40.8	50.9% (*m*) chi angles: 301.4	0.128Å	-	-
A1952	SER	50	-	Favored (51.07%) Pre-proline / -125.0,161.1	44.1% (*p*) chi angles: 54	0.073Å	-	-
A1953	PRO	50	-	Favored (3.6%) Trans-proline / -83.2,123.9	86.3% (*Cg_endo*) chi angles: 31.7	0.022Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A1954		ALA	50	-	Favored (9.56%)	-	0.063Å	-	-
A1955		VAL	50	-	Favored (72.53%) Isoleucine or valine / -125.1,127.9	99.5% (*t*) chi angles: 178.5	0.054Å	-	-
A1956		ASP	50	-	Allowed (1.71%) General / -124.9,78.5	6.2% (*m-20*) chi angles: 316.5,328.3	0.027Å	-	-
A1957		ARG	50	-	Favored (5.7%) General / 63.7,43.4	51.8% (*mmm-85*) chi angles: 294.7,282.9,293.6,280.4	0.103Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.20	Clashscore: 0.58	Outliers: 3 of 224	Poor rotamers: 0 of 186	Outliers: 4 of 203	Outliers: 0 of 226	Outliers: 11 of 226
A1958		LEU	99.99	-	Favored (55.58%) General / -67.4,144.8	53.3% (*mt*) chi angles: 293,184.8	0.046Å	-	-
A1959		CYS	50	-	Favored (10.29%) General / -138.2,114.5	84.9% (*m*) chi angles: 292.6	0.084Å	-	-
A1960		VAL	50	-	OUTLIER (0.08%) Isoleucine or valine / -156.5,-172.4	1.3% (*p*) chi angles: 85.7	0.203Å	-	-
A1961		GLY	50	-	Favored (7.48%) Glycine / 177.3,148.9	-	-	-	-
A1962		VAL	50	-	Favored (33.4%) Isoleucine or valine / -129.6,149.2	2.4% (*m*) chi angles: 318.4	0.153Å	-	-
A1963		ARG	50	-	Favored (13.6%) Pre-proline / -75.9,170.9	81.9% (*mtm180*) chi angles: 297.7,179.2,289.8,160.5	0.091Å	-	-
					Favored (9.84%)	45.1% (*Cg_endo*)			

A1964	PRO	50	-	Trans-proline / -85.8,150.3	chi angles: 35.5	0.065Å	-	-
A1965	GLY	50	-	Favored (68.82%) Glycine / 70.4,30.7	-	-	-	-
A1966	GLU	50	-	Favored (11.87%) General / -133.4,173.1	4.8% (*pt-20*) chi angles: 85.4,163.2,336	0.087Å	-	-
A1967	CYS	50	-	Favored (23.31%) General / -121.3,115.6	1.6% (*p*) chi angles: 38.6	0.037Å	-	-
A1968	PHE	50	-	Favored (47.78%) General / -114.9,141.5	43.1% (*t80*) chi angles: 189.5,273.9	0.065Å	-	-
A1969	GLY	50	-	Favored (5.75%) Glycine / -109.1,120.2	-	-	-	-
A1970	LEU	50	-	Favored (5.62%) General / -92.0,72.8	14.8% (*tp*) chi angles: 194.4,74.6	0.064Å	-	-
A1971	LEU	99.99	-	Favored (16.62%) General / -77.5,170.4	14.6% (*tp*) chi angles: 200.4,63	0.128Å	-	-
A1972	GLY	50	-	Favored (12.5%) Glycine / 128.5,168.9	-	-	-	-
A1973	VAL	50	-	Favored (2.44%) Isoleucine or valine / -55.0,149.5	9% (*p*) chi angles: 70.8	0.111Å	-	-
A1974	ASN	50	-	Favored (12.46%) General / -47.5,128.4	1.8% (*m-20*) chi angles: 300.7,37.9	0.133Å	-	-
A1975	GLY	50	-	Favored (86.19%) Glycine / 81.0,9.5	-	-	-	-

Allowed

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A1976		ALA	50	-	(0.42%) General / -78.7,41.8	-	0.049Å	-	-
A1977		GLY	50	-	Favored (61.39%) Glycine / 63.5,18.6	-	-	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.20	Clashscore: 0.58	Outliers: 3 of 224	Poor rotamers: 0 of 186	Outliers: 4 of 203	Outliers: 0 of 226	Outliers: 11 of 226
A1978		LYS	50	-	Favored (12.62%) General / -75.3,-51.7	24.4% (*mtmt*) chi angles: 313.6,193.8,291.4,157.2	0.096Å	-	-
A1979		THR	50	-	Favored (71.92%) General / -54.0,-46.9	53% (*m*) chi angles: 295.1	0.056Å	-	-
A1980		THR	50	-	Favored (69.86%) General / -53.6,-47.8	4.2% (*m*) chi angles: 317.9	0.09Å	-	-
A1981		THR	50	-	Favored (93.41%) General / -59.9,-42.3	94.5% (*m*) chi angles: 298.1	0.125Å	-	-
A1982		PHE	99.99	-	Favored (91.49%) General / -64.4,-38.6	5.9% (*m-30*) chi angles: 283.2,18.1	0.166Å	-	-
A1983		LYS	50	-	Favored (59.62%) General / -77.0,-15.5	62.7% (*mttm*) chi angles: 303.6,188.3,188.4,299.7	0.163Å	-	-
A1984		MET	99.99	-	Favored (30.88%) General / -82.1,-30.8	36.8% (*mtp*) chi angles: 296.3,150,73	0.072Å	-	-
A1985		LEU	50	-	Favored (64.39%) General / -74.0,-34.9	89.9% (*mt*) chi angles: 290.6,171.6	0.119Å	-	-
A1986		THR	50	-	Favored (81.89%) General / -67.4,-36.7	37.2% (*p*) chi angles: 52.9	0.102Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A1987		GLY	50	-	Favored (2.91%) Glycine / 99.9,41.3	-	-	-	-
A1988		ASP	50	-	Allowed (0.93%) General / -120.7,-68.1	50.4% (*m-20*) chi angles: 304.8,304.8	0.083Å	-	-
A1989		THR	50	-	Favored (2.18%) General / -72.6,97.6	43.1% (*p*) chi angles: 54.7	0.037Å	-	-
A1990		THR	50	-	Allowed (1.32%) General / -39.4,133.6	13.2% (*p*) chi angles: 45.6	0.037Å	-	-
A1991		VAL	99.99	-	Favored (14.91%) Isoleucine or valine / -66.1,144.2	22.7% (*m*) chi angles: 293.1	0.059Å	-	-
A1992		THR	50	-	Favored (26.68%) General / -82.1,-37.2	92.6% (*m*) chi angles: 300.4	0.152Å	-	-
A1993		SER	50	-	Favored (3.58%) General / -170.7,178.4	7.1% (*t*) chi angles: 196.8	0.054Å	-	-
A1994		GLY	50	-	Favored (30.43%) Glycine / 98.4,162.2	-	-	-	-
A1995		ASP	50	-	Favored (39.88%) General / -76.6,138.1	15.4% (*t70*) chi angles: 174.5,46.3	0.086Å	-	-
A1996		ALA	50	-	Favored (2.55%) General / -161.9,122.0	-	0.063Å	-	-
A1997		THR	50	-	Favored (41.63%) General / -131.7,130.2	66.6% (*p*) chi angles: 59.5	0.039Å	-	-

		Avg: 54.20	Clashscore: 0.58	Outliers: 3 of 224	Poor rotamers: 0 of 186	Outliers: 4 of 203	Outliers: 0 of 226	Outliers: 11 of 226
A1998	VAL	50	-	Favored (38.37%) Isoleucine or valine / -109.4,112.0	3.9% (*t*) chi angles: 157.2	0.068Å	-	-
A1999	ALA	50	-	Favored (21.77%) General / 58.5,32.1	-	0.083Å	-	-
A2000	GLY	50	-	Favored (17.48%) Glycine / 89.0,-23.5	-	-	-	-
A2001	LYS	50	-	Favored (40.84%) General / -67.8,129.7	55% (*mmtt*) chi angles: 306.4,288,187.1,157.9	0.063Å	-	-
A2002	SER	50	-	Favored (21.98%) General / -83.7,115.0	12.5% (*t*) chi angles: 166.3	0.05Å	-	-
A2003	ILE	50	-	Favored (8.43%) Isoleucine or valine / -55.5,-57.2	16.3% (*mt*) chi angles: 304,189.8	0.184Å	-	-
A2004	LEU	50	-	Favored (82.32%) General / -62.6,-36.3	6.4% (*tt*) chi angles: 186.1,138.8	0.113Å	-	-
A2005	THR	50	-	Favored (55.41%) General / -82.2,-14.6	16.6% (*p*) chi angles: 46.6	0.063Å	-	-
A2006	ASN	50	-	Allowed (1.9%) General / -139.5,46.4	11.3% (*m120*) chi angles: 305.4,146.7	0.051Å	-	OUTLIER(S) worst is CA-CB-CG: 7.477 σ
A2007	ILE	50	-	Favored (61.99%) Isoleucine or valine / -58.1,-37.4	24.9% (*pt*) chi angles: 61.2,181.6	0.216Å	-	-
A2008	SER	50	-	Favored (17.84%) General /	76.4% (*p*) chi angles: 58.4	0.039Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
					-54.5,-56.5				
A2009		GLU	50	-	Favored (83.37%) General / -60.6,-38.0	10.9% (*mm-40*) chi angles: 309.2,304.4,96.9	0.057Å	-	-
A2010		VAL	50	-	Favored (61.17%) Isoleucine or valine / -71.2,-36.2	54.6% (*t*) chi angles: 170.6	0.179Å	-	-
A2011		HIS	50	-	Favored (68.56%) General / -71.4,-32.5	52.2% (*m80*) chi angles: 289.1,68.9	0.143Å	-	-
A2012		GLN	50	-	Favored (3.5%) General / -70.1,2.6	14.1% (*mt-30*) chi angles: 294.3,150.1,228.2	0.063Å	-	-
A2013		ASN	50	-	Favored (5.18%) General / -131.0,12.6	8.9% (*m120*) chi angles: 296.8,163.2	0.037Å	-	OUTLIER(S) worst is CA-CB-CG: 7.98 σ
A2014		MET	99.99	-	Favored (35.34%) General / -113.9,149.3	35.3% (*tpp*) chi angles: 195,56.9,57.2	0.144Å	-	-
A2015		GLY	50	-	Favored (2.6%) Glycine / -144.1,125.9	-	-	-	-
A2016		TYR	50	-	Favored (37.17%) General / -138.6,137.6	23.1% (*t80*) chi angles: 179.7,48.7	0.085Å	-	-
A2017		CYS	50	-	Favored (50.13%) Pre-proline / -116.7,105.3	1.6% (*t*) chi angles: 159.5	0.097Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	**Ramachandran**	**Rotamer**	**Cβ deviation**	**Bond lengths**	**Bond angles**
			Avg: 54.20	Clashscore: 0.58	Outliers: 3 of 224	Poor rotamers: 0 of 186	Outliers: 4 of 203	Outliers: 0 of 226	Outliers: 11 of 226
A2018		PRO	50	-	Favored (41.24%) Trans-proline / -75.3,158.0	92.9% (*Cg_endo*) chi angles: 30.9	0.037Å	-	-
A2019		GLN	50	-	Favored (5.85%) General /	47.5% (*tt0*) chi angles: 193.4,188.7,5.9	0.052Å	-	-

				-47.2,123.7			
A2020	PHE	50	-	Favored (14.22%) General / 60.1,43.5	3.7% (*m-85*) chi angles: 263.4,71.7	0.155Å	-	-
A2021	ASP	50	-	Allowed (0.51%) General / -53.1,163.6	7.3% (*t0*) chi angles: 214.8,349.5	0.031Å	-	-
A2022	ALA	50	-	Allowed (1.11%) General / -140.0,-160.8	-	0.122Å	-	-
A2023	ILE	50	-	OUTLIER (0.08%) Isoleucine or valine / -148.7,-160.8	15.6% (*pt*) chi angles: 64.6,158.1	0.142Å	-	-
A2024	ASP	50	-	Favored (24.89%) General / -111.0,153.9	10.8% (*t0*) chi angles: 171.2,32.7	0.089Å	-	-
A2025	GLU	50	-	Favored (10.02%) General / -104.6,-30.4	42.8% (*mm-40*) chi angles: 298,288.9,293	0.033Å	-	-
A2026	LEU	50	-	Favored (11.76%) General / -82.3,-48.0	11.2% (*mp*) chi angles: 275,61.7	0.129Å	-	-
A2027	LEU	50	-	Favored (21.84%) General / -70.5,165.8	10.9% (*mp*) chi angles: 278.1,59.8	0.055Å	-	-
A2028	THR	50	-	Favored (13.1%) General / -73.9,171.6	3.2% (*p*) chi angles: 82.7	0.23Å	-	-
A2029	GLY	50	-	Favored (30.04%) Glycine / -61.2,-55.3	-	-	-	-
A2030	ARG	50	-	Favored (90.44%) General / -65.9,-39.3	31% (*ttm-85*) chi angles: 196.1,188.8,301.5,254.2	0.108Å	-	-
				Favored			

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A2031		GLU	50	-	(84.19%) General / -62.7,-47.3	62.1% (*tt0*) chi angles: 181.8,188.8,23	0.032Å	-	-
A2032		HIS	50	-	Favored (79.2%) General / -65.5,-34.8	11.8% (*t60*) chi angles: 201.1,89.5	0.128Å	-	-
A2033		LEU	50	-	Favored (87.13%) General / -63.9,-37.4	28.8% (*mt*) chi angles: 291.7,158.6	0.1Å	-	-
A2034		TYR	99.99	-	Favored (96.6%) General / -63.0,-44.2	49.7% (*t80*) chi angles: 184.5,94.5	0.086Å	-	-
A2035		LEU	50	-	Favored (74.54%) General / -59.2,-50.3	57.6% (*tp*) chi angles: 177.8,58.1	0.047Å	-	-
A2036		TYR	50	-	Favored (90.83%) General / -60.1,-46.1	65.3% (*t80*) chi angles: 169.8,75	0.066Å	-	-
A2037		ALA	50	-	Favored (58.19%) General / -76.2,-19.6	-	0.161Å	-	-
#	**Alt**	**Res**	**High B**	**Clash > 0.4Å**	**Ramachandran**	**Rotamer**	**Cβ deviation**	**Bond lengths**	**Bond angles**
			Avg: 54.20	Clashscore: 0.58	Outliers: 3 of 224	Poor rotamers: 0 of 186	Outliers: 4 of 203	Outliers: 0 of 226	Outliers: 11 of 226
A2038		ARG	50	-	Favored (69.07%) General / -69.8,-31.2	25.2% (*ttm-85*) chi angles: 178.7,153.4,285,292.2	0.159Å	-	-
A2039		LEU	50	-	Favored (78.26%) General / -66.0,-34.5	10.9% (*mp*) chi angles: 272.2,63.8	0.112Å	-	-
A2040		ARG	50	-	Favored (57.28%) General / -76.4,-30.0	32.5% (*ttt-85*) chi angles: 183.2,181.7,151.8,280.3	0.069Å	-	-
A2041		GLY	50	-	Favored (21.84%) Glycine / -165.2,152.4	-	-	-	-

A2042	VAL	50	-	Allowed (0.46%) Pre-proline / -84.1,-30.6	2.5% (*p*) chi angles: 81.8	0.247Å	-	-
A2043	PRO	50	-	Favored (4.15%) Trans-proline / -86.8,135.8	17.8% (*Cg_endo*) chi angles: 38.9	0.031Å	-	-
A2044	ALA	50	-	Favored (74.57%) General / -59.4,-35.8	-	0.126Å	-	-
A2045	GLU	50	-	Favored (8.5%) General / -54.1,-58.1	3.8% (*tm-20*) chi angles: 175.8,290.6,303.1	0.084Å	-	-
A2046	GLU	50	-	Favored (72.98%) General / -54.6,-44.2	32.6% (*tp10*) chi angles: 173.9,57.9,32.9	0.041Å	-	-
A2047	ILE	50	-	Favored (71.17%) Isoleucine or valine / -60.0,-51.6	86.7% (*mt*) chi angles: 294.5,165.4	0.099Å	-	-
A2048	GLU	50	-	Favored (70.62%) General / -70.8,-33.3	24.9% (*tp10*) chi angles: 175.3,48.5,30.2	0.119Å	-	-
A2049	LYS	50	-	Favored (85.55%) General / -59.6,-39.9	6.3% (*ttpt*) chi angles: 183,175.3,65.2,231.7	0.046Å	-	-
A2050	VAL	50	-	Favored (86.43%) Isoleucine or valine / -63.5,-39.7	54.3% (*t*) chi angles: 169.2	0.129Å	-	-
A2051	ALA	50	-	Favored (72.08%) General / -65.3,-31.1	-	0.144Å	-	-
A2052	ASN	50	-	Favored (92.22%) General / -65.1,-43.4	2.1% (*m120*) chi angles: 294.6,187	0.116Å	-	OUTLIER(S) worst is CA-CB-CG: 8.314 σ
A2053	TRP	99.99	-	Favored (79.93%) General /	9.9% (*t-105*) chi angles: 191.5,288.6	0.096Å	-	-

					-58.4,-39.5				
A2054	SER	50	-		Favored (65.02%) General / -61.1,-52.4	2.6% (*t*) chi angles: 204.2	0.109Å	-	-
A2055	ILE	50	-		Favored (76.39%) Isoleucine or valine / -64.8,-36.0	5.2% (*pt*) chi angles: 68.9,193.7	0.24Å	-	-
A2056	LYS	50	-		Favored (97.4%) General / -60.5,-42.9	15.9% (*ttpt*) chi angles: 184.8,213.2,76,188.7	0.028Å	-	-
A2057	SER	50	-		Favored (39.24%) General / -81.1,-22.1	49.3% (*m*) chi angles: 301.8	0.076Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.20	Clashscore: 0.58	Outliers: 3 of 224	Poor rotamers: 0 of 186	Outliers: 4 of 203	Outliers: 0 of 226	Outliers: 11 of 226
A2058		LEU	99.99	-	Favored (48.52%) General / -74.1,-45.5	36.5% (*mt*) chi angles: 281.8,166.6	0.075Å	-	-
A2059		GLY	50	-	Favored (26.44%) Glycine / 65.8,54.3	-	-	-	-
A2060		LEU	50	-	Favored (3.89%) General / -130.6,-11.8	91.9% (*mt*) chi angles: 293.3,177.5	0.071Å	-	-
A2061		THR	50	-	Allowed (0.54%) General / 42.5,-120.0	79.2% (*p*) chi angles: 60.3	0.302Å	-	-
A2062		VAL	50	-	Favored (48.7%) Isoleucine or valine / -60.6,-31.3	5.1% (*p*) chi angles: 76.1	0.17Å	-	-
A2063		TYR	50	-	Favored (21.98%) General / -71.0,-3.9	45.5% (*m-85*) chi angles: 308.9,291.4	0.118Å	-	-

A2064	ALA	50	-	Favored (57.1%) General / -79.8,-15.6	-	0.093Å	-	-
A2065	ASP	50	-	Favored (19.87%) General / -104.7,-7.0	18% (*m-20*) chi angles: 293.5,278.8	0.119Å	-	-
A2066	CYS	50	-	Favored (7.49%) General / -62.5,164.5	90.2% (*m*) chi angles: 295.2	0.047Å	-	-
A2067	LEU	50	-	Favored (44.79%) General / -55.3,138.7	9.4% (*mp*) chi angles: 269.9,67.2	0.075Å	-	-
A2068	ALA	50	-	Favored (70.26%) General / -61.2,-30.2	-	0.111Å	-	-
A2069	GLY	50	-	Favored (59.2%) Glycine / -73.7,-32.5	-	-	-	-
A2070	THR	50	-	Favored (60.25%) General / -75.6,-16.4	72.6% (*p*) chi angles: 59	0.188Å	-	-
A2071	TYR	50	-	Allowed (1.39%) General / -46.0,145.9	3.9% (*m-30*) chi angles: 273.1,25.1	0.115Å	-	-
A2072	SER	50	-	Favored (25.62%) General / -65.0,158.4	5.6% (*p*) chi angles: 86.9	0.055Å	-	-
A2073	GLY	50	-	Favored (69.89%) Glycine / -58.8,-32.4	-	-	-	-
A2074	GLY	50	-	Favored (96.28%) Glycine / -64.9,-43.3	-	-	-	-
A2075	ASN	50	-	Favored (86.8%) General / -59.1,-40.9	4.1% (*m-20*) chi angles: 305.1,8.9	0.136Å	-	OUTLIER(S) worst is CA-CB-CG: 6.77 σ

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A2076		LYS	50	-	Favored (98.12%) General / -63.6,-42.4	94.3% (*mttt*) chi angles: 299.6,187.9,177.2,179.9	0.133Å	-	-
A2077		ARG	50	-	Favored (55.82%) General / -75.8,-23.4	17.4% (*mmt85*) chi angles: 275.1,285.2,174,72.7	0.152Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.20	Clashscore: 0.58	Outliers: 3 of 224	Poor rotamers: 0 of 186	Outliers: 4 of 203	Outliers: 0 of 226	Outliers: 11 of 226
A2078		LYS	50	-	Favored (84.7%) General / -64.1,-36.6	54.2% (*mtmt*) chi angles: 295.3,194.8,293.7,177.5	0.162Å	-	-
A2079		LEU	50	-	Favored (74.2%) General / -70.5,-36.9	21.9% (*tp*) chi angles: 192.3,67.8	0.094Å	-	-
A2080		SER	50	-	Favored (82.58%) General / -64.4,-36.0	7.8% (*m*) chi angles: 312.3	0.095Å	-	-
A2081		THR	50	-	Favored (96.51%) General / -64.5,-41.2	99.6% (*m*) chi angles: 298.6	0.09Å	-	-
A2082		ALA	50	0.402Å O with A2086 ILE HG23	Favored (83.26%) General / -59.2,-48.0	-	0.08Å	-	-
A2083		ILE	50	-	Favored (45.28%) Isoleucine or valine / -58.5,-32.3	15.9% (*pt*) chi angles: 66.4,184.8	0.254Å	-	-
A2084		ALA	50	-	Favored (56.49%) General / -78.0,-18.0	-	0.069Å	-	-
A2085		LEU	50	-	Favored (10.36%) General / -105.2,-29.4	73.8% (*mt*) chi angles: 298.5,169.5	0.071Å	-	-
				0.402Å HG23 with	Favored (27.45%)	10.8% (*pt*)			

A2086	ILE	99.99	A2082 ALA O	Isoleucine or valine / -76.6,-36.5	chi angles: 63.1,188.8	0.2Å	-	-
A2087	GLY	50	-	Allowed (1.52%) Glycine / -75.5,23.8	-	-	-	-
A2088	CYS	50	-	Allowed (0.26%) Pre-proline / 64.9,39.7	13.9% (*m*) chi angles: 313.7	0.143Å	-	-
A2089	PRO	50	-	Favored (5.68%) Trans-proline / -81.4,127.0	94.1% (*Cg_endo*) chi angles: 32.7	0.04Å	-	-
A2090	PRO	50	-	Favored (3.01%) Trans-proline / -74.4,-36.6	60.6% (*Cg_endo*) chi angles: 27.2	0.113Å	-	-
A2091	LEU	50	-	Favored (39.03%) General / -104.3,139.6	23.3% (*tp*) chi angles: 179.4,75	0.083Å	-	-
A2092	VAL	50	-	Favored (27.93%) Isoleucine or valine / -141.3,132.7	1.4% (*p*) chi angles: 42.5	0.124Å	-	-
A2093	LEU	50	-	Favored (42.87%) General / -121.8,123.9	16.1% (*mt*) chi angles: 316.4,173.5	0.073Å	-	-
A2094	LEU	50	-	Favored (47.94%) General / -116.0,123.4	8.5% (*mt*) chi angles: 322,177.8	0.097Å	-	-
A2095	ASP	50	-	Favored (4%) General / -102.5,90.9	26.4% (*t0*) chi angles: 198.8,345.9	0.13Å	-	OUTLIER(S) worst is CA-CB-CG: 5.854 σ
A2096	GLU	50	-	Allowed (0.31%) Pre-proline / 60.5,37.7	80.1% (*mm-40*) chi angles: 293.9,296.2,320.4	0.076Å	-	-
A2097	PRO	50	-	Favored (20.35%) Trans-proline / -71.2,-27.2	35.4% (*Cg_endo*) chi angles: 36.9	0.047Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.20	Clashscore: 0.58	Outliers: 3 of 224	Poor rotamers: 0 of 186	Outliers: 4 of 203	Outliers: 0 of 226	Outliers: 11 of 226
A2098		THR	50	-	Favored (59.48%) General / -83.5,-7.6	10.8% (*p*) chi angles: 44.5	0.181Å	-	-
A2099		THR	50	-	Favored (3.78%) General / -73.2,102.9	87% (*m*) chi angles: 301.8	0.041Å	-	-
A2100		GLY	50	-	Favored (42.47%) Glycine / 104.3,6.0	-	-	-	-
A2101		MET	50	-	Favored (15%) General / -85.7,167.8	81.9% (*mtp*) chi angles: 282.5,183.6,78.2	0.047Å	-	-
A2102		ASP	50	-	Favored (3.59%) Pre-proline / -71.0,174.5	8.4% (*p-10*) chi angles: 69.9,298.1	0.064Å	-	-
A2103		PRO	50	-	Favored (13.86%) Trans-proline / -75.9,-21.8	58% (*Cg_endo*) chi angles: 26.5	0.106Å	-	-
A2104		GLN	50	-	Favored (5.34%) General / -96.1,-49.2	6.6% (*tp-100*) chi angles: 170,47.2,227.9	0.085Å	-	-
A2105		ALA	50	-	Favored (57.63%) General / -76.3,-20.0	-	0.168Å	-	-
A2106		ARG	50	-	Favored (72.74%) General / -55.3,-41.8	43.2% (*ptt85*) chi angles: 69.2,184.1,183.9,100.8	0.099Å	-	-
A2107		ARG	50	-	Favored (42.92%) General / -79.3,-31.0	7.6% (*tpm_?*) chi angles: 191.1,64.4,263.4,184.4	0.089Å	-	-
A2108		MET	50	-	Favored (89.9%) General / -60.1,-46.4	30% (*mtt*) chi angles: 288.5,162.4,162.5	0.078Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A2109		LEU	50	-	Favored (52.02%) General / -57.0,-54.0	7.4% (*tt*) chi angles: 194.2,156.9	0.071Å	-	-
A2110		TRP	99.99	-	Favored (74.64%) General / -61.7,-33.8	11.6% (*m0*) chi angles: 302.9,317	0.132Å	-	OUTLIER(S) worst is CE3-CD2-CG: 4.066 σ
A2111		ASN	50	-	Favored (70.35%) General / -69.6,-31.9	29.7% (*m-20*) chi angles: 294.9,5.6	0.138Å	-	-
A2112		VAL	50	-	Favored (17.17%) Isoleucine or valine / -76.4,-26.9	16.9% (*m*) chi angles: 305.1	0.287Å	-	-
A2113		ILE	50	-	Favored (83.57%) Isoleucine or valine / -64.3,-38.8	10.8% (*mm*) chi angles: 301.6,318.8	0.127Å	-	-
A2114		VAL	50	-	Favored (15.68%) Isoleucine or valine / -74.9,-14.2	99.2% (*t*) chi angles: 176.4	0.152Å	-	-
A2115		SER	50	-	Favored (11.95%) General / -87.3,-43.7	54.5% (*m*) chi angles: 299.8	0.085Å	-	-
A2116		ILE	50	-	Favored (42.67%) Isoleucine or valine / -68.6,-29.1	2.6% (*pp*) chi angles: 58.9,95.5	0.273Å	-	-
A2117		ILE	50	-	Favored (71.44%) Isoleucine or valine / -63.2,-35.3	16.4% (*pt*) chi angles: 55.9,159.2	0.188Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.20	Clashscore: 0.58	Outliers: 3 of 224	Poor rotamers: 0 of 186	Outliers: 4 of 203	Outliers: 0 of 226	Outliers: 11 of 226
A2118		ARG	50	-	Favored (60.88%) General /	73.7% (*mtm180*) chi angles:	0.112Å	-	-

					-73.1,-25.4	296.9,178.5,288.6,152.5			
A2119	GLU	50	-	Favored (2.48%) General / -85.4,18.9	54.7% (*mt-10*) chi angles: 301,180.1,300.8	0.05Å	-	-
A2120	GLY	50	-	Favored (78.54%) Glycine / 91.8,-4.0	-	-	-	-
A2121	ARG	50	-	Favored (30.98%) General / -78.9,152.9	17.1% (*mmt85*) chi angles: 311.9,306.5,190,71.9	0.044Å	-	-
A2122	ALA	50	-	Favored (28.75%) General / -107.2,114.6	-	0.079Å	-	-
A2123	VAL	50	-	Favored (45.2%) Isoleucine or valine / -120.5,140.2	7.6% (*p*) chi angles: 69.1	0.102Å	-	-
A2124	VAL	50	-	Favored (64.56%) Isoleucine or valine / -129.4,127.0	4.7% (*t*) chi angles: 195	0.035Å	-	-
A2125	LEU	50	-	Favored (51.02%) General / -115.5,138.4	7.9% (*mp*) chi angles: 267,68.3	0.078Å	-	-
A2126	THR	99.99	-	Favored (46.55%) General / -100.7,128.9	1.7% (*t*) chi angles: 168.6	0.166Å	-	-
A2127	SER	50	-	Favored (41.69%) General / -133.5,133.0	36.7% (*t*) chi angles: 175.9	0.074Å	-	-
A2128	HIS	50	-	Favored (75.4%) General / -68.8,-34.4	34.4% (*p-80*) chi angles: 76.3,282.4	0.096Å	-	-
A2129	SER	50	-	Favored (35.93%) General / -81.1,136.5	1.4% (*m*) chi angles: 268.2	0.044Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A2130		MET	50	-	Favored (14.25%) General / -105.8,-17.8	34% (*mtt*) chi angles: 305.6,196.2,175.2	0.083Å	-	OUTLIER(S) worst is C-N-CA: 4.056 σ
A2131		GLU	50	-	Favored (9.6%) General / -46.6,-38.4	1.5% (*mp0*) chi angles: 316.2,82.2,275.5	0.11Å	-	-
A2132		GLU	50	-	Favored (10.96%) General / -119.8,6.6	16% (*mm-40*) chi angles: 292.7,268.3,19.2	0.066Å	-	-
A2133		CYS	50	-	Favored (87.32%) General / -59.2,-41.0	22.6% (*p*) chi angles: 68.3	0.133Å	-	-
A2134		GLU	50	-	Favored (31.68%) General / -93.0,-12.1	12.7% (*pt-20*) chi angles: 65.3,197.7,131.8	0.157Å	-	-
A2135		ALA	50	-	Allowed (0.75%) General / -86.4,37.8	-	0.043Å	-	-
A2136		LEU	50	-	OUTLIER (0.03%) General / -166.3,-62.8	15.8% (*tp*) chi angles: 162.6,61.5	0.051Å	-	-
A2137		CYS	50	-	Favored (27.75%) General / -105.3,147.8	64.9% (*m*) chi angles: 287	0.033Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.20	Clashscore: 0.58	Outliers: 3 of 224	Poor rotamers: 0 of 186	Outliers: 4 of 203	Outliers: 0 of 226	Outliers: 11 of 226
A2138		THR	50	-	Favored (41.35%) General / -79.7,-31.8	23.9% (*p*) chi angles: 49.8	0.117Å	-	-
A2139		ARG	50	-	Favored (48.99%) General / -138.3,153.3	30.3% (*mtp-105*) chi angles: 281.6,178.9,60.1,250	0.06Å	-	-
A2140		LEU	99.99	-	Favored (20.27%) General / -137.6,168.1	43% (*mt*) chi angles: 305.3,169.9	0.105Å	-	-

A2141	ALA	50	-	Favored (12.95%) General / -152.0,131.4	-	0.07Å	-	-
A2142	ILE	50	-	Favored (48.7%) Isoleucine or valine / -96.3,123.8	26.6% (*pt*) chi angles: 52.2,172.4	0.137Å	-	-
A2143	MET	50	-	Favored (25.95%) General / -96.2,145.0	32.7% (*mmp*) chi angles: 307.9,293.5,103.5	0.071Å	-	-
A2144	VAL	50	-	Allowed (0.55%) Isoleucine or valine / -147.2,105.3	5.9% (*p*) chi angles: 54.9	0.102Å	-	-
A2145	LYS	50	-	Allowed (0.66%) General / 71.9,-12.6	1.8% (*tmtm?*) chi angles: 178.2,261.5,151.8,279.8	0.223Å	-	-
A2146	GLY	50	-	Favored (4.22%) Glycine / 134.9,-16.5	-	-	-	-
A2147	ALA	50	-	Favored (4.06%) General / -95.0,-177.1	-	0.055Å	-	-
A2148	PHE	99.99	-	Favored (30.77%) General / -124.1,159.1	52.4% (*p90*) chi angles: 59.4,92	0.042Å	-	-
A2149	ARG	50	-	Favored (3.1%) General / -125.5,-30.6	50.8% (*tpt85*) chi angles: 169.6,61.5,183.6,81.6	0.114Å	-	-
A2150	CYS	50	-	Favored (40.35%) General / -151.3,162.8	36.7% (*m*) chi angles: 308.2	0.101Å	-	-
A2151	MET	50	-	Favored (5.8%) General / -168.5,152.4	20.8% (*ptp*) chi angles: 66.7,190,78.2	0.032Å	-	-
A2152	GLY	50	-	Favored (32.03%) Glycine / 153.1,-169.5	-	-	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A2153		THR	50	-	Favored (37.25%) General / -79.4,137.4	4% (*p*) chi angles: 41	0.038Å	-	-
A2154		ILE	50	-	Allowed (0.71%) Isoleucine or valine / -45.9,-58.5	4% (*pt*) chi angles: 57.9,196.1	0.219Å	-	-
A2155		GLN	50	-	Favored (83.74%) General / -64.1,-36.4	7.2% (*tp60*) chi angles: 181.4,66.3,104	0.087Å	-	-
A2156		HIS	50	-	Favored (48.5%) General / -87.2,-11.9	26.6% (*t60*) chi angles: 193.3,46.2	0.176Å	-	-
A2157		LEU	50	-	Favored (65.01%) General / -66.4,-50.0	11.4% (*mt*) chi angles: 270.4,166.4	0.053Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.20	Clashscore: 0.58	Outliers: 3 of 224	Poor rotamers: 0 of 186	Outliers: 4 of 203	Outliers: 0 of 226	Outliers: 11 of 226
A2158		LYS	50	-	Favored (69.85%) General / -53.5,-46.3	13.5% (*mtpp*) chi angles: 317.7,205.4,78.5,67.8	0.142Å	-	-
A2159		SER	50	-	Favored (2.44%) General / -77.3,62.9	53.6% (*p*) chi angles: 74.3	0.075Å	-	-
A2160		LYS	50	-	Allowed (0.07%) General / -158.4,-57.8	4.5% (*tptp*) chi angles: 189.5,63.1,227,56.4	0.158Å	-	-
A2161		PHE	50	0.403Å HB2 with A2163 ASP OD1	Favored (2.37%) General / -131.7,-22.6	41.3% (*m-85*) chi angles: 310.4,286.1	0.102Å	-	-
A2162		GLY	50	-	Allowed (0.53%) Glycine / 110.3,65.1	-	-	-	-
A2163		ASP	99.99	0.403Å OD1 with A2161 PHE	-	5.9% (*m-20*)	0.05Å	-	OUTLIER(S) worst is CA-CB-CG: 7.368

HB2   chi angles: 310.1,352.5   σ

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