Viewing abca4_sm_1938-2163H-multi.table

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All-Atom Contacts	Clashscore, all atoms:	55.04		3rd percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	1	0.54%	Goal: <1%
	Ramachandran outliers	3	1.34%	Goal: <0.05%
	Ramachandran favored	210	93.75%	Goal: >98%
	MolProbity score^	2.63		40th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	1	0.49%	Goal: 0
	Bad backbone bonds:	12 / 1735	0.69%	Goal: 0%
	Bad backbone angles:	14 / 2349	0.60%	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: 55.04	Outliers: 3 of 224	Poor rotamers: 1 of 186	Outliers: 1 of 203	Outliers: 7 of 226	Outliers: 12 of 226
A1938		LEU	50	0.672Å HB3 with A1962 VAL HG22	-	2.7% (*tt*) chi angles: 172.7,167.7	0.063Å	-	-
A1939		ARG	50	-	Favored (27.18%) General / -126.9,119.6	62.5% (*ttm-85*) chi angles: 183,180.9,293.1,275.9	0.068Å	-	-
A1940		LEU	50	0.553Å HD21 with A1943 LEU HB3	Favored (56.55%) General / -113.2,128.7	8.5% (*tt*) chi angles: 187.7,159.6	0.172Å	-	-
A1941		HIS	50	-	Favored (9.68%) General / -135.1,111.4	21.4% (*t-160*) chi angles: 182.5,203.5	0.065Å	OUTLIER(S) worst is CG--ND1: 4.425 σ	-

A1942	GLU	50	0.628Å OE1 with A1957 ARG HB3	Favored (31.98%) General / 54.3,40.7	42.8% (*mm-40*) chi angles: 288.5,292.3,3	0.051Å	-	-
A1943	LEU	50	0.553Å HB3 with A1940 LEU HD21	Favored (20.24%) General / -70.3,122.8	69.2% (*tp*) chi angles: 177.7,62.1	0.024Å	-	-
A1944	THR	50	0.756Å HG23 with A1957 ARG HD2	Favored (23.04%) General / -120.3,160.4	38.8% (*p*) chi angles: 53.3	0.149Å	-	-
A1945	LYS	50	0.714Å HB3 with A1955 VAL HG12	Allowed (1.1%) General / -165.1,115.1	57.1% (*tptt*) chi angles: 181.3,65.9,182.4,182.7	0.038Å	-	-
A1946	ILE	50	0.813Å HG12 with A1992 THR HG21	Favored (29.93%) Isoleucine or valine / -93.0,134.7	35.8% (*pt*) chi angles: 66.1,174.9	0.045Å	-	-
A1947	TYR	99.99	0.722Å HD2 with A1950 THR HG22	Favored (65.83%) Pre-proline / -96.6,117.7	81.8% (*t80*) chi angles: 181.2,83.3	0.064Å	-	-
A1948	PRO	99.99	-	Allowed (0.35%) Trans-proline / -68.2,-171.4	63.6% (*Cg_endo*) chi angles: 34.1	0.06Å	-	-
A1949	GLY	99.99	-	OUTLIER (0.06%) Glycine / 63.1,-51.2	-	-	-	-
A1950	THR	99.99	0.722Å HG22 with A1947 TYR HD2	Favored (15.11%) General / -100.4,-22.3	1.5% (*t*) chi angles: 204.6	0.233Å	-	-
A1951	SER	50	-	OUTLIER (0.01%) General / 94.6,28.1	1.4% (*m*) chi angles: 323.2	0.096Å	-	-
A1952	SER	50	-	Favored (22.24%) Pre-proline / -114.5,134.9	50.5% (*m*) chi angles: 300.3	0.058Å	-	-
A1953	PRO	50	-	Allowed (1.44%) Trans-proline / -79.5,88.4	86% (*Cg_endo*) chi angles: 31.3	0.01Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A1954		ALA	50	-	Favored (78.49%) General / -64.0,-47.9	-	0.021Å	-	-
A1955		VAL	50	0.714Å HG12 with A1945 LYS HB3	Favored (52.37%) Isoleucine or valine / -110.5,134.6	10.8% (*p*) chi angles: 61.3	0.168Å	-	OUTLIER(S) worst is CG1-CB-CG2: 4.277 σ
A1956		ASP	50	-	Allowed (1.28%) General / -115.0,47.4	45.5% (*m-20*) chi angles: 300.4,294.6	0.026Å	-	-
A1957		ARG	50	0.756Å HD2 with A1944 THR HG23	OUTLIER (0.05%) General / 76.5,65.2	50.9% (*mmm-85*) chi angles: 305.4,288.8,293.3,272.5	0.061Å	-	-
#	**Alt**	**Res**	**High B**	**Clash > 0.4Å**	**Ramachandran**	**Rotamer**	**Cβ deviation**	**Bond lengths**	**Bond angles**
			Avg: 54.20	Clashscore: 55.04	Outliers: 3 of 224	Poor rotamers: 1 of 186	Outliers: 1 of 203	Outliers: 7 of 226	Outliers: 12 of 226
A1958		LEU	99.99	0.947Å HD21 with A2147 ALA HA	Favored (22.63%) General / -91.3,148.0	58.2% (*mt*) chi angles: 299.9,185.7	0.046Å	-	-
A1959		CYS	50	-	Favored (38.48%) General / -139.6,145.4	66.6% (*m*) chi angles: 302.1	0.089Å	-	-
A1960		VAL	50	0.482Å HG21 with A2141 ALA HB2	Allowed (0.17%) Isoleucine or valine / -178.4,156.7	11% (*p*) chi angles: 67	0.082Å	-	-
A1961		GLY	50	-	Favored (17.27%) Glycine / -126.3,148.8	-	-	-	-
A1962		VAL	50	0.672Å HG22 with A1938 LEU HB3	Favored (70.98%) Isoleucine or valine / -122.1,132.4	11.7% (*m*) chi angles: 307.5	0.075Å	-	-
A1963		ARG	50	0.619Å O with A1966 GLU HG2	Favored (51.93%) Pre-proline / -82.6,145.8	55% (*mmm-85*) chi angles: 296.3,298.7,292.6,279.5	0.046Å	-	-
A1964		PRO	50	-	Favored (15.6%)	81.5% (*Cg_endo*)	0.03Å	-	-

A1964	PRO	50		Trans-proline / -64.9,125.9	chi angles: 29.9	0.05Å	
A1965	GLY	50	-	Favored (62.8%) Glycine / 90.3,11.4	-	-	-	-
A1966	GLU	50	0.619Å HG2 with A1963 ARG O	Favored (9.65%) General / -110.3,168.2	20.4% (*pt-20*) chi angles: 71,171.3,28.1	0.031Å	-	-
A1967	CYS	50	0.607Å SG with A2138 THR HG23	Favored (22.86%) General / -102.0,110.8	13.7% (*p*) chi angles: 53	0.007Å	-	-
A1968	PHE	50	0.446Å CG with A1962 VAL HG12	Favored (42.97%) General / -107.8,139.1	47.5% (*t80*) chi angles: 188.2,273.4	0.087Å	-	-
A1969	GLY	50	-	Favored (6.5%) Glycine / -125.4,128.2	-	-	-	-
A1970	LEU	50	0.504Å HB3 with A1982 PHE CZ	Favored (14.8%) General / -89.2,102.1	20.2% (*tp*) chi angles: 191.6,70.9	0.027Å	-	-
A1971	LEU	99.99	0.631Å HD12 with A2127 SER O	Favored (53.65%) General / -111.4,133.6	45.3% (*tp*) chi angles: 183.4,67.2	0.076Å	-	-
A1972	GLY	50	-	Favored (17.83%) Glycine / 175.0,158.0	-	-	-	-
A1973	VAL	50	-	Allowed (0.49%) Isoleucine or valine / -59.2,168.2	12.9% (*p*) chi angles: 65.4	0.09Å	-	-
A1974	ASN	50	-	Favored (48.07%) General / -55.0,136.2	90.1% (*m-20*) chi angles: 295,325.8	0.086Å	-	-
A1975	GLY	50	-	Favored (85.93%) Glycine / 79.0,10.7	-	-	-	-
A1976	ALA	50	-	Favored (64.89%) General /	-	0.024Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A1977		GLY	50	-	-68.1,-22.1 Favored (8.7%) Glycine / 99.0,26.7	-	-	-	-
			Avg: 54.20	Clashscore: 55.04	Outliers: 3 of 224	Poor rotamers: 1 of 186	Outliers: 1 of 203	Outliers: 7 of 226	Outliers: 12 of 226
A1978		LYS	50	0.468Å O with A1982 PHE CD1	Favored (83.88%) General / -67.8,-41.0	36.1% (*mtmm*) chi angles: 298.8,184.2,302,292.4	0.034Å	-	-
A1979		THR	50	0.569Å HG22 with A1983 LYS HE2	Favored (78.51%) General / -69.2,-39.9	97% (*m*) chi angles: 298.3	0.078Å	-	-
A1980		THR	50	0.443Å O with A1984 MET HG3	Favored (97.78%) General / -62.2,-43.9	92.4% (*m*) chi angles: 300.4	0.048Å	-	-
A1981		THR	50	-	Favored (85%) General / -58.4,-47.1	63% (*m*) chi angles: 303.6	0.035Å	-	-
A1982		PHE	99.99	0.91Å CZ with A2126 THR HB	Favored (78.9%) General / -68.6,-36.6	1.7% (*m-30*) chi angles: 292.5,32.7	0.036Å	-	-
A1983		LYS	50	0.569Å HE2 with A1979 THR HG22	Favored (78.59%) General / -68.2,-35.8	67.8% (*mttm*) chi angles: 290.4,181.6,177.3,301.9	0.015Å	-	-
A1984		MET	99.99	0.628Å CE with A1991 VAL HA	Favored (79.75%) General / -68.9,-38.7	95.6% (*mtp*) chi angles: 296.6,176.4,73.3	0.02Å	-	-
A1985		LEU	50	0.653Å HD13 with A1938 LEU HD11	Favored (73.58%) General / -66.3,-32.3	93.3% (*mt*) chi angles: 296.8,172.3	0.016Å	-	-
A1986		THR	50	0.689Å HG22 with A2093 LEU HD12	Favored (55.83%) General / -79.0,-6.2	59.1% (*p*) chi angles: 62.6	0.041Å	-	-
A1987		GLY	50	-	Favored (72.13%) Glycine / 72.1,9.6	-	-	-	-
A1988		ASP	50	-	Favored (88.8%) General /	97.3% (*m-20*) chi angles: 300.4,341.4	0.073Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
					General / -66.4,-39.1	chi angles: 290.4,341.4			
A1989		THR	50	-	Favored (40.81%) General / -128.4,157.5	71.2% (*p*) chi angles: 61.9	0.039Å	-	-
A1990		THR	50	-	Favored (20.02%) General / -104.1,154.2	80.6% (*p*) chi angles: 61.4	0.031Å	-	-
A1991		VAL	99.99	0.628Å HA with A1984 MET CE	Favored (6.14%) Isoleucine or valine / -61.4,152.4	4.1% (*m*) chi angles: 312.4	0.094Å	-	-
A1992		THR	50	0.813Å HG21 with A1946 ILE HG12	Favored (31.25%) General / -81.2,-35.4	63.2% (*p*) chi angles: 56.9	0.065Å	-	-
A1993		SER	50	-	Favored (9.19%) General / -169.7,168.2	54.5% (*p*) chi angles: 73.7	0.039Å	-	-
A1994		GLY	50	-	Favored (28.62%) Glycine / 101.2,-180.0	-	-	-	-
A1995		ASP	50	-	Favored (42.99%) General / -132.4,132.6	40.8% (*t0*) chi angles: 191.3,329	0.05Å	-	-
A1996		ALA	50	-	Favored (47%) General / -122.4,126.0	-	0.062Å	-	-
A1997		THR	50	-	Favored (53.89%) General / -120.3,138.1	43.1% (*p*) chi angles: 67.4	0.02Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.20	Clashscore: 55.04	Outliers: 3 of 224	Poor rotamers: 1 of 186	Outliers: 1 of 203	Outliers: 7 of 226	Outliers: 12 of 226
A1998		VAL	50	0.636Å HG23 with A2003 ILE HD11	Favored (45.88%) Isoleucine or valine / -117.7,114.6	91.5% (*t*) chi angles: 175.4	0.034Å	-	-
A1999		ALA	50		Favored (29.61%)		0.073Å		

A1999	ALA	50	-	General / 54.6,38.2	-	0.072Å	-	-
A2000	GLY	50	-	Favored (86.35%) Glycine / 77.6,10.2	-	-	-	-
A2001	LYS	50	-	Favored (30.07%) General / -105.1,115.3	72.2% (*mmtt*) chi angles: 302.6,299.2,193.8,182.9	0.09Å	-	-
A2002	SER	50	0.602Å HB3 with A2005 THR OG1	Favored (15.52%) General / -62.5,122.3	36% (*t*) chi angles: 175.8	0.043Å	-	-
A2003	ILE	50	0.695Å O with A2007 ILE HG22	Favored (43.99%) Isoleucine or valine / -65.2,-28.2	82.2% (*mt*) chi angles: 301.2,171.6	0.085Å	OUTLIER(S) worst is C--O: 5.714 σ	-
A2004	LEU	50	-	Favored (20.39%) General / -85.7,-36.1	10% (*tt*) chi angles: 186.3,154.4	0.11Å	-	-
A2005	THR	50	0.602Å OG1 with A2002 SER HB3	Favored (30.7%) General / -80.9,-36.9	71.1% (*p*) chi angles: 63.9	0.063Å	-	-
A2006	ASN	50	-	Allowed (1.52%) General / -132.7,67.7	35.1% (*m120*) chi angles: 295.6,116	0.013Å	-	-
A2007	ILE	50	0.695Å HG22 with A2003 ILE O	Favored (78.76%) Isoleucine or valine / -62.5,-37.4	48.4% (*pt*) chi angles: 63.4,172.2	0.052Å	-	-
A2008	SER	50	-	Favored (85.42%) General / -60.7,-47.6	41.3% (*t*) chi angles: 181.3	0.02Å	-	-
A2009	GLU	50	-	Favored (96.8%) General / -63.0,-40.1	6% (*mm-40*) chi angles: 291.8,289.1,48.8	0.027Å	-	-
A2010	VAL	50	0.498Å HG21 with A2003 ILE HA	Favored (94.85%) Isoleucine or valine / -64.5,-45.7	71.4% (*t*) chi angles: 173.3	0.062Å	-	-
				Favored				

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A2011		HIS	50	-	Favored (74.09%) General / -66.1,-32.6	66.5% (*m170*) chi angles: 293.7,164.6	0.064Å	OUTLIER(S) worst is CG-- ND1: 4.64 σ	-
A2012		GLN	50	-	Favored (46.3%) General / -60.2,-18.2	84.9% (*mt-30*) chi angles: 294.3,181.7,296.9	0.016Å	-	-
A2013		ASN	50	0.8Å HD22 with A2090 PRO HG3	Favored (15.41%) General / -103.0,-17.6	28% (*m120*) chi angles: 290.5,124.3	0.041Å	-	-
A2014		MET	99.99	0.747Å HE1 with A2091 LEU HG	Favored (30.07%) General / -112.4,151.2	80.1% (*mmm*) chi angles: 292.8,309,305.8	0.097Å	-	-
A2015		GLY	50	-	Favored (3.46%) Glycine / -134.0,124.0	-	-	-	-
A2016		TYR	50	0.494Å CG with A1986 THR HG21	Favored (52.45%) General / -111.9,135.5	49.5% (*t80*) chi angles: 175.2,62	0.054Å	-	-
A2017		CYS	50	-	Favored (31.79%) Pre-proline / -124.5,103.5	50.9% (*t*) chi angles: 181.9	0.062Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.20	Clashscore: 55.04	Outliers: 3 of 224	Poor rotamers: 1 of 186	Outliers: 1 of 203	Outliers: 7 of 226	Outliers: 12 of 226
A2018		PRO	50	-	Favored (46.07%) Trans-proline / -62.1,157.1	78.6% (*Cg_endo*) chi angles: 29.8	0.044Å	-	-
A2019		GLN	50	0.679Å HG2 with A2020 PHE CD1	Favored (56.25%) General / -62.8,134.4	62.9% (*tt0*) chi angles: 185.6,181.5,354.9	0.119Å	-	-
A2020		PHE	50	0.679Å CD1 with A2019 GLN HG2	Favored (20.11%) General / 60.8,33.5	1.9% (*m-30*) chi angles: 292,30.6	0.033Å	-	-
A2021		ASP	50	-	Favored (57.02%) General / -59.7,139.7	46.3% (*t0*) chi angles: 190.1,333.7	0.055Å	-	-

A2022	ALA	50	-	Favored (8.98%) General / -111.1,169.1	-	0.059Å	-	-
A2023	ILE	50	0.847Å HD13 with A2079 LEU HD23	Favored (20.28%) Isoleucine or valine / -118.9,158.1	45.8% (*pt*) chi angles: 60.7,169.6	0.092Å	-	-
A2024	ASP	50	0.71Å OD2 with A2027 LEU HD13	Favored (7.59%) General / -64.5,117.6	25.8% (*t70*) chi angles: 193,47.2	0.041Å	-	-
A2025	GLU	50	0.473Å HA with A2068 ALA HB3	Favored (63.08%) General / -70.0,-22.9	54.3% (*mt-10*) chi angles: 296.2,182.1,296.3	0.055Å	-	-
A2026	LEU	50	0.581Å O with A2027 LEU HD12	Favored (3.83%) General / -95.5,26.5	10.9% (*mp*) chi angles: 277.8,66.7	0.092Å	-	-
A2027	LEU	50	0.71Å HD13 with A2024 ASP OD2	Favored (52.33%) General / -131.5,149.9	11.2% (*mp*) chi angles: 275.3,62.6	0.049Å	-	-
A2028	THR	50	-	Favored (45.51%) General / -64.9,151.5	40.7% (*p*) chi angles: 67.8	0.015Å	-	-
A2029	GLY	50	-	Favored (56.34%) Glycine / -52.0,-44.3	-	-	-	-
A2030	ARG	50	-	Favored (78.95%) General / -67.2,-35.1	63.5% (*ttm-85*) chi angles: 185.7,180.1,293.6,275.6	0.036Å	-	-
A2031	GLU	50	-	Favored (81.02%) General / -68.6,-39.1	72.4% (*tt0*) chi angles: 182.9,175.4,20.7	0.07Å	-	-
A2032	HIS	50	-	Favored (94.44%) General / -63.1,-39.4	81.4% (*t60*) chi angles: 185.9,62.7	0.031Å	OUTLIER(S) worst is CG--ND1: 4.387 σ	-
A2033	LEU	50	0.466Å CD2 with A2083 ILE HG22	Favored (86.44%) General / -66.7,-42.3	96.2% (*mt*) chi angles: 297.9,175.8	0.011Å	-	-

Favored

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A2034		TYR	99.99	-	Favored (98.35%) General / -62.8,-43.6	86.5% (*t80*) chi angles: 178.3,83.2	0.033Å	-	-
A2035		LEU	50	0.401Å O with A2038 ARG HB3	Favored (71.54%) General / -60.0,-51.0	50.9% (*tp*) chi angles: 183.6,64.3	0.036Å	-	-
A2036		TYR	50	0.527Å HA with A2039 LEU HD13	Favored (78.71%) General / -69.1,-39.8	83.3% (*t80*) chi angles: 182.6,80.6	0.025Å	-	-
A2037		ALA	50	0.407Å HB1 with A2050 VAL HG11	Favored (64.25%) General / -55.6,-33.9	-	0.166Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.20	Clashscore: 55.04	Outliers: 3 of 224	Poor rotamers: 1 of 186	Outliers: 1 of 203	Outliers: 7 of 226	Outliers: 12 of 226
A2038		ARG	50	0.401Å HB3 with A2035 LEU O	Favored (68.47%) General / -62.0,-26.9	59.8% (*ttm-85*) chi angles: 181.2,181,290.4,277.8	0.03Å	-	-
A2039		LEU	50	0.527Å HD13 with A2036 TYR HA	Favored (96.02%) General / -64.3,-40.5	10.6% (*mp*) chi angles: 279.4,65.9	0.03Å	-	-
A2040		ARG	50	-	Favored (47.28%) General / -78.6,-33.6	79.3% (*mtp85*) chi angles: 295,181.8,63.5,83.8	0.009Å	-	-
A2041		GLY	50	-	Favored (24.43%) Glycine / -153.3,152.9	-	-	-	-
A2042		VAL	50	0.567Å N with A2043 PRO HD2	Allowed (0.36%) Pre-proline / -91.8,-35.1	12.8% (*p*) chi angles: 65.5	0.109Å	-	-
A2043		PRO	50	0.738Å HG3 with A2046 GLU OE2	Favored (73.29%) Trans-proline / -65.1,142.3	60.9% (*Cg_endo*) chi angles: 34.4	0.054Å	-	-
A2044		ALA	50	-	Favored (88.41%) General / -62.8,-37.9	-	0.036Å	-	-
					Favored	11% (*tm-20*)			

A2045	GLU	50	-	(92.13%) General / -62.4,-45.7	11% (tm-20) chi angles: 179.5,288.4,327.2	0.074Å	-	-
A2046	GLU	50	0.738Å OE2 with A2043 PRO HG3	Favored (76.3%) General / -69.4,-41.4	45.7% (mt-10) chi angles: 291.8,183.5,73.2	0.053Å	-	-
A2047	ILE	50	0.479Å O with A2050 VAL HG12	Favored (98.9%) Isoleucine or valine / -63.1,-45.3	89.2% (mt) chi angles: 296.5,174.7	0.077Å	-	-
A2048	GLU	50	-	Favored (99.46%) General / -62.5,-42.3	37.2% (tp10) chi angles: 188.4,58.2,32	0.017Å	-	-
A2049	LYS	50	-	Favored (80.19%) General / -63.2,-48.0	39% (ttpt) chi angles: 182.2,181.6,64.4,181.8	0.035Å	-	-
A2050	VAL	50	0.658Å HG22 with A2086 ILE HD12	Favored (88.41%) Isoleucine or valine / -62.0,-40.8	8.1% (p) chi angles: 68.8	0.186Å	-	-
A2051	ALA	50	0.427Å O with A2055 ILE HG23	Favored (85.7%) General / -67.4,-40.2	-	0.01Å	-	-
A2052	ASN	50	0.459Å HA with A2055 ILE HG12	Favored (73.69%) General / -70.4,-36.0	30% (m120) chi angles: 291.1,120.7	0.056Å	-	-
A2053	TRP	99.99	0.65Å HD1 with A2086 ILE HA	Favored (85.7%) General / -67.3,-38.9	75.3% (t-105) chi angles: 181.3,258.5	0.021Å	-	-
A2054	SER	50	0.691Å O with A2058 LEU HD12	Favored (5.31%) General / -57.5,-59.3	5.1% (t) chi angles: 199.5	0.095Å	-	-
A2055	ILE	50	0.459Å HG12 with A2052 ASN HA	Favored (55.1%) Isoleucine or valine / -56.9,-37.6	43.1% (pt) chi angles: 64.8,171.5	0.064Å	-	-
A2056	LYS	50	-	Favored (81.63%) General / -67.9,-42.1	38.9% (ttpt) chi angles: 185.8,178.7,63,182	0.053Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A2057		SER	50	-	Favored (72.62%) General / -67.6,-46.4	32.7% (*t*) chi angles: 184.1	0.036Å	-	-
			Avg: 54.20	Clashscore: 55.04	Outliers: 3 of 224	Poor rotamers: 1 of 186	Outliers: 1 of 203	Outliers: 7 of 226	Outliers: 12 of 226
A2058		LEU	99.99	0.81Å HD21 with A2079 LEU HD12	Favored (80.03%) General / -56.4,-46.9	2.4% (*mp*) chi angles: 285.1,101.8	0.142Å	-	OUTLIER(S) worst is CD1-CG-CD2: 7.705 σ
A2059		GLY	50	-	Favored (94.1%) Glycine / 61.5,46.5	-	-	-	-
A2060		LEU	50	0.68Å HG with A2058 LEU HB3	Favored (57.44%) General / -92.2,1.1	41.3% (*mt*) chi angles: 294.7,187.5	0.037Å	-	-
A2061		THR	50	-	Allowed (1%) General / 56.1,-138.6	37.4% (*p*) chi angles: 68.2	0.102Å	-	-
A2062		VAL	50	-	Favored (27.26%) Isoleucine or valine / -63.3,-21.0	14.8% (*p*) chi angles: 63.8	0.114Å	-	-
A2063		TYR	50	0.421Å HB2 with A2060 LEU O	Favored (64.99%) General / -66.7,-17.7	1.3% (*m-30*) chi angles: 294.7,32	0.046Å	-	-
A2064		ALA	50	-	Favored (66.16%) General / -59.6,-27.2	-	0.025Å	-	-
A2065		ASP	50	-	Favored (59.01%) General / -85.3,-4.0	62.7% (*m-20*) chi angles: 295,302.9	0.034Å	-	-
A2066		CYS	50	-	Favored (19.71%) General / -90.4,154.4	72.2% (*m*) chi angles: 297.2	0.035Å	-	-
A2067		LEU	50	-	Favored (57.71%) General / -61.6,141.6	11% (*mp*) chi angles: 278.5,63.9	0.008Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A2068		ALA	50	0.473Å HB3 with A2025 GLU HA	Favored (69.1%) General / -61.5,-28.2	-	0.157Å	-	-
A2069		GLY	50	-	Favored (56.82%) Glycine / -57.0,-27.4	-	-	-	-
A2070		THR	50	-	Favored (46.59%) General / -86.4,-13.4	28.7% (*p*) chi angles: 70.8	0.045Å	-	-
A2071		TYR	50	-	Favored (56.59%) General / -67.6,141.9	4.9% (*m-30*) chi angles: 284.9,20.8	0.018Å	-	-
A2072		SER	50	-	Favored (13.53%) General / -74.0,171.4	53.8% (*p*) chi angles: 74.1	0.028Å	-	-
A2073		GLY	50	-	Favored (94.84%) Glycine / -59.7,-39.1	-	-	-	-
A2074		GLY	50	-	Favored (97.14%) Glycine / -65.0,-40.4	-	-	-	-
A2075		ASN	50	0.515Å HD22 with A2060 LEU CD2	Favored (85.09%) General / -67.5,-39.8	31.7% (*m120*) chi angles: 292.1,119.4	0.02Å	-	-
A2076		LYS	50	-	Favored (96.24%) General / -64.4,-42.4	39.4% (*ttpt*) chi angles: 184.4,180.9,65.3,181.6	0.038Å	-	-
A2077		ARG	50	-	Favored (98.52%) General / -61.9,-43.6	0% chi angles: 184.3,62.1,107.7,286.4	0.037Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.20	Clashscore: 55.04	Outliers: 3 of 224	Poor rotamers: 1 of 186	Outliers: 1 of 203	Outliers: 7 of 226	Outliers: 12 of 226
A2078		LYS	50	-	Favored (81.19%) General / -67.7,-36.7	46.1% (*mtmt*) chi angles: 291.5,194.6,294.9,167.4	0.052Å	-	-
				0.847Å	Favored				OUTLIER(S)

A2079	LEU	50	0.847Å HD23 with A2023 ILE HD13	Favored (89.17%) General / -62.2,-38.5	27.7% (*tp*) chi angles: 181.2,73.1	0.047Å	-	OUTLIER(S) worst is CD1-CG-CD2: 6.073 σ
A2080	SER	50	0.722Å O with A2083 ILE HG12	Favored (55.35%) General / -77.0,-37.2	71.1% (*m*) chi angles: 297.5	0.04Å	-	-
A2081	THR	50	-	Favored (77.88%) General / -69.0,-41.2	72.5% (*m*) chi angles: 296.8	0.051Å	-	-
A2082	ALA	50	0.734Å O with A2086 ILE HG23	Favored (96.1%) General / -61.9,-40.6	-	0.098Å	-	-
A2083	ILE	50	0.722Å HG12 with A2080 SER O	Favored (68.33%) Isoleucine or valine / -61.3,-35.8	8.9% (*pt*) chi angles: 70.5,187.7	0.109Å	-	OUTLIER(S) worst is CB-CG1-CD1: 4.15 σ
A2084	ALA	50	-	Favored (67.79%) General / -72.3,-34.0	-	0.027Å	-	-
A2085	LEU	50	0.698Å HD21 with A2116 ILE HD13	Favored (23.38%) General / -90.2,-20.2	9.8% (*mp*) chi angles: 274.7,55	0.02Å	-	-
A2086	ILE	99.99	0.734Å HG23 with A2082 ALA O	Favored (44.55%) Isoleucine or valine / -59.2,-30.7	22.8% (*pt*) chi angles: 55.9,180.6	0.109Å	-	OUTLIER(S) worst is CA-CB-CG2: 4.278 σ
A2087	GLY	50	-	Favored (40.07%) Glycine / -70.1,-2.6	-	-	-	-
A2088	CYS	50	-	Favored (15.63%) Pre-proline / 49.0,54.1	99.5% (*m*) chi angles: 294.5	0.054Å	-	-
A2089	PRO	50	0.901Å HG2 with A2121 ARG HH12	Favored (42.13%) Trans-proline / -73.0,146.8	54.1% (*Cg_endo*) chi angles: 25.4	0.065Å	-	-
A2090	PRO	50	0.8Å HG3 with A2013 ASN HD22	Favored (30.34%) Trans-proline / -66.8,-34.5	29.1% (*Cg_endo*) chi angles: 21	0.115Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A2091		LEU	50	0.747Å HG with A2014 MET HE1	Favored (32.56%) General / -130.3,124.5	23.2% (tp) chi angles: 167.2,70	0.241Å	-	-
A2092		VAL	50	0.908Å HG13 with A2123 VAL HG23	Favored (46.63%) Isoleucine or valine / -102.6,133.3	13.3% (p) chi angles: 65.2	0.127Å	-	-
A2093		LEU	50	0.785Å HD23 with A2124 VAL HB	Favored (14.87%) General / -117.0,107.7	83.5% (mt) chi angles: 298.4,181.7	0.042Å	-	OUTLIER(S) worst is CD1-CG-CD2: 4.132 σ
A2094		LEU	50	0.568Å HD12 with A2125 LEU HD11	Favored (49.18%) General / -114.0,123.2	45.5% (mt) chi angles: 307.8,173.9	0.022Å	-	-
A2095		ASP	50	0.787Å HA with A2126 THR HG22	Favored (13.25%) General / -96.0,101.6	25.5% (t0) chi angles: 198.2,333.9	0.038Å	-	-
A2096		GLU	50	0.516Å HB2 with A2019 GLN HG3	Favored (2.76%) Pre-proline / 61.5,53.9	68.7% (mm-40) chi angles: 303.1,287.8,345.4	0.056Å	-	-
A2097		PRO	50	0.506Å HG3 with A2125 LEU CD2	Favored (77.25%) Trans-proline / -61.0,-23.4	94.4% (Cg_endo) chi angles: 32.2	0.094Å	-	-
			Avg: 54.20	Clashscore: 55.04	Outliers: 3 of 224	Poor rotamers: 1 of 186	Outliers: 1 of 203	Outliers: 7 of 226	Outliers: 12 of 226
A2098		THR	50	0.883Å HG21 with A2110 TRP HE1	Favored (15.83%) General / -112.1,0.1	80.2% (p) chi angles: 60.3	0.024Å	-	-
A2099		THR	50	0.411Å OG1 with A2020 PHE HE1	Favored (53.15%) General / -61.7,145.2	17.9% (p) chi angles: 47.4	0.051Å	-	-
A2100		GLY	50	-	Favored (58.15%) Glycine / 62.8,17.6	-	-	-	-
A2101		MET	50	0.505Å HE2 with A2105 ALA HB1	Favored (32.32%) General /	95.5% (mtp) chi angles: 296.8,178.3,75.7	0.061Å	-	-

			HB1	-102.6,143.4				
A2102	ASP	50	0.624Å HB2 with A2103 PRO HD2	Allowed (1.41%) Pre-proline / -69.2,176.8	35.4% (*p30*) chi angles: 72.7,8.4	0.171Å	-	-
A2103	PRO	50	0.624Å HD2 with A2102 ASP HB2	Favored (47.21%) Trans-proline / -59.3,-42.7	75.7% (*Cg_endo*) chi angles: 29.7	0.086Å	-	-
A2104	GLN	50	-	Favored (72.64%) General / -67.3,-46.8	53.4% (*tt0*) chi angles: 180.7,181.5,60.3	0.025Å	-	-
A2105	ALA	50	0.505Å HB1 with A2101 MET HE2	Favored (79.85%) General / -68.8,-40.1	-	0.098Å	-	-
A2106	ARG	50	0.592Å NE with A2103 PRO HA	Favored (88.31%) General / -64.7,-37.6	40.8% (*ptt180*) chi angles: 66,180.5,179.2,179.5	0.063Å	-	-
A2107	ARG	50	-	Favored (97.4%) General / -63.9,-43.0	35.9% (*ttp-105*) chi angles: 184.3,166.3,74.1,244.5	0.031Å	-	-
A2108	MET	50	0.434Å O with A2112 VAL HG13	Favored (85.98%) General / -64.6,-37.0	63.6% (*mtt*) chi angles: 291.7,183.9,177.2	0.036Å	-	-
A2109	LEU	50	0.532Å HD22 with A2098 THR CG2	Favored (69.16%) General / -72.2,-37.7	9% (*tt*) chi angles: 191.1,152.8	0.047Å	-	-
A2110	TRP	99.99	0.883Å HE1 with A2098 THR HG21	Favored (84.14%) General / -63.9,-36.5	49.4% (*m0*) chi angles: 295.6,354.1	0.02Å	OUTLIER(S) worst is NE1--CE2: 7.458 σ	OUTLIER(S) worst is CZ2-CH2-CZ3: 5.525 σ
A2111	ASN	50	0.509Å HA with A2114 VAL HG12	Favored (95.27%) General / -64.6,-42.8	26.2% (*t-20*) chi angles: 184.2,300.2	0.03Å	-	-
A2112	VAL	50	0.518Å O with A2116 ILE HG23	Favored (98.59%) Isoleucine or valine / -62.7,-43.4	28.4% (*m*) chi angles: 301.4	0.124Å	-	-
A2113	ILE	50	1.073Å HD12 with A2116 ILE	Favored (75.51%) Isoleucine or	4% (*tp*) chi angles: 178.7,78.7	0.118Å	-	OUTLIER(S) worst is CB-CG1-CD1:

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		A2116 ILE HD11			Isoleucine or valine / -71.1,-40.4	chi angles: 178.7,78.7			CGT-CDT: 4.386 σ
A2114		VAL	50	0.509Å HG12 with A2111 ASN HA	Favored (88.12%) Isoleucine or valine / -63.8,-40.2	12.7% (*p*) chi angles: 65.5	0.117Å	-	-
A2115		SER	50	-	Favored (84.51%) General / -67.5,-38.5	37.4% (*t*) chi angles: 182.1	0.014Å	-	-
A2116		ILE	50	1.073Å HD11 with A2113 ILE HD12	Favored (77.9%) Isoleucine or valine / -68.9,-37.9	28.7% (*pt*) chi angles: 67.6,177.4	0.107Å	-	-
A2117		ILE	50	0.433Å HG12 with A2114 VAL O	Favored (76.39%) Isoleucine or valine / -69.3,-37.9	40.7% (*pt*) chi angles: 65,173.9	0.089Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.20	Clashscore: 55.04	Outliers: 3 of 224	Poor rotamers: 1 of 186	Outliers: 1 of 203	Outliers: 7 of 226	Outliers: 12 of 226
A2118		ARG	50	0.445Å HG3 with A2114 VAL O	Favored (68.48%) General / -63.4,-25.9	77.4% (*mtp85*) chi angles: 292.3,178.9,68.1,83.4	0.004Å	-	-
A2119		GLU	50	-	Favored (12.91%) General / -87.8,12.4	97.5% (*mt-10*) chi angles: 295.4,179.8,358.5	0.035Å	-	-
A2120		GLY	50	-	Favored (36.59%) Glycine / 105.9,-20.3	-	-	-	-
A2121		ARG	50	0.901Å HH12 with A2089 PRO HG2	Favored (57.94%) General / -59.6,137.7	61.1% (*ttm-85*) chi angles: 182.4,184,292.8,277.6	0.043Å	-	-
A2122		ALA	50	-	Favored (44.75%) General / -98.4,131.3	-	0.059Å	-	-
A2123		VAL	50	1.026Å HG21 with A2113 ILE HD11	Favored (69.27%) Isoleucine or valine /	9.8% (*p*) chi angles: 72.2	0.164Å	-	-

			HD11	...tttt... -127.2,132.9			
A2124	VAL	50	0.785Å HB with A2093 LEU HD23	Favored (49.76%) Isoleucine or valine / -115.4,115.6	81.3% (*t*) chi angles: 174.6	0.061Å	-	-
A2125	LEU	50	0.568Å HD11 with A2094 LEU HD12	Favored (34.94%) General / -113.9,149.6	7.5% (*mp*) chi angles: 264.8,56.4	0.102Å	-	-
A2126	THR	99.99	0.91Å HB with A1982 PHE CZ	Favored (48.45%) General / -115.5,141.1	5.3% (*t*) chi angles: 176.5	0.019Å	-	-
A2127	SER	50	0.631Å O with A1971 LEU HD12	Favored (18.15%) General / -159.4,148.4	46.8% (*t*) chi angles: 180.4	0.067Å	-	-
A2128	HIS	50	-	Favored (17.75%) General / -112.2,4.4	52.3% (*p-80*) chi angles: 62.8,274	0.042Å	OUTLIER(S) worst is CG-- ND1: 4.556 σ	OUTLIER(S) worst is CB- CG-CD2: 4.123 σ
A2129	SER	50	-	Favored (5.98%) General / -92.7,87.7	46.6% (*t*) chi angles: 180.5	0.019Å	-	-
A2130	MET	50	-	Favored (63.12%) General / -72.1,-28.2	58.7% (*mtt*) chi angles: 300,187.9,179.2	0.108Å	-	-
A2131	GLU	50	-	Favored (93.74%) General / -64.4,-39.4	52.1% (*mt-10*) chi angles: 290.6,184.8,296.3	0.05Å	-	-
A2132	GLU	50	0.743Å HB3 with A2110 TRP CH2	Favored (56.34%) General / -88.2,-7.7	71.2% (*mm-40*) chi angles: 288.8,305.7,322.7	0.187Å	-	OUTLIER(S) worst is CB- CG-CD: 4.603 σ
A2133	CYS	50	-	Favored (86.05%) General / -63.1,-37.1	21.8% (*p*) chi angles: 68.7	0.047Å	-	-
A2134	GLU	50	-	Favored (68.28%) General / -62.7,-25.7	11% (*pt-20*) chi angles: 61.2,174.5,78.9	0.138Å	-	-
A2135	ALA	50	-	Favored (20.04%) General /	-	0.05Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
					General / -94.0,14.3				
A2136		LEU	50	0.538Å HD11 with A2113 ILE HG21	Allowed (0.65%) General / -135.9,-45.9	46.8% (*tp*) chi angles: 181.7,56.8	0.058Å	-	-
A2137		CYS	50	0.521Å HA with A1967 CYS SG	Favored (26.48%) General / -101.0,147.2	63.7% (*m*) chi angles: 302.8	0.039Å	-	-
			Avg: 54.20	Clashscore: 55.04	Outliers: 3 of 224	Poor rotamers: 1 of 186	Outliers: 1 of 203	Outliers: 7 of 226	Outliers: 12 of 226
A2138		THR	50	0.607Å HG23 with A1967 CYS SG	Favored (11.9%) General / -86.0,-45.0	82.8% (*p*) chi angles: 60.5	0.026Å	-	-
A2139		ARG	50	-	Favored (50.51%) General / -134.7,149.5	42.4% (*mtp-105*) chi angles: 292.5,179.2,60.6,242.5	0.059Å	-	-
A2140		LEU	99.99	0.489Å HD21 with A2137 CYS SG	Favored (51.79%) General / -135.5,153.2	95.2% (*mt*) chi angles: 297.9,178.5	0.036Å	-	OUTLIER(S) worst is CD1-CG-CD2: 4.011 σ
A2141		ALA	50	0.482Å HB2 with A1960 VAL HG21	Favored (20.78%) General / -121.5,114.1	-	0.056Å	-	-
A2142		ILE	50	0.666Å HG13 with A2149 ARG HG3	Favored (28.92%) Isoleucine or valine / -81.7,118.1	48% (*pt*) chi angles: 62.5,169.6	0.098Å	-	-
A2143		MET	50	0.525Å HE1 with A2148 PHE HA	Favored (53.5%) General / -114.5,136.0	38.1% (*mmp*) chi angles: 293.7,302.3,107.3	0.112Å	-	OUTLIER(S) worst is CG-SD-CE: 5.069 σ
A2144		VAL	50	0.666Å HB with A2149 ARG NH1	Favored (11.43%) Isoleucine or valine / -142.1,122.5	9.9% (*p*) chi angles: 60.8	0.049Å	-	-
A2145		LYS	50	-	Favored (16.19%) General / 53.2,33.8	32.9% (*mmmt*) chi angles: 295.4,295,294.8,180.7	0.044Å	-	-
					Favored				

A2146	GLY	50	-	(72.03%) Glycine / 69.1,30.3	-	-	-	-
A2147	ALA	50	0.947Å HA with A1958 LEU HD21	Favored (52.27%) General / -127.2,140.4	-	0.066Å	-	-
A2148	PHE	99.99	0.525Å HA with A2143 MET HE1	Favored (16.33%) General / -89.5,103.7	50.5% (*p90*) chi angles: 65.8,88	0.119Å	-	-
A2149	ARG	50	0.666Å HG3 with A2142 ILE HG13	Favored (27.99%) General / -85.8,-21.9	15.7% (*ptt-85*) chi angles: 51.5,166.9,193.5,290.3	0.251Å	-	-
A2150	CYS	50	0.417Å SG with A2149 ARG O	Favored (5.21%) General / -172.5,162.1	61.3% (*m*) chi angles: 303.8	0.126Å	-	-
A2151	MET	50	-	Favored (42.34%) General / -153.4,161.4	25.9% (*ptp*) chi angles: 63.5,179.9,69.8	0.033Å	-	-
A2152	GLY	50	-	Favored (19.8%) Glycine / 141.6,-179.3	-	-	-	-
A2153	THR	50	-	Favored (37.84%) General / -68.0,156.2	23.4% (*p*) chi angles: 72.2	0.033Å	-	-
A2154	ILE	50	0.411Å HG13 with A2155 GLN N	Favored (66.82%) Isoleucine or valine / -57.6,-39.0	49.6% (*pt*) chi angles: 62.6,171.1	0.056Å	-	-
A2155	GLN	50	0.411Å N with A2154 ILE HG13	Favored (72.2%) General / -70.1,-42.8	70.7% (*tp60*) chi angles: 184.4,61.7,59.8	0.008Å	-	-
A2156	HIS	50	-	Favored (96.85%) General / -60.3,-43.0	60.8% (*m170*) chi angles: 294.5,160	0.064Å	OUTLIER(S) worst is CD2-- NE2: 4.265 σ	-
A2157	LEU	50	-	Favored (92.43%) General / -65.5,-42.3	88.4% (*mt*) chi angles: 290.3,173.5	0.005Å	-	-

| | | **High** | **Clash >** | | | **Cβ** | **Bond** | **Bond** |

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.20	Clashscore: 55.04	Outliers: 3 of 224	Poor rotamers: 1 of 186	Outliers: 1 of 203	Outliers: 7 of 226	Outliers: 12 of 226
A2158		LYS	50	0.764Å HA with A2163 ASP OD1	Favored (93.65%) General / -64.0,-39.2	61.2% (*mtpt*) chi angles: 289.7,169.5,63.3,173	0.1Å	-	-
A2159		SER	50	-	Favored (57.38%) General / -75.6,-39.7	64.6% (*m*) chi angles: 298.7	0.009Å	-	-
A2160		LYS	50	-	Favored (97.79%) General / -61.9,-41.3	40.9% (*ttmt*) chi angles: 183.6,178.5,293.1,180.1	0.016Å	-	-
A2161		PHE	50	0.449Å HB2 with A2163 ASP OD2	Favored (34.34%) General / -104.8,10.9	97% (*m-85*) chi angles: 293.4,275.7	0.026Å	-	-
A2162		GLY	50	-	Favored (26.78%) Glycine / 48.4,43.1	-	-	-	-
A2163		ASP	99.99	0.764Å OD1 with A2158 LYS HA	-	9.9% (*p30*) chi angles: 63,40.7	0.1Å	-	-

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