Viewing abca4_sm_928-1154H-multi.table

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All-Atom Contacts	Clashscore, all atoms:	53.67		3rd percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	2	1.05%	Goal: <1%
	Ramachandran outliers	0	0.00%	Goal: <0.05%
	Ramachandran favored	216	96.00%	Goal: >98%
	MolProbity score^	2.49		47th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	Bad backbone bonds:	19 / 1778	1.07%	Goal: 0%
	Bad backbone angles:	19 / 2403	0.79%	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: 53.74	Clashscore: 53.67	Outliers: 0 of 225	Poor rotamers: 2 of 190	Outliers: 0 of 205	Outliers: 10 of 227	Outliers: 14 of 227
A 928		GLY	50	-	-	-	-	-	-
A 929		VAL	50	-	Favored (42.72%) Isoleucine or valine / -138.0,132.0	59.4% (t) chi angles: 180.9	0.034Å	-	-
A 930		CYS	50	0.736Å SG with A 988 LEU HB2	Favored (19.88%) General / -129.0,116.8	27.4% (p) chi angles: 60	0.02Å	-	-
A 931		VAL	50	-	Favored (57.2%) Isoleucine or valine / -105.5,130.2	89.1% (t) chi angles: 178.8	0.077Å	-	-
				0.837Å HA with A	Favored (9.14%)	26.3% (tptp)			

A 932	LYS	50	HA with A 950 ASN OD1	(8.14%) General / -131.8,106.5	chi angles: 189.8,69.8,180.7,61	0.084A	-	-
A 933	ASN	50	0.514Å H with A 950 ASN CG	Favored (32.02%) General / 52.9,43.1	98.2% (*m-20*) chi angles: 289,336.3	0.039Å	-	-
A 934	LEU	50	0.445Å O with A 946 VAL HG22	Favored (17.15%) General / -71.8,120.3	67% (*tp*) chi angles: 176.8,61.9	0.026Å	-	-
A 935	VAL	50	0.664Å HG13 with A 983 THR OG1	Favored (22.85%) Isoleucine or valine / -120.6,158.6	9% (*p*) chi angles: 70.8	0.118Å	-	-
A 936	LYS	50	0.729Å HB3 with A 946 VAL HG12	Favored (2.12%) General / -161.9,118.7	50.6% (*tptt*) chi angles: 179.8,67.1,187.4,187.6	0.025Å	-	-
A 937	ILE	50	0.884Å HG12 with A 983 THR HG21	Favored (36.11%) Isoleucine or valine / -97.2,134.2	36.4% (*pt*) chi angles: 65.9,174.8	0.037Å	-	-
A 938	PHE	99.99	0.504Å CE1 with A 945 ALA CB	Favored (40.28%) General / -75.2,131.3	3.1% (*m-30*) chi angles: 290.1,23.3	0.071Å	-	-
A 939	GLU	99.99	0.55Å N with A 940 PRO HD2	Favored (4.98%) Pre-proline / -73.4,-39.6	11.2% (*pm0*) chi angles: 67.2,294.2,354.8	0.066Å	-	-
A 940	PRO	99.99	0.55Å HD2 with A 939 GLU N	Favored (39.96%) Trans-proline / -67.4,-27.8	72.2% (*Cg_endo*) chi angles: 33.4	0.047Å	-	-
A 941	CYS	99.99	0.542Å HB2 with A 943 ARG NH1	Favored (2.23%) General / -140.0,26.6	15.7% (*p*) chi angles: 73.5	0.136Å	-	-
A 942	GLY	50	-	Favored (17.83%) Glycine / 49.8,32.4	-	-	-	-
A 943	ARG	50	0.542Å NH1 with A 941 CYS HB2	Favored (22.49%) Pre-proline / -114.7,133.8	81% (*mtt85*) chi angles: 290.1,184.9,181.4,80.1	0.073Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 944		PRO	50	-	Allowed (1.08%) Trans-proline / -83.1,89.7	91.2% (*Cg_endo*) chi angles: 32	0.021Å	-	-
A 945		ALA	50	0.504Å CB with A 938 PHE CE1	Favored (64.6%) General / -72.0,-43.7	-	0.08Å	-	-
A 946		VAL	50	0.729Å HG12 with A 936 LYS HB3	Favored (55.48%) Isoleucine or valine / -106.0,131.5	10.2% (*p*) chi angles: 61	0.167Å	-	OUTLIER(S) worst is CG1-CB-CG2: 4.003 σ
A 947		ASP	50	0.464Å O with A 948 ARG HB3	Allowed (1.08%) General / -113.1,47.9	44.9% (*m-20*) chi angles: 299.7,293.8	0.036Å	-	-
			Avg: 53.74	Clashscore: 53.67	Outliers: 0 of 225	Poor rotamers: 2 of 190	Outliers: 0 of 205	Outliers: 10 of 227	Outliers: 14 of 227
A 948		ARG	50	0.464Å HB3 with A 947 ASP O	Allowed (0.12%) General / 73.2,70.6	51.1% (*ttm-85*) chi angles: 175.4,191.2,298.4,280.9	0.087Å	-	-
A 949		LEU	99.99	1.085Å HD21 with A1137 ARG HA	Favored (24.53%) General / -97.3,147.1	59.2% (*mt*) chi angles: 296.7,185.5	0.034Å	-	-
A 950		ASN	50	0.837Å OD1 with A 932 LYS HA	Favored (40.14%) General / -138.2,143.1	25% (*m-80*) chi angles: 288.1,264.6	0.16Å	-	-
A 951		ILE	50	0.518Å HG12 with A1131 ALA HB2	Allowed (0.23%) Isoleucine or valine / -177.1,155.8	7% (*tp*) chi angles: 187.4,53.5	0.075Å	-	-
A 952		THR	50	-	Favored (47.9%) General / -133.2,141.0	76.8% (*p*) chi angles: 61.7	0.076Å	-	-
A 953		PHE	50	0.584Å HD2 with A1114 ILE HG22	Favored (55.35%) General / -120.0,132.0	1.6% (*m-30*) chi angles: 293.9,29.7	0.072Å	-	-
A 954		TYR	50	0.744Å H with A 957 GLN NE2	Favored (24.99%) General /	1.4% (*m-30*) chi angles: 294.6,30.5	0.016Å	-	-

					-90.5,145.3		
A 955	GLU	50	0.405Å O with A 956 ASN HB3	Favored (57.49%) General / -61.4,135.0	43.5% (*tt0*) chi angles: 180.1,177.1,56.8	0.075Å	-	-
A 956	ASN	50	0.405Å HB3 with A 955 GLU O	Allowed (0.32%) General / 88.4,2.4	20.7% (*t-20*) chi angles: 184.7,292.2	0.056Å	-	-
A 957	GLN	50	0.759Å HE22 with A1129 ARG HH11	Favored (11.18%) General / -106.6,165.6	13.8% (*pt20*) chi angles: 66.2,178,20.5	0.06Å	-	-
A 958	ILE	50	-	Favored (42.66%) Isoleucine or valine / -101.8,114.9	72.8% (*mt*) chi angles: 297.6,178.6	0.082Å	-	-
A 959	THR	50	0.473Å HB with A 953 PHE CD2	Favored (44.65%) General / -110.3,140.3	29.3% (*m*) chi angles: 307.4	0.026Å	-	-
A 960	ALA	50	0.793Å HB3 with A1130 ILE HG22	Favored (34.46%) General / -119.0,119.5	-	0.047Å	-	-
A 961	PHE	99.99	0.806Å HZ with A1133 ILE HD12	Favored (13.13%) General / -88.7,100.5	69.8% (*t80*) chi angles: 187,78.1	0.108Å	-	OUTLIER(S) worst is CA- CB-CG: 4.812 σ
A 962	LEU	50	0.425Å CD2 with A1117 THR HB	Favored (50.45%) General / -111.0,136.1	85.4% (*mt*) chi angles: 299.3,172.7	0.049Å	-	-
A 963	GLY	50	-	Favored (18.06%) Glycine / 173.7,158.5	-	-	-	-
A 964	HIS	50	-	Favored (2.06%) General / -62.0,170.6	63.8% (*m170*) chi angles: 295.7,163.3	0.024Å	OUTLIER(S) worst is CG-- ND1: 4.532 σ	-
A 965	ASN	50	-	Favored (55.06%) General / -56.7,137.0	90.7% (*m-20*) chi angles: 294.5,324.8	0.078Å	-	-
A 966	GLY	50	-	Favored (86.05%) Glycine / 79.3,10.4	-	-	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 967		ALA	50	0.457Å O with A1133 ILE HD13	Favored (64.5%) General / -68.5,-22.9	-	-	0.024Å	-	-
			Avg: 53.74	Clashscore: 53.67	Outliers: 0 of 225	Poor rotamers: 2 of 190	Outliers: 0 of 205	Outliers: 10 of 227	Outliers: 14 of 227
A 968		GLY	50	-	Favored (7.91%) Glycine / 100.3,27.1	-	-	-	-
A 969		LYS	50	0.589Å HA with A 961 PHE CE2	Favored (87.92%) General / -65.8,-43.6	36.8% (*mtmm*) chi angles: 302.5,190.8,292.9,297	0.016Å	-	-
A 970		THR	50	-	Favored (79.21%) General / -68.9,-40.3	97.6% (*m*) chi angles: 299.2	0.051Å	-	-
A 971		THR	50	-	Favored (99.16%) General / -62.1,-43.3	91.7% (*m*) chi angles: 300.5	0.052Å	-	-
A 972		THR	50	-	Favored (68.84%) General / -59.0,-51.7	61.9% (*m*) chi angles: 303.7	0.024Å	-	-
A 973		LEU	50	0.422Å HD13 with A 969 LYS O	Favored (80.38%) General / -61.8,-36.2	11.1% (*mp*) chi angles: 274.1,63.3	0.026Å	-	-
A 974		SER	50	0.577Å O with A 977 THR HG22	Favored (73.03%) General / -70.2,-34.6	69.1% (*m*) chi angles: 297.1	0.039Å	-	-
A 975		ILE	50	-	Favored (85.81%) Isoleucine or valine / -67.8,-42.0	82.6% (*mt*) chi angles: 294,175.5	0.083Å	-	-
A 976		LEU	50	0.8Å HD23 with A 987 VAL HG11	Favored (73.56%) General / -63.2,-32.2	89% (*mt*) chi angles: 298.1,180.2	0.024Å	-	-
A 977		THR	99.99	0.85Å HG21 with A1007 MET	Favored (58.24%) General /	9% (*t*) chi angles: 193	0.123Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			SD		-80.4,-6.6				
A 978		GLY	50	-	Favored (77.82%) Glycine / 72.6,14.2	-	-	-	-
A 979		LEU	50	0.528Å HB2 with A 977 THR HG23	Favored (76.13%) General / -69.8,-37.0	10% (*tp*) chi angles: 205.7,49.2	0.045Å	-	-
A 980		LEU	50	0.822Å HD12 with A 981 PRO HD2	Favored (48.72%) Pre-proline / -131.1,143.3	33% (*tp*) chi angles: 188.3,64.7	0.059Å	-	-
A 981		PRO	50	0.822Å HD2 with A 980 LEU HD12	Favored (17.79%) Trans-proline / -81.3,151.3	63.8% (*Cg_endo*) chi angles: 34.1	0.045Å	-	-
A 982		PRO	50	0.414Å HD3 with A 981 PRO HA	Favored (44.25%) Trans-proline / -64.3,159.3	55.9% (*Cg_exo*) chi angles: 334.4	0.132Å	-	-
A 983		THR	50	0.884Å HG21 with A 937 ILE HG12	Favored (24.94%) General / -83.7,-34.1	46.5% (*p*) chi angles: 55.3	0.064Å	-	-
A 984		SER	50	0.459Å OG with A 935 VAL HG12	Favored (11.1%) General / -168.3,168.9	24.7% (*p*) chi angles: 78.9	0.062Å	-	-
A 985		GLY	50	-	Favored (29.3%) Glycine / 100.4,-179.1	-	-	-	-
A 986		THR	50	-	Favored (45.38%) General / -133.2,136.1	98.4% (*m*) chi angles: 299	0.078Å	-	-
A 987		VAL	50	0.8Å HG11 with A 976 LEU HD23	Favored (69.22%) Isoleucine or valine / -127.2,127.3	40.2% (*t*) chi angles: 184.9	0.084Å	-	OUTLIER(S) worst is CA-CB-CG1: 4.275 σ
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 53.74	Clashscore: 53.67	Outliers: 0 of 225	Poor rotamers: 2 of 190	Outliers: 0 of 205	Outliers: 10 of 227	Outliers: 14 of 227
A 988		LEU	50	0.736Å HB2 with A	Favored (53.45%) General /	10.6% (*mp*) chi angles: 279.9,61.5	0.068Å	-	-

			930 CYS SG	General / -121.7,139.5	chi angles: 279.9,61.3			
A 989	VAL	50	0.677Å HG23 with A 994 ILE HD11	Favored (41.72%) Isoleucine or valine / -118.4,113.4	96% (*t*) chi angles: 176	0.045Å	-	-
A 990	GLY	50	-	Favored (80.39%) Glycine / 57.4,37.2	-	-	-	-
A 991	GLY	50	-	Favored (85.8%) Glycine / 76.7,10.8	-	-	-	-
A 992	ARG	50	-	Favored (30.19%) General / -107.8,115.5	41.1% (*mmt180*) chi angles: 295.3,294.9,181.3,179.2	0.051Å	-	-
A 993	ASP	50	0.661Å HB3 with A 996 THR OG1	Favored (21.32%) General / -61.9,124.6	51.6% (*t0*) chi angles: 187.6,335.1	0.059Å	-	-
A 994	ILE	50	0.677Å HD11 with A 989 VAL HG23	Favored (61.22%) Isoleucine or valine / -65.5,-33.1	61.6% (*mt*) chi angles: 302.4,179.1	0.103Å	-	-
A 995	GLU	50	0.634Å HG2 with A 993 ASP OD1	Favored (47.15%) General / -78.1,-36.9	12.3% (*pt-20*) chi angles: 59.5,184.1,65.3	0.095Å	-	-
A 996	THR	50	0.661Å OG1 with A 993 ASP HB3	Favored (28.12%) General / -81.8,-36.6	65% (*p*) chi angles: 63	0.06Å	-	-
A 997	SER	50	-	Allowed (1.57%) General / -133.7,65.9	43.9% (*m*) chi angles: 302.6	0.015Å	-	-
A 998	LEU	50	0.654Å HG with A 994 ILE O	Favored (81.68%) General / -62.5,-36.1	32.8% (*mt*) chi angles: 280.4,168.5	0.075Å	-	-
A 999	ASP	50	-	Favored (77.71%) General / -60.4,-49.4	46.1% (*t0*) chi angles: 187.9,330.7	0.025Å	-	-
				Favored (92.23%)				

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A1000		ALA	50	-	(92.23%) General / -62.9,-38.8	-	0.038Å	-	-
A1001		VAL	50	0.407Å HG21 with A 994 ILE HA	Favored (95.77%) Isoleucine or valine / -64.2,-45.6	72.5% (*t*) chi angles: 173.2	0.067Å	-	-
A1002		ARG	50	-	Favored (73.13%) General / -66.3,-32.0	85.3% (*mtm-85*) chi angles: 283.3,186.9,292.6,261.7	0.071Å	-	-
A1003		GLN	50	-	Favored (46.45%) General / -60.6,-17.5	83.4% (*mt-30*) chi angles: 295.7,181.1,295.5	0.019Å	-	-
A1004		SER	50	-	Favored (13.82%) General / -104.4,-20.2	68% (*m*) chi angles: 296.9	0.02Å	-	-
A1005		LEU	50	1.076Å HD11 with A1084 ILE HG13	Favored (28.82%) General / -114.7,154.2	56.4% (*tp*) chi angles: 180.4,65.4	0.104Å	-	-
A1006		GLY	50	0.459Å N with A1005 LEU HG	Favored (4.54%) Glycine / -132.5,126.5	-	-	-	-
A1007		MET	99.99	0.85Å SD with A 977 THR HG21	Favored (52.82%) General / -114.4,136.6	19.7% (*ttt*) chi angles: 184.9,189.8,185.1	0.043Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 53.74	Clashscore: 53.67	Outliers: 0 of 225	Poor rotamers: 2 of 190	Outliers: 0 of 205	Outliers: 10 of 227	Outliers: 14 of 227
A1008		CYS	50	-	Favored (31.28%) Pre-proline / -124.5,104.4	53% (*t*) chi angles: 181.1	0.048Å	-	-
A1009		PRO	50	-	Favored (46.93%) Trans-proline / -62.5,157.3	80.3% (*Cg_endo*) chi angles: 29.8	0.036Å	-	-
A1010		GLN	50	-	Favored (58.51%) General / -63.6,138.4	65.8% (*tt0*) chi angles: 182.3,179.8,358.5	0.078Å	-	-
					Favored				

A1011	HIS	50	-	Favored (21.81%) General / 55.4,33.9	52.3% (*m170*) chi angles: 298.6,159.1	0.037Å	OUTLIER(S) worst is CD2-- NE2: 4.475 σ	-
A1012	ASN	50	-	Favored (55.97%) General / -60.0,141.3	24% (*t-20*) chi angles: 185.6,297.7	0.063Å	-	-
A1013	ILE	50	0.75Å C with A1014 LEU HD12	Favored (10.45%) Isoleucine or valine / -116.2,166.3	37.2% (*pt*) chi angles: 65.6,167.7	0.032Å	-	-
A1014	LEU	50	0.75Å HD12 with A1013 ILE C	Favored (44.11%) General / -124.5,151.9	9.3% (*mp*) chi angles: 283.7,67.1	0.045Å	-	OUTLIER(S) worst is CD1-CG-CD2: 5.231 σ
A1015	PHE	50	0.766Å CD2 with A1018 LEU HD13	Favored (3.78%) General / -60.6,115.7	59% (*t80*) chi angles: 188.8,82.4	0.074Å	-	OUTLIER(S) worst is CA-CB-CG: 4.368 σ
A1016	HIS	50	0.451Å HA with A1059 ALA HB3	Favored (64.9%) General / -68.2,-24.1	64% (*m170*) chi angles: 295.4,162.8	0.046Å	OUTLIER(S) worst is CG--ND1: 4.481 σ	-
A1017	HIS	50	0.615Å HB2 with A1015 PHE CE2	Favored (3.04%) General / -95.7,28.4	97.5% (*m-70*) chi angles: 294.3,287.8	0.091Å	OUTLIER(S) worst is CG--ND1: 4.684 σ	-
A1018	LEU	50	0.766Å HD13 with A1015 PHE CD2	Favored (52.2%) General / -131.7,150.3	8.7% (*mp*) chi angles: 267.7,56.4	0.069Å	-	-
A1019	THR	50	-	Favored (45.43%) General / -65.3,151.8	43.4% (*p*) chi angles: 67.2	0.008Å	-	-
A1020	VAL	50	0.681Å HG13 with A1070 LEU HD13	Favored (11.47%) Isoleucine or valine / -48.4,-51.0	48.7% (*t*) chi angles: 168.4	0.105Å	-	-
A1021	ALA	50	0.499Å O with A1024 MET HB2	Favored (88.93%) General / -62.4,-38.3	-	0.037Å	-	-
A1022	GLU	50	-	Favored (89.83%) General / -65.9,-38.9	73.2% (*tt0*) chi angles: 183.4,175.5,19.9	0.075Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A1023		HIS	50	0.526Å CD2 with A1014 LEU HD23	Favored (90.84%) General / -63.1,-38.4	81.3% (*t60*) chi angles: 186.3,63.2	0.046Å	OUTLIER(S) worst is CG--ND1: 4.784 σ	OUTLIER(S) worst is CA-CB-CG: 4.272 σ
A1024		MET	50	0.865Å HB3 with A1045 MET SD	Favored (83.28%) General / -66.5,-44.1	22.6% (*mmp*) chi angles: 284.8,313.1,92.2	0.207Å	-	OUTLIER(S) worst is N-CA-CB: 4.872 σ
A1025		LEU	50	0.481Å HD13 with A1021 ALA O	Favored (99.7%) General / -62.2,-43.0	11.2% (*mp*) chi angles: 275,62.5	0.068Å	-	-
A1026		PHE	50	-	Favored (64.77%) General / -59.0,-52.7	28.7% (*t80*) chi angles: 178.8,51.9	0.06Å	-	-
A1027		TYR	50	0.523Å HA with A1030 LEU HD13	Favored (78.58%) General / -69.2,-39.6	81.8% (*t80*) chi angles: 183,80.8	0.029Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 53.74	Clashscore: 53.67	Outliers: 0 of 225	Poor rotamers: 2 of 190	Outliers: 0 of 205	Outliers: 10 of 227	Outliers: 14 of 227
A1028		ALA	50	-	Favored (65.38%) General / -56.8,-32.2	-	0.041Å	-	-
A1029		GLN	50	-	Favored (68.92%) General / -62.4,-27.2	54.6% (*tt0*) chi angles: 186.1,180,53.2	0.024Å	-	-
A1030		LEU	50	0.523Å HD13 with A1027 TYR HA	Favored (95.67%) General / -64.4,-40.4	10.6% (*mp*) chi angles: 279.4,65.7	0.031Å	-	-
A1031		LYS	50	-	Favored (45.27%) General / -79.0,-33.1	30.4% (*mtpp*) chi angles: 295,184.3,62.7,64.5	0.012Å	-	-
A1032		GLY	50	-	Favored (28.14%) Glycine / -153.8,158.5	-	-	-	-
A1033		LYS	50	-	Favored (12.11%) General / -106.6,-24.6	32.7% (*mmmt*) chi angles: 294,294.9,295,180.6	0.026Å	-	-

A1034	SER	50	-	Favored (57.61%) General / -66.1,138.3	0.1% chi angles: 114.5	0.05Å	-	-
A1035	GLN	50	-	Favored (90.99%) General / -62.4,-38.8	82.1% (*mt-30*) chi angles: 298.2,179.2,295	0.056Å	-	-
A1036	GLU	50	-	Favored (94.12%) General / -61.7,-45.4	11.1% (*tm-20*) chi angles: 179.4,288.2,327.5	0.078Å	-	-
A1037	GLU	50	-	Favored (75.96%) General / -69.3,-42.1	43.7% (*mt-10*) chi angles: 290.7,182.2,81.5	0.034Å	-	-
A1038	ALA	50	-	Favored (92.96%) General / -62.3,-45.5	-	0.034Å	-	-
A1039	GLN	50	0.595Å HE21 with A1043 GLU HG3	Favored (99.6%) General / -61.6,-42.9	71.1% (*tp60*) chi angles: 184,64.4,59.1	0.003Å	-	-
A1040	LEU	50	-	Favored (82.21%) General / -63.3,-47.4	53% (*tp*) chi angles: 183.9,62.4	0.02Å	-	-
A1041	GLU	50	-	Favored (95.2%) General / -60.1,-44.2	53% (*mt-10*) chi angles: 296.7,181.6,292.8	0.034Å	-	-
A1042	MET	50	0.924Å HA with A1045 MET SD	Favored (74.81%) General / -66.5,-33.0	22% (*ptp*) chi angles: 73.2,180.7,64.7	0.198Å	-	-
A1043	GLU	50	0.595Å HG3 with A1039 GLN HE21	Favored (36.95%) General / -80.5,-32.1	90.7% (*mt-10*) chi angles: 295.1,188.6,343.8	0.045Å	-	-
A1044	ALA	50	-	Favored (89.64%) General / -65.3,-43.9	-	0.031Å	-	-
A1045	MET	50	0.924Å SD with A1042 MET HA	Favored (97%) General / -64.1,-42.4	7.2% (*ptp*) chi angles: 42.2,201.4,66.8	0.195Å	-	OUTLIER(S) worst is CG-SD-CE: 4.599 σ

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A1046		LEU	50	0.925A HA with A1055 ARG CZ	Favored (74.76%) General / -54.9,-45.6	7% (*tt*) chi angles: 188.6,164.1	0.159Å	-	-
A1047		GLU	50	-	Favored (78.41%) General / -69.0,-40.9	76.2% (*tt0*) chi angles: 180,171.2,16.7	0.146Å	-	-
			Avg: 53.74	Clashscore: 53.67	Outliers: 0 of 225	Poor rotamers: 2 of 190	Outliers: 0 of 205	Outliers: 10 of 227	Outliers: 14 of 227
A1048		ASP	50	0.466Å HA with A1107 TYR OH	Favored (33.19%) General / -66.3,-53.7	35.3% (*t0*) chi angles: 192.5,325.4	0.051Å	-	-
A1049		THR	50	0.673Å HB with A1055 ARG NH2	Favored (83.37%) General / -59.0,-39.9	7% (*m*) chi angles: 315	0.02Å	-	-
A1050		GLY	50	-	Favored (93.75%) Glycine / 60.7,46.8	-	-	-	-
A1051		LEU	50	0.647Å HG with A1049 THR HG22	Favored (57.36%) General / -91.4,1.1	78% (*mt*) chi angles: 293.1,180.3	0.054Å	-	-
A1052		HIS	50	0.629Å CG with A1053 HIS H	Allowed (1.2%) General / 55.8,-136.5	16.2% (*t-160*) chi angles: 182.4,210.8	0.138Å	OUTLIER(S) worst is CD2--NE2: 4.577 σ	-
A1053		HIS	50	0.629Å H with A1052 HIS CG	Favored (63.68%) General / -69.5,-20.2	63.3% (*m170*) chi angles: 295.2,162	0.013Å	OUTLIER(S) worst is CG--ND1: 4.385 σ	-
A1054		LYS	50	-	Favored (62.75%) General / -63.0,-17.9	46.4% (*mtpt*) chi angles: 297.9,182.3,76,189.6	0.038Å	-	-
A1055		ARG	50	0.925Å CZ with A1046 LEU HA	Favored (65.66%) General / -59.5,-26.9	59% (*ttm-85*) chi angles: 183.8,174.3,299.1,268	0.042Å	-	-
A1056		ASN	50	-	Favored (58.92%) General / -85.5,-3.6	32% (*m120*) chi angles: 291.9,116.5	0.034Å	-	-
					Favored				

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A1057		GLU	50	-	(22.08%) General / -88.0,152.4	53.7% (*mm-40*) chi angles: 290.8,292.1,360	0.043Å	-	-
A1058		GLU	50	-	Favored (57.84%) General / -62.5,142.7	52% (*mt-10*) chi angles: 297.4,182.1,291.2	0.024Å	-	-
A1059		ALA	50	0.904Å HA with A1062 LEU HD13	Favored (68.55%) General / -61.0,-27.7	-	0.027Å	-	-
A1060		GLN	50	0.401Å HB3 with A1016 HIS HB3	Favored (66.87%) General / -60.5,-26.5	19.7% (*pt20*) chi angles: 61.5,179.9,61.9	0.048Å	-	-
A1061		ASP	50	-	Favored (41.16%) General / -82.1,-18.9	33.2% (*t0*) chi angles: 194.7,328.3	0.043Å	-	-
A1062		LEU	50	0.904Å HD13 with A1059 ALA HA	Favored (58.36%) General / -65.2,142.4	10.6% (*mp*) chi angles: 279.9,61.7	0.01Å	-	-
A1063		SER	50	-	Favored (11.68%) General / -72.7,171.9	85.2% (*p*) chi angles: 68.2	0.031Å	-	-
A1064		GLY	50	0.691Å O with A1067 GLN HG2	Favored (94.9%) Glycine / -61.2,-38.0	-	-	-	-
A1065		GLY	50	-	Favored (97.02%) Glycine / -64.9,-40.1	-	-	-	-
A1066		MET	50	0.487Å HE1 with A1062 LEU HG	Favored (74.39%) General / -70.5,-38.1	97.4% (*mtp*) chi angles: 293.6,174.9,67	0.106Å	-	-
A1067		GLN	50	0.691Å HG2 with A1064 GLY O	Favored (92.59%) General / -65.3,-39.5	14.1% (*pt20*) chi angles: 73.4,184.8,49.1	0.053Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 53.74	Clashscore: 53.67	Outliers: 0 of 225	Poor rotamers: 2 of 190	Outliers: 0 of 205	Outliers: 10 of 227	Outliers: 14 of 227
A1068		ARG	50		Favored (95.84%)	0%	0.015Å		

A1068	ARG	50	-	(~~~~%) General / -63.8,-43.6	chi angles: 182.5,64.4,106.3,284.5	0.015Å	-	-
A1069	LYS	50	0.54Å HA with A1072 VAL HG22	Favored (80.16%) General / -67.6,-36.1	46.8% (*mtmt*) chi angles: 291.6,194.7,294.9,168.1	0.049Å	-	-
A1070	LEU	50	0.707Å O with A1074 ILE HG23	Favored (88.44%) General / -63.0,-37.8	29% (*tp*) chi angles: 187.5,55.7	0.049Å	-	-
A1071	SER	50	0.756Å O with A1074 ILE HG12	Favored (55.34%) General / -76.3,-38.8	19.7% (*m*) chi angles: 306.1	0.098Å	-	-
A1072	VAL	50	0.54Å HG22 with A1069 LYS HA	Favored (80.83%) Isoleucine or valine / -68.2,-39.2	34.3% (*m*) chi angles: 299	0.092Å	-	-
A1073	ALA	50	0.713Å O with A1077 VAL HG13	Favored (96.73%) General / -62.4,-40.5	-	0.1Å	-	-
A1074	ILE	50	0.756Å HG12 with A1071 SER O	Favored (81.02%) Isoleucine or valine / -63.0,-38.1	7.8% (*pt*) chi angles: 67.3,190.9	0.119Å	-	OUTLIER(S) worst is CB- CG1-CD1: 4.415 σ
A1075	ALA	50	-	Favored (67.47%) General / -70.3,-30.5	-	0.053Å	-	-
A1076	PHE	50	0.688Å CE1 with A1083 VAL HG21	Favored (18.44%) General / -95.5,-21.2	1.8% (*m-30*) chi angles: 291.1,33.7	0.014Å	-	-
A1077	VAL	50	0.789Å HG11 with A1045 MET HB3	Favored (45.13%) Isoleucine or valine / -59.4,-30.8	19.6% (*m*) chi angles: 292.4	0.075Å	-	OUTLIER(S) worst is CA- CB-CG1: 4.73 σ
A1078	GLY	50	-	Favored (44.95%) Glycine / -67.6,-6.9	-	-	-	-
A1079	ASP	50	-	Favored (5.3%) General / 48.9,58.5	56.2% (*t0*) chi angles: 184.7,339.9	0.033Å	-	-

A1080	ALA	50	-	Favored (42.89%) General / -71.9,152.1	-	0.063Å	-	-
A1081	LYS	50	-	Favored (72.78%) General / -71.0,-38.3	30.3% (*mtpp*) chi angles: 290.9,185.9,64.9,64.5	0.01Å	-	-
A1082	VAL	50	0.644Å O with A1005 LEU HD12	Favored (64.34%) Isoleucine or valine / -124.2,135.2	2.7% (*p*) chi angles: 50.2	0.129Å	-	-
A1083	VAL	50	0.688Å HG21 with A1076 PHE CE1	Favored (43.65%) Isoleucine or valine / -112.4,137.8	8.3% (*p*) chi angles: 68.7	0.105Å	-	-
A1084	ILE	50	1.076Å HG13 with A1005 LEU HD11	Favored (26.52%) Isoleucine or valine / -118.9,109.3	19.8% (*mt*) chi angles: 302.1,189	0.037Å	-	-
A1085	LEU	50	0.551Å HD11 with A1076 PHE HZ	Favored (45.74%) General / -116.9,122.9	51.9% (*mt*) chi angles: 307,174.6	0.058Å	-	-
A1086	ASP	50	-	Favored (15.66%) General / -96.8,103.7	27.7% (*t0*) chi angles: 197.8,340.7	0.06Å	-	-
A1087	GLU	50	-	Favored (3.73%) Pre-proline / 60.3,54.2	63.9% (*mm-40*) chi angles: 305.8,286.2,344.1	0.04Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 53.74	Clashscore: 53.67	Outliers: 0 of 225	Poor rotamers: 2 of 190	Outliers: 0 of 205	Outliers: 10 of 227	Outliers: 14 of 227
A1088		PRO	50	-	Favored (70.03%) Trans-proline / -59.8,-22.9	68.9% (*Cg_endo*) chi angles: 28.1	0.095Å	-	-
A1089		THR	50	0.837Å HG21 with A1101 TRP NE1	Favored (15.12%) General / -115.2,6.7	67.6% (*p*) chi angles: 63.1	0.021Å	-	-
					Favored				

A1090	SER	50	-	Favored (54.35%) General / -66.1,146.7	65.7% (*p*) chi angles: 71.1	0.096Å	-	-
A1091	GLY	50	-	Favored (67.11%) Glycine / 64.7,21.4	-	-	-	-
A1092	VAL	50	0.664Å CG2 with A1096 SER HB2	Favored (10.24%) Isoleucine or valine / -105.4,148.2	4.6% (*p*) chi angles: 77	0.179Å	-	-
A1093	ASP	50	0.643Å HB2 with A1094 PRO HD2	Favored (3.18%) Pre-proline / -73.4,175.8	33% (*p30*) chi angles: 73.3,7.4	0.179Å	-	-
A1094	PRO	50	0.643Å HD2 with A1093 ASP HB2	Favored (59.98%) Trans-proline / -59.4,-41.2	72.9% (*Cg_endo*) chi angles: 29.5	0.078Å	-	-
A1095	TYR	50	-	Favored (73.52%) General / -68.0,-45.7	86.8% (*t80*) chi angles: 180.8,80.5	0.011Å	-	-
A1096	SER	50	0.664Å HB2 with A1092 VAL CG2	Favored (55.75%) General / -76.9,-29.3	14% (*m*) chi angles: 309.7	0.113Å	-	-
A1097	ARG	50	0.65Å HB3 with A1092 VAL CG1	Favored (92.9%) General / -65.6,-40.6	38.3% (*ptt180*) chi angles: 56,186.6,184.7,180.1	0.123Å	-	-
A1098	ARG	50	-	Favored (99.56%) General / -62.8,-42.0	35.7% (*ttp-105*) chi angles: 184.4,166,74.6,244.2	0.024Å	-	-
A1099	SER	50	-	Favored (83.64%) General / -66.4,-36.8	71.6% (*m*) chi angles: 295.7	0.04Å	-	-
A1100	ILE	99.99	0.404Å HG13 with A1096 SER O	Favored (80.24%) Isoleucine or valine / -69.4,-44.2	90.4% (*mt*) chi angles: 298.9,169.9	0.059Å	-	-
A1101	TRP	99.99	0.837Å NE1 with A1089 THR HG21	Favored (86.04%) General / -59.5,-40.2	48.3% (*m0*) chi angles: 294.8,355.7	0.033Å	OUTLIER(S) worst is NE1--CE2: 6.381 σ	OUTLIER(S) worst is CZ2-CH2-CZ3: 6.089 σ

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A1102		ASP	50	-	Favored (93%) General / -62.0,-45.6	43.8% (*t0*) chi angles: 185.6,330.1	0.018Å	-	-
A1103		LEU	50	0.407Å O with A1107 TYR HD2	Favored (80.86%) General / -57.5,-47.8	94.4% (*mt*) chi angles: 293.5,175.8	0.018Å	-	-
A1104		LEU	50	-	Favored (88.39%) General / -66.2,-42.8	58.9% (*mt*) chi angles: 302,185.4	0.039Å	-	-
A1105		LEU	50	0.529Å HD13 with A1101 TRP O	Favored (96.43%) General / -61.3,-44.9	11.1% (*mp*) chi angles: 274.2,63.3	0.048Å	-	-
A1106		LYS	50	-	Favored (95.47%) General / -63.4,-44.1	38.8% (*ttpt*) chi angles: 185,181.9,63.4,181.6	0.028Å	-	-
A1107		TYR	99.99	0.466Å OH with A1048 ASP HA	Favored (5.33%) General / -79.0,70.2	97.2% (*m-85*) chi angles: 296.3,279.6	0.019Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 53.74	Clashscore: 53.67	Outliers: 0 of 225	Poor rotamers: 2 of 190	Outliers: 0 of 205	Outliers: 10 of 227	Outliers: 14 of 227
A1108		ARG	99.99	-	Allowed (1.75%) General / -135.0,-19.7	30.5% (*ptt-85*) chi angles: 67.2,173.9,178.8,279.9	0.04Å	-	-
A1109		SER	99.99	-	Favored (54.11%) General / -50.1,-46.9	29.7% (*t*) chi angles: 172.7	0.061Å	-	-
A1110		GLY	99.99	-	Favored (26.17%) Glycine / -112.4,-2.1	-	-	-	-
A1111		ARG	50	0.485Å HD3 with A1083 VAL HG11	Favored (55%) General / -119.0,129.2	59.9% (*ttm-85*) chi angles: 192.7,178.4,293.2,280.3	0.065Å	-	-
A1112		THR	50	-	Favored (44.56%) General / -97.9,128.5	37.2% (*m*) chi angles: 306.1	0.108Å	-	-
				0.462Å HG13 with	Favored (75.22%)	35.6% (*mt*)			

A1113	ILE	50	HG12 with A1083 VAL HG12	Isoleucine or valine / -122.4,129.5	33.6% (*mt*) chi angles: 308.9,179.9	0.028Å	-	-
A1114	ILE	50	0.683Å HG12 with A1084 ILE HG12	Favored (50.2%) Isoleucine or valine / -115.3,115.7	12.2% (*pt*) chi angles: 74.1,163.7	0.087Å	-	-
A1115	MET	50	-	Favored (32.97%) General / -118.2,154.0	12.8% (*ptp*) chi angles: 59.2,185.7,48.7	0.058Å	-	-
A1116	SER	50	-	Favored (44.38%) General / -112.2,142.7	85.7% (*p*) chi angles: 61.2	0.086Å	-	-
A1117	THR	50	0.74Å HG22 with A1119 HIS H	Favored (20.39%) General / -157.8,147.9	97.8% (*m*) chi angles: 299.1	0.057Å	-	-
A1118	HIS	50	-	Favored (17.19%) General / -112.1,3.3	52.9% (*p-80*) chi angles: 63.1,274.4	0.04Å	OUTLIER(S) worst is CG--ND1: 4.446 σ	OUTLIER(S) worst is CB-CG-CD2: 4.226 σ
A1119	HIS	99.99	0.74Å H with A1117 THR HG22	Favored (7.08%) General / -90.9,88.5	98.3% (*m-70*) chi angles: 295.6,289.1	0.007Å	OUTLIER(S) worst is CG--ND1: 4.615 σ	-
A1120	MET	50	-	Favored (62.39%) General / -72.7,-27.9	62.9% (*mtt*) chi angles: 297.4,185.3,181.6	0.119Å	-	-
A1121	ASP	50	-	Favored (94.12%) General / -64.8,-39.8	99.3% (*m-20*) chi angles: 287.8,347.6	0.069Å	-	-
A1122	GLU	50	0.732Å HB3 with A1101 TRP CH2	Favored (57.17%) General / -87.8,-7.6	69.5% (*mm-40*) chi angles: 288,306.4,322.2	0.196Å	-	OUTLIER(S) worst is CB-CG-CD: 4.949 σ
A1123	ALA	50	-	Favored (88.14%) General / -60.5,-39.5	-	0.057Å	-	-
A1124	ASP	50	-	Favored (67.31%) General / -58.5,-30.8	63.3% (*m-20*) chi angles: 291.6,306.8	0.033Å	-	-
				Favored				

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A1125		LEU	50	-	(18.09%) General / -92.8,14.2	10.3% (*mp*) chi angles: 280.8,66.5	0.017Å	-	-
A1126		LEU	50	0.449Å HD12 with A1105 LEU CD1	Allowed (0.59%) General / -136.7,-44.2	50.1% (*tp*) chi angles: 181.6,57.6	0.059Å	-	-
A1127		GLY	50	-	Favored (17.06%) Glycine / -100.1,144.8	-	-	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 53.74	Clashscore: 53.67	Outliers: 0 of 225	Poor rotamers: 2 of 190	Outliers: 0 of 205	Outliers: 10 of 227	Outliers: 14 of 227
A1128		ASP	50	0.408Å O with A1144 PRO HD3	Favored (12.89%) General / -85.7,-44.0	59.2% (*m-20*) chi angles: 301.1,302.4	0.042Å	-	-
A1129		ARG	50	0.759Å HH11 with A 957 GLN HE22	Favored (51.53%) General / -135.2,152.4	42.2% (*mtp-105*) chi angles: 291.9,178.3,60.3,242.3	0.076Å	-	-
A1130		ILE	50	0.793Å HG22 with A 960 ALA HB3	Favored (22.79%) Isoleucine or valine / -140.3,154.5	39.2% (*pt*) chi angles: 66,173.1	0.058Å	-	-
A1131		ALA	50	0.518Å HB2 with A 951 ILE HG12	Favored (19.37%) General / -122.5,113.5	-	0.082Å	-	-
A1132		ILE	50	-	Favored (38.16%) Isoleucine or valine / -78.0,128.6	30.5% (*pt*) chi angles: 68.5,169.2	0.069Å	-	-
A1133		ILE	50	0.806Å HD12 with A 961 PHE HZ	Favored (51.3%) Isoleucine or valine / -122.8,138.9	2.1% (*tt*) chi angles: 191.5,195.9	0.057Å	-	OUTLIER(S) worst is CB-CG1-CD1: 5.1 σ
A1134		ALA	50	0.667Å O with A1137 ARG HG2	Favored (13.95%) General / -144.0,124.5	-	0.096Å	-	-
A1135		GLN	50	0.515Å HB2 with A1137 ARG	Favored (17.36%) General /	19.4% (*mm100*) chi angles:	0.023Å	-	-

				A1137 ARG NH1	General / 53.4,34.1	296.6,296.5,98.6		
A1136	GLY	50	0.72Å HA2 with A1133 ILE HD11	Favored (70.07%) Glycine / 72.3,27.3	-	-	-	-
A1137	ARG	50	1.085Å HA with A 949 LEU HD21	Favored (52.09%) General / -128.2,140.1	32.2% (*ptt-85*) chi angles: 69,178.1,174.7,276.1	0.13Å	-	-
A1138	LEU	99.99	0.706Å HG with A 949 LEU HD22	Favored (17.32%) General / -87.8,105.3	86.1% (*mt*) chi angles: 292.1,177.9	0.032Å	-	-
A1139	TYR	50	-	Favored (30.26%) General / -84.1,-24.6	75.8% (*t80*) chi angles: 185.5,76.8	0.11Å	-	-
A1140	CYS	50	-	Favored (10.02%) General / -169.3,161.4	77.8% (*m*) chi angles: 299.2	0.089Å	-	-
A1141	SER	50	-	Favored (39.21%) General / -155.4,158.8	31.6% (*t*) chi angles: 175	0.056Å	-	-
A1142	GLY	50	-	Favored (25.05%) Glycine / 146.1,-176.4	-	-	-	-
A1143	THR	50	0.541Å OG1 with A1146 PHE CD1	Favored (87.69%) Pre-proline / -70.3,158.4	17.4% (*p*) chi angles: 74.6	0.032Å	-	-
A1144	PRO	50	0.483Å HD2 with A1143 THR HB	Favored (84.26%) Trans-proline / -61.3,-35.5	84.5% (*Cg_endo*) chi angles: 31.6	0.032Å	-	-
A1145	LEU	50	-	Favored (73.66%) General / -70.7,-38.6	10.2% (*tt*) chi angles: 183.8,153.8	0.096Å	-	-
A1146	PHE	50	0.541Å CD1 with A1143 THR OG1	Favored (91.42%) General / -65.7,-42.1	2.6% (*m-30*) chi angles: 289.1,29.8	0.032Å	-	-
A1147	LEU	50	-	Favored (89.26%) General / -65.5,-43.7	88% (*mt*) chi angles: 290.6,174.4	0.013Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 53.74	Clashscore: 53.67	Outliers: 0 of 225	Poor rotamers: 2 of 190	Outliers: 0 of 205	Outliers: 10 of 227	Outliers: 14 of 227
A1148		LYS	50	-	Favored (88.67%) General / -65.5,-38.1	59.7% (*mtpt*) chi angles: 288.5,168.2,63.8,170.8	0.037Å	-	-
A1149		ASN	50	-	Favored (63.1%) General / -74.1,-39.9	30.4% (*m120*) chi angles: 290.9,117.2	0.042Å	-	-
A1150		CYS	50	-	Favored (95.26%) General / -61.8,-40.5	49.4% (*t*) chi angles: 182.3	0.008Å	-	-
A1151		PHE	50	0.449Å O with A1153 THR HG23	Favored (33.3%) General / -105.4,10.8	96.6% (*m-85*) chi angles: 292.7,276.2	0.022Å	-	-
A1152		GLY	50	-	Favored (30.14%) Glycine / 48.8,43.2	-	-	-	-
A1153		THR	50	0.449Å HG23 with A1151 PHE O	Favored (46.14%) General / -114.5,142.6	65.1% (*p*) chi angles: 57.1	0.032Å	-	-
A1154		GLY	99.99	-	-	-	-	-	-

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