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All-Atom Contacts	Clashscore, all atoms:	42.95		6th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	1	0.67%	Goal: <1%
	Ramachandran outliers	6	3.47%	Goal: <0.05%
	Ramachandran favored	162	93.64%	Goal: >98%
	MolProbity score^	2.53		45th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	3	1.88%	Goal: 0
	Bad backbone bonds:	12 / 1380	0.87%	Goal: 0%
	Bad backbone angles:	29 / 1876	1.55%	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: 56.86	Clashscore: 42.95	Outliers: 6 of 173	Poor rotamers: 1 of 149	Outliers: 3 of 160	Outliers: 6 of 175	Outliers: 18 of 175
C 871		VAL	50	-	-	16.6% (*m*) chi angles: 290.8	0.086Å	-	-
C 872		GLU	50	0.554Å CG with C 988 VAL HB	Favored (6.12%) Pre-proline / -154.3,131.6	10.7% (*pt-20*) chi angles: 59.5,174.4,79.6	0.081Å	-	-
C 873		PRO	50	-	OUTLIER (0.05%) Trans-proline / -109.7,148.4	24.8% (*Cg_endo*) chi angles: 38	0.08Å	-	-
C 874		GLU	50	0.519Å OE1 with C 876 PHE CZ	Favored (9.25%) General / -162.7,142.4	45.3% (*tt0*) chi angles: 179.9,179.7,63.7	0.027Å	-	-
C 875		TYR	50		Favored (26.33%)	1.4% (*m-30*)	0.051Å		

C 875	TYR	50	-	(36.22%) General / -90.0,130.1	chi angles: 294.6,30.5	0.031Å	-	-
C 876	PHE	50	0.519Å CZ with C 874 GLU OE1	Favored (46.11%) General / -118.4,123.8	88.1% (m-85) chi angles: 290.4,268.3	0.038Å	-	-
C 877	GLU	50	-	Favored (32.49%) General / -80.4,-37.3	49.8% (mm-40) chi angles: 290.9,290.9,1.8	0.013Å	-	-
C 878	GLN	50	0.591Å HB2 with C 939 GLN NE2	Allowed (1.64%) General / -119.1,81.0	18.2% (mm100) chi angles: 297.6,293.8,97.4	0.047Å	-	-
C 879	VAL	50	-	Favored (38.93%) Isoleucine or valine / -123.8,142.9	78.6% (t) chi angles: 172.6	0.079Å	-	-
C 880	THR	50	-	Favored (53.83%) General / -117.0,127.1	86% (m) chi angles: 301.7	0.032Å	-	-
C 881	LEU	50	0.746Å HB3 with C 932 MET HE1	Favored (35.51%) General / -107.3,143.4	19.4% (mt) chi angles: 286.8,190	0.167Å	-	-
C 882	TYR	99.99	0.86Å CE2 with C 977 ILE HG21	Favored (8.9%) General / -127.3,106.0	79.7% (t80) chi angles: 178.8,265.3	0.126Å	-	OUTLIER(S) worst is CB-CG-CD2: 4.66 σ
C 883	PHE	50	0.589Å CD1 with C 932 MET SD	Favored (51.65%) General / -104.1,127.8	31.8% (m-85) chi angles: 277,86.3	0.066Å	-	-
C 884	SER	50	0.694Å HB2 with C 975 ILE HD11	Favored (51.27%) General / -135.6,152.5	83.9% (p) chi angles: 68.7	0.048Å	-	-
C 885	ASP	50	0.591Å O with C 975 ILE HD12	Favored (29.62%) General / -147.5,146.8	8.3% (p-10) chi angles: 70.7,300.6	0.042Å	-	-
C 886	ILE	50	-	Favored (22%) Isoleucine or valine / -72.0,121.3	63.1% (mt) chi angles: 303.9,166.8	0.08Å	-	-
				Favored (25.78%)	88.6% (t)			

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
C 887		VAL	50	-	Isoleucine or valine / -61.8,130.2	88.6% (*t*) chi angles: 177.8	0.054Å	-	-
C 888		GLY	50	-	Favored (91.79%) Glycine / 64.8,35.3	-	-	-	-
C 889		PHE	50	-	Favored (80.93%) General / -66.5,-45.0	87.9% (*t80*) chi angles: 175.7,75.8	0.057Å	-	-
C 890		THR	50	-	Favored (71.73%) General / -63.3,-30.6	65.7% (*p*) chi angles: 57.1	0.094Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 56.86	Clashscore: 42.95	Outliers: 6 of 173	Poor rotamers: 1 of 149	Outliers: 3 of 160	Outliers: 6 of 175	Outliers: 18 of 175
C 891		THR	50	-	Favored (65.15%) General / -72.8,-41.2	80.9% (*p*) chi angles: 61.3	0.031Å	-	-
C 892		ILE	50	-	Favored (96.47%) Isoleucine or valine / -61.6,-46.5	90.2% (*mt*) chi angles: 294.5,174	0.031Å	-	-
C 893		SER	50	-	Favored (79.78%) General / -62.0,-35.8	33.1% (*t*) chi angles: 183.8	0.034Å	-	-
C 894		ALA	50	-	Favored (24.64%) General / -83.9,-33.8	-	0.018Å	-	-
C 895		MET	50	-	Favored (17.99%) General / -98.8,-18.4	65.1% (*mtt*) chi angles: 292.3,182.8,177.7	0.031Å	-	-
C 896		SER	99.99	0.575Å HB2 with C 900 GLU OE2	Favored (22.93%) General / -108.2,153.6	1% chi angles: 98.9	0.304Å	-	OUTLIER(S) worst is N-CA-CB: 6.161 σ
C 897		GLU	50	0.806Å O with C 900 GLU HG2	Favored (67.99%) Pre-proline / -56.9,144.4	4.7% (*pt-20*) chi angles: 89.2,199.7,27.9	0.171Å	-	OUTLIER(S) worst is CB-CG-CD: 4.628 σ

C 898	PRO	50	-	Favored (93.96%) Trans-proline / -55.5,-38.5	98.3% (Cg_exo) chi angles: 329.4	0.044Å	-	-
C 899	ILE	50	-	Favored (96.27%) Isoleucine or valine / -60.4,-45.7	51.2% (mm) chi angles: 302.2,300.6	0.029Å	-	-
C 900	GLU	99.99	0.983Å HB2 with C 966 ARG HD3	Favored (73.81%) General / -70.1,-35.0	11.1% ($pt-20$) chi angles: 77.1,200.8,26.3	0.113Å	-	-
C 901	VAL	50	-	Favored (92.28%) Isoleucine or valine / -64.0,-47.0	63.2% (t) chi angles: 180	0.019Å	-	-
C 902	VAL	50	-	Favored (79.13%) Isoleucine or valine / -67.8,-37.8	33.9% (m) chi angles: 299.3	0.089Å	-	-
C 903	ASP	50	-	Favored (99.35%) General / -62.4,-42.3	43.7% ($t0$) chi angles: 189.8,330.5	0.03Å	-	-
C 904	LEU	50	0.589Å HD13 with C 964 ARG O	Favored (75.98%) General / -62.7,-49.2	57.5% (tp) chi angles: 180.7,60	0.033Å	-	-
C 905	LEU	50	-	Favored (81.04%) General / -58.9,-48.5	76.7% (mt) chi angles: 288.4,175	0.023Å	-	-
C 906	ASN	50	-	Favored (91.52%) General / -63.9,-38.5	43.2% ($m-20$) chi angles: 275.2,312.7	0.051Å	-	-
C 907	ASP	99.99	-	Favored (88.11%) General / -61.6,-46.9	90.3% ($m-20$) chi angles: 294.3,341.2	0.071Å	-	-
C 908	LEU	50	0.702Å HD21 with C 973 VAL HG21	Favored (4.9%) General / -63.3,-59.3	16.6% (mt) chi angles: 275.7,164.4	0.057Å	-	-
C 909	TYR	50	-	Favored (75.43%) General /	22% ($m-30$) chi angles: 295.6,341.1	0.06Å	-	-

					-59.3,-36.4				
C 910		THR	50	-	Favored (82.05%) General / -68.2,-40.5	86.9% (*m*) chi angles: 301.2	0.049Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 56.86	Clashscore: 42.95	Outliers: 6 of 173	Poor rotamers: 1 of 149	Outliers: 3 of 160	Outliers: 6 of 175	Outliers: 18 of 175
C 911		LEU	99.99	-	Favored (97.77%) General / -63.3,-40.6	39.5% (*tp*) chi angles: 186,59.2	0.037Å	-	-
C 912		PHE	50	0.601Å CZ with C 956 ILE HG23	Favored (75.6%) General / -69.5,-41.7	17.5% (*m-30*) chi angles: 300.5,342.1	0.028Å	-	-
C 913		ASP	50	0.732Å O with C 916 ILE HG12	Favored (95.41%) General / -62.2,-40.2	87.1% (*m-20*) chi angles: 295.1,337.4	0.065Å	-	-
C 914		ALA	50	-	Favored (76.48%) General / -62.7,-34.1	-	0.037Å	-	-
C 915		ILE	50	0.73Å HD11 with C 956 ILE HD13	Favored (11.69%) Isoleucine or valine / -82.2,-16.9	32.1% (*pt*) chi angles: 66.1,176.9	0.153Å	-	-
C 916		ILE	50	0.732Å HG12 with C 913 ASP O	Favored (83.05%) Isoleucine or valine / -57.9,-42.7	10% (*pt*) chi angles: 74.8,182.4	0.076Å	-	-
C 917		GLY	50	-	Favored (85.74%) Glycine / -64.6,-47.3	-	-	-	-
C 918		SER	50	-	Favored (67.95%) General / -61.8,-26.1	27.2% (*t*) chi angles: 185.5	0.017Å	-	-
C 919		HIS	50	0.542Å HE1 with C 955 ASP OD2	Favored (17.82%) General / -110.1,-0.7	62.9% (*m170*) chi angles: 294.9,161.5	0.032Å	OUTLIER(S) worst is CG-- ND1: 4.995 σ	-
C 920		ASP	50	-	Favored (9.05%)	32.8% (*t70*)	0.075Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
C 920		ASP	50		General / 57.9,51.4	chi angles: 187.4,69.3	0.075Å		
C 921		VAL	50	-	Favored (24.02%) Isoleucine or valine / -120.6,154.8	35.8% (*m*) chi angles: 297.7	0.062Å	-	-
C 922		TYR	50	0.695Å CE2 with C 937 LEU HB3	Favored (44.83%) General / -108.4,138.4	94.3% (*m-85*) chi angles: 292.7,278.9	0.014Å	-	-
C 923		LYS	50	-	Favored (43.94%) General / -71.1,131.7	39.4% (*ttpt*) chi angles: 184.7,180.6,64.3,180.8	0.066Å	-	-
C 924		VAL	50	-	Favored (50.54%) Isoleucine or valine / -114.3,136.5	84.7% (*t*) chi angles: 174.9	0.076Å	-	-
C 925		GLU	50	-	Favored (58.24%) General / -66.0,140.0	56% (*mm-40*) chi angles: 303.7,307.7,303.7	0.025Å	-	-
C 926		THR	50	-	Favored (24.62%) General / -137.5,166.1	77.2% (*p*) chi angles: 58.6	0.035Å	-	-
C 927		ILE	50	-	Favored (26.72%) Isoleucine or valine / -92.4,135.7	89.8% (*mt*) chi angles: 299.6,171.8	0.082Å	-	-
C 928		GLY	50	-	Favored (35.28%) Glycine / 70.3,-142.2	-	-	-	-
C 929		ASP	50	-	Favored (57.39%) General / -85.6,-9.4	6.5% (*p-10*) chi angles: 56.8,280	0.065Å	-	-
C 930		ALA	50	-	Favored (56.07%) General / -62.4,144.2	-	0.037Å	-	-
			Avg: 56.86	Clashscore: 42.95	Outliers: 6 of 173	Poor rotamers: 1 of 149	Outliers: 3 of 160	Outliers: 6 of 175	Outliers: 18 of 175

C 931	TYR	50	-	Favored (38.33%) General / -118.0,120.6	53.7% (*t80*) chi angles: 187.5,270.5	0.041Å	-	-
C 932	MET	50	0.746Å HE1 with C 881 LEU HB3	Favored (54.04%) General / -125.3,137.8	18% (*tpt*) chi angles: 179.7,64.9,191.6	0.113Å	-	-
C 933	VAL	50	-	Favored (28.35%) Isoleucine or valine / -136.3,151.2	16.2% (*m*) chi angles: 290.6	0.056Å	-	-
C 934	ALA	50	-	Favored (52.56%) General / -131.4,147.4	-	0.148Å	-	-
C 935	SER	50	0.616Å HB2 with C 949 ILE HG12	Favored (41.68%) General / -117.0,148.2	12.1% (*t*) chi angles: 191.1	0.067Å	-	-
C 936	GLY	99.99	-	Favored (4.79%) Glycine / 101.4,33.6	-	-	OUTLIER(S) worst is C--O: 6.31 σ	-
C 937	LEU	99.99	0.795Å HD11 with C 996 TYR CE2	OUTLIER (0.08%) Pre-proline / -100.7,3.6	8.1% (*tt*) chi angles: 191.1,158.4	0.215Å	-	OUTLIER(S) worst is N-CA-CB: 4.967 σ
C 938	PRO	99.99	0.826Å HG2 with C 940 ARG N	Allowed (1.03%) Trans-proline / -66.6,-51.1	7.4% (*Cg_endo*) chi angles: 9.8	0.208Å	-	OUTLIER(S) worst is C-N-CA: 7.085 σ
C 939	GLN	50	0.591Å NE2 with C 878 GLN HB2	Favored (21.02%) General / -84.8,113.0	48% (*tp60*) chi angles: 170.1,75.5,58.7	0.227Å	-	OUTLIER(S) worst is N-CA-CB: 4.133 σ
C 940	ARG	99.99	0.965Å HE with C 944 ARG H	Favored (10.46%) General / 47.9,54.1	45.5% (*mtp180*) chi angles: 290.7,180.8,86.6,168.4	0.08Å	-	OUTLIER(S) worst is CB-CG-CD: 4.167 σ
C 941	ASN	99.99	0.646Å ND2 with C 938 PRO HB3	Favored (8.06%) General / -83.3,82.9	57.4% (*p30*) chi angles: 63.5,12.5	0.061Å	-	OUTLIER(S) worst is OD1-CG-ND2: 6.725 σ
C 942	GLY	99.99	-	Favored (5.76%) Glycine / 122.1,-28.8	-	-	-	-

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C 943		GLN	99.99	0.718Å HA with C 944 ARG HB3	Favored (2.74%) General / -128.6,-172.6	12.1% (*pm0*) chi angles: 75.7,272.1,2	0.152Å	-	OUTLIER(S) worst is C-N-CA: 6.698 σ
C 944		ARG	50	0.965Å H with C 940 ARG HE	OUTLIER (0%) General / 94.9,40.0	0% chi angles: 132.6,229.3,311.1,287.2	0.377Å	-	OUTLIER(S) worst is C-CA-CB: 6.471 σ
C 945		HIS	50	0.624Å HD2 with C 940 ARG CD	Favored (53.69%) General / -54.6,-30.3	24.2% (*p80*) chi angles: 63,93.5	0.04Å	OUTLIER(S) worst is CG--ND1: 6.93 σ	OUTLIER(S) worst is CG-CD2-NE2: 7.26 σ
C 946		ALA	50	-	Favored (68.29%) General / -72.4,-38.7	-	0.111Å	-	-
C 947		ALA	50	0.695Å HB3 with C 944 ARG HG3	Favored (73.65%) General / -70.7,-37.8	-	0.09Å	-	-
C 948		GLU	50	-	Favored (95.81%) General / -60.2,-43.7	36.8% (*mm-40*) chi angles: 289.6,291.2,6.9	0.027Å	-	-
C 949		ILE	50	0.616Å HG12 with C 935 SER HB2	Favored (88.42%) Isoleucine or valine / -66.5,-41.4	19.9% (*mm*) chi angles: 287.8,300	0.097Å	-	-
C 950		ALA	50	-	Favored (93.1%) General / -64.3,-39.0	-	0.041Å	-	-
			Avg: 56.86	Clashscore: 42.95	Outliers: 6 of 173	Poor rotamers: 1 of 149	Outliers: 3 of 160	Outliers: 6 of 175	Outliers: 18 of 175
C 951		ASN	50	-	Favored (83.71%) General / -67.9,-39.3	33.1% (*m120*) chi angles: 293.3,118.3	0.024Å	-	-
C 952		MET	50	0.678Å O with C 956 ILE HG12	Favored (99.22%) General / -61.0,-42.8	15.4% (*tpt*) chi angles: 180.7,63.9,176.1	0.043Å	-	-
C 953		SER	50	-	Favored (86.52%) General / -59.8,-47.2	24.9% (*t*) chi angles: 186	0.107Å	-	-

C 954	LEU	50	-	Favored (91.97%) General / -65.6,-42.0	75.2% (*mt*) chi angles: 287.9,168.1	0.013Å	-	-
C 955	ASP	50	0.542Å OD2 with C 919 HIS HE1	Favored (92.72%) General / -64.1,-38.9	53.3% (*m-20*) chi angles: 293.9,298.4	0.039Å	-	-
C 956	ILE	50	0.73Å HD13 with C 915 ILE HD11	Favored (93%) Isoleucine or valine / -61.9,-42.0	48% (*mm*) chi angles: 299.6,299.5	0.015Å	-	-
C 957	LEU	50	0.617Å O with C 960 VAL HG22	Favored (97.8%) General / -61.3,-41.9	85% (*mt*) chi angles: 294.2,179.4	0.074Å	-	-
C 958	SER	50	-	Favored (81.79%) General / -68.3,-38.7	48.8% (*m*) chi angles: 300.5	0.055Å	-	-
C 959	ALA	50	-	Favored (94.13%) General / -65.3,-40.6	-	0.153Å	-	-
C 960	VAL	50	0.979Å HB with C 973 VAL HG23	Favored (70.89%) Isoleucine or valine / -62.2,-35.8	33% (*m*) chi angles: 300.1	0.089Å	-	-
C 961	GLY	50	0.906Å HA2 with C 972 PRO HB3	Favored (25.92%) Glycine / -50.9,-32.2	-	-	-	-
C 962	THR	50	-	Favored (46.2%) General / -79.1,-21.8	29.5% (*p*) chi angles: 70.6	0.054Å	-	-
C 963	PHE	99.99	0.65Å CE2 with C 908 LEU HA	Favored (36.74%) General / -104.2,141.2	21.2% (*m-30*) chi angles: 295.1,324.8	0.06Å	-	-
C 964	ARG	50	0.589Å O with C 904 LEU HD13	Favored (33.66%) General / -107.4,144.9	86.1% (*mmt-85*) chi angles: 293.4,291,178.9,278.7	0.124Å	-	-
C 965	MET	50	0.795Å HG2 with C 969 PRO HD3	Favored (22.09%) General / -70.9,166.0	13.4% (*ptp*) chi angles: 72.8,191.1,54.3	0.065Å	-	-
			0.983Å	Favored				OUTLIER(S)

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
C 966		ARG	99.99	0.985Å HD3 with C 900 GLU HB2	Favored (58.1%) General / -54.0,-33.8	35.6% (*tpt85*) chi angles: 183.7,67.4,162.6,83.9	0.041Å	-	OUTLIER(S) worst is CA-CB-CG: 4.913 σ
C 967		HIS	50	-	Favored (4.98%) General / -82.2,11.8	82.2% (*m-70*) chi angles: 293.2,304.5	0.034Å	OUTLIER(S) worst is CD2--NE2: 4.27 σ	OUTLIER(S) worst is CB-CG-CD2: 4.898 σ
C 968		MET	99.99	-	Favored (6%) Pre-proline / 39.5,55.6	24.3% (*ptp*) chi angles: 65.8,173.7,68.3	0.095Å	-	-
C 969		PRO	99.99	0.795Å HD3 with C 965 MET HG2	Favored (18.94%) Trans-proline / -72.1,170.5	7.9% (*Cg_endo*) chi angles: 40.7	0.077Å	-	-
C 970		GLU	99.99	-	Allowed (1.41%) General / -80.1,15.8	8.2% (*pm0*) chi angles: 66.6,292,345.1	0.04Å	-	-

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			Avg: 56.86	Clashscore: 42.95	Outliers: 6 of 173	Poor rotamers: 1 of 149	Outliers: 3 of 160	Outliers: 6 of 175	Outliers: 18 of 175
C 971		VAL	99.99	0.786Å HB with C 972 PRO HD2	Allowed (0.43%) Pre-proline / -115.5,-177.3	27.2% (*m*) chi angles: 296.1	0.1Å	-	-
C 972		PRO	99.99	0.906Å HB3 with C 961 GLY HA2	OUTLIER (0%) Trans-proline / -50.2,-98.8	34.9% (*Cg_endo*) chi angles: 22.3	0.347Å	-	OUTLIER(S) worst is C-N-CA: 9.231 σ
C 973		VAL	50	0.979Å HG23 with C 960 VAL HB	OUTLIER (0%) Isoleucine or valine / 18.4,129.0	6.3% (*m*) chi angles: 309.6	0.175Å	-	OUTLIER(S) worst is N-CA-C: 5.856 σ
C 974		ARG	50	-	Favored (40.38%) General / -104.0,138.6	93.7% (*mtt-85*) chi angles: 297.2,175.3,175.2,277.3	0.052Å	-	-
C 975		ILE	50	0.694Å HD11 with C 884 SER HB2	Favored (17.02%) Isoleucine or valine / -115.3,151.9	6% (*tp*) chi angles: 180.3,73	0.091Å	-	-
C 976		ARG	50	0.438Å HB3 with C 885 ASP OD1	Favored (45.18%) General / -118.2,123.3	23% (*ttm-85*) chi angles: 200.7,184.5,304.6,250	0.163Å	-	-
C 977		ILE	50	0.86Å HG21 with C	Favored (30.27%) Isoleucine or	11.8% (*mt*)	0.214Å		OUTLIER(S) worst is CA-

C 977	ILE	50	HG21 with C 882 TYR CE2	Isoleucine or valine / -125.7,148.1	chi angles: 292.3,145.2	0.214Å	-	CB-CG2: 5.068 σ
C 978	GLY	50	-	Favored (14.61%) Glycine / -129.6,143.4	-	-	-	-
C 979	LEU	50	-	Favored (54.74%) General / -122.4,135.7	10.8% (*mp*) chi angles: 273.4,58	0.1Å	-	-
C 980	HIS	50	0.69Å HB2 with C1009 MET SD	Favored (15.49%) General / -154.8,137.7	13% (*t60*) chi angles: 187.2,38.2	0.177Å	OUTLIER(S) worst is CG--ND1: 4.758 σ	OUTLIER(S) worst is CB-CG-CD2: 5.021 σ
C 981	SER	50	-	Favored (49.16%) General / -115.9,140.5	49.1% (*m*) chi angles: 300.7	0.07Å	-	-
C 982	GLY	50	-	Favored (32.09%) Glycine / 170.5,168.3	-	-	-	-
C 983	PRO	50	0.419Å HA with C 876 PHE O	Favored (49.45%) Trans-proline / -67.5,139.5	80.8% (*Cg_endo*) chi angles: 29.8	0.039Å	-	-
C 984	CYS	50	-	Favored (32.12%) General / -144.7,164.1	30.2% (*p*) chi angles: 63.1	0.084Å	-	-
C 985	VAL	50	0.616Å HG13 with C 999 PHE CD1	Favored (18.76%) Isoleucine or valine / -109.6,143.9	2.7% (*p*) chi angles: 50.2	0.132Å	-	-
C 986	ALA	50	-	Favored (54.65%) General / -122.3,133.5	-	0.053Å	-	-
C 987	GLY	50	-	Favored (14.24%) Glycine / -108.3,137.7	-	-	-	-
C 988	VAL	50	0.554Å HB with C 872 GLU CG	Favored (74.85%) Isoleucine or valine / -118.6,126.0	85.2% (*t*) chi angles: 174.9	0.055Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
C 989		VAL	50	-	Favored (71.98%) Isoleucine or valine / -115.2,129.1	59.8% (*t*) chi angles: 181	0.059Å	-	-
C 990		GLY	50	-	Favored (25.27%) Glycine / 85.5,155.6	-	-	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 56.86	Clashscore: 42.95	Outliers: 6 of 173	Poor rotamers: 1 of 149	Outliers: 3 of 160	Outliers: 6 of 175	Outliers: 18 of 175
C 991		LEU	50	-	Favored (4.39%) General / -111.5,-40.4	9% (*tt*) chi angles: 183.1,157.9	0.066Å	-	-
C 992		THR	50	-	Favored (38.65%) General / -58.6,-55.2	69.4% (*p*) chi angles: 57.6	0.03Å	-	-
C 993		MET	50	-	Favored (17.97%) Pre-proline / -138.4,85.6	83.6% (*mmm*) chi angles: 289.3,286.2,289.8	0.039Å	-	-
C 994		PRO	50	-	Favored (99.27%) Trans-proline / -59.2,142.5	73.8% (*Cg_endo*) chi angles: 28.8	0.061Å	-	-
C 995		ARG	50	-	Favored (54.52%) General / -120.2,136.8	83.5% (*mtp180*) chi angles: 295.4,175.1,63.5,182.3	0.14Å	-	-
C 996		TYR	50	0.795Å CE2 with C 937 LEU HD11	Favored (55.9%) General / -113.8,127.2	1.6% (*m-30*) chi angles: 292.8,33.2	0.03Å	-	-
C 997		CYS	50	-	Favored (46.28%) General / -116.9,142.9	80% (*m*) chi angles: 299.6	0.072Å	-	-
C 998		LEU	50	0.405Å CD1 with C 881 LEU HD21	Favored (51.93%) General / -117.3,138.2	84.5% (*mt*) chi angles: 300.6,180.2	0.044Å	-	-
C 999		PHE	50	0.616Å CD1 with C 985 VAL HG13	Favored (46.19%) General / -141.0,155.4	2% (*p90*) chi angles: 34.5,92.7	0.152Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
C1000		GLY	50	-	Favored (9.77%) Glycine / 130.5,159.7	-	-	-	-
C1001		ASP	50	-	Favored (67.94%) General / -55.7,-37.1	42.7% (*t0*) chi angles: 189.3,328.9	0.011Å	-	-
C1002		THR	50	-	Favored (68.68%) General / -65.7,-27.9	63.9% (*p*) chi angles: 62.9	0.025Å	-	-
C1003		VAL	50	-	Favored (71.68%) Isoleucine or valine / -71.2,-45.4	61.3% (*t*) chi angles: 181.3	0.047Å	-	-
C1004		ASN	50	-	Favored (98.27%) General / -62.4,-41.0	25.5% (*t-20*) chi angles: 186.9,298.7	0.037Å	-	-
C1005		THR	50	-	Favored (91.45%) General / -65.6,-39.4	73% (*p*) chi angles: 58	0.031Å	-	-
C1006		ALA	50	-	Favored (90.83%) General / -63.1,-38.4	-	0.029Å	-	-
C1007		SER	50	0.423Å O with C1010 GLU HB3	Favored (83.52%) General / -66.0,-36.5	32.5% (*t*) chi angles: 184.2	0.022Å	-	-
C1008		ARG	50	-	Favored (68.94%) General / -68.7,-30.3	84% (*mtp180*) chi angles: 292,181.3,65.1,185.1	0.034Å	-	-
C1009		MET	50	0.698Å SD with C1021 ASN HB2	Favored (78.66%) General / -64.2,-34.7	62.5% (*mtt*) chi angles: 294.9,187.2,186.9	0.061Å	-	OUTLIER(S) worst is CG-SD-CE: 5.829 σ
C1010		GLU	50	0.459Å OE1 with C 883 PHE HB3	Favored (69.41%) General / -65.0,-49.6	43.5% (*tt0*) chi angles: 179.1,198.3,339.7	0.106Å	-	-
			Avg:	Clashscore:	Outliers: 6 of	Poor rotamers: 1 of	Outliers:	Outliers: 6	Outliers: 18

		56.86	42.95	173	149	3 of 160	of 175	of 175
C1011	SER	50	-	Favored (81.82%) General / -61.9,-36.6	51.1% (*m*) chi angles: 301.5	0.057Å	-	-
C1012	THR	50	-	Favored (57.61%) General / -80.3,-6.2	51.1% (*p*) chi angles: 55.8	0.063Å	-	-
C1013	GLY	50	-	Favored (37.01%) Glycine / -69.5,173.5	-	-	-	-
C1014	LEU	50	0.608Å HB3 with C1017 ARG HD2	Favored (60.46%) Pre-proline / -124.7,148.8	9.7% (*tt*) chi angles: 186.6,155.8	0.102Å	-	-
C1015	PRO	50	0.533Å HD2 with C1014 LEU HG	Favored (28.03%) Trans-proline / -48.7,135.4	68.7% (*Cg_exo*) chi angles: 327.7	0.079Å	-	-
C1016	TYR	50	0.415Å CD2 with C1016 TYR O	Favored (10.4%) General / 64.5,16.7	81.8% (*t80*) chi angles: 181.8,82.8	0.069Å	-	-
C1017	ARG	50	0.608Å HD2 with C1014 LEU HB3	Favored (41.14%) General / -123.0,152.2	96.3% (*mtt-85*) chi angles: 293.9,181.3,179.1,275.9	0.045Å	-	-
C1018	ILE	50	0.405Å HG13 with C 957 LEU HD11	Favored (18.78%) Isoleucine or valine / -110.3,105.4	59.3% (*mt*) chi angles: 304.3,166.2	0.079Å	-	-
C1019	HIS	50	-	Favored (30.73%) General / -86.1,122.9	22.8% (*t-160*) chi angles: 183.3,200.4	0.071Å	OUTLIER(S) worst is CG-- ND1: 5.053 σ	-
C1020	VAL	50	-	Favored (71.24%) Isoleucine or valine / -114.5,124.5	59.6% (*t*) chi angles: 181.7	0.058Å	-	-
C1021	ASN	50	0.698Å HB2 with C1009 MET SD	Favored (13.81%) General / -61.4,158.7	60.4% (*t30*) chi angles: 189.7,48	0.191Å	-	-
C1022	LEU	50	0.746Å HA with	Favored (72.2%)	92% (*mt*)	0.097Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
C1022		LEU	50	C1025 VAL HG12	General / -63.7,-31.1	chi angles: 293.1,177.3	0.097Å		
C1023		SER	50	0.586Å HB3 with C1021 ASN HD22	Favored (83.25%) General / -67.9,-41.0	43.4% (*t*) chi angles: 181	0.024Å	-	-
C1024		THR	50	-	Favored (65.11%) General / -73.6,-38.5	24.8% (*m*) chi angles: 308.9	0.021Å	-	-
C1025		VAL	50	0.746Å HG12 with C1022 LEU HA	Favored (78.88%) Isoleucine or valine / -61.0,-38.1	7.8% (*p*) chi angles: 69	0.098Å	-	-
C1026		GLY	50	-	Favored (99.15%) Glycine / -61.2,-40.9	-	-	-	-
C1027		ILE	50	-	Favored (18.12%) Isoleucine or valine / -74.0,-21.7	7.9% (*tp*) chi angles: 181.9,67.2	0.187Å	-	-
C1028		LEU	50	-	Favored (14.28%) General / -99.2,-26.1	88.4% (*mt*) chi angles: 291,174.9	0.028Å	-	-
C1029		ARG	50	-	Favored (70.88%) General / -58.5,-34.5	54.3% (*ptt85*) chi angles: 63.5,179.5,181.8,83.1	0.081Å	-	-
C1030		ALA	99.99	-	Favored (8.91%) General / -123.1,24.4	-	0.058Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 56.86	Clashscore: 42.95	Outliers: 6 of 173	Poor rotamers: 1 of 149	Outliers: 3 of 160	Outliers: 6 of 175	Outliers: 18 of 175
C1031		LEU	99.99	0.794Å HD21 with C 944 ARG NH1	Favored (2.13%) General / -108.3,85.5	6.7% (*tt*) chi angles: 185.1,164.8	0.072Å	-	-
C1032		ASP	99.99	-	Favored (2.1%) General / 51.1,63.8	34.8% (*t70*) chi angles: 181.4,71.1	0.058Å	-	-
C1033		SER	99.99		OUTLIER (0.01%)	33.4% (*t*)			

C1033	SER	99.99	-	(0.01%) General / -62.0,55.5	55.4% (t) chi angles: 183.6	0.114A	-	-
C1034	GLY	50	-	Favored (73.92%) Glycine / -67.7,-23.0	-	-	-	-
C1035	TYR	50	-	Favored (44.36%) General / -66.3,130.8	97.7% (m-85) chi angles: 294.4,275.8	0.028Å	-	-
C1036	GLN	50	-	Favored (56.11%) General / -114.9,128.1	19.5% (pt20) chi angles: 59.1,180,63.8	0.021Å	-	-
C1037	VAL	50	-	Favored (24.93%) Isoleucine or valine / -121.6,151.0	11.7% (p) chi angles: 61.8	0.084Å	-	-
C1038	GLU	50	-	Favored (30.98%) General / -117.0,117.9	10.4% (pt-20) chi angles: 56.4,175.8,72.9	0.056Å	-	-
C1039	LEU	50	-	Favored (56.73%) General / -62.8,144.2	97.1% (mt) chi angles: 296.3,176.7	0.017Å	-	-
C1040	ARG	50	-	Allowed (0.38%) General / -109.2,-100.7	78.3% (mtp180) chi angles: 297.8,187.9,72.2,186.9	0.07Å	-	-
C1041	GLY	50	-	Favored (41.31%) Glycine / -176.0,168.9	-	-	-	-
C1042	ARG	50	-	Favored (72.26%) General / -71.1,-38.2	22.6% (tpt180) chi angles: 188.5,74.1,189.4,180.6	0.075Å	-	-
C1043	THR	50	-	Favored (67.81%) General / -65.7,-26.5	72.3% (p) chi angles: 59	0.027Å	-	-
C1044	GLU	50	-	Favored (59.25%) General / -86.5,-4.9	46.3% (mt-10) chi angles: 293,174.4,276.4	0.054Å	-	-
C1045	LEU	99.99	-	-	84.9% (mt) chi angles: 290.2,175	0.016Å	-	-

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