



Viewing iqcb1_swissmodel_292-319_FFX1H-multi.table

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All-Atom Contacts	Clashscore, all atoms:	0	100 th 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	1	3.85%	Goal: <0.05%
	Ramachandran favored	24	92.31%	Goal: >98%
	MolProbity score [^]	0.97		100 th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	1	3.70%	Goal: 0
	Bad backbone bonds:	0 / 241	0.00%	Goal: 0%
	Bad backbone angles:	2 / 321	0.62%	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: 51.79	Clashscore: 0	Outliers: 1 of 26	Poor rotamers: 0 of 24	Outliers: 1 of 27	Outliers: 0 of 28	Outliers: 2 of 28
C 292	GLN	50	-	-	17.7% (<i>mp0</i>) chi angles: 305.7,79.7,335.1	0.118Å	-	-
C 293	LYS	50	-	Favored (60.76%) General / -53.4,-35.9	99.3% (<i>mttt</i>) chi angles: 293.8,183.2,178.4,180.3	0.144Å	-	-
C 294	LEU	50	-	Favored (72.63%) General / -59.2,-34.8	46.8% (<i>mt</i>) chi angles: 307.6,183.4	0.117Å	-	-
C 295	HIS	50	-	Favored (72.61%) General / -65.1,-31.4	3.6% (<i>t-160</i>) chi angles: 202.3,153.1	0.127Å	-	-

C 296	GLN	50	-	Favored (87.77%) General / -66.4,-42.4	35.7% (<i>mt-30</i>) chi angles: 305.9,172.9,254.4	0.074Å	-	-
C 297	ALA	50	-	Favored (86.89%) General / -66.2,-38.0	-	0.068Å	-	-
C 298	ALA	50	-	Favored (93.97%) General / -60.9,-40.7	-	0.086Å	-	-
C 299	CYS	50	-	Favored (57.15%) General / -76.9,-35.8	26% (<i>p</i>) chi angles: 58.3	0.203Å	-	-
C 300	LEU	50	-	Favored (69.43%) General / -60.6,-51.4	7% (<i>tt</i>) chi angles: 180.9,140.5	0.062Å	-	-
C 301	ILE	50	-	Favored (95.82%) Isoleucine or valine / -62.8,-42.3	7.6% (<i>pt</i>) chi angles: 64.2,191.5	0.202Å	-	-
C 302	GLN	50	-	Favored (77.08%) General / -62.5,-34.5	86.4% (<i>mt-30</i>) chi angles: 292.6,171.2,4.4	0.095Å	-	-
C 303	ALA	50	-	Favored (87.42%) General / -62.1,-46.8	-	0.063Å	-	-
C 304	TYR	50	-	Favored (88.99%) General / -65.3,-38.1	64.1% (<i>m-85</i>) chi angles: 288.6,288.5	0.121Å	-	-
C 305	TRP	50	-	Favored (98.68%) General / -61.4,-43.5	29.3% (<i>m0</i>) chi angles: 307.2,335.4	0.122Å	-	OUTLIER(S) worst is CE3- CD2-CG: 4.225 σ
C 306	LYS	50	-	Favored (96.64%) General / -64.4,-41.3	99.1% (<i>mttt</i>) chi angles: 293.6,180.6,179.2,182.2	0.112Å	-	-
C 307	GLY	50	-	Favored (97.99%) Glycine / -64.1,-40.4	-	-	-	-

C 308	PHE	50	-	Favored (60.94%) General / -75.3,-32.1	1.1% (<i>p90</i>) chi angles: 64.1,57.3	0.266Å	-	OUTLIER(S) worst is CA-CB- CG: 7.507 σ	
C 309	GLN	50	-	Favored (83.68%) General / -67.8,-40.7	24.2% (<i>mm100</i>) chi angles: 289.4,295.6,106	0.14Å	-	-	
C 310	THR	50	-	Favored (91.21%) General / -65.9,-41.7	33% (<i>p</i>) chi angles: 51.8	0.148Å	-	-	
C 311	ARG	50	-	Favored (73.17%) General / -63.2,-31.9	35.4% (<i>mmt180</i>) chi angles: 286.5,293.4,188.6,175.1	0.172Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 51.79	Clashscore: 0	Outliers: 1 of 26	Poor rotamers: 0 of 24	Outliers: 1 of 27	Outliers: 0 of 28	Outliers: 2 of 28
C 312	LYS	50	-	Favored (97.01%) General / -64.0,-42.9	83.8% (<i>mttt</i>) chi angles: 292.6,165.8,193.3,175.8	0.112Å	-	-	
C 313	ARG	50	-	Favored (68.54%) General / -69.2,-30.4	28.5% (<i>tpt180</i>) chi angles: 176.7,55.6,171.2,177.7	0.151Å	-	-	
C 314	LEU	50	-	Favored (75.56%) General / -58.4,-37.5	3.2% (<i>tt</i>) chi angles: 189,133.2	0.107Å	-	-	
C 315	LYS	50	-	Favored (49.82%) General / -75.6,-43.1	27.1% (<i>tptp</i>) chi angles: 183.3,52.2,165.1,62.6	0.161Å	-	-	
C 316	LYS	50	-	Favored (5.25%) General / -81.5,62.2	17.6% (<i>tptp</i>) chi angles: 194.1,81,188.4,81.4	0.071Å	-	-	
C 317	LEU	50	-	OUTLIER (0.02%) Pre-proline / -142.3,-58.7	18.7% (<i>mt</i>) chi angles: 275.9,168	0.2Å	-	-	
C 318	PRO	50	-	Allowed (1.05%) Trans-proline /	13.4% (<i>Cg_endo</i>) chi angles: 39.6	0.051Å	-	-	

-90.0,49.7

C
319

SER 99.99

-

-

59.6% (*m*)
chi angles: 291.8

0.117Å

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