

Viewing iqcb1_swissmodel_292-319H-multi.table

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	Clashscore, all atoms: 22.45			26 th percentile* (N=1784, all resolutions)			
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.						
	Poor rotamers	0	0.00%	Goal: <1%			
	Ramachandran outliers	0	0.00%	Goal: <0.05%			
II I	Ramachandran favored	26	100.00%	Goal: >98%			
Protein Geometry	MolProbity score [^]	1.84		83 rd percentile [*] (N=27675, 0Å - 99Å)			
	Cβ deviations >0.25Å	1	3.70%	Goal: 0			
	Bad backbone bonds:	2 / 241	0.83%	Goal: 0%			
	Bad backbone angles:	4/321	1.25%	Goal: <0.1%			

In the two column results, the left column gives the raw count, right column gives the percentage.

[^] 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	C β deviation	Bond lengths	Bond angles
			Avg: 51.79		Outliers: 0 of 26	Poor rotamers: 0 of 24	Outliers: 1 of 27	Outliers: 1 of 28	Outliers: 2 of 28
C 292	<u>.</u>	GLN		-	-	81.2% (<i>mt-30</i>) chi angles: 299.2,178.3,295.2	0.041Å	-	-
C 293	;	LYS	50	-	Favored (80.4%) General / -63.6,-47.7	28% (<i>tptp</i>) chi angles: 185.9,62.1,182.5,65.2	0.017Å	-	-
C 294	ļ	LEU	50	-	Favored (75.4%) General / -61.9,-34.1	95.3% (<i>mt</i>) chi angles: 295,176.7	0.018Å	-	-
C 295		HIS	50	-	Favored (74.09%) General / -66.6,-47.0	21.9% (<i>t-160</i>) chi angles: 183.5,202.5	0.049Å	OUTLIER(S) worst is CG ND1: 4.416 σ	-

^{* 100&}lt;sup>th</sup> 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.

C 296	GLN	50	-	Favored (86.28%) General / -64.7,-37.1	84.4% (<i>mt-30</i>) chi angles: 295,181.8,296.9	0.037Å	-	-
C 297	ALA	50	-	Favored (86.79%) General / -66.1,-37.9	-	0.031Å	-	-
C 298	ALA	50	0.52Å O with C 301 ILE HG12	Favored (77.29%) General / -66.9,-45.7	-	0.01Å	-	-
C 299	CYS	50	-	Favored (77.7%) General / -66.4,-34.3	24.4% (p) chi angles: 67.6	0.052Å	-	-
C 300	LEU	50	-	Favored (77.11%) General / -65.9,-46.8	10.2% (tt) chi angles: 187.2,153.6	0.063Å	-	-
C 301	ILE	50	0.52Å HG12 with C 298 ALA O	Favored (78.78%) Isoleucine or valine / -65.5,-36.9	31.1% (<i>pt</i>) chi angles: 67.5,175.8	0.098Å	-	-
C 302	GLN	50	-	Favored (75.36%) General / -69.6,-35.4	91.2% (<i>mt-30</i>) chi angles: 291.8,166,332.7	0.009Å	-	-
C 303	ALA	50	-	Favored (74.35%) General / -70.2,-40.7	-	0.025Å	-	-
C 304	TYR	50	-	Favored (80.76%) General / -67.0,-35.8	46.6% (<i>m</i> -85) chi angles: 280.6,272.3	0.089Å	-	-
C 305	TRP	50	1.11Å HA with C 308 PHE CE2	Favored (72.39%) General / -58.0,-50.7	41.5% (<i>m0</i>) chi angles: 291.9,9.9	0.339Å	-	-
C 306	LYS	50	0.461Å O with C 310 THR HG23	Favored (71.97%) General / -69.5,-32.8	98.6% (<i>mttt</i>) chi angles: 296.7,180.3,178.8,181.6	0.045Å	-	-
C 307	GLY	50	-	Favored (60.93%) Glycine /	-	-	-	-

				-66.6,-48.7				
C 308	PHE	50	1.11Å CE2 with C 305 TRP HA	Favored (61.64%) General / -75.0,-38.7	52.4% (<i>p90</i>) chi angles: 63.5,87.1	0.095Å	-	-
C 309	GLN	50	0.44Å HG3 with C 308 PHE CE1	Favored (87.43%) General / -63.4,-37.5	84.8% (<i>mt-30</i>) chi angles: 298,187.1,342	0.044Å	-	-
C 310	THR	50	0.461Å HG23 with C 306 LYS O	Favored (83.24%) General / -67.4,-37.5	70% (p) chi angles: 59.7	0.062Å	-	-
C 311	ARG	50	-	Favored (74.5%) General / -68.6,-33.7	89.1% (<i>mtm-85</i>) chi angles: 283.9,184.8,285.4,277	0.064Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg:	Clashscore:	Outliers: 0 of	Poor rotamers: 0 of	Outliers:	Outliers: 1	Outliers: 2
		51.79	22.45	26	24	1 of 27	of 28	of 28
C 312	LYS	50	-	Favored (78.9%) General / -68.9,-41.0	30.7% (<i>mtpp</i>) chi angles: 294.1,182.7,66,63.5	0.047Å	-	-
C 313	ARG	50	-	Favored (80.56%) General / -67.5,-43.6	61.5% (ttm-85) chi angles: 181.5,182.3,293.5,276.9	0.055Å	-	-
C 314	LEU	50	0.798Å O with C 318 PRO HD3	Favored (69.43%) General / -65.2,-28.5	10.4% (tt) chi angles: 185.4,151.2	0.105Å	-	OUTLIER(S) worst is CA-C- O: 4.623 σ
C 315	LYS	50	0.533Å C with C 318 PRO HD2	Favored (63.07%) General / -74.1,-32.2	83% (tttt) chi angles: 186.6,189,182.8,182.8	0.06Å	-	-
C 316	LYS	50	-	Favored (95.25%) General / -64.7,-42.7	28.6% (<i>tptp</i>) chi angles: 184.5,64.1,181.5,65.6	0.042Å	-	-
C 317	, LEU	50	0.401Å N with C 318 PRO HD2	Favored (87.53%) Pre-proline / -60.4,-50.0	97.4% (<i>mt</i>) chi angles: 297.4,178.1	0.113Å	-	-
С			0.798Å HD3 with C	Favored (27.76%)	94.7% (<i>Cg_endo</i>)	o		OUTLIER(S) worst is N-

318 PRO 50 314 LEU O Trans-proline / chi angles: 32.3 0.104A - CD-CG: 5.416 σ

C 319 SER 99.99 - - 32.9% (t) chi angles: 183.9 0.036Å - -

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