Viewing cnga3_mb_352-407_FFX1H-multi.table

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All-Atom Contacts	Clashscore, all atoms:	1.14		99th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	3	5.88%	Goal: <1%
	Ramachandran outliers	0	0.00%	Goal: <0.05%
	Ramachandran favored	51	94.44%	Goal: >98%
	MolProbity score^	1.79		86th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	4	7.69%	Goal: 0
	Bad backbone bonds:	0 / 451	0.00%	Goal: 0%
	Bad backbone angles:	5 / 620	0.81%	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: 79.37	Clashscore: 1.14	Outliers: 0 of 54	Poor rotamers: 3 of 51	Outliers: 4 of 52	Outliers: 0 of 56	Outliers: 5 of 56
352		TYR	20.32	0.616Å N with 355 SER HG	-	59.7% (*m-85*) chi angles: 305.5,267.6	0.257Å	-	-
353		ILE	61.82	-	Favored (79.89%) Isoleucine or valine / -63.5,-37.5	10.3% (*tp*) chi angles: 193,59.6	0.221Å	-	-
354		TYR	86.1	-	Favored (83.91%) General / -62.7,-36.7	53.6% (*p90*) chi angles: 64.1,89.9	0.098Å	-	-
355		SER	24.93	0.616Å HG with 352 TYR N	Favored (34.99%) General / -81.1,0.7	44% (*p*) chi angles: 76.1	0.213Å	-	-

356	LEU 33.81	-	Favored (41.89%) General / -79.4,-29.6	54.6% (*tp*) chi angles: 183.2,61.5	0.085Å	-	-
357	TYR 31.98	-	Favored (29.9%) General / -81.6,-35.7	60.2% (*t80*) chi angles: 186.8,267.2	0.096Å	-	-
358	TRP 47.15	-	Favored (94.59%) General / -60.7,-41.2	43.7% (*t90*) chi angles: 165.8,75.1	0.189Å	-	OUTLIER(S) worst is CE3-CD2-CG: 4.837 σ
359	SER 70.49	-	Favored (90.15%) General / -62.0,-38.9	23.7% (*p*) chi angles: 51	0.156Å	-	-
360	THR 101.68	-	Favored (83.71%) General / -63.9,-36.4	3% (*p*) chi angles: 39.9	0.241Å	-	-
361	LEU 140.84	-	Favored (46.16%) General / -79.3,-21.4	2.9% (*pp*) chi angles: 68.3,97.8	0.235Å	-	-
362	THR 115.28	-	Favored (31.15%) General / -83.7,-24.7	1.8% (*p*) chi angles: 37.5	0.199Å	-	-
363	LEU 59.01	-	Favored (71.07%) General / -71.1,-34.3	48.8% (*mt*) chi angles: 290.1,162.6	0.116Å	-	-
364	THR 62.69	-	Favored (32.04%) General / -89.8,-15.6	45% (*p*) chi angles: 55.1	0.128Å	-	-
365	THR 78.89	-	Favored (24.19%) General / 56.4,44.6	14.2% (*p*) chi angles: 45.9	0.228Å	-	-
366	ILE 127.75	-	Favored (4.57%) Isoleucine or valine / -92.7,-30.8	9.5% (*tp*) chi angles: 190.2,57.9	0.252Å	-	-
367	GLY 29.72	-	Favored (59.34%) Glycine / 72.8,34.5	-	-	-	-
368	GLU 47.73	-	Favored (96.34%) General / -62.8,-40.1	16% (*mt-10*) chi angles: 300.6,154.6,95.9	0.088Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
369		THR	46.35	-	Favored (2.27%) Pre-proline / -105.0,175.2	44.7% (*p*) chi angles: 66.6	0.033Å	-	-
370		PRO	65.92	-	Favored (12.26%) Trans-proline / -61.2,165.6	1.4% (*Cg_exo*) chi angles: 321.4	0.09Å	-	-
371		PRO	74.35	-	Favored (6.69%) Trans-proline / -83.4,177.1	35.4% (*Cg_endo*) chi angles: 36.9	0.067Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 79.37	Clashscore: 1.14	Outliers: 0 of 54	Poor rotamers: 3 of 51	Outliers: 4 of 52	Outliers: 0 of 56	Outliers: 5 of 56
372		PRO	73.95	-	Favored (13.53%) Trans-proline / -46.9,140.0	0% chi angles: 314.9	0.122Å	-	-
373		VAL	102.16	-	Favored (4.89%) Isoleucine or valine / -111.0,-22.6	31.2% (*m*) chi angles: 300.8	0.15Å	-	-
374		LYS	76.31	-	Favored (33.9%) General / -117.0,152.8	27.9% (*tttt*) chi angles: 199.2,197.1,160.1,204.1	0.071Å	-	OUTLIER(S) worst is C-N-CA: 4.464 σ
375		ASP	86.09	-	Allowed (0.13%) General / -33.1,-67.0	0.3% chi angles: 37,85.1	0.1Å	-	-
376		GLU	71.39	-	Favored (62.9%) General / -52.2,-41.8	8.9% (*pt-20*) chi angles: 51.7,171.7,290.2	0.133Å	-	-
377		GLU	64.27	-	Favored (85.01%) General / -67.5,-39.7	82.1% (*mt-10*) chi angles: 301.8,167.7,338.3	0.051Å	-	-
378		TYR	126.42	-	Favored (87.3%) General / -66.6,-38.6	86.5% (*t80*) chi angles: 175.7,75	0.112Å	-	-
379		LEU	35.87	-	Favored (79.4%) General / -61.7,-35.9	84.4% (*mt*) chi angles: 302.2,178.7	0.123Å	-	-
380		PHE	46.4	-	Favored (99.17%) General / -62.9,-43.3	26.1% (*t80*) chi angles: 194,98.9	0.112Å	-	-
381		VAL	90.99	-	Favored (57.95%) Isoleucine or valine	0.8% chi angles: 87.8	0.305Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
					/ -64.5,-32.5				
382		VAL	26.31	-	Favored (67.03%) Isoleucine or valine / -59.8,-36.6	75.1% (*t*) chi angles: 174.1	0.109Å	-	-
383		VAL	27.69	-	Favored (9.45%) Isoleucine or valine / -76.2,-56.0	93% (*t*) chi angles: 175.6	0.096Å	-	-
384		ASP	89.99	-	Favored (36.59%) General / -79.1,-38.3	12.2% (*p-10*) chi angles: 74.8,335.6	0.226Å	-	-
385		PHE	128.95	-	Favored (70.09%) General / -68.2,-30.9	73.1% (*t80*) chi angles: 178.1,248.1	0.112Å	-	-
386		LEU	46.02	-	Favored (14.05%) General / -91.8,-35.5	66.7% (*mt*) chi angles: 305.8,178.4	0.154Å	-	-
387		VAL	104.04	-	Allowed (0.84%) Isoleucine or valine / -131.8,-24.8	23.3% (*m*) chi angles: 302.5	0.186Å	-	-
388		GLY	44.31	-	Favored (92.06%) Glycine / -66.3,-36.7	-	-	-	-
389		VAL	97.06	-	Favored (38.47%) Isoleucine or valine / -55.2,-36.1	15.7% (*m*) chi angles: 290	0.148Å	-	-
390		LEU	82.64	-	Favored (77.69%) General / -62.6,-48.8	10.6% (*mp*) chi angles: 272.8,57	0.092Å	-	-
391		ILE	84.04	-	Favored (47.83%) Isoleucine or valine / -72.7,-34.6	8.2% (*tt*) chi angles: 206.3,174.2	0.264Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 79.37	Clashscore: 1.14	Outliers: 0 of 54	Poor rotamers: 3 of 51	Outliers: 4 of 52	Outliers: 0 of 56	Outliers: 5 of 56
392		PHE	104.66	-	Favored (60.67%) General /	20.9% (*m-85*) chi angles: 275.6,74	0.206Å	-	-

			-74.7,-28.2				
393	ALA 31.16	-	Favored (91.66%) General / -62.6,-38.9	-	0.073Å	-	-
394	THR 27.03	-	Favored (73.65%) General / -68.3,-33.1	20% (*m*) chi angles: 310.4	0.124Å	-	-
395	ILE 129.78	-	Favored (78.63%) Isoleucine or valine / -65.9,-36.9	89.8% (*mt*) chi angles: 291.1,167.8	0.138Å	-	-
396	VAL 40.15	-	Favored (78.84%) Isoleucine or valine / -68.6,-38.3	84.2% (*t*) chi angles: 174.8	0.108Å	-	-
397	GLY 85.56	-	Allowed (1.86%) Glycine / 132.0,-116.4	-	-	-	-
398	ASN 234.3	-	Favored (36.24%) General / -141.2,162.1	5.1% (*m120*) chi angles: 285.5,172.5	0.08Å	-	OUTLIER(S) worst is CA-CB-CG: 8.355 σ
399	VAL 312.24	-	Favored (28.29%) Isoleucine or valine / -139.3,161.4	6.5% (*p*) chi angles: 74.5	0.116Å	-	-
400	GLY 237.9	-	Favored (20.91%) Glycine / 100.9,147.6	-	-	-	-
401	SER 107.83	-	Favored (72.7%) General / -61.4,-32.8	74.1% (*p*) chi angles: 58.1	0.139Å	-	-
402	MET 61.05	-	Favored (62.25%) General / -54.4,-34.9	67.1% (*mtt*) chi angles: 293.1,177.3,179.2	0.121Å	-	-
403	ILE 39.23	-	Favored (4.63%) Isoleucine or valine / -97.7,-34.1	85.4% (*mt*) chi angles: 298.9,167	0.139Å	-	-
404	SER 66.61	-	Favored (4.03%) General / -79.9,10.6	53.1% (*p*) chi angles: 74.6	0.117Å	-	-
			Favored (3.82%)	10.2% (*m120*)			OUTLIER(S) worst is CA-

405	ASN 55.67	-	General / -134.3,24.8	chi angles: 304,152	0.034Å	-	CB-CG: 7.013 σ
406	MET 62.26	-	Favored (12.05%) General / -116.2,-3.1	42.4% (*ttm*) chi angles: 189.2,194.6,286.5	0.048Å	-	-
407	ASN 17.55	-	-	11.7% (*m-80*) chi angles: 303.4,262.4	0.07Å	-	OUTLIER(S) worst is CA-CB-CG: 4.02 σ

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