

Viewing cnga3_mb_352-407Hmulti.table

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All-Atom	Clashscore, all atoms: 86.36			0 th percentile* (N=1784, all resolutions)		
Contacts	Clashscore is the number	of seriou	us steric ove	erlaps (> 0.4 Å) per 1000 atoms.		
	Poor rotamers	1	1.96%	Goal: <1%		
	Ramachandran outliers	0	0.00%	Goal: <0.05%		
II .	Ramachandran favored	54	100.00%	Goal: >98%		
Protein Geometry	MolProbity score [^]	2.63		40 th percentile [*] (N=27675, 0Å - 99Å)		
geometry	Cβ deviations >0.25Å	0	0.00%	Goal: 0		
	Bad backbone bonds:	0 / 451	0.00%	Goal: 0%		
	Bad backbone angles:	9 / 620	1.45%	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	Cβ deviation	Bond lengths	Bond angles
		Avg: 79.37	Clashscore: 86.36	Outliers: 0 of 54	Poor rotamers: 1 of 51	Outliers: 0 of 52	Outliers: 0 of 56	Outliers: 9 of 56
352	. TYR	20.32	-	-	97.8% (<i>m</i> -85) chi angles: 295.6,272	0.104Å	-	-
353	ILE	61.82	0.528Å HG23 with 354 TYR N	Favored (95.64%) Isoleucine or valine /-61.2,-43.0	10.5% (<i>tp</i>) chi angles: 188.4,65.5	0.042Å	-	-
354	TYR	86.1	0.528Å N with 353 ILE HG23	Favored (90.92%) General / -66.0,-41.7	88.6% (<i>m-85</i>) chi angles: 298.9,85.7	0.065Å	-	OUTLIER(S) worst is CA- CB-CG: 4.848 σ
355	S SER	24.93	-	Favored (95.52%) General / -60.6,-41.8	84.6% (<i>p</i>) chi angles: 68.4	0.099Å	-	-

^{* 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.

356	LEU 33.81	-	Favored (92.58%) General / -65.5,-40.0	60.6% (<i>tp</i>) chi angles: 180.2,60.9	0.093Å	-	-
357	TYR 31.98	0.734Å O with 360 THR HG22	Favored (99.38%) General / -63.1,-43.1	43.7% (<i>t80</i>) chi angles: 182.5,276.9	0.06Å	-	-
358	TRP 47.15	0.654Å O with 362 THR HG23	Favored (98.96%) General / -62.1,-43.4	87.8% (<i>t</i> 90) chi angles: 185.1,88.7	0.09Å	-	-
359	SER 70.49	0.404Å O with 363 LEU HG	Favored (99.7%) General / -62.4,-42.8	47.8% (<i>t</i>) chi angles: 179.9	0.099Å	-	-
360	THR 101.68	0.734Å HG22 with 357 TYR O	Favored (77.46%) General / -66.5,-46.1	12.2% (<i>t</i>) chi angles: 191.4	0.056Å	-	-
361	LEU 140.84	0.935Å HD13 with 367 GLY HA2	Favored (83.48%) General / -65.8,-36.4	3.5% (<i>pp</i>) chi angles: 65.6,72.9	0.054Å	-	-
362	THR 115.28	0.817Å N with 361 LEU HD12	Favored (70.57%) General / -67.1,-47.6	78.6% (p) chi angles: 60.2	0.074Å	-	-
363	LEU 59.01	0.59Å HD13 with 392 PHE CD1	Favored (96.2%) General / -64.3,-40.5	84.5% (<i>mt</i>) chi angles: 295.4,180.2	0.116Å	-	-
364	THR 62.69	0.403Å HG23 with 360 THR O	Favored (61.3%) General / -72.1,-22.6	74.1% (p) chi angles: 60	0.048Å	-	OUTLIER(S) worst is C-N-CA: 4.118σ
365	THR 78.89	0.688Å HG22 with 385 PHE CZ	Favored (2.28%) General / 75.4,18.7	21.5% (<i>p</i>) chi angles: 72.8	0.141Å	-	-
366	ILE 127.75	0.704Å CG2 with 361 LEU HB2	Favored (86.97%) Isoleucine or valine / -66.5,-46.2	10.4% (<i>tp</i>) chi angles: 187.7,64.6	0.057Å	-	-
367	GLY 29.72	0.935Å HA2 with 361 LEU HD13	Favored (93.73%) Glycine / 59.0,46.4	-	-	-	-
			Favored	92.2% (mt-10)			

368	GLU 47.73	-	(82.96%) General / -68.1,-39.1	chi angles: 294.7,188,358.8	0.119Å	-	-
369	THR 46.35	0.509Å OG1 with 361 LEU HD21	Favored (12.86%) Pre-proline / -83.3,170.9	58.4% (p) chi angles: 62.5	0.057Å	-	-
370	PRO 65.92	-	Favored (50.24%) Trans-proline / -70.9,160.2	74.5% (<i>Cg_exo</i>) chi angles: 332.3	0.105Å	-	-
371	PRO 74.35	-	Favored (31.47%) Trans-proline / -75.2,165.2	13.2% (<i>Cg_endo</i>) chi angles: 15.8	0.117Å	-	-
# Al	t Res High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
	Avg: 79.37	Clashscore: 86.36	Outliers: 0 of 54	Poor rotamers: 1 of 51		•	
372	PRO 73.95	0.822Å HB3 with 377 GLU HB3	Favored (36.34%) Trans-proline / -67.6,135.5	81% (<i>Cg_exo</i>) chi angles: 332	0.138Å	-	-
373	VAL 102.16	0.566Å HG23 with 374 LYS N	Favored (34.88%) Isoleucine or valine /-76.4,-40.6	27% (m) chi angles: 296.3	0.057Å	-	-
374	LYS 76.31	0.775Å HB3 with 377 GLU CG	Favored (34.81%) General / -77.6,149.6	78.5% (tttt) chi angles: 192.3,164.8,182.7,176.3	0.081Å	-	-
375	ASP 86.09	-	Favored (90.48%) General / -64.8,-44.3	13.7% (<i>p-10</i>) chi angles: 58.5,304.2	0.067Å	-	OUTLIER(S) worst is CA- CB-CG: 4.327 σ
376	GLU 71.39	0.629Å HG3 with 377 GLU N	Favored (83.38%) General / -64.1,-36.2	5.1% (<i>pt-20</i>) chi angles: 72,155.4,342.9	0.171Å	-	-
377	GLU 64.27	0.822Å HB3 with 372 PRO HB3	Favored (93.17%) General / -59.5,-44.0	60.4% (<i>mm-40</i>) chi angles: 294.3,280.1,348.7	0.091Å	-	-
378	TYR 126.42	0.7Å O with 381 VAL HG12	Favored (84.41%) General / -67.4,-41.8	38.7% (<i>t80</i>) chi angles: 194.1,73.6	0.056Å	-	-

379	LEU 35.87	-	Favored (81.82%) General / -65.0,-46.4	85.7% (<i>mt</i>) chi angles: 296,180.3	0.102Å	-	-
380	PHE 46.4	0.68Å CE2 with 384 ASP HB3	Favored (95.39%) General / -65.0,-41.4	65.1% (<i>t80</i>) chi angles: 185.2,86.8	0.077Å	-	OUTLIER(S) worst is CA- CB-CG: 6.375 σ
381	VAL 90.99	0.813Å HA with 384 ASP OD2	Favored (82.81%) Isoleucine or valine / -61.3,-39.5	12.9% (p) chi angles: 65.4	0.078Å	-	-
382	VAL 26.31	0.528Å N with 381 VAL HG13	Favored (84.47%) Isoleucine or valine /-60.0,-49.3	74.2% (t) chi angles: 174	0.089Å	-	-
383	VAL 27.69	-	Favored (94.37%) Isoleucine or valine /-65.5,-43.6	70.2% (t) chi angles: 173.6	0.064Å	-	-
384	ASP 89.99	0.813Å OD2 with 381 VAL HA	Favored (83.45%) General / -63.6,-36.3	4.5% (<i>p30</i>) chi angles: 60.5,49.5	0.134Å	-	-
385	PHE 128.95	0.75Å O with 389 VAL HG13	Favored (86.83%) General / -64.1,-45.9	31.7% (<i>t80</i>) chi angles: 193.8,275	0.087Å	-	OUTLIER(S) worst is CA- CB-CG: 4.929 σ
386	LEU 46.02	-	Favored (71.95%) General / -62.7,-50.2	68.6% (<i>mt</i>) chi angles: 302.2,183.8	0.101Å	-	-
387	VAL 104.04	0.598Å HG23 with 388 GLY N	Favored (61.65%) Isoleucine or valine / -70.9,-47.6	29.2% (<i>m</i>) chi angles: 296.8	0.06Å	-	-
388	GLY 44.31	0.614Å O with 392 PHE HD1	Favored (73.25%) Glycine / -69.9,-36.3	-	-	-	-
389	VAL 97.06	0.75Å HG13 with 385 PHE O	Favored (85.38%) Isoleucine or valine / -58.9,-42.2	27.6% (<i>m</i>) chi angles: 295.7	0.064Å	-	-
390	LEU 82.64	0.647Å HD12 with 389 VAL HG23	Favored (79.89%) General / -60.6,-48.9	4.8% (<i>mp</i>) chi angles: 296.7,67.2	0.135Å	-	-

391		ILE	84.04	0.707Å HG23 with 392 PHE CD1	Favored (90.07%) Isoleucine or valine /-66.1,-45.6	20% (tt) chi angles: 191.4,166.1	0.046Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C β deviation	Bond lengths	Bond angles
			Avg: 79.37	Clashscore: 86.36	Outliers: 0 of 54	Poor rotamers: 1 of 51	Outliers: 0 of 52	Outliers: 0 of 56	Outliers: 9 of 56
392	F	PHE	104.66	0.856Å O with 396 VAL HG23	Favored (86.78%) General / -66.8,-38.5	90.8% (<i>m-85</i>) chi angles: 291.2,87.4	0.146Å	-	OUTLIER(S) worst is CA- CB-CG: 9.977 σ
393	F	ALA	31.16	-	Favored (99.76%) General / -62.8,-42.5	-	0.068Å	-	-
394	Т	THR	27.03	-	Favored (99.43%) General / -63.2,-42.7	85.7% (<i>m</i>) chi angles: 301.6	0.097Å	-	-
395		ILE	129.78	0.801Å HG22 with 392 PHE O	Favored (79.26%) Isoleucine or valine /-61.6,-38.0	0.1% chi angles: 199.9,294.2	0.04Å	-	-
396	\	√AL	40.15	0.856Å HG23 with 392 PHE O	Favored (63.79%) Isoleucine or valine /-55.4,-41.7	83.2% (<i>t</i>) chi angles: 174.8	0.091Å	-	OUTLIER(S) worst is C-N- CA: 4.172 σ
397	(GLY	85.56	-	Favored (22.75%) Glycine / 161.8,-152.3	-	-	-	-
398	A	ASN	234.3	0.874Å HB3 with 403 ILE HG21	Favored (27.32%) General / -116.7,156.3	22.9% (<i>m120</i>) chi angles: 291.6,135.3	0.125Å	-	-
399	\	√AL	312.24	0.666Å H with 403 ILE HD12	Favored (23.27%) Isoleucine or valine /-139.1,151.3	10.3% (p) chi angles: 61	0.086Å	-	-
400	(GLY	237.9	0.456Å N with 399 VAL HG22	Favored (26.29%) Glycine / 93.1,150.2	-	-	-	-
401	Š	SER	107.83	-	Favored (71.22%) General /	68.6% (<i>m</i>) chi angles: 298	0.151Å	-	-

402	MET 61.05	-	-66.6,-30.9 Favored (83.21%) General / -61.9,-47.8	66.1% (<i>mtt</i>) chi angles: 297.4,181.4,182.3	0.081Å	-	-
403	ILE 39.23	0.874Å HG21 with 398 ASN HB3	Favored (84.01%) Isoleucine or valine / -68.1,-45.0	96.8% (<i>mt</i>) chi angles: 297.3,173.2	0.082Å	-	-
404	SER 66.61	-	Favored (95.94%) General / -60.7,-41.8	48% (<i>t</i>) chi angles: 179.7	0.074Å	-	-
405	ASN 55.67	-	Favored (74.52%) General / -63.6,-32.9	62.6% (<i>m</i> -20) chi angles: 277.4,322.2	0.085Å	-	OUTLIER(S) worst is CA- CB-CG: 5.48 σ
406	MET 62.26	-	Favored (87.59%) General / -58.4,-42.8	43.6% (<i>ttm</i>) chi angles: 193.2,180.2,301.1	0.1Å	-	-
407	ASN 17.55	-	-	69.7% (<i>m-80</i>) chi angles: 288.2,298.7	0.115Å	-	OUTLIER(S) worst is CA- CB-CG: 4.409 σ

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