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All-Atom Contacts	Clashscore, all atoms:	1.21		99th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	4	3.85%	Goal: <1%
	Ramachandran outliers	4	3.45%	Goal: <0.05%
	Ramachandran favored	87	75.00%	Goal: >98%
	MolProbity score$^\wedge$	2.08		72nd percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	1	0.93%	Goal: 0
	Bad backbone bonds:	0 / 906	0.00%	Goal: 0%
	Bad backbone angles:	9 / 1235	0.73%	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.

$^\wedge$ 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: 60.17	Clashscore: 1.21	Outliers: 4 of 116	Poor rotamers: 4 of 104	Outliers: 1 of 107	Outliers: 0 of 118	Outliers: 8 of 118
A 307		SER	50	-	-	28.1% (*t*) chi angles: 185.3	0.047Å	-	-
A 308		LYS	99.99	-	Favored (41.42%) Pre-proline / -54.2,123.3	15.4% (*mtpt*) chi angles: 300,212.8,77.9,193.4	0.079Å	-	-
A 309		PRO	50	-	Allowed (0.22%) Trans-proline / -95.0,-22.2	9.7% (*Cg_endo*) chi angles: 40.3	0.017Å	-	-
A 310		CYS	50	0.435Å HA with A 335 GLN O	Favored (23.86%) General / -87.6,150.2	30.7% (*p*) chi angles: 65.6	0.043Å	-	-

A 311	HIS	50	-	Allowed (0.21%) General / -97.5,-131.9	2.4% (*m80*) chi angles: 327.5,103.3	0.278Å	-	OUTLIER(S) worst is C-N-CA: 4.73 σ
A 312	ASN	50	-	Allowed (0.16%) General / -32.3,114.8	2% (*m-20*) chi angles: 298.1,37	0.053Å	-	OUTLIER(S) worst is C-N-CA: 6.416 σ
A 313	ASN	50	-	OUTLIER (0%) General / 49.5,-19.4	35.9% (*m-20*) chi angles: 305.2,343.7	0.205Å	-	-
A 314	ALA	50	-	Favored (7.69%) General / -52.2,147.5	-	0.063Å	-	-
A 315	THR	50	-	Favored (17.8%) General / -86.3,163.2	40.3% (*p*) chi angles: 53.7	0.098Å	-	-
A 316	CYS	50	-	Favored (39.06%) General / -124.4,122.9	36.7% (*t*) chi angles: 174.4	0.101Å	-	-
A 317	GLU	50	-	Favored (7.45%) General / -106.4,97.7	3.6% (*mp0*) chi angles: 307.2,56.4,65.3	0.056Å	-	-
A 318	ASP	50	-	Favored (49.48%) General / -65.1,132.6	3% (*m-20*) chi angles: 288.7,34.2	0.048Å	-	-
A 319	SER	50	-	Favored (9.24%) General / -132.7,175.5	30.2% (*t*) chi angles: 172.9	0.11Å	-	-
A 320	VAL	50	-	Favored (29.93%) Isoleucine or valine / -64.5,133.6	1.7% (*p*) chi angles: 83.8	0.094Å	-	-
A 321	ASP	50	-	Allowed (0.71%) General / 61.4,3.0	3.1% (*m-20*) chi angles: 319.8,327.8	0.12Å	-	-
A 322	ASN	99.99	-	Favored (41.09%) General / -152.3,162.5	36.5% (*m-80*) chi angles: 293.2,268.1	0.1Å	-	-
A 323	TYR	99.99	-	Favored (3.88%) General / -147.5,106.8	65.7% (*m-85*) chi angles: 306.2,282.4	0.104Å	-	-
A 324	THR	50	-	Favored (27.26%) General /	60.9% (*p*) chi angles: 56.6	0.172Å	-	-

-80.0,156.2

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 325		CYS	50	0.421Å SG with A 310 CYS HB3	Allowed (1%) General / -113.4,76.8	60.3% (*m*) chi angles: 304.3	0.039Å	-	-
A 326		HIS	50	-	Allowed (1.64%) General / -69.5,101.6	3% (*t-80*) chi angles: 157.5,272.6	0.114Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 60.17	Clashscore: 1.21	Outliers: 4 of 116	Poor rotamers: 4 of 104	Outliers: 1 of 107	Outliers: 0 of 118	Outliers: 8 of 118
A 327		CYS	50	-	Favored (2.75%) General / -64.4,172.2	25.8% (*m*) chi angles: 310.9	0.065Å	-	-
A 328		TRP	50	-	Allowed (1.72%) Pre-proline / -117.6,176.2	65.4% (*m95*) chi angles: 306.4,96	0.068Å	-	OUTLIER(S) worst is CE3-CD2-CG: 4.164 σ
A 329		PRO	50	-	Favored (5.45%) Trans-proline / -70.1,118.0	56% (*Cg_endo*) chi angles: 25.8	0.015Å	-	-
A 330		GLY	50	-	Favored (6.04%) Glycine / 128.6,-15.0	-	-	-	-
A 331		TYR	50	-	Favored (29.5%) General / -136.7,128.7	10.1% (*m-85*) chi angles: 320.3,291.3	0.065Å	-	-
A 332		THR	50	-	Allowed (1.22%) General / -137.8,-161.8	7.4% (*t*) chi angles: 193.8	0.214Å	-	-
A 333		GLY	50	-	Favored (32.67%) Glycine / 89.8,-166.3	-	-	-	-
A 334		ALA	50	-	Favored (29.92%) General / -85.7,-20.1	-	0.063Å	-	-
A 335		GLN	50	0.435Å O with A 310 CYS HA	Allowed (1.16%) General / -146.5,26.4	7.4% (*mm-40*) chi angles: 293.7,285.1,255.1	0.04Å	-	-
A 336		CYS	50	-	Favored (7.43%) General / 54.1,56.1	41.1% (*m*) chi angles: 307.4	0.174Å	-	OUTLIER(S) worst is C-N-CA: 5.304 σ

A 337	GLU	50	-	Favored (12.42%) General / -112.4,-18.6	7.2% (*pm0*) chi angles: 73.5,289.9,35.6	0.093Å	-	OUTLIER(S) worst is CB-CG-CD: 4.515 σ
A 338	ILE	50	-	Allowed (1.7%) Isoleucine or valine / -107.4,91.2	39% (*mt*) chi angles: 306.7,181.3	0.037Å	-	-
A 339	ASP	50	-	Favored (4.22%) General / -65.8,171.6	3% (*m-20*) chi angles: 294.5,30.4	0.082Å	-	-
A 340	LEU	50	-	Favored (12.86%) General / -82.5,172.6	1.1% (*mp*) chi angles: 244.6,68.5	0.11Å	-	-
A 341	ASN	50	-	Allowed (0.66%) General / -168.3,114.1	9.3% (*t-20*) chi angles: 172.2,295.3	0.065Å	-	-
A 342	GLU	50	-	Favored (59.26%) General / -79.0,-14.3	45.4% (*mp0*) chi angles: 298.1,71.7,14.4	0.114Å	-	-
A 343	CYS	50	-	Favored (60.21%) General / -72.2,-10.8	32.2% (*m*) chi angles: 309.7	0.121Å	-	-
A 344	ASN	50	-	Favored (64.88%) General / -55.8,-34.1	52.1% (*p-10*) chi angles: 65,357.3	0.129Å	-	-
A 345	SER	50	-	Favored (52.28%) General / -94.3,-2.4	12.2% (*t*) chi angles: 191.1	0.074Å	-	-
A 346	ASN	50	-	Favored (4.67%) Pre-proline / 53.7,48.2	7% (*m120*) chi angles: 308.2,155	0.036Å	-	OUTLIER(S) worst is CA-CB-CG: 6.741 σ

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 60.17	Clashscore: 1.21	Outliers: 4 of 116	Poor rotamers: 4 of 104	Outliers: 1 of 107	Outliers: 0 of 118	Outliers: 8 of 118
A 347		PRO	50	-	Allowed (1.89%) Trans-proline / -81.6,45.1	0.1% chi angles: 46.1	0.086Å	-	-
A 348		CYS	50	-	Favored (47.77%) General /	96.1% (*m*) chi angles: 294	0.111Å	-	-

				-128.8,153.1				
A 349	GLN	50	-	Favored (6.72%) General / -116.8,173.3	4.4% (*tt0*) chi angles: 207.1,193.3,252.8	0.105Å	-	-
A 350	SER	50	-	Favored (4.83%) General / 55.9,21.3	74% (*m*) chi angles: 295.1	0.106Å	-	-
A 351	ASN	50	-	Allowed (1.74%) General / 74.6,24.3	12% (*m-80*) chi angles: 314.6,279.1	0.14Å	-	-
A 352	GLY	50	-	Favored (52.71%) Glycine / -77.8,165.8	-	-	-	-
A 353	GLU	50	-	Favored (38.95%) General / -113.0,146.5	0% chi angles: 164.5,267.6,40.4	0.121Å	-	-
A 354	CYS	50	-	Favored (13.38%) General / -115.5,165.1	49.9% (*t*) chi angles: 186.5	0.06Å	-	-
A 355	VAL	50	-	Allowed (1.52%) Isoleucine or valine / -98.1,169.4	1.1% (*p*) chi angles: 86.4	0.104Å	-	-
A 356	GLU	50	-	Favored (19.27%) General / -119.2,112.2	38.1% (*tt0*) chi angles: 178,179.2,93.2	0.088Å	-	-
A 357	LEU	50	-	Favored (4.45%) General / -143.2,-175.2	65.2% (*mt*) chi angles: 289.9,179.9	0.06Å	-	-
A 358	SER	50	-	Allowed (1.17%) General / -96.5,51.2	30.6% (*t*) chi angles: 173.1	0.068Å	-	-
A 359	SER	50	-	OUTLIER (0%) General / 96.3,36.6	29.7% (*t*) chi angles: 185	0.208Å	-	-
A 360	GLU	50	-	Favored (39.43%) General / -144.5,151.6	8.9% (*tp10*) chi angles: 174.9,59.7,96.4	0.077Å	-	-
A 361	LYS	50	-	Allowed (0.28%) General / -157.4,32.4	0% chi angles: 57.3,146.1,265.2,65	0.208Å	-	-
A				Favored (7.36%)	21% (*mm100*)			

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
362		GLN	50	-	General / -126.2,9.4	chi angles: 301.3,310.4,139.1	0.12Å	-	-
363	A	TYR	99.99	-	Favored (20.99%) General / -50.4,128.9	6.3% (*t80*) chi angles: 165.7,45.5	0.042Å	-	-
364	A	GLY	99.99	-	Favored (2.07%) Glycine / -88.2,95.2	-	-	-	-
365	A	ARG	99.99	-	Favored (56.35%) General / -59.7,140.6	53.3% (*mtm180*) chi angles: 290,180.3,288.8,204.9	0.034Å	-	-
366	A	ILE	99.99	-	Favored (21.06%) Isoleucine or valine / -140.4,151.3	1.3% (*mt*) chi angles: 266,155.9	0.164Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 60.17	Clashscore: 1.21	Outliers: 4 of 116	Poor rotamers: 4 of 104	Outliers: 1 of 107	Outliers: 0 of 118	Outliers: 8 of 118
367	A	THR	99.99	-	Favored (2.11%) General / -139.4,31.1	52.8% (*p*) chi angles: 65.6	0.093Å	-	-
368	A	GLY	99.99	-	Favored (45.96%) Glycine / -54.5,134.8	-	-	-	-
369	A	LEU	99.99	-	Favored (13.55%) Pre-proline / -134.7,98.3	26.8% (*mt*) chi angles: 310,170.2	0.045Å	-	-
370	A	PRO	99.99	-	Favored (3.67%) Trans-proline / -91.2,149.1	24.3% (*Cg_endo*) chi angles: 38	0.056Å	-	-
371	A	SER	99.99	-	Allowed (0.33%) General / -140.3,-150.7	22.2% (*p*) chi angles: 80	0.139Å	-	-
372	A	SER	99.99	-	Favored (15.75%) General / -106.0,-12.6	30.5% (*p*) chi angles: 52.2	0.047Å	-	-
373	A	PHE	99.99	-	Favored (3.87%) General / -132.1,1.1	15.9% (*m-30*) chi angles: 309.4,311.1	0.043Å	-	-
					Allowed				

#	Alt	Res	High	Clash >	Ramachandran	Rotamer	Cβ	Bond	Bond angles
A 374		SER	99.99	-	(0.89%) General / -178.1,154.6	16.6% (*t*) chi angles: 189.6	0.039Å	-	-
A 375		TYR	99.99	-	Favored (3.91%) General / -145.8,104.9	61.7% (*m-85*) chi angles: 305,87.1	0.063Å	-	-
A 376		HIS	99.99	-	Favored (22.41%) General / -89.0,151.2	10.7% (*t-80*) chi angles: 164.3,273.3	0.052Å	-	-
A 377		GLU	99.99	-	Favored (39.59%) General / -152.2,163.3	7.9% (*tp10*) chi angles: 185.4,48.7,92.9	0.068Å	-	OUTLIER(S) worst is C-N-CA: 4.811 σ
A 378		ALA	99.99	-	OUTLIER (0.04%) General / 179.1,114.1	-	0.036Å	-	-
A 379		SER	99.99	-	Favored (10.69%) General / -101.2,166.6	24.4% (*p*) chi angles: 51.1	0.066Å	-	-
A 380		GLY	99.99	-	Allowed (0.4%) Glycine / -153.1,60.2	-	-	-	-
A 381		TYR	99.99	-	Favored (12.78%) General / -49.0,137.6	96% (*m-85*) chi angles: 294.1,268.1	0.087Å	-	-
A 382		VAL	99.99	-	Favored (3.53%) Isoleucine or valine / -85.2,154.4	15% (*m*) chi angles: 289.4	0.123Å	-	-
A 383		CYS	50	-	Favored (50.01%) General / -60.6,131.2	99% (*m*) chi angles: 294.6	0.068Å	-	-
A 384		ILE	50	-	Favored (41.6%) Isoleucine or valine / -88.3,126.1	12.4% (*tt*) chi angles: 199.1,175	0.138Å	-	-
A 385		CYS	50	-	Favored (22.1%) General / -83.6,157.9	15.7% (*m*) chi angles: 313.2	0.04Å	-	-
A 386		GLN	50	-	Favored (91.41%) Pre-proline / -72.6,154.8	62.9% (*mm-40*) chi angles: 289.5,296.2,342.2	0.057Å	-	-

		B Avg: 60.17	0.4Å Clashscore: 1.21	Outliers: 4 of 116	Poor rotamers: 4 of 104	deviation Outliers: 1 of 107	lengths Outliers: 0 of 118	Outliers: 8 of 118
A 387	PRO	50	-	Favored (7.05%) Trans-proline / -53.5,120.0	3.6% (*Cg_exo*) chi angles: 321.8	0.057Å	-	-
A 388	GLY	50	-	Favored (11.06%) Glycine / 121.0,-6.2	-	-	-	-
A 389	PHE	50	-	Favored (51.12%) General / -134.4,154.9	45.7% (*m-85*) chi angles: 308.9,92.7	0.04Å	-	-
A 390	THR	50	-	Allowed (0.24%) General / -127.6,-134.8	15.2% (*p*) chi angles: 46.1	0.205Å	-	-
A 391	GLY	50	-	Favored (45.45%) Glycine / 63.9,-155.3	-	-	-	-
A 392	ILE	50	-	Favored (9.83%) Isoleucine or valine / -120.8,-10.7	45.1% (*pt*) chi angles: 62,174.6	0.197Å	-	-
A 393	HIS	50	-	Favored (10.87%) General / -120.5,9.2	52% (*m80*) chi angles: 305.6,82.1	0.084Å	-	-
A 394	CYS	50	-	Allowed (1.28%) General / 74.1,30.0	1.8% (*m*) chi angles: 328.6	0.158Å	-	-
A 395	GLU	50	-	Favored (13.52%) General / -97.2,-29.5	2.9% (*pm0*) chi angles: 70.8,279.3,61.5	0.171Å	-	-
A 396	GLU	50	-	Favored (28.01%) General / -83.0,147.7	36.9% (*tt0*) chi angles: 190.2,178.1,61.4	0.144Å	-	-
A 397	ASP	50	-	Favored (30.52%) General / -89.8,139.5	35.8% (*t0*) chi angles: 183,207.1	0.044Å	-	-
A 398	VAL	50	-	Favored (2.79%) Isoleucine or valine / -78.9,98.6	8.8% (*p*) chi angles: 73.2	0.205Å	-	-

A	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 399	ASN	50	-	Favored (4.59%) General / -78.7,89.6	59.2% (*t30*) chi angles: 191.6,49.7	0.095Å	-	-
A 400	GLU	50	-	Favored (70.74%) General / -59.6,-32.8	1.9% (*mp0*) chi angles: 275.7,59.1,79.1	0.103Å	-	-
A 401	CYS	50	-	Favored (4.79%) General / -51.2,-25.1	57.7% (*m*) chi angles: 285.4	0.178Å	-	-
A 402	SER	50	-	Favored (63.81%) General / -55.2,-34.4	16.5% (*m*) chi angles: 307.6	0.089Å	-	-
A 403	SER	50	-	Favored (45.35%) General / -78.7,-27.9	82.8% (*p*) chi angles: 69.3	0.12Å	-	-
A 404	ASN	50	-	Favored (2.5%) Pre-proline / 54.3,45.8	39.8% (*m-80*) chi angles: 295.3,269.6	0.059Å	-	-
A 405	PRO	50	-	Allowed (0.52%) Trans-proline / -79.9,28.4	0.2% chi angles: 44.2	0.054Å	-	-
A 406	CYS	50	-	Favored (10.8%) General / -85.1,72.2	91% (*m*) chi angles: 293.4	0.058Å	-	-

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			Avg: 60.17	Clashscore: 1.21	Outliers: 4 of 116	Poor rotamers: 4 of 104	Outliers: 1 of 107	Outliers: 0 of 118	Outliers: 8 of 118
A 407		GLN	50	-	Favored (37.19%) General / -56.5,128.7	8.8% (*tp-100*) chi angles: 184.7,54.9,258.7	0.036Å	-	OUTLIER(S) worst is C-N-CA: 4.177 σ
A 408		ASN	50	-	OUTLIER (0.02%) General / 104.1,-2.8	26% (*m-20*) chi angles: 303.8,354	0.206Å	-	-
A 409		GLY	50	-	Favored (9.34%) Glycine / 96.4,28.1	-	-	-	-
A 410		GLY	50	-	Favored (54.42%) Glycine / -80.0,171.5	-	-	-	-
					Favored				

A 411	THR	50	-	(26.87%) General / -92.4,142.9	85.1% (*m*) chi angles: 301.4	0.052Å	-	-
A 412	CYS	50	-	Favored (33.54%) General / -99.9,140.8	2.3% (*t*) chi angles: 208.1	0.043Å	-	-
A 413	GLU	50	-	Favored (51.13%) General / -128.7,142.1	35.3% (*tt0*) chi angles: 192.8,174.4,74.6	0.134Å	-	-
A 414	ASN	50	-	Favored (35.89%) General / -113.7,148.7	6.1% (*t30*) chi angles: 207,72.6	0.131Å	-	-
A 415	LEU	50	-	Favored (8.85%) Pre-proline / -134.9,171.5	14% (*mt*) chi angles: 315.8,168.4	0.048Å	-	-
A 416	PRO	50	-	Allowed (0.59%) Trans-proline / -66.5,102.3	9.5% (*Cg_endo*) chi angles: 11	0.03Å	-	-
A 417	GLY	50	-	Favored (5.47%) Glycine / 92.0,39.4	-	-	-	-
A 418	ASN	50	-	Allowed (0.77%) General / -171.5,132.8	23.5% (*t-20*) chi angles: 172.6,255.2	0.115Å	-	-
A 419	TYR	50	-	Favored (47.18%) General / -107.8,136.6	44.1% (*p90*) chi angles: 55.2,269.8	0.047Å	-	-
A 420	THR	50	-	Favored (8.22%) General / -115.5,100.7	24.2% (*m*) chi angles: 291.4	0.058Å	-	-
A 421	CYS	50	-	Favored (12.86%) General / -63.1,121.1	76.5% (*m*) chi angles: 296.4	0.073Å	-	-
A 422	HIS	50	-	Allowed (0.92%) General / -104.6,70.0	2.6% (*m80*) chi angles: 288.9,42.8	0.03Å	-	-
A 423	CYS	50	-	Favored (24.16%) Pre-proline / -104.4,161.0	71.4% (*m*) chi angles: 297.3	0.09Å	-	-

| A 424 | PRO 99.99 | - | - | 10.4% (*Cg_endo*) chi angles: 40.2 | 0.074Å | - | - |