Viewing lrat_mb_48-171_FFX1H-multi.table

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All-Atom Contacts	Clashscore, all atoms:	0		100th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	12	11.11%	Goal: <1%
	Ramachandran outliers	7	5.74%	Goal: <0.05%
	Ramachandran favored	91	74.59%	Goal: >98%
	MolProbity score^	2.09		71st percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	2	1.72%	Goal: 0
	Bad backbone bonds:	0 / 1008	0.00%	Goal: 0%
	Bad backbone angles:	16 / 1367	1.17%	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: 121.40	Clashscore: 0	Outliers: 7 of 122	Poor rotamers: 12 of 108	Outliers: 2 of 116	Outliers: 0 of 124	Outliers: 16 of 124
48		GLY	19.77	-	-	-	-	-	-
49		ASP	40.91	-	Favored (36.37%) General / -132.8,128.2	7.2% (*m-20*) chi angles: 312.5,98.4	0.1Å	-	-
50		VAL	40.19	-	Favored (5.65%) Isoleucine or valine / -83.3,147.7	87.8% (*t*) chi angles: 177.2	0.107Å	-	-
51		LEU	89.53	-	Favored (32.89%) General / -131.4,161.2	0.8% chi angles: 310.2,315.6	0.136Å	-	-
					Favored	14.6% (*tt0*)			

52	GLU	66.24	-	(43.22%) General / -121.8,149.5	chi angles: 197.2,198.8,254.6	0.08Å	-	-
53	VAL	115.58	-	Favored (8.39%) Pre-proline / -149.5,66.6	8.7% (p) chi angles: 60	0.174Å	-	-
54	PRO	97.7	-	Favored (17.94%) Trans-proline / -75.7,171.6	0.4% chi angles: 43.1	0.086Å	-	-
55	ARG	94.79	-	Allowed (1.62%) General / -124.4,-167.3	1.4% ($mmt85$) chi angles: 315.2,297.5,147.1,118.9	0.153Å	-	-
56	THR	125.76	-	Allowed (0.36%) General / -68.4,90.0	30% (p) chi angles: 51.2	0.027Å	-	-
57	HIS	102.68	-	Allowed (0.71%) General / 77.4,26.1	26.6% (t-80) chi angles: 203.8,296.6	0.129Å	-	-
58	LEU	109.81	-	Favored (36.97%) General / -131.7,127.5	5% (mp) chi angles: 279.2,87.6	0.063Å	-	-
59	THR	133.72	-	Favored (7.3%) General / -84.7,179.7	30.3% (p) chi angles: 51.3	0.041Å	-	OUTLIER(S) worst is C-N-CA: 5.306 σ
60	HIS	72.48	-	OUTLIER (0%) General / 141.1,138.1	7.2% ($m80$) chi angles: 267,72.7	0.178Å	-	OUTLIER(S) worst is N-CA-CB: 4.144 σ
61	TYR	127.89	-	Favored (4.14%) General / -112.8,178.9	56.3% (m-85) chi angles: 300.5,78.5	0.09Å	-	OUTLIER(S) worst is C-N-CA: 4.753 σ
62	GLY	40.23	-	Favored (23.09%) Glycine / -135.8,170.5	-	-	-	-
63	ILE	59.43	-	Allowed (0.53%) Isoleucine or valine / -149.3,109.8	17.9% (tt) chi angles: 195,166.8	0.181Å	-	OUTLIER(S) worst is C-N-CA: 4.227 σ
64	TYR	91.16	-	Favored (49.59%) General / -71.8,143.3	9.5% ($t80$) chi angles: 203.6,65.7	0.057Å	-	OUTLIER(S) worst is C-N-CA: 4.039 σ

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
65		LEU	181.96	-	Favored (2.1%) General / -139.1,41.7	1.5% (*tt*) chi angles: 191,128.9	0.088Å	-	-
66		GLY	43.05	-	Favored (49.13%) Glycine / 77.0,179.8	-	-	-	OUTLIER(S) worst is C-N-CA: 4.239 σ
67		ASP	62.4	-	OUTLIER (0.01%) General / -15.8,99.4	5.1% (*t70*) chi angles: 165.1,46.9	0.047Å	-	-

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			Avg: 121.40	Clashscore: 0	Outliers: 7 of 122	Poor rotamers: 12 of 108	Outliers: 2 of 116	Outliers: 0 of 124	Outliers: 16 of 124
68		ASN	105.13	-	Allowed (0.11%) General / 65.6,-16.1	23.9% (*m-80*) chi angles: 277.5,269.4	0.095Å	-	-
69		ARG	70.79	-	Favored (31.61%) General / -85.3,124.2	1.1% (*mtt-85*) chi angles: 306.1,129.1,205.8,241.2	0.082Å	-	OUTLIER(S) worst is CD-NE-CZ: 4.137 σ
70		VAL	103.07	-	Favored (17.8%) Isoleucine or valine / -143.0,161.0	0.8% chi angles: 340.1	0.183Å	-	-
71		ALA	56.32	-	Favored (2.55%) General / -116.6,-174.3	-	0.031Å	-	-
72		HIS	105.13	-	OUTLIER (0.01%) General / 154.0,159.3	0.3% chi angles: 46.7,197.1	0.146Å	-	-
73		MET	100.8	-	Favored (7.02%) General / -63.3,117.7	12.9% (*mtm*) chi angles: 308.1,214.6,294.3	0.036Å	-	-
74		MET	162.56	-	Favored (2.72%) Pre-proline / -65.3,172.1	13.9% (*mtt*) chi angles: 279.1,194.2,149.7	0.095Å	-	-
75		PRO	169.97	-	Favored (3.48%) Trans-proline / -46.1,147.6	0% chi angles: 314.9	0.067Å	-	-

76	ASP 306.78	-	Allowed (0.42%) General / -176.0,140.6	54.2% (*t0*) chi angles: 186.8,11.7	0.067Å	-	-
77	ILE 145.25	-	OUTLIER (0.03%) Isoleucine or valine / -172.2,116.8	10.5% (*tt*) chi angles: 176.7,160.8	0.087Å	-	-
78	LEU 139.88	-	Favored (60.17%) General / -74.2,-11.0	19.5% (*tp*) chi angles: 183.5,49	0.098Å	-	-
79	LEU 138.96	-	Favored (58.36%) General / -75.5,-21.0	6.3% (*tt*) chi angles: 185.2,138.5	0.092Å	-	-
80	ALA 216.28	-	Favored (23.22%) General / -81.1,163.3	-	0.039Å	-	-
81	LEU 209.12	-	Allowed (0.15%) General / -135.6,-131.7	71.9% (*mt*) chi angles: 302.7,173.4	0.15Å	-	-
82	THR 185.98	-	Favored (7.25%) General / -87.0,85.3	43.3% (*p*) chi angles: 54.8	0.022Å	-	-
83	ASP 215.57	-	Allowed (0.71%) General / -133.1,-155.9	5.1% (*p30*) chi angles: 44.3,36.7	0.229Å	-	OUTLIER(S) worst is C-CA-CB: 4.288 σ
84	ASP 231.79	-	Allowed (1.02%) General / -69.7,97.0	10.4% (*p-10*) chi angles: 49,320.5	0.176Å	-	OUTLIER(S) worst is CA-CB-CG: 4.983 σ
85	MET 286.26	-	Allowed (0.38%) General / -35.2,117.0	57.2% (*mtt*) chi angles: 294,190,179.2	0.044Å	-	-
86	GLY 65.7	-	Favored (4.11%) Glycine / 128.3,-29.3	-	-	-	-
87	ARG 191.23	-	Favored (10.99%) General / -76.0,173.7	12.3% (*mmt-85*) chi angles: 316.4,305,171.8,297.1	0.083Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 121.40	Clashscore: 0	Outliers: 7 of 122	Poor rotamers: 12 of 108	Outliers: 2 of 116	Outliers: 0 of 124	Outliers: 16 of 124
88		THR	152.15	-	Allowed (0.57%) General / 177.8,173.4	10% (*t*) chi angles: 181	0.107Å	-	-
89		GLN	104.76	-	Favored (15.92%) General / -109.3,-5.4	2.8% (*mm-40*) chi angles: 312.2,283,249	0.072Å	-	-
90		LYS	93.54	-	Favored (12.32%) General / -146.9,125.3	38.7% (*mmtm*) chi angles: 299.5,296.8,164.4,296.6	0.081Å	-	-
91		VAL	144.05	-	Allowed (0.16%) Isoleucine or valine / -54.1,168.2	22% (*m*) chi angles: 303	0.06Å	-	-
92		VAL	109.11	-	Favored (14.03%) Isoleucine or valine / -136.9,114.8	12.1% (*p*) chi angles: 62.1	0.104Å	-	-
93		SER	100.09	-	Favored (55.81%) General / -68.4,139.8	15.3% (*t*) chi angles: 190	0.134Å	-	-
94		ASN	89.7	-	Favored (10.91%) General / -164.1,150.0	15.5% (*t-20*) chi angles: 206.6,345	0.105Å	-	-
95		LYS	199.01	-	Favored (28.89%) General / -100.1,144.7	6.8% (*mmmm*) chi angles: 281.6,281.4,300.7,304.7	0.135Å	-	-
96		ARG	120.86	-	Favored (5.1%) General / -172.8,163.7	60.9% (*ttt180*) chi angles: 180.2,166.1,175.5,161.2	0.076Å	-	-
97		LEU	114.45	-	Favored (3.28%) General / -76.9,69.9	71% (*mt*) chi angles: 304,181.5	0.061Å	-	-
98		ILE	102.18	-	Favored (21.12%) Isoleucine or valine / -76.5,-32.2	3.4% (*mt*) chi angles: 276.5,141.1	0.18Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
99		LEU	118.92	-	Favored (89.43%) General / -59.6,-46.3	31.5% (*tp*) chi angles: 187.7,57.2	0.114Å	-	-
100		GLY	45.65	-	Favored (27.74%) Glycine / -83.7,-31.1	-	-	-	-
101		VAL	48.1	-	Favored (3.65%) Isoleucine or valine / -100.0,-32.7	60% (*t*) chi angles: 181.1	0.134Å	-	-
102		ILE	111.72	-	Favored (3.01%) Isoleucine or valine / -118.0,-25.2	50.7% (*mm*) chi angles: 302,299.7	0.134Å	-	-
103		VAL	69.6	-	Allowed (1.92%) Isoleucine or valine / -73.7,-61.0	39.6% (*t*) chi angles: 166.3	0.061Å	-	OUTLIER(S) worst is C-N-CA: 4.163 σ
104		LYS	147.47	-	Allowed (0.46%) General / 69.6,-60.9	1.3% (*tpmp?*) chi angles: 186.7,68.5,259.1,77.6	0.212Å	-	-
105		VAL	48.5	-	Allowed (0.17%) Isoleucine or valine / -145.3,-12.3	1.8% (*t*) chi angles: 205.4	0.101Å	-	-
106		ALA	47.63	-	Favored (39.91%) General / -76.9,142.8	-	0.044Å	-	-
107		SER	34.83	-	Favored (24.9%) General / -50.5,132.0	46.1% (*m*) chi angles: 302.3	0.06Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 121.40	Clashscore: 0	Outliers: 7 of 122	Poor rotamers: 12 of 108	Outliers: 2 of 116	Outliers: 0 of 124	Outliers: 16 of 124
108		ILE	149.89	-	Favored (48.13%) Isoleucine or valine / -132.7,140.2	0% chi angles: 182.4,264.5	0.089Å	-	-
109		ARG	71.55	-	Favored (10.81%) General /	14.4% (*ptt-85*) chi angles: 62.9,157.6,193.5,282.2	0.037Å	-	-

				-141.1,174.1			
110	VAL	110.2	-	Favored (4.03%) Isoleucine or valine / -83.7,150.9	18.2% (*m*) chi angles: 291.8	0.085Å	-	-
111	ASP	70.98	-	Allowed (0.86%) General / -151.0,51.8	9.2% (*m-20*) chi angles: 288.4,93.5	0.032Å	-	-
112	THR	83.35	-	Favored (7.56%) General / -81.0,79.9	34.6% (*p*) chi angles: 52.2	0.043Å	-	-
113	VAL	63.91	-	Favored (95.24%) Isoleucine or valine / -59.8,-44.9	54.5% (*t*) chi angles: 170	0.157Å	-	-
114	GLU	108.53	-	Favored (27.34%) General / -83.5,-30.3	11.8% (*mm-40*) chi angles: 309.4,323.2,297.9	0.155Å	-	-
115	ASP	58.89	-	Favored (36.62%) General / -50.0,-38.3	0.7% chi angles: 304.2,47.9	0.166Å	-	-
116	PHE	51.85	-	Favored (32.69%) General / -83.4,-22.6	47.9% (*p90*) chi angles: 66.1,86.7	0.144Å	-	-
117	ALA	39.75	-	Favored (21.19%) General / -80.6,-43.0	-	0.078Å	-	-
118	TYR	96.87	-	Allowed (0.06%) General / 177.8,131.6	6.5% (*t80*) chi angles: 194.7,222.2	0.057Å	-	-
119	GLY	43.94	-	Allowed (0.37%) Glycine / 162.1,-43.3	-	-	-	-
120	ALA	207	-	Favored (16.09%) General / -68.0,166.4	-	0.023Å	-	-
121	ASN	172.2	-	Favored (3.28%) General /	34.9% (*m-20*) chi angles: 295.7,3.2	0.076Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
					-127.1,91.2				
122		ILE	130.78	-	Favored (16.83%) Isoleucine or valine / -57.5,139.6	9.9% (*tp*) chi angles: 194.8,69.8	0.131Å	-	-
123		LEU	105.23	-	Favored (85.56%) General / -58.5,-47.0	2.7% (*tm?*) chi angles: 189.8,275	0.09Å	-	-
124		VAL	97.35	-	Allowed (1.08%) Isoleucine or valine / -93.6,77.0	14.2% (*m*) chi angles: 289.1	0.137Å	-	-
125		ASN	150.15	-	Favored (26.85%) General / -52.7,139.3	43.3% (*t30*) chi angles: 180.3,35.5	0.081Å	-	-
126		HIS	200.48	-	OUTLIER (0.02%) General / -170.1,24.7	26% (*t-80*) chi angles: 204.9,294.9	0.058Å	-	-
127		LEU	275.59	-	Favored (6.03%) General / -129.2,17.6	12.5% (*tp*) chi angles: 201.8,69.7	0.087Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 121.40	Clashscore: 0	Outliers: 7 of 122	Poor rotamers: 12 of 108	Outliers: 2 of 116	Outliers: 0 of 124	Outliers: 16 of 124
128		ASP	178.19	-	Favored (2.42%) General / -71.4,101.5	4.1% (*m-20*) chi angles: 305.7,256.7	0.065Å	-	-
129		GLU	91.62	-	Favored (87.98%) General / -59.9,-40.2	46.3% (*mt-10*) chi angles: 289.9,179.4,249.1	0.101Å	-	OUTLIER(S) worst is C-N-CA: 4.768 σ
130		SER	195.77	-	OUTLIER (0%) General / 123.7,-172.2	8.7% (*t*) chi angles: 193.6	0.214Å	-	-
131		LEU	240.75	-	Allowed (0.11%) General / 53.8,-162.8	14.6% (*mt*) chi angles: 317.5,177.2	0.172Å	-	-
132		GLN	252.3	-	Allowed (1.19%) General /	0% chi angles: 195.3,224.7,239.8	0.057Å	-	-

			-95.0,48.9			
133	LYS 320.84	-	Favored (9.45%) General / -82.8,77.9	23.7% (*mtpt*) chi angles: 300.8,200.2,83.3,195.2	0.083Å	-	OUTLIER(S) worst is C-N-CA: 4.396 σ
134	LYS 153.7	-	Favored (49.34%) General / -133.2,143.6	0% chi angles: 256.5,69.7,230.9,64.5	0.09Å	-	-
135	ALA 44.8	-	Favored (25.42%) General / -63.7,125.8	-	0.027Å	-	-
136	LEU 131.58	-	Favored (21.45%) General / -58.7,151.2	17.9% (*tp*) chi angles: 191,51.7	0.1Å	-	-
137	LEU 47.71	-	Favored (15.28%) General / -50.0,126.9	48.2% (*mt*) chi angles: 306.8,183.9	0.052Å	-	-
138	ASN 98.48	-	Favored (72.7%) General / -61.8,-32.4	1.4% (*t-20*) chi angles: 219.2,285	0.246Å	-	-
139	GLU 78.09	-	Favored (70.58%) General / -57.1,-51.1	2% (*tm-20*) chi angles: 206.4,306.8,307.8	0.036Å	-	-
140	GLU 48.07	-	Favored (93.34%) General / -65.2,-42.8	12.3% (*tp10*) chi angles: 163.7,46.7,31.3	0.139Å	-	-
141	VAL 95.19	-	Favored (72.51%) Isoleucine or valine / -67.8,-35.5	7.4% (*p*) chi angles: 58.9	0.296Å	-	-
142	ALA 36.19	-	Favored (87.53%) General / -66.1,-38.1	-	0.061Å	-	-
143	ARG 92.96	-	Favored (91.08%) General / -63.8,-38.4	15.1% (*ttm-85*) chi angles: 198.8,144.9,293.1,284.7	0.045Å	-	-
144	ARG 144.09	-	Favored (72.96%) General /	20.7% (*ttm180*) chi angles:	0.065Å	-	-

	-67.2,-32.1	195.4,179.1,291.7,202.7			

#	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
145	ALA	38.34	-	Favored (63.38%) General / -56.2,-31.3	-	0.065Å	-	-
146	GLU	67.61	-	Favored (14.38%) General / -99.5,-25.6	95.6% (*mt-10*) chi angles: 290,168.7,354.5	0.065Å	-	-
147	LYS	65.08	-	Favored (69.32%) General / -71.9,-39.6	55.7% (*mtmt*) chi angles: 295.9,178.3,296.3,185.2	0.11Å	-	-

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148		LEU	67.3	-	Favored (7.71%) General / -87.8,81.0	29.7% (*mt*) chi angles: 311.3,183.2	0.076Å	-	-
149		LEU	113.68	-	Favored (28.08%) General / -145.3,140.9	0.7% chi angles: 222.3,170.5	0.118Å	-	-
150		GLY	119.03	-	Favored (50.28%) Glycine / 71.7,-153.4	-	-	-	-
151		PHE	260.89	-	Favored (5.26%) General / -79.8,91.1	0.8% chi angles: 31.2,71.2	0.104Å	-	-
152		THR	311	-	Favored (10.03%) Pre-proline / -161.0,144.9	10% (*t*) chi angles: 181	0.083Å	-	-
153		PRO	236.03	-	Favored (67.91%) Trans-proline / -52.6,-35.6	57.6% (*Cg_exo*) chi angles: 327	0.08Å	-	-
154		TYR	48.95	-	Favored (8.18%) General / -72.0,0.9	15.4% (*m-85*) chi angles: 316.7,103.3	0.067Å	-	OUTLIER(S) worst is C-N-CA: 4.33 σ
155		SER	151.91	-	Favored (4.61%)	40.4% (*t*)	0.108Å	-	-

			General / -130.9,6.3	chi angles: 181.4			
156	LEU 156.92	-	Favored (4.57%) General / -131.2,29.9	12.2% (*tp*) chi angles: 199.9,73.5	0.075Å	-	-
157	LEU 152.31	-	Allowed (0.83%) General / -64.7,178.0	7.7% (*mp*) chi angles: 287.6,67.7	0.074Å	-	-
158	TRP 230.38	-	Favored (13.37%) General / -113.6,-6.4	4.2% (*t90*) chi angles: 199.1,348.5	0.082Å	-	OUTLIER(S) worst is CE3- CD2-CG: 4.419 σ
159	ASN 387.79	-	OUTLIER (0.04%) General / 170.1,-179.9	8.6% (*p30*) chi angles: 55,82	0.097Å	-	-
160	ASN 289.26	-	Allowed (0.98%) General / 67.2,50.6	11.1% (*m-80*) chi angles: 269.8,270.3	0.17Å	-	-
161	CYS 154.33	-	Favored (71.6%) General / -59.9,-33.3	26.6% (*t*) chi angles: 190.3	0.144Å	-	OUTLIER(S) worst is C-N- CA: 6.29 σ
162	GLU 117.13	-	Allowed (1.27%) General / -39.7,-58.7	24.5% (*mp0*) chi angles: 293.8,73.1,340.1	0.063Å	-	OUTLIER(S) worst is CB- CG-CD: 6.349 σ
163	HIS 62.73	-	Favored (22.17%) General / -93.0,-18.9	77.5% (*m80*) chi angles: 294.1,91.9	0.212Å	-	-
164	PHE 69.17	-	Favored (72.77%) General / -58.7,-50.8	7.3% (*t80*) chi angles: 168.3,102	0.049Å	-	-
165	VAL 53.03	-	Favored (78.33%) Isoleucine or valine / -67.5,-37.2	30.4% (*m*) chi angles: 294.8	0.231Å	-	-
166	THR 37.87	-	Favored (68.99%) General / -63.5,-50.6	0.8% chi angles: 210.4	0.268Å	-	-
167	TYR 41.1	-	Favored (64.89%)	29.5% (*t80*) chi angles: 165,65.6	0.068Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 121.40	Clashscore: 0	Outliers: 7 of 122	Poor rotamers: 12 of 108	Outliers: 2 of 116	Outliers: 0 of 124	Outliers: 16 of 124
168		CYS	50.61	-	General / -53.4,-40.1 Favored (16.99%) General / -49.2,-35.2	63.7% (*m*) chi angles: 286.7	0.119Å	-	-
169		ARG	198.4	-	Favored (21.83%) General / -108.4,17.7	6.6% (*ptm105*) chi angles: 73.4,175.5,292.7,95.8	0.174Å	-	-
170		TYR	89.72	-	Favored (2.99%) General / -124.8,-33.0	7.2% (*m-85*) chi angles: 322,297.9	0.164Å	-	-
171		GLY	19.75	-	-	-	-	-	-

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