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All-Atom	Clashscore, all atoms:	1.52		99 th percentile* (N=1784, all resolutions)		
Contacts	Clashscore is the number	of serious s	steric ove	rlaps (> 0.4 Å) per 1000 atoms.		
i	Poor rotamers	5	4.35%	Goal: <1%		
	Ramachandran outliers	4	3.05%	Goal: <0.05%		
	Ramachandran favored	113 86.26%		Goal: >98%		
Protein Geometry	MolProbity score [^]	2.01		75 th percentile [*] (N=27675, 0Å - 99Å)		
Geometry	Cβ deviations >0.25Å	4	3.28%	Goal: 0		
	Bad backbone bonds:	0 / 1038 0.00%		Goal: 0%		
	Bad backbone angles:	10 / 1403 0.71%		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:	Clashscore:	Outliers: 4 of	Poor rotamers: 5 of	Outliers:	Outliers:	Outliers: 10
			54.96	1.52	131	115	4 of 122	0 of 133	of 133
A 4		SER	50	-	-	6.3% (p) chi angles: 44.3	0.153Å	-	-
A 5		HIS	50	-	Favored (37.35%) General / -96.0,135.8	46.9% (<i>p-80</i>) chi angles: 65.1,270.9	0.1Å	-	OUTLIER(S) worst is CA- CB-CG: 4.625 σ
A 6		SER	50	-	Favored (44.44%) General / -67.7,153.1	74.3% (m) chi angles: 294.1	0.059Å	-	-
A 7		GLY	50	-	Favored (21.05%) Glycine / -130.2,169.6 Favored	-	-	-	-
ΛΩ		\/ \/ I	50		(29.72%)	84.6% (t)	0 075 Å		

^{* 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.

Λ 0	V∕\L	JU	-	Isoleucine or valine / -123.3,145.8	chi angles: 177.5	U.U/ J/\	-	-
A 9	ASN	50	0.432Å HB2 with C2019 DGU OP2	Favored (4.6%) General / -104.3,178.3	24.2% (<i>p30</i>) chi angles: 52.9,40.4	0.096Å	-	OUTLIER(S) worst is CA- CB-CG: 4.258 σ
A 10	GLN	50	-	Favored (61.89%) General / -72.3,-17.2	32.8% (<i>mt-30</i>) chi angles: 282.7,177.6,110.3	0.076Å	-	-
A 11	LEU	50	-	Favored (47.83%) General / -80.6,-18.6	4.7% (mp) chi angles: 302.1,92.9	0.101Å	-	-
A 12	GLY	50	-	Favored (57.21%) Glycine / 96.5,8.7	-	-	-	-
A 13	GLY	50	-	Favored (46.47%) Glycine / -89.0,-177.0	-	-	-	-
A 14	VAL	50	-	Favored (33.85%) Isoleucine or valine / -128.3,150.2	6.7% (<i>m</i>) chi angles: 286.2	0.042Å	-	-
A 15	PHE	50	-	Favored (2.8%) General / -143.4,-168.4	18.5% (<i>p90</i>) chi angles: 72.5,285.6	0.069Å	-	-
A 16	VAL	50	-	Favored (48.48%) Isoleucine or valine / -136.5,136.7	75.8% (<i>t</i>) chi angles: 174.1	0.07Å	-	-
A 17	ASN	50	-	Favored (36.23%) General / -76.4,152.3	19.7% (<i>t30</i>) chi angles: 203.6,58.1	0.026Å	-	-
A 18	GLY	50	-	Favored (36.66%) Glycine / 55.4,24.0	-	-	-	-
A 19	ARG	50	-	Favored (37.88%) Pre-proline / -148.6,159.8	27.2% (mmm180) chi angles: 293.6,302.3,292.9,177.7	0.037Å	-	-
A 20	PR∩	50	-	Favored	5.5% (<i>Cg_exo</i>)	∩ ∩44Å	_	-

1140	1 NO	50		(1/.33/0) Trans-proline/ -79.5,144.0	chi angles: 356.4	0.011/1		
A 21	LEU	50	-	Favored (67.54%) Pre-proline / -56.7,125.3	17.1% (<i>tp</i>) chi angles: 195.9,68.2	0.057Å	-	-
A 22	PRO	50	-	Favored (48.38%) Trans-proline / -55.2,148.7	0.1% chi angles: 318.2	0.055Å	-	-
A 23	ASP	50	-	Allowed (0.45%) General / -48.2,-21.2	9.3% (<i>m-20</i>) chi angles: 307.3,353.7	0.137Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C β deviation	Bond lengths	Bond angles
		Avg: 54.96	Clashscore: 1.52	Outliers: 4 of 131	Poor rotamers: 5 of 115		Outliers:	Outliers: 10 of 133
A 24	SER	50	-	Favored (56.54%) General / -50.4,-46.4	52.8% (<i>p</i>) chi angles: 54.9	0.08Å	-	-
A 25	THR	50	-	Favored (14.07%) General / -95.9,-29.6	1.2% (<i>m</i>) chi angles: 326.4	0.112Å	-	-
A 26	ARG	50	-	Favored (78.55%) General / -63.7,-34.7	10.1% (<i>mtp85</i>) chi angles: 310.3,184.5,104.2,85	0.151Å	-	-
A 27	GLN	50	-	Favored (82.99%) General / -60.8,-37.8	2.3% (<i>tp60</i>) chi angles: 172.3,68.3,111.4	0.059Å	-	-
A 28	LYS	50	-	Favored (71.98%) General / -71.0,-35.4	26.3% (mmmt) chi angles: 308.3,314.8,301.5,180.5	0.163Å	-	-
A 29	ILE	50	-	Favored (97.3%) Isoleucine or valine / -62.9,-42.7	54.8% (<i>mt</i>) chi angles: 303.8,179.8	0.196Å	-	-
A 30	VAL	50	-	Favored (51.38%) Isoleucine or valine / -70.4,-32.8	1.4% (<i>p</i>) chi angles: 85.1	0.247Å	-	-

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A 31	GLU	50	-	Favored (96.79%) General / -61.3,-44.7	31.6% (<i>mt-10</i>) chi angles: 276.4,179,48.6	0.087Å	-	-
A 32	LEU	50	-	Favored (3.35%) General / -87.9,-56.4	29.3% (<i>mt</i>) chi angles: 305.8,189.2	0.129Å	-	-
A 33	ALA	50	-	Favored (97.84%) General / -63.8,-40.9	-	0.104Å	-	-
A 34	HIS	50	-	Favored (29.98%) General / -71.9,-4.8	2.1% (<i>t-80</i>) chi angles: 213.6,312.9	0.063Å	-	-
A 35	SER	50	-	Favored (20.28%) General / -96.1,-18.3	10.3% (<i>p</i>) chi angles: 83.7	0.112Å	-	-
A 36	GLY	50	-	Allowed (0.47%) Glycine / 134.1,29.0	-	-	-	-
A 37	ALA	50	-	Favored (45.61%) General / -122.3,147.9	-	0.051Å	-	-
A 38	ARG	50	-	Favored (23.49%) Pre-proline / -81.3,168.6	72.9% (mtm180) chi angles: 299.1,180.4,299.9,155.2	0.068Å	-	-
A 39	PRO	50	-	Favored (12.93%) Trans-proline / -53.4,-50.7	2.9% (<i>Cg_exo</i>) chi angles: 321.7	0.043Å	-	-
A 40	CYS	50	-	Favored (80.35%) General / -64.9,-35.2	1.5% (<i>p</i>) chi angles: 86.7	0.212Å	-	-
A 41	ASP	50	-	Favored (97.61%) General / -64.0,-41.3	30.8% (<i>m-20</i>) chi angles: 308.4,323.6	0.156Å	-	-
A 42	ILE	50	-	Favored (15.03%) Isoleucine or valine /	7.1% (pt) chi angles: 63.7,150.6	0.319Å	-	-

A 43	SER	50	-	-70.3,-29.0 Favored (76.8%) General / -58.5,-49.6	5.8% (t) chi angles: 161.3	0.027Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C β deviation	Bond lengths	Bond angles
		Avg: 54.96	Clashscore: 1.52	Outliers: 4 of 131	Poor rotamers: 5 of 115	Outliers: 4 of 122		Outliers: 10 of 133
A 44	ARG	50	-	Favored (60.23%) General / -76.0,-14.3	29.5% (<i>ttp-105</i>) chi angles: 200.2,176.7,64.2,254.3	0.065Å	-	-
A 45	ILE	50	-	Favored (11.36%) Isoleucine or valine / -113.9,-13.4	16.7% (<i>mt</i>) chi angles: 305.4,188.8	0.246Å	-	-
A 46	LEU	50	-	Favored (16.78%) General / -102.9,-13.8	77.5% (<i>mt</i>) chi angles: 299.1,170.8	0.122Å	-	-
A 47	GLN	50	-	Allowed (0.86%) General / 70.5,42.6	36.4% (<i>mt-30</i>) chi angles: 305,179.3,252.6	0.153Å	-	-
A 48	VAL	50	-	Favored (27.59%) Isoleucine or valine / -123.2,151.5	53.3% (<i>t</i>) chi angles: 170.4	0.135Å	-	-
A 49	SER	50	-	Favored (26.7%) General / -64.3,157.2	82.8% (<i>p</i>) chi angles: 69.3	0.037Å	-	-
A 50	ASN	50	-	Favored (94.73%) General / -65.2,-41.2	43.3% (<i>m-80</i>) chi angles: 308.6,293.1	0.111Å	-	-
A 51	GLY	50	0.404Å HA3 with C2019 DGU O6	Favored (62.65%) Glycine / -71.7,-34.7	-	-	-	-
Λ Γ 2	CVC	FO		Favored (99.94%) General /	43.6% (<i>t</i>) chi angles: 176.2	0.055Å		
A 52	CYS	50	-	-63.0,-43.0 Allowed	em angles. 170.2	U.USSA	-	-
				moweu				

A 53	VAL	50	-	(1.01%) Isoleucine or valine / -45.2,-56.1	2.6% (<i>t</i>) chi angles: 153.6	0.162Å	-	-
A 54	SER	50	-	Favored (49.71%) General / -87.1,-11.6	73% (<i>m</i>) chi angles: 293.8	0.232Å	-	-
A 55	LYS	50	-	Favored (59.31%) General / -73.2,-10.0	50.7% (<i>mtmt</i>) chi angles: 286.7,186.9,283.4,195.4	0.207Å	-	-
A 56	ILE	50	-	Favored (3.94%) Isoleucine or valine / -91.4,-57.9	3.3% (<i>mp</i>) chi angles: 291.6,76.2	0.158Å	-	-
A 57	LEU	50	-	Favored (76.36%) General / -55.9,-42.7	81.9% (<i>mt</i>) chi angles: 299.7,181.7	0.217Å	-	-
A 58	GLY	50	-	Favored (92.64%) Glycine / -60.2,-37.2	-	-	-	-
A 59	ARG	50	-	Favored (50.28%) General / -77.5,-23.4	72.7% (mtm180) chi angles: 293.6,182.2,276.7,184.9	0.131Å	-	-
A 60	TYR	50	-	Favored (75.44%) General / -70.0,-37.1	87.7% (<i>t80</i>) chi angles: 182.5,77.7	0.128Å	-	-
A 61	TYR	50	-	Favored (69.77%) General / -58.3,-33.7	20.4% (<i>m-30</i>) chi angles: 298.8,340.4	0.124Å	-	-
A 62	GLU	50	-	Allowed (0.22%) General / -95.7,-91.4	15.1% (<i>tm-20</i>) chi angles: 185.7,274.5,326.8	0.209Å	-	OUTLIER(S) worst is C-CA- CB: 4.073 σ
A 63	THR	50	-	Favored (78.65%) General / -57.7,-40.1	3.4% (<i>p</i>) chi angles: 40.5	0.136Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg:	Clashscore:	Outliers: 4 of			Outliers:	Outliers: 10

		J4.7U	1.32	131	113	4 UI 122	U UI 133	UI 133
A 64	GLY	50	-	Favored (35.73%) Glycine / 102.4,11.6	-	-	-	-
A 65	SER	50	-	Favored (34.11%) General / -65.9,128.0	17.5% (<i>t</i>) chi angles: 189.3	0.066Å	-	-
A 66	ILE	50	-	Favored (7.75%) Isoleucine or valine / -89.1,-18.7	45.3% (<i>pt</i>) chi angles: 61.5,168.4	0.192Å	-	-
A 67	ARG	50	-	Favored (90.12%) Pre-proline / -73.3,152.3	18.7% (mmm180) chi angles: 277.3,292,303.6,169	0.074Å	-	-
A 68	PRO	50	-	Allowed (0.98%) Trans-proline / -84.5,-171.3	0.4% chi angles: 43.3	0.118Å	-	-
A 69	ARG	50	-	OUTLIER (0.03%) General / -75.3,-152.1	85% (<i>mtm180</i>) chi angles: 295.5,178.1,281.5,173.6	0.15Å	-	-
A 70	ALA	50	-	Favored (50.65%) General / -125.2,129.7	-	0.096Å	-	-
A 71	ILE	50	-	Favored (5.57%) Isoleucine or valine / -78.2,150.3	38.8% (<i>mt</i>) chi angles: 292.7,154.7	0.107Å	-	-
A 72	GLY	50	0.451Å HA2 with C2013 DAD H2	Favored (40.9%) Glycine / 80.5,169.7	-	-	-	-
A 73	GLY	50	-	Favored (3.12%) Glycine / 97.3,113.7	-	-	-	-
A 74	SER	50	-	Allowed (0.12%) General / -81.5,-154.8	15.7% (<i>p</i>) chi angles: 81.7	0.229Å	-	-
		~ ^		Favored	30.3% (<i>mmtm</i>)	~ ~ · · · ⁹		

A 75	LYS	50	-	(43.00 /o) Pre-proline / -140.8,163.4	chi angles: 307.7,299.6,162.4,307.1	0.041A	-	-
A 76	PRO	50	-	Allowed (0.12%) Trans-proline / -55.6,103.9	0.1% chi angles: 318.5	0.06Å	-	-
A 77	ARG	50	-	Favored (19.73%) General / -88.4,-30.1	83.7% (mtm180) chi angles: 284.1,174,283,177.5	0.178Å	-	-
A 78	VAL	50	-	Allowed (0.93%) Isoleucine or valine / -126.7,-31.6	8.4% (<i>m</i>) chi angles: 309	0.182Å	-	-
A 79	ALA	50	-	Allowed (0.96%) General / -79.1,49.6	-	0.042Å	-	-
A 80	THR	50	-	Favored (3.75%) Pre-proline / -56.0,161.3	66.3% (<i>p</i>) chi angles: 63	0.07Å	-	-
A 81	PRO	50	-	Favored (30.44%) Trans-proline / -47.7,-39.8	0.1% chi angles: 318.2	0.093Å	-	-
A 82	GLU	50	-	Favored (41.42%) General / -79.7,-32.4	43.4% (tt0) chi angles: 185.3,155,354.6	0.236Å	-	-
A 83	VAL	50	-	Favored (86.64%) Isoleucine or valine / -58.8,-42.8	18.8% (<i>t</i>) chi angles: 162.5	0.107Å	-	-
# A	It Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 54.96		Outliers: 4 of 131 Favored	Poor rotamers: 5 of 115		Outliers:	•
A 84	VAL	50	-	(96.71%) Isoleucine or valine / -60.7,-46.0	79.8% (<i>t</i>) chi angles: 174.5	0.072Å	-	-
A 85				Favored				

				General / -59.9,-36.9	em ungres. 255.0			
A 86	LYS	50	-	Favored (61.98%) General / -72.8,-44.1	68.9% (<i>mmtt</i>) chi angles: 284.4,292.3,176.6,186.6	0.086Å	-	-
A 87	ILE	50	-	Favored (57.67%) Isoleucine or valine / -68.6,-33.0	10.6% (<i>mt</i>) chi angles: 298.6,144.4	0.249Å	-	-
A 88	ALA	50	-	Favored (81.25%) General / -57.6,-47.8	-	0.072Å	-	-
A 89	GLN	50	-	Favored (74.71%) General / -55.6,-48.5	28.2% (tt0) chi angles: 188.5,197.7,311.8	0.053Å	-	-
A 90	TYR	50	-	Favored (53.82%) General / -71.4,-47.9	4.2% (<i>m-30</i>) chi angles: 315.6,325.1	0.113Å	-	-
A 91	LYS	50	0.415Å NZ with C2004 DTY OP1	Favored (60.65%) General / -75.0,-15.0	62% (<i>mmtt</i>) chi angles: 291.2,279.4,180.4,168.4	0.104Å	-	-
A 92	ARG	50	-	Favored (13.47%) General / -109.9,-18.1	37.8% (<i>mtp180</i>) chi angles: 304.6,158.2,76.1,167.4	0.159Å	-	-
A 93	GLU	50	-	Favored (13.63%) General / -91.9,-36.1	9.2% (<i>pt-20</i>) chi angles: 88,182.9,346.4	0.139Å	-	-
A 94	CYS	50	-	Favored (26.81%) Pre-proline / -139.2,79.1	38.5% (<i>t</i>) chi angles: 187.7	0.048Å	-	-
A 95	PRO	50	-	Favored (7.67%) Trans-proline /	11% (<i>Cg_exo</i>) chi angles: 323	0.106Å	-	-
A 96	SER	50	-	-46.1,-30.6 Favored (9.55%) General / -85.4,79.2	91.3% (<i>p</i>) chi angles: 65.2	0.056Å	-	-
		F-0		Favored (21.21%)	19.3% (<i>mt</i>)	0 001 9		

A 9/	ILE	50	-	Isoleucine or valine / -145.8,139.2	chi angles: 286.2,185	0.08TA	-	-
A 98	РНЕ	50	-	Favored (8.85%) General / -93.9,171.4	50.2% (<i>m-85</i>) chi angles: 307.3,292.8	0.049Å	-	-
A 99	ALA	50	-	Favored (86.75%) General / -60.4,-39.3	-	0.095Å	-	-
A 100	TRP	50	-	Favored (75.18%) General / -70.0,-36.7	63.3% (<i>p-90</i>) chi angles: 53.7,271.7	0.176Å	-	-
A 101	GLU	50	-	Favored (83.01%) General / -60.9,-37.7	47.6% (<i>mt-10</i>) chi angles: 291.4,187.9,281.3	0.103Å	-	-
A 102	ILE	50	-	Favored (34.07%) Isoleucine or valine / -71.7,-29.4	61.2% (<i>mt</i>) chi angles: 301.1,179.9	0.31Å	-	-
			0.51 %	Favored				
A 103	ARG	50	0.51Å CZ with A 119 SER HA	(89.18%) General / -61.3,-39.1	34.1% (<i>ttt180</i>) chi angles: 208.2,168.1,188.7,168.6	0.146Å	-	-
	ARG Alt Res		CZ with A 119 SER HA Clash >	(89.18%) General /	chi angles: 208.2,168.1,188.7,168.6	Сβ	Bond lengths	- Bond angles
		High B	CZ with A 119 SER HA Clash > 0.4Å Clashscore:	(89.18%) General / -61.3,-39.1 Ramachandran	chi angles: 208.2,168.1,188.7,168.6	Cβ deviation	lengths Outliers: 0	angles
		High B Avg:	CZ with A 119 SER HA Clash > 0.4Å Clashscore:	(89.18%) General / -61.3,-39.1 Ramachandran Outliers: 4 of	chi angles: 208.2,168.1,188.7,168.6 Rotamer Poor rotamers: 5 of	C β deviation Outliers:	lengths Outliers: 0	angles Outliers: 10
# /	Alt Res	High B Avg: 54.96	CZ with A 119 SER HA Clash > 0.4Å Clashscore:	(89.18%) General / -61.3,-39.1 Ramachandran Outliers: 4 of 131 Favored (52.71%) General /	chi angles: 208.2,168.1,188.7,168.6 Rotamer Poor rotamers: 5 of 115 25.8% (<i>m-20</i>)	Cβ deviation Outliers: 4 of 122	lengths Outliers: 0	angles Outliers: 10
# /	Alt Res ASP	High B Avg: 54.96	CZ with A 119 SER HA Clash > 0.4Å Clashscore:	(89.18%) General / -61.3,-39.1 Ramachandran Outliers: 4 of 131 Favored (52.71%) General / -81.0,-16.7 Favored (98.11%) General /	chi angles: 208.2,168.1,188.7,168.6 Rotamer Poor rotamers: 5 of 115 25.8% (m-20) chi angles: 284.1,13.2 9.4% (mmt180) chi angles:	Cβ deviation Outliers: 4 of 122 0.155Å	lengths Outliers: 0	angles Outliers: 10

A 108	SER	50	-	Favored (12.25%) General / -97.7,-31.4	80.2% (p) chi angles: 60.1	0.166Å	-	-
A 109	GLU	50	-	Favored (53.03%) General / -77.2,-26.9	21.2% (<i>mt-10</i>) chi angles: 284.1,205.4,26.3	0.115Å	-	-
A 110	GLY	50	-	Favored (8.45%) Glycine / 88.9,35.1	-	-	-	-
A 111	VAL	50	-	Favored (17.34%) Isoleucine or valine / -83.5,-42.1	97.5% (<i>t</i>) chi angles: 176.2	0.079Å	-	-
A 112	CYS	50	-	Favored (8.32%) General / -98.5,171.2	73% (<i>m</i>) chi angles: 298.1	0.026Å	-	-
A 113	THR	50	-	Allowed (0.19%) General / -101.6,-114.6	0.8% chi angles: 31.3	0.281Å	-	OUTLIER(S) worst is C-CA- CB: 4.208 σ
A 114	ASN	50	-	Allowed (1.59%) General / -141.8,33.6	9.6% (<i>m120</i>) chi angles: 293.3,161.4	0.043Å	-	OUTLIER(S) worst is CA- CB-CG: 9.14 σ
A 115	ASP	50	-	Allowed (0.06%) General / -164.0,17.1	2.6% (<i>p30</i>) chi angles: 38.9,8.4	0.074Å	-	OUTLIER(S) worst is CA- CB-CG: 5.631 σ
A 116	ASN	50	-	OUTLIER (0.03%) General / -169.0,36.2	28% (<i>p30</i>) chi angles: 51.4,9.2	0.048Å	-	-
A 117	ILE	50	-	Favored (64.6%) Pre-proline/	7.4% (<i>tp</i>) chi angles: 185.1,73	0.063Å	-	-
A 118	PRO	50	-	-98.4,113.9 Favored (52.71%) Trans-proline / -53.8,144.9	24.3% (<i>Cg_exo</i>) chi angles: 324.6	0.089Å	-	-
A 119	SER	50	0.51Å HA with A 103 ARG CZ	Favored (4.62%) General / -89.0,-174.8	21.2% (<i>p</i>) chi angles: 80.2	0.114Å	-	-

A 120	VAL	50	-	Favored (18.54%) Isoleucine or valine / -74.3,-52.9	45% (<i>t</i>) chi angles: 183.7	0.102Å	-	-
A 121	SER	50	-	Favored (82.25%) General / -68.2,-40.9	8.7% (<i>t</i>) chi angles: 193.5	0.096Å	-	-
A 122	SER	50	-	Favored (90.5%) General / -65.1,-38.4	75.4% (<i>m</i>) chi angles: 294.6	0.12Å	-	-
A 123	ILE	50	-	Favored (84.97%) Isoleucine or valine / -63.3,-39.4	43.1% (<i>mt</i>) chi angles: 298,184.3	0.256Å	-	-
# A	lt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C β deviation	Bond lengths	Bond angles
		Avg: 54.96	Clashscore: 1.52	Outliers: 4 of 131	Poor rotamers: 5 of 115	Outliers: 4 of 122		Outliers: 10 of 133
A 124	ASN	50	-	Favored (69.16%) General / -71.3,-32.9	28.8% (<i>m-20</i>) chi angles: 287.1,10.5	0.115Å	-	-
A 125	ARG	50	-	Favored (90.95%) General / -59.0,-42.8	39.9% (<i>ttp85</i>) chi angles: 184.5,162.1,52.7,64.3	0.091Å	-	-
A 126	VAL	50	-	Favored (96.86%) Isoleucine or valine / -64.5,-43.2	95.5% (<i>t</i>) chi angles: 175.9	0.083Å	-	-
A 127	LEU	50	-	Favored (73.5%) General / -57.3,-38.1	89.1% (<i>mt</i>) chi angles: 299.4,179.4	0.155Å	-	-
A 120				г 1				
A 128	ARG	50	-	Favored (59.49%) General / -74.6,-25.8	83.9% (<i>mtm-85</i>) chi angles: 297.3,195.6,295.2,290.2	0.222Å	-	-
A 129	ARG ASN	50 50	-	(59.49%) General /	chi angles:		-	-

A 130	LEU	50	-	(60.81%) General / -73.9,-19.1	40% (IIII) chi angles: 299.6,164.4	0.096Å	-	-
A 131	ALA	50	-	Favored (68.02%) General / -63.5,-24.9	-	0.104Å	-	-
A 132	SER	50	-	OUTLIER (0%) General / -73.9,-121.6	19% (<i>p</i>) chi angles: 80.8	0.233Å	-	OUTLIER(S) worst is C-CA- CB: 4.091 σ
A 133	GLU	50	-	Allowed (1.28%) General / 52.8,-118.1	2.5% (tt0) chi angles: 200.4,215.3,285.8	0.181Å	-	OUTLIER(S) worst is C-N-CA: 8.07σ
A 134	LYS	50	-	OUTLIER (0%) General / -31.6,8.8	2% (<i>pttm</i>) chi angles: 62.2,229.2,174.3,285.4	0.051Å	-	OUTLIER(S) worst is N-CA- C: 4.811 σ
A 135	GLN	50	-	Favored (16.08%) General / -114.1,5.6	35.5% (<i>mt-30</i>) chi angles: 292.4,167.6,104.9	0.091Å	-	-
A 136	GLN	99.99	-	-	5.2% (<i>tp-100</i>) chi angles: 177.7,46.8,205.9	0.085Å	-	OUTLIER(S) worst is CB- CG-CD: 4.209 σ
B1001	DAD	100.5	-	-	-	-	_	-
B1002	DAD	102.72	-	-	-	-	-	-
B1003	DGU	95.24	-	-	-	-	-	-
B1004	DCY	83.06	-	-	-	-	-	-
B1005	DAD	74.41	-	-	-	-	_	-
B1006	DTY	64.72	-	-	-	-	-	-
B1007	DTY	55.15	-	-	-	-	-	-
# /	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	$\begin{array}{c} C\beta \\ \text{deviation} \end{array}$	Bond lengths	Bond angles
		Avg:	Clashscore:	Outliers: 4 of	Poor rotamers: 5 of	Outliers:	Outliers:	Outliers: 10
		54.96	1.52	131	115	4 of 122	0 of 133	of 133
B1008	DTY	63.52	-	-	-	-	-	-
B1009	DTY	50.43	-	-	-	-	-	-
B1010	DCY	60.49	-	-	-	-	-	-
B1011	DAD	62.65	-	-	-	-	-	-
B1012	DCY	60.46	-	-	-	-	-	-
B1013	DGU	62.87	-	-	-	-	-	-
B1014	DCY	66.18	-	-	-	-	-	-
B1015	DAD	53.92	-	-	-	-	-	-
B1016	DTY	60.67	-	-	-	-	-	-

B1017	DGU	53.38	_	_	_	_	_	_
B1017		45.88	_	_	_	_	_	_
B1019		45.01						
B1013		47.07	-	-	-	-	_	-
B1020	DGU		-	-	-	-	-	-
B1021		69.79	-	-	-	-	-	-
			-	-	-	-	-	-
B1023	DAD		-	-	-	-	-	-
B1024		89.37	-	-	-	-	-	-
B1025		84.51	-	-	-	-	-	-
B1026		87.98	-	-	-	-	-	_
C2001	DIY	75.67	- Cl. I	-	-	-	- 5 I	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg:	Clashscore:	Outliers: 4 of	Poor rotamers: 5 of	Outliers:	Outliers:	Outliers: 10
		54.96	1.52	131	115	4 of 122	0 of 133	of 133
C2002	DTY	77.07	-	-	-	-	-	-
C2003	DCY	78.78	-	-	-	-	-	-
60004	DTV.	10.01	0.415Å					
C2004	DIY	48.81	OP1 with A 91 LYS NZ	-	-	-	-	-
C2005	DGU	57.01	-	_	_	_	_	-
C2006		69.23	_	_	_	_	_	_
C2007		76.12	-	-	_	-	-	_
C2008		80.78	-	-	_	-	-	_
C2009		74.88	-	-	_	-	-	_
C2010	DCY	75.39	-	-	_	-	-	_
C2011	DTY	73.29	-	-	_	-	-	_
C2012		61.25	-	-	_	-	-	_
			0.451Å					
C2013	DAD	63.28	H2 with A 72 GLY HA2	-	-	-	-	-
C2014	DTY	61.51	-	-	-	-	-	-
C004 F	D.C.L.	40.05						
C2015		43.87	-	-	-	-	-	-
C2016		43.32	-	-	-	-	-	-
C2017		43.75	-	-	-	-	-	-
C2018	DTY	44.55	-	-	-	-	-	-
C2019	DGU	51.15	0.432Å OP2 with A 9 ASN HB2	-	-	-	-	-
C2020	DAD	67.99	-	-	-	-	-	-
C2021	DAD	76.69	-	-	-	-	-	-
			~! !			~~	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C β deviation	Bond lengths	Bond angles
			Avg:	Clashscore:	Outliers: 4 of	Poor rotamers: 5 of	Outliers:	Outliers:	Outliers: 10
			54.96	1.52	131	115	4 of 122	0 of 133	of 133
C2022		DAD	70.65	-	-	-	-	-	-
C2023	3	DAD	68.53	-	-	-	-	-	-
C2024	Ļ	DTY	68.92	-	-	-	-	-	-
C2025	5 1	DGU	68.54	-	-	-	-	-	-
C2026	•	DCY	62.68	-	-	-	-	-	-

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